

Supporting Information for

Characterization of the Structure and Reactivity of Monocopper-Oxygen
Complexes Supported by β -Diketimate and Anilido-Imine Ligands

Benjamin F. Gherman, William B. Tolman, Christopher J. Cramer*

Department of Chemistry and Supercomputer Institute,

University of Minnesota,

207 Pleasant St. SE

Minneapolis, MN 55455

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Table S1. C–H bond dissociation energies (kcal/mol) computed by density functional methods and corresponding literature values.^a

	computed	literature
methane	103.4	104.9
cyclohexane	95.5	95.5
acetonitrile	96.2	93.9
toluene	87.4	89.8
phenol	83.5	86.5
isopropylbenzene	82.5	84.4
1,4-cyclohexadiene	71.2	73.0

^(a) Lide, D. R. *Handbook of Chemistry and Physics, 85th Edition*; CRC Press: Boca Raton, 2004.

Table S2. Electronic energies (hartrees), thermal enthalpies (kcal/mol), entropies (cal/mol·K), zero-point energies (kcal/mol), CASPT2 corrections (kcal/mol), and solvation energies (kcal/mol) for all computed species.

small molecules

	electronic energy	thermal enthalpy		entropy		zero-point energy	CASPT2 correction	solvation energy (THF)	
		25 °C	223 K	25 °C	223 K			25 °C	223 K
O ₂ triplet	-150.3201	2.075	1.551	49.010	46.985	2.370	0.00	-0.0519	-0.0519
MeCN	-132.7592	2.852	1.986	60.113	56.776	28.526	0.00	-6.9584	-7.3939
THF	-232.4602	3.716	2.479	75.014	70.266	73.465	0.00	-2.5032	-2.6951

L¹ system.

	electronic energy	thermal enthalpy		entropy		zero-point energy	CASPT2 correction	solvation energy (H ₂ O, 25 °C)	solvation energy (THF)	
		25 °C	223 K	25 °C	223K				25 °C	223 K
L ¹ CuO ₂ side-on singlet	-1585.8902	13.777	8.321	154.900	133.941	191.082	-16.38	-4.8479	-6.0812	-6.7107
L ¹ CuO ₂ end-on singlet	-1585.8642	14.268	8.727	159.531	138.238	190.312	-27.00	-3.9495	-5.8207	-6.3416
L ¹ CuO ₂ end-on singlet → L ¹ CuO ₂ side-on singlet transition state	-1585.8609	13.864	8.463	155.703	134.952	189.993	-24.93	n/a	-5.7290	-7.2641
L ¹ CuO ₂ side-on triplet	-1585.9051	14.188	8.647	159.116	137.824	190.315	0.00	n/a	-5.1559	-5.5401
L ¹ CuO ₂ end-on triplet	-1585.8918	14.465	8.888	166.195	144.762	189.941	0.00	n/a	-4.0611	-4.4054
L ¹ CuO ₂ H ⁺ side-on singlet	-1586.2749	14.270	8.653	156.808	135.230	198.133	1.82	-37.5831	-34.5269	-36.2392
L ¹ CuO ₂ H ⁺ end-on singlet	-1586.2759	14.384	8.735	157.941	136.235	198.057	-13.11	-36.6512	-34.1143	-35.8267
L ¹ CuO ₂ H ⁺ side-on triplet	-1586.2756	14.655	8.972	164.605	142.768	197.082	0.00	-40.4327	-34.8372	-36.6741
L ¹ CuO ₂ H ⁺ end-on triplet	-1586.2780	14.347	8.763	162.280	140.826	196.782	0.00	n/a	-35.6292	-37.4182
L ¹ CuO ₂ H ₂ ²⁺ end-on singlet	-1586.5230	14.713	n/a	160.612	n/a	204.845	0.00	-134.0637	n/a	n/a

L ¹ CuO ₂ H ₂ ²⁺ end-on triplet	-1586.5187	14.852	n/a	164.989	n/a	204.292	0.00	n/a	n/a	n/a
L ¹ CuO ₂ H ₂ ⁺ end-on doublet	-1586.8749	14.624	n/a	161.303	n/a	204.985	0.00	n/a	n/a	n/a
L ¹ CuO ₂ ⁻ side-on doublet	-1585.9619	14.043	8.556	157.552	136.470	188.436	0.00	n/a	-43.0961	-45.8229
L ¹ CuO ₂ ⁻ end-on doublet	-1585.9618	14.823	9.173	167.568	145.852	188.310	0.00	n/a	-39.7786	-42.1935
L ¹ CuO ₂ ⁻ end-on doublet → L ¹ CuO ₂ ⁻ side-on doublet transition state	-1585.9557	13.825	8.461	158.134	137.525	188.086	0.00	n/a	-40.8516	-43.4402
L ¹ CuO ₂ H side-on doublet	-1586.5142	14.392	8.754	160.413	138.750	197.695	0.00	n/a	-8.1250	-8.8360
L ¹ CuO ₂ H end-on doublet	-1586.5142	14.081	8.542	157.314	136.030	197.384	0.00	n/a	-7.0050	-7.6144
L ¹ CuO ₂ H end-on singlet → L ¹ CuO ₂ H side-on singlet transition state	-1586.5086	14.093	8.560	157.815	136.558	197.248	0.00	n/a	-7.9568	-8.6709
L ¹ CuO singlet	-1510.6751	13.366	8.151	153.179	133.144	188.482	-23.47	-11.4455	-10.8632	-11.8299
L ¹ CuO triplet	-1510.7026	13.389	8.146	153.766	133.625	188.177	0.00	n/a	-7.0355	-7.6597
L ¹ CuOH ⁺ singlet	-1511.1411	13.842	8.400	154.361	133.455	194.665	0.00	-38.3395	-34.7015	-36.4818
L ¹ CuOH ₂ ²⁺ singlet	-1511.4427	14.815	n/a	164.707	n/a	201.842	0.00	-130.6186	n/a	n/a
L ¹ CuO ⁻ doublet	-1510.7809	13.715	n/a	157.932	n/a	186.702	0.00	n/a	-43.3361	n/a
L ¹ CuOH doublet	-1511.3815	13.679	n/a	154.321	n/a	195.183	0.00	n/a	-7.0047	n/a
L ¹ CuOH ₂ ⁺ doublet	-1511.7934	13.756	n/a	155.397	n/a	201.653	0.00	n/a	n/a	n/a

L² system.

	electronic energy	thermal enthalpy		entropy		zero-point energy	CASPT2 correction	solvation energy (H ₂ O, 25 °C)	solvation energy (THF)	
		25 °C	223 K	25 °C	223K				25 °C	223 K
L ² Cu	-1549.8644	12.865	7.649	147.499	198.970	198.970	0.00	n/a	-5.4887	-5.9647
L ² Cu(MeCN)	-1682.6617	16.130	9.782	174.803	150.418	228.194	0.00	n/a	-7.9065	-8.4112
L ² Cu(THF)	-1782.3542	16.693	10.085	180.837	155.470	273.042	0.00	n/a	-4.6675	-5.0834
L ² Cu(MeCN)O ₂ singlet	-1832.9607	16.745	10.075	176.410	150.785	231.872	-26.12	n/a	-8.8594	-9.1149
L ² Cu(MeCN)O ₂ triplet	-1832.9781	18.380	11.321	197.951	170.821	231.094	0.00	n/a	-7.9158	-8.4523
L ² Cu(THF)O ₂ singlet	-1932.6444	19.013	11.613	198.188	169.763	276.626	-38.19	n/a	-7.0091	-7.5666

$L^2Cu(THF)O_2$ triplet	-1932.6795	18.857	n/a	200.406	n/a	275.900	n/a	n/a	n/a	n/a
$L^2Cu(MeCN) + O_2 \rightarrow L^2Cu(MeCN)O_2$ transition state (triplet)	-1832.9788	17.832	10.910	189.642	163.041	230.997	0.00	n/a	-8.0499	-8.6704
$L^2Cu(MeCN) \rightarrow L^2Cu(THF)$ transition state	-1915.1188	20.147	12.374	208.400	178.539	301.708	0.00	n/a	-8.6462	-9.1580
L^2CuO_2 side-on singlet	-1700.2019	13.442	7.929	149.160	127.997	202.858	-26.97	-5.4046	-6.3088	-6.9956
L^2CuO_2 end-on singlet	-1700.1796	14.747	8.880	162.482	139.948	202.481	-32.20	-5.8909	-7.2416	-7.8237
L^2CuO_2 end-on singlet $\rightarrow L^2CuO_2$ side-on singlet transition state	-1700.1773	13.956	8.365	157.987	136.518	201.875	-32.79	n/a	-8.1526	-8.8205
L^2CuO_2 side-on triplet	-1700.2164	14.387	8.644	162.632	140.578	202.146	0.00	-3.9195	-5.6088	-6.1359
L^2CuO_2 end-on triplet	-1700.2070	14.904	9.006	166.394	143.740	202.200	0.00	n/a	-4.9780	-5.4416
$L^2CuO_2H^+$ side-on singlet (isomer #1)	-1700.5936	14.816	8.870	161.572	138.736	210.377	-11.11	-38.3621	-34.7751	-36.5792
$L^2CuO_2H^+$ side-on singlet (isomer #2)	-1700.5982	14.795	8.848	160.978	138.136	210.407	-10.79	-37.9820	-34.9640	-36.7454
$L^2CuO_2H^+$ end-on singlet	-1700.5962	14.431	8.586	157.237	134.794	210.094	-15.94	-35.8150	-34.3664	-36.1198
$L^2CuO_2H^+$ end-on singlet $\rightarrow L^2CuO_2H^+$ side-on singlet (isomer #1) transition state	-1700.5853	14.329	8.574	159.053	136.954	209.226	-13.53	n/a	-34.8908	-36.6779
$L^2CuO_2H^+$ end-on singlet $\rightarrow L^2CuO_2H^+$ side-on singlet (isomer #2) transition state	-1700.5835	13.844	8.239	154.405	132.883	210.407	-13.37	n/a	-33.5922	-35.4105
$L^2CuO_2H^+$ side-on triplet (isomer #1)	-1700.6015	14.979	8.999	166.415	143.449	209.919	0.00	-38.2805	-36.3519	-38.2969
$L^2CuO_2H^+$ side-on triplet (isomer #2)	-1700.6016	14.428	8.593	159.650	137.242	209.817	0.00	n/a	-34.7713	-36.7094
$L^2CuO_2H^+$ end-on triplet	-1700.6052	15.146	9.121	168.194	145.052	209.692	0.00	n/a	-34.8434	-36.6234
$L^2CuO_2H_2^{2+}$ end-on singlet	-1700.8545	15.110	n/a	162.271	n/a	217.403	0.00	-131.0950	n/a	n/a
$L^2CuO_2H_2^{2+}$ end-on triplet	-1700.8516	15.106	n/a	164.984	n/a	217.206	0.00	n/a	n/a	n/a
$L^2CuO_2H_2^+$ end-on doublet	-1701.1934	15.152	n/a	164.406	n/a	217.022	0.00	n/a	n/a	n/a
$L^2CuO_2^-$ side-on doublet	-1700.2758	14.220	8.532	159.294	137.452	200.252	0.00	n/a	-41.9266	-44.6265
$L^2CuO_2^-$ end-on doublet	-1700.2818	15.369	9.389	173.978	151.008	200.480	0.00	n/a	-39.4119	-41.8127

L ² CuO ₂ ⁻ end-on doublet → L ² CuO ₂ ⁻ side-on doublet transition state	-1700.2723	14.261	8.562	160.533	138.649	200.047	0.00	n/a	-40.5477	-43.1552
L ² CuO ₂ H side-on doublet (isomer #1)	-1700.8301	14.871	8.909	163.627	140.729	209.918	0.00	n/a	7.9592	-8.6454
L ² CuO ₂ H side-on doublet (isomer #2)	-1700.8288	14.919	8.947	164.277	141.342	209.813	0.00	n/a	-8.6973	-9.4760
L ² CuO ₂ H end-on doublet	-1700.8305	14.587	8.714	160.840	138.289	209.548	0.00	n/a	-7.5248	-8.1858
L ² CuO ₂ H end-on singlet → L ² CuO ₂ H side-on singlet transition state (isomer #1)	-1700.8213	14.377	8.621	160.881	138.776	208.967	0.00	n/a	-8.0544	-8.7996
L ² CuO ₂ H end-on singlet → L ² CuO ₂ H side-on singlet transition state (isomer #1)	-1700.8210	14.064	8.326	155.347	133.319	208.925	0.00	n/a	-8.8643	-9.6899
L ² CuO singlet	-1624.9913	13.919	8.360	157.568	136.219	200.471	-31.50	-12.6761	-11.5908	-12.6346
L ² CuO triplet	-1625.0195	13.929	8.345	157.703	136.259	200.201	0.00	n/a	-7.6945	-8.5300
L ² CuOH ⁺ singlet	-1625.4666	14.277	8.481	157.033	134.966	207.386	0.00	-38.1608	-34.9913	-36.8026
L ² CuOH ₂ ²⁺ singlet	-1625.7734	14.894	n/a	161.327	n/a	214.781	0.00	-128.3313	n/a	n/a
L ² CuO ⁻ doublet	-1625.0997	13.634	n/a	153.480	n/a	198.728	0.00	n/a	-43.3901	n/a
L ² CuOH doublet	-1625.6984	14.209	n/a	158.056	n/a	207.245	0.00	n/a	-7.1900	n/a
L ² CuOH ₂ ⁺ doublet	-1626.1144	14.221	n/a	158.233	n/a	213.925	0.00	n/a	n/a	n/a

L¹ Cu/O structures in reactions with substrates: substrate-bound complexes

	electronic energy	thermal enthalpy (25 °C)	zero-point energy	CASPT2 correction
L ¹ CuO ₂ side-on				
MeCN	-1718.6532	16.629	216.608	-16.38
methane	-1626.4149	16.168	219.337	-16.38
dopamine	-2102.5709	21.327	305.983	-16.38
formylglycine	-1983.1124	18.622	239.105	-16.38
cyclohexane	-1821.7882	17.956	298.158	-16.38
toluene	-1857.4702	17.717	271.475	-16.38
phenol	-1893.3757	17.837	256.924	-16.38
isopropylbenzene	-1936.1023	19.801	307.388	-16.38
cyclohexadiene	-1819.3220	17.666	267.801	-16.38

L¹CuO₂ end-on

MeCN	-1718.6298	17.120	215.838	-27.00
methane	-1626.3897	16.659	218.567	-27.00
dopamine	-2102.5498	21.818	305.213	-27.00
formylglycine	-1983.1020	19.113	238.335	-27.00
cyclohexane	-1821.7632	18.447	297.388	-27.00
toluene	-1857.4453	18.208	270.705	-27.00
phenol	-1893.3760	18.328	256.154	-27.00
isopropylbenzene	-1936.0772	20.292	306.618	-27.00
cyclohexadiene	-1819.2967	18.157	267.031	-27.00

L¹CuO₂H⁺

MeCN	-1719.0331	17.236	223.583	-13.11
methane	-1626.8026	16.775	226.312	-13.11
dopamine	-2102.9861	21.934	312.958	-13.11
formylglycine	-1983.6207	19.229	246.080	-13.11
cyclohexane	-1822.1760	18.563	305.133	-13.11
toluene	-1857.8635	18.324	278.450	-13.11
phenol	-1893.7641	18.444	263.899	-13.11
isopropylbenzene	-1936.4874	20.408	314.363	-13.11
cyclohexadiene	-1819.7174	18.273	274.776	-13.11

L¹CuO

MeCN	-1643.4434	16.218	214.008	-23.47
methane	-1551.2020	15.757	216.737	-23.47
dopamine	-2027.3734	20.916	303.383	-23.47
formylglycine	-1907.9147	18.211	236.505	-23.47
cyclohexane	-1746.5752	17.545	295.558	-23.47
toluene	-1782.2583	17.306	268.875	-23.47
phenol	-1818.1984	17.426	254.324	-23.47
isopropylbenzene	-1860.8926	19.390	304.788	-23.47
cyclohexadiene	-1744.1095	17.255	265.201	-23.47

L¹CuOH⁺

MeCN	-1643.9166	16.694	220.191	0.00
methane	-1551.6662	16.233	222.920	0.00
dopamine	-2027.8311	21.392	309.566	0.00
formylglycine	-1908.4927	18.687	242.688	0.00
cyclohexane	-1747.0395	18.021	301.741	0.00
toluene	-1782.7212	17.782	275.058	0.00
phenol	n/a	n/a	n/a	n/a
isopropylbenzene	-1861.3521	19.866	310.971	0.00
cyclohexadiene	-1744.5742	17.731	271.384	0.00

L¹ Cu/O structures in reactions with substrates: H-abstraction transition states

	electronic energy	thermal enthalpy (25 °C)	zero-point energy
L ¹ CuO ₂ side-on	-1718.6053	16.374	215.636
MeCN	-1626.3600	15.708	215.331
methane	-2102.5317	21.462	301.413
dopamine	-1983.0990	18.896	234.400
formylglycine	-1821.7440	17.607	293.539
cyclohexane	-1857.4315	18.647	267.483
toluene	-1893.3504	17.940	253.047
phenol	-1936.0574	19.771	302.121
isopropylbenzene	-1819.2982	17.139	263.834
cyclohexadiene	-1718.6053	16.374	215.636
L ¹ CuO ₂ end-on			
MeCN	-1718.5942	16.610	215.220
methane	-1626.3527	15.339	214.937
dopamine	-2102.5282	21.469	301.501
formylglycine	-1983.0896	19.013	234.251
cyclohexane	-1821.7428	18.235	293.536
toluene	-1857.4194	18.221	267.265
phenol	-1893.3463	16.967	255.096
isopropylbenzene	-1936.0504	19.801	302.223
cyclohexadiene	-1819.2852	17.390	263.424
L ¹ CuO ₂ H ⁺			
MeCN	-1718.9623	16.952	222.553
methane	-1626.7233	16.725	222.719
dopamine	-2102.9322	20.718	309.932
formylglycine	-1983.5856	18.079	242.777
cyclohexane	-1822.1226	17.712	300.683
toluene	-1857.8170	18.184	274.830
phenol	-1893.7540	17.819	261.737
isopropylbenzene	-1936.4365	19.696	309.460
cyclohexadiene	-1819.6864	17.661	271.054
L ¹ CuO			
MeCN	-1643.4525	15.085	214.010
methane	-1551.2092	14.961	213.283
dopamine	-2027.3616	19.267	298.973
formylglycine	-1907.9240	17.628	233.476
cyclohexane	-1746.5902	16.762	292.513
toluene	-1782.2716	17.406	265.523
phenol	-1818.1867	16.579	251.255
isopropylbenzene	-1860.9042	18.728	300.983
cyclohexadiene	-1744.1320	16.945	261.988

L^1CuOH^+			
MeCN	-1643.8628	16.485	219.672
methane	-1551.6225	15.146	219.614
dopamine	-2027.8249	20.594	306.647
formylglycine	-1908.4748	17.687	239.285
cyclohexane	-1747.0170	17.929	298.129
toluene	-1782.7096	17.954	272.717
phenol	-1818.6474	17.168	258.184
isopropylbenzene	-1861.3231	19.913	307.179
cyclohexadiene	-1744.5726	17.389	268.977

Substrates.

	electronic energy	thermal enthalpy (25 °C)	zero-point energy
MeCN	-132.7592	2.852	25.526
methane	-40.5240	2.391	28.255
dopamine	-516.6803	7.550	114.901
formylglycine	-397.2249	4.845	48.023
cyclohexane	-235.8972	4.179	107.076
toluene	-271.5785	3.940	80.393
phenol	-307.4781	4.060	65.842
isopropylbenzene	-350.2107	6.024	116.306
cyclohexadiene	-233.4306	3.889	76.719

Figure S1. Correlation between computed and literature values for C–H bond dissociation energies of substrates based upon data in Table S1.

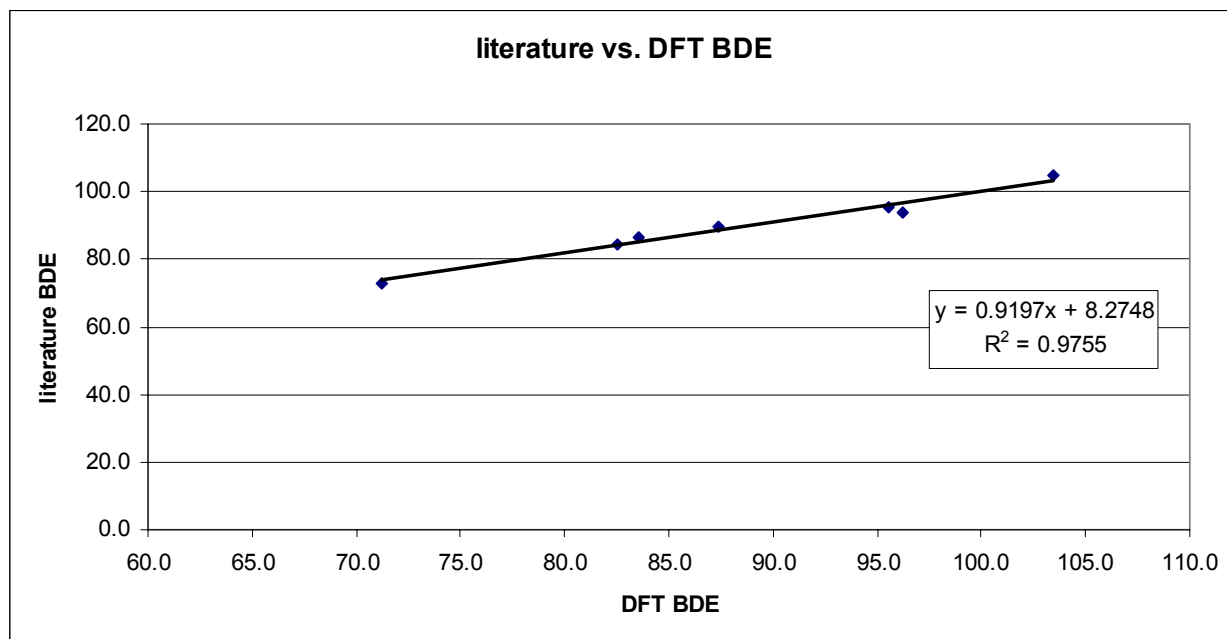


Figure S2. Linear correlation between the CASPT2 energy correction and Cu–O bond length in the singlet (a) side-on and (b) end-on 1:1 Cu-O₂ adducts supported by L².

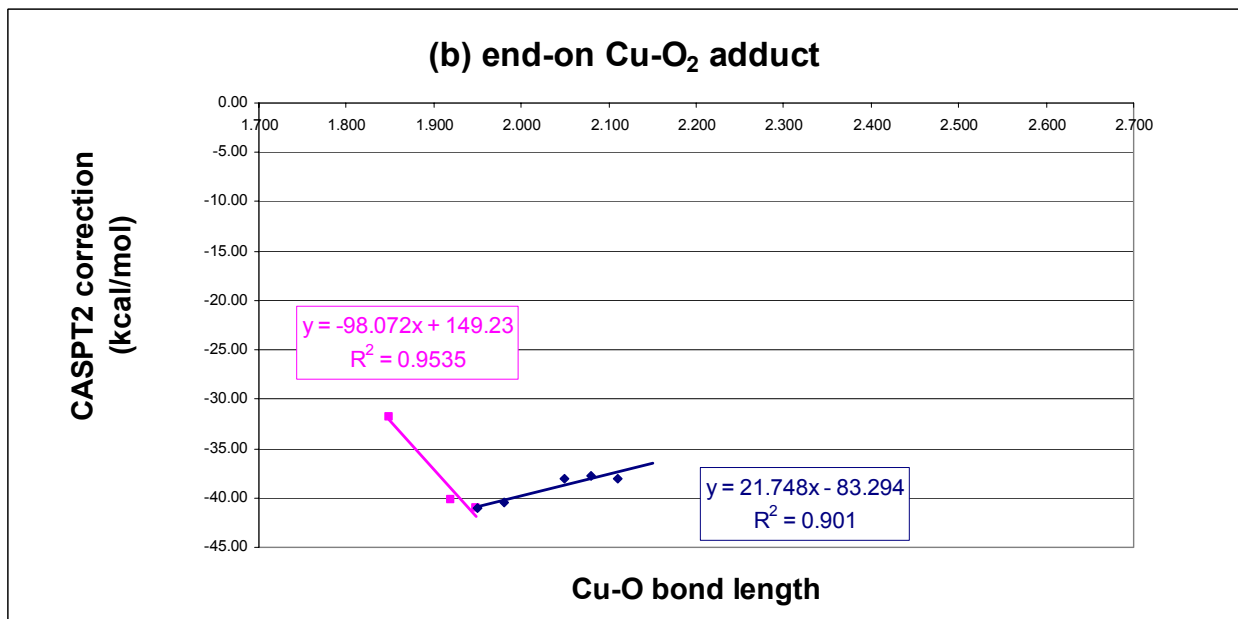
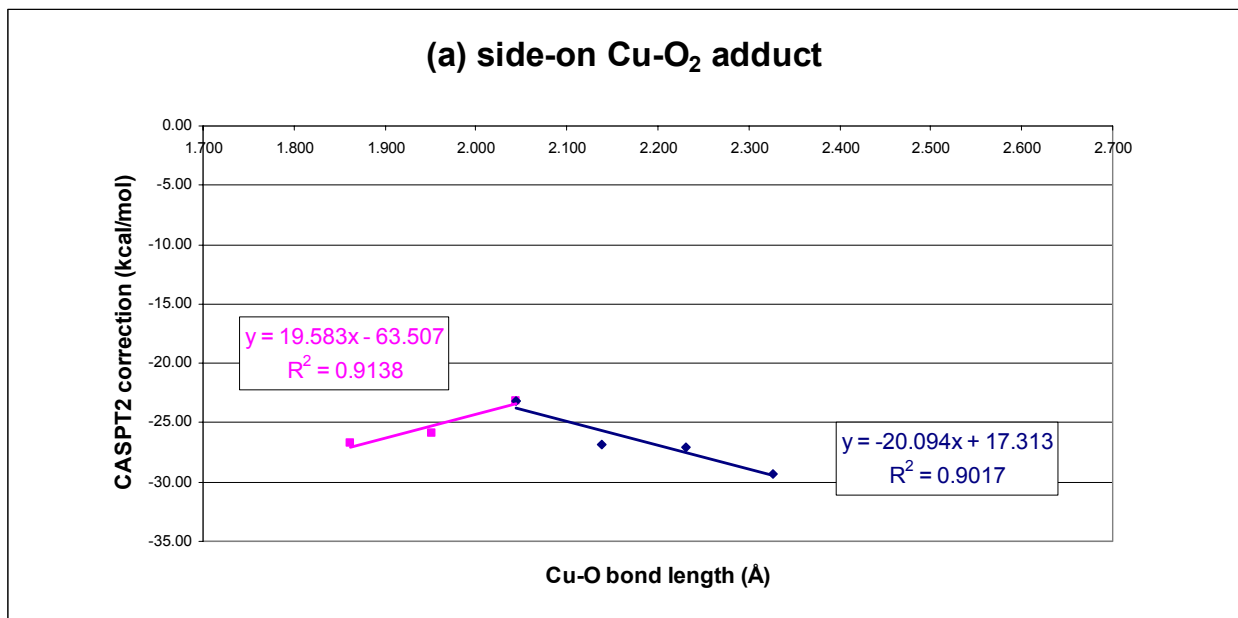


Figure S3. Optimized geometries for (a) L^2CuO and (b) L^2CuOH^+ . Hydrogen atoms on L^2 are omitted for clarity. Distances are measured in Å. Pink stands for Cu; gray, C; blue, N; yellow, S; red, O; white, H.

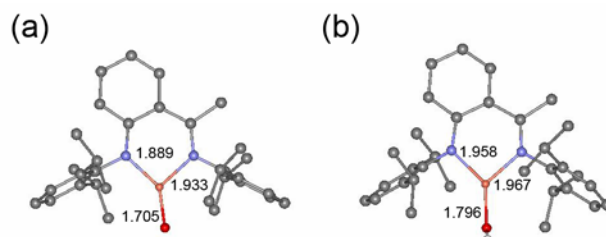


Figure S4. Key frontier orbitals showing partial occupation in the singlet L^1CuO CASSCF wave function. Occupation numbers are shown in parentheses. Orange represents C, blue N, red O, white H, and yellow Cu.

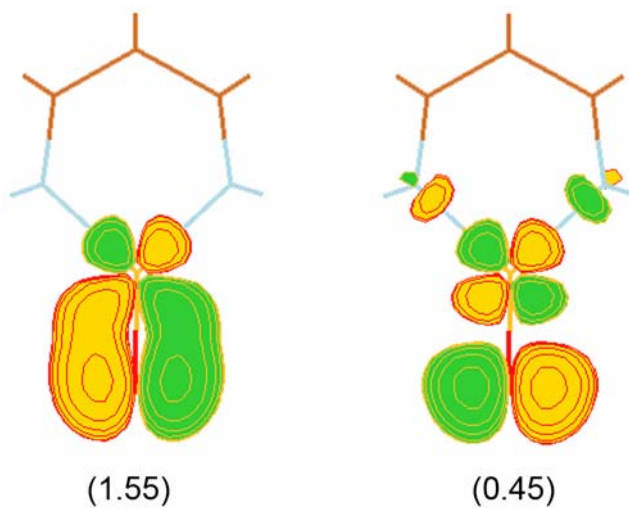


Figure S5. Optimized geometries for (a) end-on $L^2CuO_2H^+$ and (b) side-on $L^2CuO_2H^+$ isomers. Hydrogen atoms on L^2 are omitted for clarity. Distances are measured in Å. Pink stands for Cu; gray, C; blue, N; yellow, S; red, O; white, H.

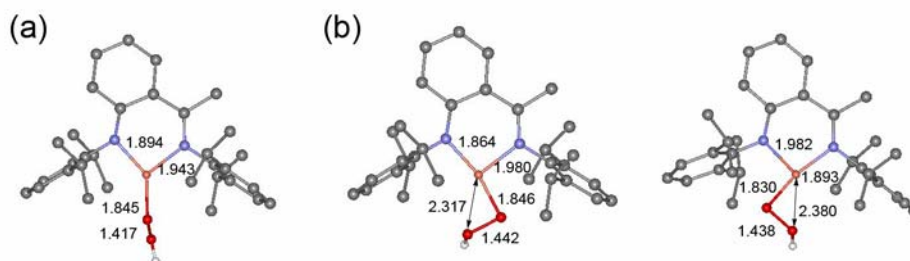


Figure S6. Key frontier orbitals showing partial occupation in the singlet end-on $L^1CuO_2H^+$ CASSCF wave function. Occupation numbers are shown in parentheses. Orange represents C, blue N, red O, white H, and yellow Cu.

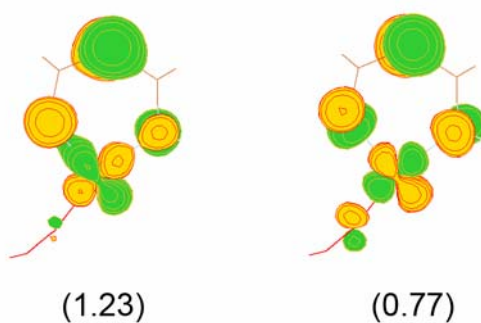
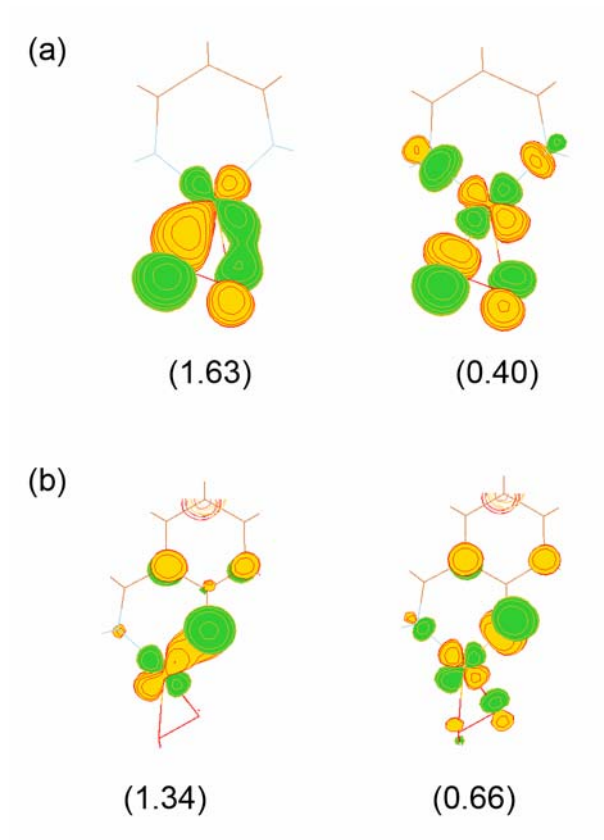


Figure S7. Key frontier orbitals showing partial occupation in the singlet side-on (a) $L^1\text{CuO}_2\text{H}^+$ and (b) $L^2\text{CuO}_2\text{H}^+$ CASSCF wave functions. Occupation numbers are shown in parentheses. Orange represents C, blue N, red O, white H, and yellow Cu.



Atomic Coordinates for Computed Structures.

β -diketiminato Cu/O structures

1. L^1CuO_2 side-on singlet

Cu	-.5758635651	-.5834236022	.0138496438
O	.1762387641	-2.2476472803	-.3865500627
O	-1.1777005354	-2.3189886612	-.3138871007
N	.8194449426	.7032326449	.2263509595
N	-2.0850856479	.5385699780	.3326851982
C	1.7246025666	2.9474128940	.6526827409
C	.5659826254	1.9794276976	.5146153160
C	-.7242778094	2.5014975336	.7071267402
C	-1.9571582723	1.8320355900	.6269944377
C	-3.2037747255	2.6544801764	.8858608956
C	2.1651049221	.2441474512	.0250621731
C	2.8873052804	-.2740816224	1.1219947780
C	4.1924022009	-.7274530326	.8990846160
C	4.7652091895	-.6832733689	-.3685337581
C	4.0274905262	-.1955084582	-1.4438128410
C	2.7193140991	.2700114296	-1.2744136551
C	2.2631048398	-.3972270764	2.5082129261
C	3.1339207510	.2238757262	3.6140111306
C	1.9357770380	-1.8715533544	2.8194907971
C	1.9080277891	.7250619328	-2.4831666200
C	1.4577475615	-.4957347417	-3.3114199014
C	2.6529903690	1.7453735654	-3.3609494204
C	-3.3790013479	-.0813641741	.2742682799
C	-3.9285534575	-.6507564366	1.4444403559
C	-5.1842268827	-1.2613103365	1.3532939045
C	-5.8719137478	-1.3216484561	.1441313723
C	-5.3005492110	-.7818092914	-1.0048094412
C	-4.0474670405	-.1601956187	-.9676578631
C	-3.1634079923	-.6679213942	2.7640776811
C	-2.6181245450	-2.0828519204	3.0466526765
C	-3.9937665759	-.1477080623	3.9494637355
C	-3.4120731190	.3580846023	-2.2540233516
C	-4.3418659616	1.2894267165	-3.0503112131
C	-2.9279451741	-.8202620589	-3.1228415080
H	1.3648781726	3.9472328913	.8994553135
H	2.3020353940	2.9996528932	-.2754902791
H	2.4169883747	2.6186943574	1.4340460179
H	-.7755307126	3.5546492085	.9467725579
H	-2.9443296412	3.6933832484	1.0941891586
H	-3.7657337522	2.2543227834	1.7355253229
H	-3.8767253540	2.6244509296	.0232573104
H	4.7642930904	-1.1301894690	1.7296793747
H	5.7800855536	-1.0389317837	-.5207933439
H	4.4713575832	-.1857543951	-2.4347237826
H	1.3157322819	.1496380738	2.4951773428
H	2.6156077419	.1721822163	4.5774278206
H	3.3591520564	1.2755914392	3.4081308763
H	4.0866318546	-.3039860095	3.7263627844
H	1.4153837808	-1.9553856310	3.7803059674
H	2.8510576156	-2.4706842777	2.8793682093
H	1.3032775412	-2.3044097213	2.0390171245
H	1.0038646608	1.2161767497	-2.1118752177
H	.8018545788	-.1840976774	-4.1321435307
H	.9210551111	-1.2169495046	-2.6882748384
H	2.3219547069	-1.0094499879	-3.7471025307
H	1.9998346046	2.0982669750	-4.1660818117
H	3.5412898690	1.3090015338	-3.8292769391
H	2.9763743181	2.6170584984	-2.7822931523
H	-5.6237099890	-1.7082546550	2.2399139646

H	-6.8457499647	-1.8001086803	.0949587003
H	-5.8299242269	-.8551950773	-1.9500983128
H	-2.3010199057	-.0032592653	2.6570441313
H	-1.9961216680	-2.0817707917	3.9489211657
H	-2.0191439213	-2.4472880236	2.2072990394
H	-3.4388280524	-2.7913974610	3.2044834073
H	-3.3769876489	-.1098510267	4.8536395288
H	-4.8488159113	-.7968483219	4.1645820329
H	-4.3797071846	.8598524731	3.7618607304
H	-2.5293224652	.9416143869	-1.9769348890
H	-3.8180179539	1.6879416458	-3.9256987549
H	-4.6792713735	2.1368832067	-2.4443380539
H	-5.2317657094	.7646495011	-3.4130172853
H	-2.3964655181	-.4531091402	-4.0081392372
H	-3.7745793739	-1.4256003833	-3.4654422780
H	-2.2576503836	-1.4742979327	-2.5577068941

2. $L^1\text{CuO}_2$ end-on singlet

Cu	-.9423573291	-.6007871627	.1056138644
O	-.7945812617	-3.3092063659	.6387233586
O	-.8018423473	-2.1306868433	1.1400556720
N	.5507774409	.2902579528	-.7569843158
N	-2.3454579617	.5995343359	-.4432107677
C	1.6311096499	2.1208255474	-1.9832189288
C	.4031511500	1.4481973901	-1.3984030308
C	-.8301872639	2.1012864483	-1.5799802570
C	-2.1093381004	1.7014583680	-1.1520420918
C	-3.2778046780	2.5911604723	-1.5304443228
C	1.8211718904	-.3453804551	-.6071531944
C	2.5768300809	-.1056917764	.5653939243
C	3.7940321732	-.7745146191	.7208138540
C	4.2559680774	-1.6661904488	-.2444798781
C	3.4900743920	-1.9116744134	-1.3801824791
C	2.2633082382	-1.2698879917	-1.5838636495
C	2.0566478305	.8069433422	1.6702226410
C	3.0909740664	1.8528935251	2.1195101426
C	1.5600489862	-.0256970363	2.8691711611
C	1.4262763997	-1.6087979153	-2.8129324824
C	.8649283317	-3.0409982977	-2.7153707702
C	2.2051317058	-1.4180018332	-4.1269775754
C	-3.6634788941	.2042174120	-.0586012711
C	-4.1729936385	.6017805252	1.2008755661
C	-5.4434131080	.1515248849	1.5742430268
C	-6.1904371629	-.6751671039	.7393106485
C	-5.6655322803	-1.0783203604	-.4860368806
C	-4.3999875540	-.6577550758	-.9062923129
C	-3.3426550431	1.4432035107	2.1639309741
C	-2.7530363200	.5567669019	3.2795138906
C	-4.1257165250	2.6247194956	2.7600569676
C	-3.8043441371	-1.1790693142	-2.2091091330
C	-4.7907772284	-1.1357139298	-3.3885103407
C	-3.2504077135	-2.6055055808	-2.0124954495
H	1.3686144529	3.0618764928	-2.4680078104
H	2.1176707287	1.4715446992	-2.7172147302
H	2.3711051496	2.3212693765	-1.2023136061
H	-.7899313262	3.0327200068	-2.1291697251
H	-2.9439743039	3.4514888444	-2.1117376756
H	-3.7961418485	2.9508022263	-.6358457984
H	-4.0147668523	2.0344909393	-2.1175246370
H	4.3862454818	-.6014487515	1.6146142739
H	5.2044079615	-2.1767478995	-.1055329506
H	3.8458696633	-2.6229592834	-2.1198780999
H	1.1958301056	1.3514773416	1.2720759682
H	2.6477104248	2.5304350583	2.8571059015

H	3.4457343250	2.4552596247	1.2768354922
H	3.9650291347	1.3873425737	2.5869277320
H	1.1125822123	.6236585563	3.6300621369
H	2.3888330066	-.5697946838	3.3355501240
H	.8127849016	-.7653011275	2.5663504299
H	.5731554891	-.9250609854	-2.8343750144
H	.2224514100	-3.2590599590	-3.5758729910
H	.2773326354	-3.1803985116	-1.8030177409
H	1.6743461060	-3.7794900890	-2.7062683819
H	1.5517470338	-1.6073339267	-4.9853464648
H	3.0516997732	-2.1089298813	-4.2004416680
H	2.5988086034	-.4004580248	-4.2197880464
H	-5.8514680831	.4461492667	2.5365215938
H	-7.1752868732	-1.0137654816	1.0474339239
H	-6.2461326999	-1.7388764985	-1.1225661618
H	-2.5024695646	1.8593255421	1.6008129557
H	-2.1091090421	1.1462136482	3.9417563308
H	-2.1577328576	-.2649886574	2.8689555609
H	-3.5490951230	.1134220346	3.8876824081
H	-3.4634329477	3.2458690538	3.3723356298
H	-4.9453913473	2.2892850969	3.4040936142
H	-4.5553659988	3.2574268343	1.9766299632
H	-2.9588498445	-.5354791104	-2.4687275071
H	-4.2808874076	-1.4219453631	-4.3142998449
H	-5.2094756286	-.1337264065	-3.5278190704
H	-5.6257460309	-1.8306058923	-3.2510368453
H	-2.7739075455	-2.9623613753	-2.9324051129
H	-4.0577800889	-3.3016438359	-1.7591812410
H	-2.5108117937	-2.6578721154	-1.2076741099

3. L^1CuO_2 end-on singlet \rightarrow L^1CuO_2 side-on singlet transition state

Cu	-1.0101241724	-.5478095149	.1887209534
O	-.9045348756	-2.9824519006	.5563341077
O	-.4128340112	-1.9639623879	1.2023700419
N	.5550664308	.2692470984	-.6689859108
N	-2.3728440878	.6110186823	-.4561218110
C	1.6531046729	2.0948615822	-1.8875991865
C	.4138433125	1.4244757435	-1.3211781064
C	-.8114400416	2.0834944992	-1.5489352583
C	-2.1117348155	1.6968274253	-1.1776445986
C	-3.2628821077	2.5702485156	-1.6313618390
C	1.8315056938	-.3645797913	-.5329179565
C	2.6590800144	-.0661729273	.5752624642
C	3.8896441310	-.7219704300	.6808656005
C	4.2953437276	-1.6577957663	-.2669869855
C	3.4563127428	-1.9649862344	-1.3337902848
C	2.2134940765	-1.3399214025	-1.4853443162
C	2.2183762488	.8949557859	1.6737842929
C	3.2489777006	2.0042216340	1.9456657790
C	1.8934890749	.1214819860	2.9672279996
C	1.3101059278	-1.7390469062	-2.6483871518
C	.8688303941	-3.2103613141	-2.5314302932
C	1.9707035904	-1.4726755691	-4.0136439369
C	-3.6905184953	.1790089449	-.1089924139
C	-4.1907621919	.4866360066	1.1816695645
C	-5.4390674471	-.0230193745	1.5500806343
C	-6.1763070149	-.8232199184	.6813953399
C	-5.6637760417	-1.1364550403	-.5745435864
C	-4.4190674122	-.6556606366	-.9935438517
C	-3.3943754031	1.3395880005	2.1632659743
C	-2.8752295570	.4851344343	3.3365019899
C	-4.1943041751	2.5484182164	2.6747258828
C	-3.8520329703	-1.0952819665	-2.3396875017
C	-4.8089726111	-.8077563109	-3.5090726003

C	-3.4637325363	-2.5866156817	-2.3024103542
H	1.3884646869	2.9862748137	-2.4574056481
H	2.2050695119	1.4104898060	-2.5374206696
H	2.3366053691	2.3837440397	-1.0834193595
H	-.7434594894	3.0055129833	-2.1109538319
H	-2.9015318706	3.4791673588	-2.1137773408
H	-3.8986682423	2.8460067946	-.7846794382
H	-3.8982968750	2.0306342700	-2.3410172553
H	4.5375159804	-.5029475221	1.5246688902
H	5.2557438542	-2.1550500740	-.1667016048
H	3.7665046348	-2.7107581191	-2.0602269496
H	1.2953688053	1.3787947528	1.3418396016
H	2.8664450929	2.7017990160	2.6983586666
H	3.4779914480	2.5755352137	1.0402923452
H	4.1909536712	1.5960258060	2.3265823718
H	1.4890784280	.7963675712	3.7299980874
H	2.7948021408	-.3470744092	3.3777486601
H	1.1656313676	-.6726092068	2.7794878520
H	.4084442071	-1.1227081829	-2.5956345583
H	.1725464172	-3.4644895395	-3.3386578023
H	.3746470074	-3.3991558762	-1.5735779315
H	1.7258600169	-3.8888917467	-2.6067059555
H	1.2823142263	-1.7276674244	-4.8266097181
H	2.8760597625	-2.0745270175	-4.1462335101
H	2.2521300620	-.4209325923	-4.1281304696
H	-5.8379434479	.2058179708	2.5340947755
H	-7.1427593909	-1.2127128364	.9870998239
H	-6.2348976021	-1.7793709121	-1.2380350033
H	-2.5182831569	1.7231925013	1.6344406208
H	-2.2764803390	1.0956250938	4.0217217879
H	-2.2482141650	-.3397042783	2.9830750736
H	-3.7016761892	.0495706165	3.9084497278
H	-3.5698477737	3.1686884462	3.3264210223
H	-5.0681683187	2.2372170355	3.2567871353
H	-4.5500833020	3.1730652430	1.8491845509
H	-2.9346472180	-.5270781051	-2.5179480277
H	-4.3369134636	-1.0778608913	-4.4596881873
H	-5.0846169859	.2507194772	-3.5562461866
H	-5.7342241469	-1.3877234708	-3.4263213616
H	-2.9907442489	-2.8831728108	-3.2453352140
H	-4.3466982275	-3.2184467793	-2.1559267271
H	-2.7651225878	-2.7978222570	-1.4869007011

4. $L^1\text{CuO}_2$ side-on triplet

Cu	-.5737837235	-.6010130188	.0219552473
O	.1681039121	-2.4613926505	-.3839657700
O	-1.1324312075	-2.5279637244	-.3152140814
N	.8421810809	.7112239409	.2200482177
N	-2.1099885563	.5413824331	.3362336967
C	1.7205135492	2.9676824886	.6369459492
C	.5723123158	1.9852987951	.5034939678
C	-.7256473765	2.4973633335	.6897117647
C	-1.9665613209	1.8369827550	.6160850202
C	-3.2040450327	2.6766679921	.8695012617
C	2.1874699867	.2592724253	.0217578825
C	2.9083299453	-.2792634324	1.1119052527
C	4.1983830510	-.7693287419	.8793095856
C	4.7655264423	-.7390983918	-.3913838760
C	4.0367078228	-.2208326304	-1.4584856810
C	2.7437966161	.2826713847	-1.2788481673
C	2.2988920989	-.3784887471	2.5072343906
C	3.1796174199	.2772765229	3.5854087315
C	1.9923123040	-1.8450959836	2.8680565355
C	1.9510243670	.7901089111	-2.4802789146

C	1.5007895177	-.3851539403	-3.3706208080
C	2.7200646946	1.8360633147	-3.3055703840
C	-3.4033651815	-.0721650609	.2784889788
C	-3.9553715296	-.6463474395	1.4466184119
C	-5.1922658598	-1.2925860619	1.3483658890
C	-5.8677926696	-1.3810314939	.1342000413
C	-5.3032385066	-.8253510386	-1.0104489784
C	-4.0684780801	-.1685528410	-.9654000396
C	-3.2139414766	-.6196039394	2.7802295791
C	-2.6733360990	-2.0196485509	3.1327234195
C	-4.0718576012	-.0612095044	3.9287861223
C	-3.4516498706	.3813871110	-2.2482954506
C	-4.3970615109	1.3331502688	-3.0019021937
C	-2.9842611096	-.7654933286	-3.1657442829
H	1.3547820278	3.9660430345	.8797385583
H	2.2956429656	3.0213742839	-.2926797184
H	2.4174172438	2.6488298453	1.4179495453
H	-.7769335446	3.5530117924	.9223965189
H	-2.9380271898	3.7166014888	1.0627083880
H	-3.7652123139	2.2933166306	1.7273310972
H	-3.8814482078	2.6404371919	.0108859445
H	4.7641463879	-1.1888079582	1.7062891641
H	5.7680799193	-1.1248181686	-.5512661958
H	4.4767095388	-.2138615102	-2.4515290729
H	1.3464309273	.1587812565	2.4917410111
H	2.6793443906	.2403846108	4.5590736608
H	3.3869704972	1.3266543668	3.3520259915
H	4.1416177268	-.2354143745	3.6903116401
H	1.4902345000	-1.9060037915	3.8401028493
H	2.9120410057	-2.4372208300	2.9267389438
H	1.3471023623	-2.3114756667	2.1173666566
H	1.0474557307	1.2754556933	-2.1011277464
H	.8658772916	-.0286423270	-4.1894635403
H	.9378661600	-1.1266017294	-2.7957484152
H	2.3640754369	-.8964003038	-3.8105046934
H	2.0855757559	2.2254386764	-4.1089421720
H	3.6143454256	1.4096993433	-3.7722153133
H	3.0390675779	2.6812342140	-2.6870337350
H	-5.6284854293	-1.7429780521	2.2352565440
H	-6.8264347972	-1.8883508027	.0788355890
H	-5.8254183942	-.9109027244	-1.9590717252
H	-2.3510411335	.0427239994	2.6667679475
H	-2.0788924617	-1.9832843751	4.0525274180
H	-2.0435810989	-2.4163450303	2.3308227253
H	-3.4934596051	-2.7288802683	3.2892012865
H	-3.4771557824	.0092264434	4.8458146659
H	-4.9317852308	-.7040296911	4.1443321964
H	-4.4542522894	.9380756189	3.6965848858
H	-2.5646634882	.9568434425	-1.9689120855
H	-3.8923660889	1.7534963721	-3.8784304077
H	-4.7200700721	2.1646431426	-2.3671127801
H	-5.2957228431	.8175690567	-3.3566389697
H	-2.4766043649	-.3683423046	-4.0519283644
H	-3.8337562359	-1.3677986234	-3.5058844805
H	-2.2936657153	-1.4351629148	-2.6444058550

5. L^1CuO_2 end-on triplet

Cu	-.9525798912	-.6980306113	-.0280093359
O	-1.0239781749	-3.5917464299	.3124613461
O	-.9747805089	-2.4372421603	.8076578858
N	.5968542129	.2491365252	-.7328598537
N	-2.3988284141	.5136154998	-.4817688378
C	1.6214187784	2.1202435189	-1.9526134946
C	.4120685928	1.3962360655	-1.3881442996

C	-.8419704913	2.0097086803	-1.5924239920
C	-2.1316625544	1.6211780847	-1.1742282971
C	-3.2763088141	2.5493006059	-1.5384276677
C	1.9030911407	-.3026519665	-.5332569269
C	2.6179612495	.0208491251	.6461032804
C	3.8677281112	-.5716718275	.8545598554
C	4.4060129941	-1.4671531313	-.0656470021
C	3.6851705326	-1.7906278649	-1.2111184919
C	2.4303487106	-1.2260716505	-1.4670551980
C	2.0325353956	.9480232192	1.7069199778
C	2.9968717787	2.0754718061	2.1139057575
C	1.5826584075	.1411217732	2.9405378311
C	1.6522643312	-1.6499911063	-2.7093738027
C	1.1972269725	-3.1189376655	-2.6017803268
C	2.4473375737	-1.4241336932	-4.0082396991
C	-3.7226321438	.1875415315	-.0502137934
C	-4.1427816296	.5914396582	1.2398533434
C	-5.4102681202	.1995772800	1.6825432264
C	-6.2466592680	-.5748847272	.8823356688
C	-5.8156477778	-.9755820929	-.3790332591
C	-4.5563312975	-.6105224707	-.8680516326
C	-3.2143797737	1.3790366025	2.1593747019
C	-2.5488697884	.4394404764	3.1845099680
C	-3.9120495345	2.5521918923	2.8673302222
C	-4.0928577107	-1.1158022557	-2.2310207318
C	-5.0943275037	-.7996064346	-3.3555346345
C	-3.7918217231	-2.6270885698	-2.1827928245
H	1.3284559513	3.0430295682	-2.4547096743
H	2.1562596736	1.4871717611	-2.6670590039
H	2.3332908686	2.3645837218	-1.1581237339
H	-.8071808763	2.9352244217	-2.1525124142
H	-2.9178544140	3.4199655803	-2.0888538726
H	-3.7978336386	2.8929262126	-.6395515633
H	-4.0188710989	2.0290270712	-2.1513793527
H	4.4260689020	-.3322700215	1.7552493544
H	5.3788919752	-1.9156884906	.1135353981
H	4.1008920506	-2.5021496974	-1.9189038478
H	1.1412727633	1.4176246187	1.2822202692
H	2.5071682807	2.7577796232	2.8170322468
H	3.3204017586	2.6592492858	1.2460882636
H	3.8947008042	1.6870232646	2.6063630097
H	1.1058619956	.7948060818	3.6794826141
H	2.4360838874	-.3483795904	3.4225861317
H	.8675948954	-.6404199036	2.6644829709
H	.7517111788	-1.0319357344	-2.7639028976
H	.5920354871	-3.3985609310	-3.4714053857
H	.6005067272	-3.2892895003	-1.7010136570
H	2.0575596569	-3.7960353640	-2.5609290817
H	1.8348523592	-1.6819817657	-4.8789464266
H	3.3480544062	-2.0461443920	-4.0435948138
H	2.7612829287	-.3807154279	-4.1130869487
H	-5.7464538869	.4996234713	2.6706768201
H	-7.2280953256	-.8688235938	1.2431057514
H	-6.4667564591	-1.5903197953	-.9936727822
H	-2.4163347396	1.8002020116	1.5418771176
H	-1.8349948078	.9877123381	3.8093349117
H	-2.0108196403	-.3763678241	2.6910583729
H	-3.2982099179	-.0139087367	3.8428156648
H	-3.1808230218	3.1404842881	3.4318626691
H	-4.6718498514	2.2102247353	3.5779669082
H	-4.4019610945	3.2185039662	2.1500611933
H	-3.1567459323	-.6049112679	-2.4735055357
H	-4.6851979948	-1.1061944907	-4.3241061601
H	-5.3185206668	.2707772751	-3.4057089073

H	-6.0417045316	-1.3312982028	-3.2177993851
H	-3.4049499659	-2.9744598255	-3.1474241001
H	-4.6978509814	-3.2002340720	-1.9569421106
H	-3.0520091980	-2.8663727539	-1.4133735202
6. L ¹ CuO ₂ H ⁺ side-on singlet			
Cu	.1138449054	-.9000304850	.0770233636
O	.0638555829	-3.1886062970	.3431853025
O	-1.0598128097	-2.3100481589	.1585101557
N	1.6241818477	.1950025205	.2433410609
N	-1.2377987257	.4838091902	-.2500335075
C	2.8939118010	2.2957960993	.1970280123
C	1.5980085602	1.5199071435	.1966384453
C	.3929358584	2.2492231764	.1373586715
C	-.9108678896	1.7660958213	-.0195730855
C	-2.0289158069	2.7903969024	-.0006387789
C	2.7959394275	-.5986680122	.0892242245
C	3.2818414073	-1.2913936048	1.2328400901
C	4.4317266344	-2.0697305528	1.0794116914
C	5.0623749587	-2.1901347611	-.1562960593
C	4.5489863996	-1.5353392855	-1.2774171219
C	3.4135245686	-.7311330818	-1.1885030854
C	2.6265323514	-1.1636501550	2.6023166244
C	3.5090836442	-.3424568108	3.5633034825
C	2.2792803633	-2.5381192513	3.2046154294
C	2.8075111882	-.1149379755	-2.4452064328
C	1.9450562470	-1.1621099447	-3.1826644913
C	3.8552512879	.4871932807	-3.3965260337
C	-2.5485301324	-.0176732857	-.2100952346
C	-3.2948549905	-.0720559556	1.0078140928
C	-4.6044074965	-.5403586931	.93777301580
C	-5.1593756609	-.9689879619	-.2705339641
C	-4.3989851611	-.9692239047	-1.4392414794
C	-3.0768324362	-.5298239902	-1.4341076981
C	-2.6794771145	.2608542595	2.3609837497
C	-2.3839782064	-1.0419943090	3.1387553155
C	-3.5515700980	1.2060950946	3.2060884046
C	-2.2552397771	-.5465561536	-2.7136114464
C	-2.7671820385	.5001217420	-3.7231970904
C	-2.2135114158	-1.9523819788	-3.3401498436
H	.1096151214	-3.6674933859	-.5049299486
H	2.7367047985	3.3016920688	.5889607261
H	3.2803733677	2.3905720876	-.8236683909
H	3.6563024251	1.7889081380	.7919735888
H	.4903793953	3.3248461067	.1982772915
H	-1.6307027935	3.7871717000	-.1928516968
H	-2.5199725406	2.8027825481	.9766785984
H	-2.7874852726	2.5529113527	-.7491620217
H	4.8416772896	-2.5876088888	1.9399191921
H	5.9529815006	-2.8034428536	-.2517996984
H	5.0429690638	-1.6602029922	-2.2345750427
H	1.6878218482	-.6143171581	2.4757427077
H	3.0089023324	-.2266780025	4.5296896738
H	3.7170270460	.6570365201	3.1683228735
H	4.4690600805	-.8376672940	3.7400545500
H	1.7520873700	-2.4046407088	4.1542504582
H	3.1767461361	-3.1296946802	3.4097044739
H	1.6358462351	-3.1156803992	2.5350744516
H	2.1382461786	.6972367588	-2.1459550013
H	1.4740623219	-.7209850693	-4.0666631800
H	1.1473134479	-1.5550031162	-2.5398559421
H	2.5548616174	-2.0107493669	-3.5084728548
H	3.3555413379	1.0174582426	-4.2123575903
H	4.4861514573	-.2822914099	-3.8511452200

H	4.5103952562	1.1957534898	-2.8808039063
H	-5.2007359024	-.5929424519	1.8419896602
H	-6.1844852626	-1.3254058514	-.2946907514
H	-4.8408169956	-1.3249600390	-2.3640212502
H	-1.7195424693	.7595229383	2.1920173606
H	-1.8644610748	-.8119413537	4.0745337641
H	-1.7703465259	-1.7263353500	2.5476888478
H	-3.3143307299	-1.5609833644	3.3899103979
H	-3.0218048503	1.4773404751	4.1239759703
H	-4.4907708115	.7299640066	3.5022485751
H	-3.8027307716	2.1290375744	2.6740824392
H	-1.2300902592	-.2700005147	-2.4520704624
H	-2.1379520771	.5011483001	-4.6186639672
H	-2.7534192488	1.5092158964	-3.2993426902
H	-3.7934657568	.2822323121	-4.0350172791
H	-1.5375725228	-1.9587426169	-4.2011110678
H	-3.1983268511	-2.2707802906	-3.6952439389
H	-1.8627905016	-2.6918564072	-2.6143677365

7. $L^1\text{CuO}_2\text{H}^+$ end-on singlet

Cu	-.4548859826	.2738169294	.0083886634
O	-2.7584463657	-.7542230048	1.0019469870
O	-2.1783448095	.4592468971	.6006673661
N	.6167028406	-.6566739906	1.3798036126
N	.9536849230	.6492784417	-1.1736550639
C	2.7283132117	-.9091722916	2.6229274218
C	1.9495423449	-.5153658987	1.3836433270
C	2.7025333314	-.0772745930	.2816942302
C	2.2372703963	.3912585631	-.9613094734
C	3.2429918530	.6143381271	-2.0657770260
C	-.1369718407	-1.0372392471	2.5018334893
C	-.3157530465	-.1691531910	3.6214781060
C	-1.0558041452	-.6506843102	4.6971396007
C	-1.6145601968	-1.9347065811	4.6832323903
C	-1.4720228352	-2.7547620963	3.5692078785
C	-.7625074080	-2.3228303573	2.4437616915
C	.1906732991	1.2687406518	3.6316252119
C	.9563856953	1.6260396546	4.9182947336
C	-.9829747890	2.2481034344	3.4101830516
C	-.5639782875	-3.2417985521	1.2483630935
C	-1.8163721566	-4.0599577230	.8974871478
C	.6474069747	-4.1724461514	1.4780585755
C	.3450255548	.9300631485	-2.4192326252
C	-.1883186108	2.2419905013	-2.6006302050
C	-.8328223631	2.5194025466	-3.8055662185
C	-.9767811881	1.5395210446	-4.7862754989
C	-.4797395238	.2509035925	-4.5796575023
C	.1868591822	-.0896309195	-3.4045189787
C	-.0469500296	3.3241784680	-1.5371831536
C	-1.4150704147	3.6557153943	-.9075560411
C	.6343988081	4.5912155809	-2.0855879554
C	.6155275721	-1.5313388809	-3.1604388298
C	1.4162691112	-2.1228047348	-4.3342322927
C	-.6165609303	-2.4049006154	-2.8407191682
H	-3.2091226465	-.5000787539	1.8268971467
H	3.7581641571	-1.1559230296	2.3621083790
H	2.2693893824	-1.7624905957	3.1252481109
H	2.7525361259	-.0788092115	3.3351104501
H	3.7772993792	-.1386391907	.3921274105
H	4.2293133485	.8228475828	-1.6483922281
H	2.9402620449	1.4418319901	-2.7105749992
H	3.3273797173	-.2815075817	-2.6897905526
H	-1.2093255192	-.0178582329	5.5648418738
H	-2.1750498366	-2.2852890924	5.5444851968

H	-1.9257299329	-3.7391629791	3.5692734363
H	.8784496298	1.3967614309	2.7899655956
H	1.3794629501	2.6313509912	4.8333862446
H	1.7746036487	.9279416005	5.1202532473
H	.2984510847	1.6243742470	5.7923937496
H	-.6106226736	3.2754712669	3.3462134430
H	-1.6890272225	2.1998243796	4.2457157348
H	-1.5307750105	2.0167925806	2.4922701716
H	-.3287649384	-2.6090272674	.3870880357
H	-1.6447904767	-4.6104775418	-.0322506771
H	-2.6852590298	-3.4127833092	.7548696216
H	-2.0557950340	-4.8007287843	1.6665803379
H	.8024516825	-4.8124941320	.6040749878
H	.4828248597	-4.8206615582	2.3445451587
H	1.5695578134	-3.6095975908	1.6500148911
H	-1.2286408046	3.5139393405	-3.9819907989
H	-1.4879934828	1.7760441181	-5.7141246210
H	-.6280204504	-.5024577692	-5.3458754699
H	.5965447218	2.9329098902	-.7437239226
H	-1.2932790608	4.4010649222	-.1152540747
H	-1.8934078734	2.7713764977	-.4735299231
H	-2.1032044896	4.0683466096	-1.6522091005
H	.7909120134	5.3102159582	-1.2758081318
H	.0238152511	5.0836440645	-2.8485018827
H	1.6082234285	4.3633967219	-2.5299055214
H	1.2615324652	-1.5564491928	-2.2780061903
H	1.7740384851	-3.1238413785	-4.0754642858
H	2.2838883924	-1.5050716596	-4.5863238454
H	.8041066886	-2.2194225090	-5.2358019305
H	-.3069198961	-3.4299086571	-2.6129822061
H	-1.3045178923	-2.4408056164	-3.6911568230
H	-1.1757850588	-2.0178787235	-1.9817459077

8. $L^1CuO_2H^+$ end-on singlet \rightarrow $L^1CuO_2H^+$ side-on singlet transition state

Cu	-.4703934119	-.0176285872	.1769449099
O	-2.8675510791	.4384097036	.8564398299
O	-2.2668299699	-.1170462076	-.3131707743
N	.7661603121	-.7170169919	1.4116025388
N	.8536935180	.6817718017	-1.1012645806
C	2.8959764024	-.8624737415	2.6197637136
C	2.0786062515	-.5041188222	1.4009841563
C	2.7368964645	.0013390936	.2717084155
C	2.1573330428	.4547615921	-.9296081456
C	3.1106898291	.7203274195	-2.0775795430
C	-.0475619914	-1.0533067558	2.5017283396
C	-.2583284327	-.1546862943	3.5972235779
C	-1.0422493118	-.6083707201	4.6535564517
C	-1.6240616506	-1.8786842336	4.6334518006
C	-1.4736290742	-2.7166123923	3.5275598520
C	-.7137738367	-2.3238429369	2.4298341462
C	.2454250200	1.2825050328	3.5854399060
C	.9996694337	1.6628020610	4.8720271447
C	-.9342763642	2.2517517184	3.3449610340
C	-.5282100951	-3.2426802276	1.2311930479
C	-1.8013372678	-4.0256278882	.8724138278
C	.6698929663	-4.1911950090	1.4450399721
C	.2740897290	.9591612894	-2.3646613367
C	-.2274331009	2.2761365313	-2.5751579997
C	-.8243278572	2.5607180782	-3.8024499175
C	-.9513131518	1.5822807969	-4.7875365918
C	-.4657256285	.2942732464	-4.5644344039
C	.1534704691	-.0520670292	-3.3634828616
C	-.0966703748	3.3660884292	-1.5210219386
C	-1.4733334710	3.7177356035	-.9228249989

C	.6055738610	4.6208763470	-2.0744562204
C	.5872307450	-1.4950166576	-3.1369195458
C	1.4072097573	-2.0607692000	-4.3122861477
C	-.6430512792	-2.3849136969	-2.8560217239
H	-3.6776697008	.8421715781	.5042977255
H	3.9212149389	-1.1038229877	2.3353557951
H	2.4569483082	-1.7117930076	3.1477885960
H	2.9294859264	-.0174349140	3.3147768102
H	3.8178587026	.0148481368	.3148397979
H	4.1089123407	.9394489879	-1.6957107155
H	2.7675692107	1.5490402243	-2.6989162700
H	3.1853098981	-.1664880821	-2.7156944707
H	-1.2184743236	.0403958619	5.5046713248
H	-2.2189700727	-2.2086212713	5.4794822422
H	-1.9594778807	-3.6854021338	3.5251469360
H	.9370851589	1.4007906609	2.7451801671
H	1.4099425412	2.6725074007	4.7786041378
H	1.8251011980	.9768290826	5.0842893099
H	.3358473474	1.6609541084	5.7416491579
H	-.5656028254	3.2785016514	3.2572226047
H	-1.6396036001	2.2182361613	4.1814719612
H	-1.4897535494	2.0011741743	2.4364804170
H	-.2828582790	-2.6131826851	.3696435070
H	-1.6452186526	-4.5641814665	-.0669071635
H	-2.6569498557	-3.3571173686	.7414428378
H	-2.0566532875	-4.7715057259	1.6312417109
H	.8110153868	-4.8223604681	.5622489710
H	.5035027285	-4.8456985445	2.3063058472
H	1.5986090030	-3.6380066581	1.6147935663
H	-1.1953609681	3.5616724578	-3.9958852703
H	-1.4309649584	1.8224552674	-5.7313869878
H	-.5814820348	-.4552269909	-5.3397321140
H	.5249587577	2.9749116481	-.7108630212
H	-1.3608585196	4.4642054220	-.1302075066
H	-1.9594652885	2.8345713016	-.4972251268
H	-2.1402342516	4.1339371504	-1.6847384767
H	.7597453294	5.3499082503	-1.2733129330
H	.0108429054	5.1098168151	-2.8522513821
H	1.5822392557	4.3783331914	-2.5049388287
H	1.2235475150	-1.5325698454	-2.2474264204
H	1.7795862278	-3.0588428455	-4.0631114703
H	2.2662084678	-1.4277191118	-4.5560579751
H	.8026113637	-2.1592699168	-5.2188061258
H	-.3261096623	-3.4088527064	-2.6326658923
H	-1.3034113113	-2.4198689400	-3.7282627606
H	-1.2331804640	-2.0107649547	-2.0133997918

9. $L^1\text{CuO}_2\text{H}^+$ side-on triplet

Cu	.0552083774	-1.0169292916	.0587008731
O	.2899017481	-3.1874145723	.2330632173
O	-1.0027816724	-2.5650994615	.0781537098
N	1.6478732995	.1089344457	.1175837462
N	-1.2997577685	.4585327019	-.0427070801
C	2.8987912006	2.2307820752	.1656290031
C	1.6204077356	1.4251188892	.1525635443
C	.3885210802	2.1578099263	.1786545713
C	-.9736005323	1.7290353441	.0960092132
C	-2.0273490123	2.8112108662	.1493667882
C	2.8933656690	-.6139411183	.0247080121
C	3.4074843816	-1.2153431925	1.1944786077
C	4.5949912886	-1.9476548763	1.0758663039
C	5.2332625933	-2.0969516966	-.1517601311
C	4.6885586765	-1.5163835521	-1.2957472295
C	3.5121077532	-.7627002775	-1.2404810148

C	2.7275648651	-1.0783044375	2.5536166589
C	3.6118410309	-.3105423316	3.5550727197
C	2.3167079088	-2.4509120533	3.1211174013
C	2.8770362861	-.2255827349	-2.5206544487
C	2.0026020082	-1.3141453421	-3.1752291780
C	3.8986327224	.3263187891	-3.5290184819
C	-2.6556079218	.0147591211	-.1104697477
C	-3.4544818908	-.0285044639	1.0609125796
C	-4.7603245968	-.5048709769	.9277753416
C	-5.2599288892	-.9219749738	-.3042642087
C	-4.4416015345	-.9073978190	-1.4319488157
C	-3.1186587576	-.4669562793	-1.3591783344
C	-2.8920208977	.2726201011	2.4463541135
C	-2.5927257432	-1.0502451722	3.1860564264
C	-3.8071215254	1.1787778013	3.2881028916
C	-2.2377116951	-.4643717465	-2.6032453104
C	-2.6790211749	.6215248019	-3.6052082625
C	-2.1844226188	-1.8510539608	-3.2687117071
H	.4078086434	-3.6702533820	-.6077322419
H	2.7122695693	3.2602710391	.4718486214
H	3.3490775784	2.2489319658	-.8330479669
H	3.6327086659	1.7803788968	.8384189773
H	.5119618435	3.2322243578	.2499755747
H	-1.6197743875	3.7688695440	-.1774804476
H	-2.3890473697	2.9331863023	1.1758031818
H	-2.8865437479	2.5504910248	-.4704982288
H	5.0242864106	-2.4063821249	1.9606374534
H	6.1530427017	-2.6693374539	-.2206296114
H	5.1870491209	-1.6556954778	-2.2489239498
H	1.8103242799	-.4913102730	2.4187744398
H	3.0811612963	-.1766000732	4.5026554831
H	3.8904855825	.6803390391	3.1789013797
H	4.5367518549	-.8580799790	3.7658105287
H	1.7853559335	-2.3219705315	4.0687183788
H	3.1927369809	-3.0777531876	3.3172365688
H	1.6635782164	-2.9927010699	2.4312865483
H	2.2115648792	.6037121264	-2.2562005070
H	1.5125403760	-.9293905335	-4.0754100503
H	1.2198815332	-1.6669636656	-2.4921208075
H	2.6086788932	-2.1802333354	-3.4607971609
H	3.3787533403	.8102125639	-4.3609303656
H	4.5208365116	-.4652627510	-3.9563043180
H	4.5621180426	1.0625274638	-3.0698143304
H	-5.3936195575	-.5686598140	1.8065644705
H	-6.2832791240	-1.2755012488	-.3810748046
H	-4.8367849753	-1.2471964810	-2.3833789853
H	-1.9359319722	.7932932845	2.3272564097
H	-2.1010088739	-.8494557630	4.1436614230
H	-1.9503742806	-1.7063163686	2.5898477394
H	-3.5190030117	-1.5961583077	3.3911198904
H	-3.3184884728	1.4300436224	4.2342153994
H	-4.7511169025	.6838991167	3.5335789230
H	-4.0487790831	2.1128320009	2.7705241715
H	-1.2159523198	-.2155476481	-2.2911959111
H	-2.0132656575	.6334687635	-4.4745209546
H	-2.6655489153	1.6187598106	-3.1533439975
H	-3.6962766305	.4346596297	-3.9643375642
H	-1.4759307503	-1.8405624002	-4.1043177709
H	-3.1585398043	-2.1452707386	-3.6709464609
H	-1.8713678263	-2.6149627187	-2.5500749029
10. L ¹ CuO ₂ H ⁺ end-on triplet			
Cu	-.5457138474	.2101667185	.1514892111
O	-3.0975783194	-.7526189601	.0666770149

O	-2.3961559751	.4365309278	.2459919437
N	.6989970909	-.4816135916	1.5549193750
N	.8315696935	.4541386715	-1.2332798204
C	2.8865658122	-1.2141399398	2.4542647446
C	2.0034926075	-.6146819971	1.3828920757
C	2.6570944295	-.1803493352	.1930479874
C	2.1250580585	.3160859296	-1.0423494999
C	3.1113553716	.6647614362	-2.1334794767
C	.0060824690	-1.0249009309	2.6728867082
C	-.6052437830	-.1076126489	3.5700017368
C	-1.3139395166	-.6289078195	4.6528355317
C	-1.4570448988	-2.0043610629	4.8261438124
C	-.8952254020	-2.8873492699	3.9055084238
C	-.1515316301	-2.4318220365	2.8150652552
C	-.4376088837	1.3994743466	3.4179477991
C	.5314685194	1.9581341815	4.4795953187
C	-1.7857382750	2.1401498047	3.4449070729
C	.3265510767	-3.4303742080	1.7649944844
C	-.8683781297	-3.9297976838	.9244222088
C	1.0965867132	-4.6160594095	2.3732687355
C	.2978185001	.9506330877	-2.4762648420
C	.1058783266	2.3426629477	-2.6327184394
C	-.4870989830	2.7817685744	-3.8203428097
C	-.8779307518	1.8819916681	-4.8093547838
C	-.6929777919	.5153617560	-4.6204608884
C	-.1129112528	.0141534329	-3.4502121179
C	.4485681348	3.3324030415	-1.5228517219
C	-.8191572168	3.7057270338	-.7257419932
C	1.1602527822	4.5954407028	-2.0347635688
C	.0321278782	-1.4922249475	-3.2509715288
C	.8201013014	-2.1597589013	-4.3929133487
C	-1.3463538882	-2.1594029370	-3.0704702443
H	-4.0227971413	-.4655060258	.1784616373
H	3.8657854421	-.7311589011	2.4531085507
H	3.0447741712	-2.2813551429	2.2684174322
H	2.4345306606	-1.1119623645	3.4414839763
H	3.7370933461	-.2719372315	.2147504963
H	4.1385446875	.4826626382	-1.8169684610
H	3.0111259972	1.7156302260	-2.4192121873
H	2.9080415493	.0725885427	-3.0307036350
H	-1.7575393689	.0488322360	5.3745970315
H	-2.0164853618	-2.3891929169	5.6729456659
H	-1.0506108619	-3.9536351410	4.0313461588
H	.0197260453	1.5887032828	2.4394545498
H	.6815008690	3.0320704917	4.3326521319
H	1.5088583939	1.4683346853	4.4309722757
H	.1352347679	1.8087317083	5.4886958124
H	-1.6279104734	3.2096143191	3.2742131776
H	-2.2893929757	2.0351179667	4.4103914670
H	-2.4584324546	1.7644898065	2.6681014340
H	1.0046653733	-2.9173066158	1.0765549963
H	-.5206286725	-4.5935727637	.1264174282
H	-1.4171402521	-3.0998183615	.4685996925
H	-1.5739103591	-4.4912700547	1.5450559211
H	1.4906824309	-5.2544160402	1.5767933419
H	.4503244270	-5.2396087391	2.9980177553
H	1.9356552922	-4.2855928075	2.9932633389
H	-.6497420083	3.8435803263	-3.9722820680
H	-1.3330876548	2.2465763539	-5.7246299385
H	-1.0083246361	-.1781576593	-5.3934823135
H	1.1360251341	2.8396469835	-.8261448688
H	-.5685139102	4.3648142424	.1118846593
H	-1.3301117952	2.8222625861	-.3255204341
H	-1.5383151437	4.2282903020	-1.3646826303

H	1.4717069089	5.2178161619	-1.1903802835
H	.5051396580	5.2063719339	-2.6629681210
H	2.0504165191	4.3478861815	-2.6213910723
H	.5961413892	-1.6613779173	-2.3271419245
H	.9629434364	-3.2240151373	-4.1818383800
H	1.8072810355	-1.7050815445	-4.5255054203
H	.2897786899	-2.0830923382	-5.3470543950
H	-1.2279525318	-3.2306649905	-2.8775540163
H	-1.9583766463	-2.0475752284	-3.9713637371
H	-1.9007519711	-1.7205694816	-2.2348295219

11. $L^1\text{CuO}_2\text{H}_2^{2+}$ end-on singlet

H	-3.0254150550	-1.5778717909	1.5459890792
C	2.8235354578	.3785072151	-2.0985486882
C	-.6441013240	-1.2270311851	2.4024633475
C	-.7775652194	-.2175033355	3.3977572749
C	-1.6880997499	-.4508880496	4.4367733888
C	-2.4560457984	-1.6088412071	4.4920536753
C	-2.3290303878	-2.5901653227	3.4977996135
C	-1.4283965433	-2.4334583167	2.4380415944
C	-.0667977023	1.1283906049	3.3327206777
C	.7084590508	1.4433202583	4.6275102693
C	-1.0781458470	2.2527678813	3.0166758841
C	-1.1711843384	-3.5654925560	1.4449356766
C	-2.3791722905	-4.4860693429	1.2130689923
C	.0449907474	-4.4031694803	1.9050632556
C	-.1650523674	.7037689596	-2.3360435995
C	-.9275573450	1.9444335510	-2.3136854047
C	-1.6242973438	2.2875790518	-3.4649514421
C	-1.6211464123	1.4491204709	-4.5815687918
C	-.9391828289	.2199040664	-4.5737880986
C	-.2075224288	-.1946333793	-3.4748819010
C	-.8714736891	2.8974112975	-1.1334399321
C	-2.2736312497	3.3661360468	-.7005246377
C	.0479021529	4.0998622813	-1.4504532144
C	.3738468543	-1.5980849539	-3.4229270821
C	1.1725270787	-1.9639437858	-4.6874004446
C	-.7620791711	-2.6173326258	-3.1700552119
C	2.2813172910	-1.2483905400	2.5499870932
C	1.4973091717	-.9240332667	1.2973790127
C	2.2642722117	-.5169772934	.1738508782
C	1.8161632596	.0577093621	-1.0174367704
H	-4.3892289796	-.9886722045	.8913886027
H	3.1721688709	-1.8234437945	2.2839418989
H	1.6880919925	-1.8139014791	3.2679919766
H	2.6235295500	-.3270684568	3.0320782756
H	3.3371570482	-.6325917682	.2703745774
H	3.7720575494	.6708317081	-1.6433960872
H	2.4697623722	1.1896912072	-2.7376271455
H	3.0148965327	-.4961329867	-2.7278322662
H	-1.8093943316	.2998586644	5.2099886338
H	-3.1519186399	-1.7594959899	5.3112981226
H	-2.9088897467	-3.5029393558	3.5767106925
H	.6540580866	1.1060992830	2.5100340820
H	1.2709228743	2.3728788011	4.5041954357
H	1.4130946877	.6495903851	4.8904818757
H	.0346932647	1.5832617010	5.4774715164
H	-.5520737414	3.2052606932	2.9038056225
H	-1.8044848326	2.3703708862	3.8263974623
H	-1.6353496663	2.0515915698	2.0958894224
H	-.9037773114	-3.1072695022	.4835209463
H	-2.1486668145	-5.1913420809	.4108596719
H	-3.2795834562	-3.9381111988	.9163562574
H	-2.6179089502	-5.0815667299	2.0988899604

H	.2403014559	-5.2028350216	1.1854065006
H	-.1503969597	-4.8645909478	2.8776480391
H	.9526945237	-3.8012224048	1.9929107652
H	-2.1688220969	3.2237975107	-3.5054953663
H	-2.1712242965	1.7432364384	-5.4704104852
H	-1.0083519674	-.4208393089	-5.4454159824
H	-.4199923681	2.3667871901	-.2889127384
H	-2.1865491112	3.9845847553	.1971984836
H	-2.9293606062	2.5199896744	-.4715683582
H	-2.7597829472	3.9768450469	-1.4660138218
H	.1180971633	4.7487266229	-.5730117139
H	-.3494327652	4.6945373421	-2.2780278269
H	1.0591711219	3.7790271497	-1.7174969419
H	1.0537326657	-1.6684835912	-2.5701262728
H	1.6454395708	-2.9402036254	-4.5529588130
H	1.9553779169	-1.2306746170	-4.9011936074
H	.5296178518	-2.0351696403	-5.5688770594
H	-.3455596785	-3.6241688409	-3.0767164883
H	-1.4811166623	-2.6213841548	-3.9940727508
H	-1.3144461186	-2.3896116895	-2.2494571171
N	.1758506396	-1.0524414551	1.2646901853
N	.5329651398	.4155827393	-1.1846373568
O	-3.4790021112	-1.2905628403	.6928459595
O	-2.8114132484	-.0406602556	.2253615782
Cu	-.9266839464	-.2527496884	-.1733253224

12. $L^1\text{CuO}_2\text{H}_2^{2+}$ end-on triplet

H	-2.9543400257	-1.7591302614	1.5770061435
C	2.7647709150	.7466142005	-1.9680918914
C	-.6282831547	-1.2420819767	2.5136688077
C	-.9298615744	-.4129521916	3.6228804500
C	-1.8265575662	-.9163037741	4.5774206114
C	-2.4255692685	-2.1616988019	4.4342201337
C	-2.1303641364	-2.9615543267	3.3211291109
C	-1.2271097198	-2.5322680463	2.3393417238
C	-.4136631229	1.0132892737	3.7633494437
C	.2802710555	1.2509024638	5.1177610416
C	-1.5628407305	2.0214608129	3.5436545734
C	-.7951701331	-3.4549837228	1.1984686296
C	-1.8511813725	-4.4947316168	.7931660431
C	.5271002551	-4.1700888656	1.5587722197
C	-.1532031415	.6712151821	-2.5141870456
C	-.3705614754	2.0629034903	-2.7809833674
C	-1.0043244774	2.3799511028	-3.9767381999
C	-1.4202564358	1.3830324496	-4.8688237275
C	-1.2147238310	.0322383931	-4.5786367925
C	-.5906208593	-.3629691907	-3.3984249209
C	-.0024197790	3.1322961084	-1.7617678624
C	-1.1279645605	3.2688175137	-.7111301586
C	.3120633033	4.4993343485	-2.3893027853
C	-.3643092549	-1.8383135518	-3.0966111088
C	.3948581645	-2.5530904014	-4.2313459727
C	-1.7026781489	-2.5430834270	-2.7948050703
C	2.3028575994	-.8947333710	2.6776434940
C	1.4635767360	-.5616230954	1.4685526438
C	2.1741829465	-.0448417414	.3331047734
C	1.7119793160	.3424494802	-.9677476530
H	-4.3490960886	-1.1897063490	.9648374445
H	3.2011479059	-1.4401384311	2.3754314159
H	1.7500775367	-1.4875564692	3.4050848032
H	2.6326311407	.0303255020	3.1643831799
H	3.2472770985	.0382331841	.4720074180
H	3.4593003419	1.4644278167	-1.5227664153
H	2.3308045208	1.1750352304	-2.8700199724

H	3.3518088668	-.1365352265	-2.2482087022
H	-2.0737729559	-.3055260679	5.4388258328
H	-3.1178250227	-2.5233978260	5.1876415494
H	-2.5753740323	-3.9472803764	3.2431241432
H	.3264482408	1.1944952499	2.9776432412
H	.7008910462	2.2597144345	5.1459083625
H	1.0909351055	.5376757924	5.2929962311
H	-.4215471108	1.1694123668	5.9524224738
H	-1.1738244466	3.0432880543	3.5644543056
H	-2.3164485339	1.9372206786	4.3324049605
H	-2.0657710312	1.8595914393	2.5847117171
H	-.5945725673	-2.8240362103	.3197832236
H	-1.5091251545	-5.0349121283	-.0932868793
H	-2.8184188920	-4.0441070810	.5485007138
H	-2.0100439780	-5.2425701366	1.5753490525
H	.8516955344	-4.8009702443	.7266472613
H	.3880066333	-4.8117867480	2.4338414108
H	1.3336404089	-3.4679782711	1.7846690138
H	-1.1846803734	3.4182189024	-4.2275583293
H	-1.9087363872	1.6651407115	-5.7959889855
H	-1.5345177037	-.7194634444	-5.2920058700
H	.8994234950	2.8053245581	-1.2312224260
H	-.8573838174	4.0095878688	.0463941178
H	-1.3242520157	2.3198096817	-.1888295935
H	-2.0652125622	3.5826953045	-1.1793540900
H	.6956300955	5.1752071185	-1.6208952531
H	-.5797025264	4.9693620423	-2.8135744281
H	1.0662179467	4.4195421993	-3.1771954206
H	.2602584412	-1.9107890701	-2.1984014648
H	.6139100643	-3.5844935719	-3.9413221569
H	1.3415942919	-2.0547329089	-4.4579968577
H	-.1946266305	-2.5902367185	-5.1516886747
H	-1.5288673963	-3.5944392331	-2.5470388323
H	-2.3720186762	-2.5111915962	-3.6593907150
H	-2.2313492134	-2.0748783860	-1.9554193574
N	.1626132517	-.7564143718	1.4361421369
N	.4386642512	.2852569512	-1.2884458060
O	-3.4112416710	-1.3850250379	.7596287287
O	-2.8388066267	-.0288579240	.5170111157
Cu	-1.0072878059	-.1156403512	-.0852792644

13. $L^1\text{CuO}_2\text{H}_2^+$ end-on doublet

H	-2.7781333096	-1.5786764813	1.7155396028
C	2.7264702419	.4916400481	-2.0575726472
C	-.6400924890	-1.2906539688	2.4911247339
C	-.8609300514	-.3265930314	3.5095540897
C	-1.7105407104	-.6703592267	4.5687008295
C	-2.3465300415	-1.9072224165	4.6283830329
C	-2.1414783633	-2.8419902865	3.6136118162
C	-1.2944177035	-2.5619851868	2.5265387478
C	-.2725706046	1.0793295449	3.4531728683
C	.5132347325	1.4372693054	4.7279224140
C	-1.3807347673	2.1189849623	3.1851189208
C	-.9946180840	-3.6293405726	1.4724489318
C	-2.1997761171	-4.5189580462	1.1272198527
C	.1996281547	-4.5000798666	1.9165409734
C	-.1324814315	.7552424674	-2.4738556733
C	-.6427442769	2.0788548757	-2.5823766490
C	-1.2336899330	2.4554031779	-3.7900449098
C	-1.3397675063	1.5577448816	-4.8500895109
C	-.8609378340	.2533647506	-4.7183096356
C	-.2539901674	-.1803899724	-3.5397420465
C	-.5560914434	3.0686331987	-1.4265228753
C	-1.9462003579	3.2960272910	-.7997034219

C	.0864191120	4.4045365298	-1.8402068166
C	.1548725774	-1.6393296681	-3.3722278011
C	.8421707986	-2.2277763028	-4.6150814556
C	-1.0714216546	-2.4866944312	-2.9719970426
C	2.2586584764	-1.2420852875	2.5544387025
C	1.4537266331	-.8749873779	1.3238395082
C	2.1872087223	-.4147101581	.2110864593
C	1.7120623619	.1303438843	-.9949417612
H	-4.2340378389	-.9298094133	1.4521902893
H	3.2210586826	-1.6676910255	2.2629120287
H	1.7334115104	-1.9522695596	3.1941053992
H	2.4640545572	-.3451639496	3.1486547491
H	3.2641621091	-.4623538973	.3113677401
H	3.7199419810	.6031747581	-1.6213220326
H	2.4494211161	1.4200167968	-2.5625104828
H	2.7791390489	-.2922697899	-2.8206780780
H	-1.8880052639	.0541148992	5.3570486138
H	-2.9980764422	-2.1457082177	5.4629493170
H	-2.6305605345	-3.8083871759	3.6706140636
H	.4224857694	1.1249862818	2.6106113546
H	.9839882272	2.4182783219	4.6138488897
H	1.2977687226	.7059335994	4.9433050956
H	-.1404640651	1.4896860861	5.6041401251
H	-.9434887162	3.1153446157	3.0665156406
H	-2.0884497085	2.1648910938	4.0196176593
H	-1.9441029482	1.8774258082	2.2789758397
H	-.6919468475	-3.1062536625	.5585018135
H	-1.9405576340	-5.1793699745	.2951608640
H	-3.0747535613	-3.9347105845	.8228244847
H	-2.4936999934	-5.1609425066	1.9633699405
H	.4302069387	-5.2453181032	1.1492514297
H	-.0309180311	-5.0310290770	2.8459233667
H	1.0986322113	-3.9018893270	2.0838050338
H	-1.6156978884	3.4645068480	-3.9051943049
H	-1.80444077356	1.8706900748	-5.7798493131
H	-.9722509007	-.4368313041	-5.5474500465
H	.0839206881	2.6266546606	-.6574460438
H	-1.8726400802	3.9712720857	.0589142797
H	-2.3970416074	2.3570562538	-.4556725544
H	-2.6379717875	3.7428406375	-1.5211422871
H	.2042632669	5.0506790734	-.9648071955
H	-.5278965926	4.9460993148	-2.5660576145
H	1.0745935734	4.2520641714	-2.2846143898
H	.8684871195	-1.7040171075	-2.5459731602
H	1.2161933499	-3.2319131886	-4.3942850069
H	1.6882284546	-1.6127074146	-4.9365336515
H	.1537773102	-2.3182934145	-5.4606855163
H	-.7810134711	-3.5280979587	-2.7989752695
H	-1.8324288699	-2.4705391468	-3.7586457066
H	-1.5398620754	-2.1074084586	-2.0551917734
N	.1256335206	-.9841370703	1.3327592031
N	.4205138906	.3608068575	-1.2270604118
O	-3.4194684653	-1.2364829773	1.0101896103
O	-2.8471021934	.0450614517	.4687146896
Cu	-.9969926879	-.1525583946	-.0823135473

14. $L^1CuO_2^-$ side-on doublet

Cu	-.5710400384	-.6386244775	-.0069238258
O	.2251534609	-2.3991980358	-.4260718774
O	-1.1939457007	-2.4811539811	-.3569285495
N	.8603922018	.7605634256	.2189707788
N	-2.1315451752	.5876745423	.3411052456
C	1.7153963946	3.0290718766	.6528925839
C	.5784384549	2.0264025633	.5045946276

C	-.7265080169	2.5349494885	.6890542883
C	-1.9744136427	1.8766728173	.6177672031
C	-3.2025815293	2.7381721906	.8812056721
C	2.2075341024	.3380869812	.0436052789
C	2.9319702709	-.1796376358	1.1438698950
C	4.2524792388	-.5964357505	.9457805672
C	4.8498866561	-.5345939754	-.3107667137
C	4.1058903778	-.0872929851	-1.3999853613
C	2.7825454526	.3402500839	-1.2499173985
C	2.2470661707	-.3904625304	2.4887728682
C	3.0912748439	.0649757260	3.6897598789
C	1.8270162143	-1.8696756997	2.6236424355
C	1.9368240675	.6858097137	-2.4700011757
C	1.4561184849	-.6157961404	-3.1471237186
C	2.6466704320	1.6101574003	-3.4721372539
C	-3.4296593849	.0070429758	.2986255061
C	-3.9776491705	-.5796583762	1.4647238954
C	-5.2518155524	-1.1528424128	1.3958410282
C	-5.9710103830	-1.1776931172	.2033083375
C	-5.3947441889	-.6578994372	-.9532137768
C	-4.1235951311	-.0741761265	-.9325906232
C	-3.1457584444	-.6935423037	2.7368861157
C	-2.5322870458	-2.1076158080	2.8236520454
C	-3.9211324765	-.3391758114	4.0158808458
C	-3.4485647914	.3571534843	-2.2290294754
C	-4.3576950912	1.1836729900	-3.1523184721
C	-2.8890176637	-.8856218835	-2.9542369930
H	1.3367779645	4.0253174291	.8910351306
H	2.3044365564	3.0888612356	-.2683731245
H	2.4079700939	2.7188226457	1.4423377860
H	-.7781979515	3.5922779100	.9211028220
H	-2.9239968626	3.7749522429	1.0812352698
H	-3.7696200027	2.3564948591	1.7368229105
H	-3.8845852953	2.7166198231	.0247528779
H	4.8163595735	-.9931956646	1.7860545351
H	5.8788506005	-.8587724293	-.4454328501
H	4.5557890238	-.0866951849	-2.3893707232
H	1.3315448844	.2072347877	2.4846861692
H	2.5174362566	-.0421587708	4.6176780150
H	3.3929744352	1.1146112042	3.5974579399
H	4.0020997915	-.5346558504	3.8021411935
H	1.2222496481	-2.0187801580	3.5272475701
H	2.7138656362	-2.5115584646	2.7020256317
H	1.2502774535	-2.1951919886	1.7498373842
H	1.0477763020	1.2119037323	-2.1116592580
H	.7476221777	-.3917834538	-3.9547699105
H	.9725612326	-1.2821559498	-2.4228446498
H	2.3071972763	-1.1530283829	-3.5851610731
H	1.9629807092	1.8827085181	-4.2845579830
H	3.5169084541	1.1267527902	-3.9311829957
H	2.9920877137	2.5348673843	-2.9957283074
H	-5.6803643556	-1.6042331451	2.2869003557
H	-6.9618847253	-1.6238154186	.1695904173
H	-5.9348760144	-.7223807199	-1.8942276221
H	-2.3168464188	.0140079914	2.6490073048
H	-1.8350255385	-2.1747494891	3.6685182451
H	-1.9995315793	-2.3628956200	1.8998335060
H	-3.3208084584	-2.8555354979	2.9774385935
H	-3.2516454194	-.3664589014	4.8835367264
H	-4.7338457931	-1.0480348871	4.2128174118
H	-4.3603260361	.6633536213	3.9584463562
H	-2.5960983609	.9860103280	-1.9582654851
H	-3.7950344268	1.5269283542	-4.0282761370
H	-4.7594929254	2.0658720496	-2.6408116781

H	-5.2070308616	.5981258228	-3.5232512337
H	-2.2931425000	-.5878625337	-3.8264806354
H	-3.7107842166	-1.5209777966	-3.3089480587
H	-2.2638573128	-1.4857663645	-2.2821048415

15. L¹CuO₂⁻ end-on doublet

Cu	-.9003828525	-.5124898981	.3464797224
O	-.9635945791	-3.1436991678	.7044544861
O	-.7938186233	-2.0765098299	1.5118461256
N	.6122818963	.3666112931	-.7049017473
N	-2.3586793093	.6263950647	-.4225616659
C	1.6113679463	2.1233648894	-2.1127601090
C	.4227019137	1.4648855353	-1.4231287806
C	-.8335412212	2.0874824802	-1.6157071314
C	-2.1192314353	1.6791353096	-1.1955471530
C	-3.2892416900	2.5211522762	-1.6879298235
C	1.8759600704	-.2715122497	-.6368225418
C	2.7003129982	-.0743348242	.4990170527
C	3.9208327134	-.7517015383	.5788422795
C	4.3309095073	-1.6278871039	-.4231536639
C	3.4904381442	-1.8588106747	-1.5093174731
C	2.2596607348	-1.2064104096	-1.6331733892
C	2.2227339818	.7899837715	1.6595284266
C	3.2735445825	1.8118727333	2.1239662579
C	1.7572296103	-.1005997980	2.8294745773
C	1.3136775534	-1.5805541213	-2.7699932984
C	.6761845471	-2.9588137090	-2.4988476936
C	1.9862677919	-1.5469543168	-4.1532583797
C	-3.6790237681	.2093391834	-.1145878256
C	-4.2575623788	.5684602654	1.1291899061
C	-5.5370915062	.1006354652	1.4432201647
C	-6.2444157918	-.7200242780	.5674856300
C	-5.6502128353	-1.1075158677	-.6307503665
C	-4.3721675128	-.6667819241	-.9893795037
C	-3.4549154041	1.3657154423	2.1500750983
C	-2.8801809542	.4205321392	3.2254624908
C	-4.2529241483	2.5113350763	2.7932612068
C	-3.7088371696	-1.2079111761	-2.2524299109
C	-4.5948875099	-1.0736875843	-3.5031402610
C	-3.2689356037	-2.6713821916	-2.0413384732
H	1.3272894232	3.0701780986	-2.5773725218
H	2.0251259797	1.4691106760	-2.8877368635
H	2.4210456905	2.3085566004	-1.3991664822
H	-.8117979795	2.9891069698	-2.2171190851
H	-2.9430982089	3.4014527195	-2.2338409131
H	-3.9152146899	2.8479156128	-.8509105814
H	-3.9377858692	1.9370645502	-2.3500318767
H	4.5551781944	-.6015532615	1.4489752708
H	5.2842283635	-2.1446610948	-.3461864202
H	3.7877147617	-2.5769147629	-2.2696914459
H	1.3508183863	1.3479870969	1.3081148864
H	2.8603451477	2.4520598651	2.9123599221
H	3.5987498137	2.4558530248	1.2992744213
H	4.1646121198	1.3234474914	2.5355615732
H	1.3366162887	.5124022095	3.6367727900
H	2.6015108302	-.6666438574	3.2429112490
H	.9979957083	-.8189827137	2.5060322604
H	.5029443226	-.8476787295	-2.7794729137
H	-.0452442647	-3.2088631288	-3.2870527671
H	.1549868657	-2.9751396025	-1.5358183963
H	1.4425431308	-3.7437577425	-2.4844882943
H	1.2490364821	-1.7489187484	-4.9392047498
H	2.7725521799	-2.3055780855	-4.2432197962
H	2.4417392852	-.5717413111	-4.3588782099

H	-5.9833017228	.3724637704	2.3965097608
H	-7.2390741561	-1.0735634788	.8272012874
H	-6.1830924511	-1.7822613408	-1.2963052578
H	-2.6073224809	1.8090361233	1.6206148897
H	-2.2383133222	.9727313137	3.9233664859
H	-2.2891675980	-.3820903883	2.7738292414
H	-3.6894135779	-.0422438667	3.8039446324
H	-3.6066324858	3.0991593567	3.4555299147
H	-5.0865718124	2.1399669145	3.4006648049
H	-4.6676056995	3.1861652111	2.0362918562
H	-2.8031358280	-.6211094430	-2.4261612748
H	-4.0468432549	-1.4037747313	-4.3934164648
H	-4.9121380986	-.0374379087	-3.6655155052
H	-5.4986868105	-1.6900247966	-3.4313441217
H	-2.7597854498	-3.0498021895	-2.9366248901
H	-4.1383736918	-3.3137569873	-1.8537686366
H	-2.5836891634	-2.7678252836	-1.1920153902

16. $L^1CuO_2^-$ end-on doublet \rightarrow $L^1CuO_2^-$ side-on doublet transition state

Cu	-.9232303104	-.8084060842	-.1034807729
O	-.2299449701	-2.9057072829	.8004965895
O	-1.5338139515	-2.5054901233	.7305293519
N	.6024606153	.2442211773	-.8065890947
N	-2.4242475607	.5292874440	-.5410528460
C	1.6138166115	2.1587746783	-1.9779536591
C	.4088689621	1.4074929292	-1.4243715787
C	-.8453310408	2.0288481512	-1.6161260624
C	-2.1430349853	1.6444693394	-1.1993071473
C	-3.2696164564	2.6122206093	-1.5431661000
C	1.9178295748	-.2649521735	-.6192958716
C	2.6465979912	.0701854965	.5494297426
C	3.9270281701	-.4639195860	.7259719569
C	4.4876775788	-1.3270296330	-.2121788879
C	3.7446208930	-1.6913270813	-1.3325853869
C	2.4599035387	-1.1840478832	-1.5515167746
C	2.0074519200	.9084875705	1.6510971386
C	2.9232987697	2.0202006761	2.1881045920
C	1.5251210803	-.0127336091	2.7904140722
C	1.6128091336	-1.6981352299	-2.7089348094
C	1.0257047711	-3.0780269485	-2.3447894063
C	2.3656535544	-1.7460251005	-4.0481044434
C	-3.7427443763	.2285936643	-.1234233159
C	-4.1699292302	.6032810463	1.1761893368
C	-5.4595067230	.2595497008	1.5917901275
C	-6.3191583488	-.4604190032	.7647599099
C	-5.8724286575	-.8732107953	-.4884231633
C	-4.5917394339	-.5515382240	-.9492639404
C	-3.1933692852	1.2609466600	2.1439921798
C	-2.6069453577	.1923003076	3.0901094924
C	-3.7992447418	2.4316697182	2.9339120756
C	-4.0835501445	-1.1147088893	-2.2721343929
C	-5.0891119532	-.9703910213	-3.4259722260
C	-3.6573246750	-2.5864574686	-2.0896597177
H	1.3101726292	3.0791247431	-2.4809613497
H	2.1692166644	1.5370721150	-2.6882565148
H	2.3167748993	2.4147566261	-1.1779985873
H	-.8043178011	2.9700318208	-2.1521637285
H	-2.9021202493	3.4674967912	-2.1143197880
H	-3.7539696298	2.9820988084	-.6327099476
H	-4.0496567445	2.1109553290	-2.1258828821
H	4.4892391420	-.2118147514	1.6217048291
H	5.4856361817	-1.7305969447	-.0597602939
H	4.1647538966	-2.3977840727	-2.0438297284
H	1.1219520731	1.3878541288	1.2257942666

H	2.3872613830	2.6309696707	2.9240103722
H	3.2670065349	2.6815327449	1.3850102741
H	3.8107751985	1.6152084009	2.6881271493
H	.9725906257	.5586345998	3.5465436778
H	2.3771792156	-.4953610661	3.2847294529
H	.8726767586	-.8017159991	2.4050125828
H	.7734698272	-1.0076361721	-2.8281211022
H	.3065669003	-3.4050844881	-3.1064819422
H	.5280305226	-3.0525586907	-1.3678331226
H	1.8251703772	-3.8288207360	-2.2927111903
H	1.6858626212	-2.0495096483	-4.8528374273
H	3.1881676850	-2.4707466889	-4.0305574676
H	2.7878480439	-.7693164311	-4.3107637404
H	-5.7917324194	.5453535325	2.5866404191
H	-7.3197025407	-.7177853227	1.1032794852
H	-6.5274232396	-1.4721641770	-1.1160726854
H	-2.3650285945	1.6584465512	1.5516129080
H	-1.8132197176	.6188525486	3.7157895085
H	-2.1931647335	-.6504722001	2.5275118199
H	-3.3868489584	-.2018991263	3.7536620801
H	-3.0298206829	2.9123491929	3.5493706677
H	-4.5957671904	2.1026337075	3.6114749868
H	-4.2224236893	3.1903943334	2.2661240879
H	-3.1866690632	-.5509739190	-2.5433474902
H	-4.6404339767	-1.3171744146	-4.3641667352
H	-5.4009466049	.0710807883	-3.5631950589
H	-5.9922050130	-1.5691747438	-3.2594916123
H	-3.2198397953	-2.9791996295	-3.0165159551
H	-4.5239858064	-3.2094604866	-1.8349211782
H	-2.9205428989	-2.6849362399	-1.2860869514

17. L¹CuO₂H side-on doublet

Cu	.0325870670	-.9485488531	.0578286344
O	.4105117406	-3.0611009730	.1811295173
O	-.9704895664	-2.5653876497	.0590984855
N	1.6210408392	.1375149138	.0745658127
N	-1.2934680765	.4770304351	-.0140838449
C	2.8803775564	2.2479308297	.1407064858
C	1.5787994771	1.4714626134	.0986083438
C	.3875595610	2.2175896121	.0810482573
C	-.9449110890	1.7599388333	.0088175760
C	-2.0322047549	2.8163254248	-.0477626187
C	2.8619599841	-.5825264055	.0456267820
C	3.4356128031	-1.0346482621	1.2575291030
C	4.6079473813	-1.7965414193	1.1966922326
C	5.2009683903	-2.1174077705	-.0206269911
C	4.6155235972	-1.6828953364	-1.2061276734
C	3.4448933465	-.9155425744	-1.2001659309
C	2.7762883332	-.7679358663	2.6063502112
C	3.7368844683	-.1180232104	3.6167685431
C	2.1711003198	-2.0651147787	3.1797047585
C	2.8036869635	-.5065856388	-2.5233788909
C	2.1650052544	-1.7228616157	-3.2211293438
C	3.7907666668	.2015875751	-3.4675588566
C	-2.6582109337	.0576743696	-.1133967900
C	-3.3977717968	-.1928729536	1.0655305963
C	-4.7210607598	-.6290974901	.9374709572
C	-5.2976104124	-.8321178752	-.3129078917
C	-4.5421514411	-.6231305280	-1.4631885349
C	-3.2149686167	-.1874115863	-1.3894744902
C	-2.7662965556	-.0732582839	2.4483077834
C	-2.5240318768	-1.4741736291	3.0459177464
C	-3.5885473368	.8026895765	3.4081810327
C	-2.3800730799	-.0662434788	-2.6597161471

C	-3.0501411564	.7974134139	-3.7407414411
C	-2.0371414929	-1.4679465355	-3.2043401528
H	.5691629878	-3.4494585106	-.6939474474
H	2.6943014966	3.3198907490	.2142020719
H	3.4751877424	2.0588915889	-.7585534222
H	3.4933083023	1.9373705800	.9919355455
H	.5095619175	3.2924621565	.1054606681
H	-1.6078171485	3.8190165746	.0145929214
H	-2.7474986929	2.6830095707	.7689631275
H	-2.6014921313	2.7334551813	-.9790056265
H	5.0579861523	-2.1524469914	2.1187695909
H	6.1100046800	-2.7113079808	-.0457718682
H	5.0727770930	-1.9480635870	-2.1549718183
H	1.9524977198	-.0676175401	2.4408273058
H	3.2063755111	.1144741554	4.5458723009
H	4.1618241067	.8129713741	3.2279594341
H	4.5697334759	-.7824903788	3.8718815148
H	1.6333141855	-1.8597758716	4.1114442473
H	2.9568103127	-2.7968323343	3.3991336542
H	1.4754775367	-2.5264354802	2.4738126057
H	1.9980691864	.1982264391	-2.3006416692
H	1.6675831486	-1.4227889439	-4.1496115412
H	1.4152929356	-2.1978255546	-2.5794453537
H	2.9179788405	-2.4791400090	-3.4683668434
H	3.2745395573	.5413625385	-4.3715764353
H	4.6015541254	-.4638023313	-3.7821318911
H	4.2456292443	1.0745266398	-2.9894254236
H	-5.3041273538	-.8264680447	1.8320822120
H	-6.3255202023	-1.1741127356	-.3903658950
H	-4.9851268477	-.8170290980	-2.4356527845
H	-1.7887953195	.4017738109	2.3266283983
H	-1.9885950074	-1.3977328610	3.9988776887
H	-1.9411199288	-2.0940181727	2.3595115592
H	-3.4743930353	-1.9856903169	3.2358581900
H	-3.0648770003	.9102616871	4.3639125440
H	-4.5690386365	.3632078851	3.6199952510
H	-3.7548343900	1.8046267914	2.9994561512
H	-1.4368768935	.4181499216	-2.3923624006
H	-2.3863510041	.9051793580	-4.6051830576
H	3.2845032476	1.7993545564	-3.3672090340
H	-3.9831252466	.3497842710	-4.0982751958
H	-1.3482685500	-1.3965124329	-4.0535083729
H	-2.9397424681	-1.9836460886	-3.5475583922
H	-1.5808787353	-2.0841447082	-2.4253000631

18. L¹CuO₂H end-on doublet

Cu	-.5158226797	.2647096650	.1639317038
O	-3.0566136142	-.6426024495	-.0469051775
O	-2.3355529339	.5292648635	.3651952640
N	.6705421713	-.5159209827	1.5041105095
N	.8286553822	.5421100901	-1.1954304177
C	2.8427102993	-1.0670319213	2.5107869216
C	1.9955699905	-.5335059452	1.3709535664
C	2.6771507107	-.0906371091	.2216553602
C	2.1333801560	.3753594461	-.9888241011
C	3.1024372590	.6932999904	-2.1105473272
C	.0168585044	-1.0541192547	2.6576819873
C	-.3749976472	-.1817661225	3.7005151652
C	-1.0522528650	-.7180050836	4.8005496168
C	-1.3490588850	-2.0761924405	4.8741274452
C	-.9827348094	-2.9182451374	3.8282410512
C	-.3064519178	-2.4321899428	2.7038851187
C	-.1199723863	1.3193080512	3.6230800528
C	.6352300595	1.8554276585	4.8512017601

C	-1.4421376297	2.0830646065	3.4086992291
C	.0100479284	-3.3791782043	1.5502365543
C	-1.2844783313	-3.8123518496	.8331869932
C	.8201095300	-4.6094897184	1.9970970730
C	.2966642563	.9353853505	-2.4640361792
C	-.0058013501	2.2993744397	-2.6906946548
C	-.5793444879	2.6606469554	-3.9136629545
C	-.8599667281	1.7061577146	-4.8882378704
C	-.5839338480	.3647374199	-4.6404281800
C	-.0125277666	-.0498318528	-3.4322821871
C	.2157841045	3.3441872449	-1.6032816606
C	-1.1220153718	3.6917517249	-.9182684492
C	.9181375015	4.6121573182	-2.1143921345
C	.2011413454	-1.5371271418	-3.1678834633
C	1.0315543458	-2.2225728876	-4.2678203134
C	-1.1511101684	-2.2540434375	-2.9786026634
H	-3.9341488713	-.4491105448	.3183980789
H	3.9053833313	-.9426713755	2.2987368581
H	2.6440297040	-2.1299870810	2.6783010646
H	2.6050505688	-.5524102872	3.4464849029
H	3.7568091802	-.1522229837	.2611495392
H	4.1355968422	.5928368920	-1.7754842179
H	2.9470497120	1.7103257295	-2.4831412247
H	2.9456494568	.0204275336	-2.9595693809
H	-1.3572856256	-.0599407244	5.6091194757
H	-1.8735531905	-2.4748756825	5.7377218333
H	-1.2354720935	-3.9734638565	3.8796395397
H	.5101341111	1.5021583399	2.7481139303
H	.8492126330	2.9227374542	4.7292410406
H	1.5870459841	1.3339181146	4.9968548617
H	.0495550266	1.7406402214	5.7695980602
H	-1.2507365197	3.1545015153	3.2799149484
H	-2.1065094889	1.9633641360	4.2720821239
H	-1.9725615508	1.7151045171	2.5252768230
H	.6161812840	-2.8310319267	.8238357531
H	-1.0499942762	-4.4362516165	-.0368013596
H	-1.8593352940	-2.9459495952	.4941100493
H	-1.9244435780	-4.3991589478	1.5019541082
H	1.0769856286	-5.2293046360	1.1312970338
H	.2521471001	-5.2368597273	2.6923247133
H	1.7520417386	-4.3238692328	2.4957354164
H	-.8174138911	3.7029792862	-4.1033661358
H	-1.3047723713	2.0055783103	-5.8327907098
H	-.8271069935	-.3779594145	-5.3947922514
H	.8648918172	2.8968259147	-.8448625324
H	-.9581164450	4.3690113842	-.0723338641
H	-1.6357135649	2.7978028150	-.5513861762
H	-1.7980787902	4.1899170652	-1.6225309141
H	1.1282998128	5.2891805961	-1.2796118396
H	.2995030887	5.1619874267	-2.8315395253
H	1.8674217944	4.3745891381	-2.6055209160
H	.7548114422	-1.6340580620	-2.2298478895
H	1.2184951676	-3.2691659237	-4.0045045394
H	2.0001480991	-1.7318178687	-4.4093874249
H	.5122534842	-2.2152805628	-5.2321559335
H	-.9936279231	-3.3104415982	-2.7336704392
H	-1.7504384778	-2.2077475144	-3.8948784919
H	-1.7368435673	-1.7991249106	-2.1742210122

19. L^1CuO_2H end-on singlet \rightarrow L^1CuO_2H side-on singlet transition state

Cu	-.5162337327	.2007757311	.2916876560
O	-2.7873661549	-.5445613602	-.0431986215
O	-2.1943504813	.7854286101	-.2666648278
N	.7204569648	-.5434598445	1.5441607449

N	.7617161160	.5451798075	-1.1727897171
C	2.9300635967	-1.0602786581	2.4811055378
C	2.0425304498	-.5297092030	1.3737680562
C	2.6655875766	-.0580313343	.2073738509
C	2.0708573345	.4067837514	-.9859959177
C	3.0127490065	.7556463853	-2.1239998391
C	.0822406580	-1.1009338679	2.6973240960
C	-.3355473732	-.2307899522	3.7346482802
C	-1.0415614294	-.7719669013	4.8142020948
C	-1.3352005155	-2.1319087764	4.8748455635
C	-.9332002410	-2.9727430633	3.8406027056
C	-.2290082875	-2.4826563116	2.7354281051
C	-.0708058057	1.2698418988	3.6600825195
C	.4509219762	1.8547810979	4.9826545843
C	-1.3303473041	2.0262788359	3.1890176801
C	.1239813205	-3.4217687779	1.5858648404
C	-1.1406816740	-3.8056291395	.7913206336
C	.8761265756	-4.6797159797	2.0551485916
C	.2087793290	.9457600932	-2.4295556243
C	-.0715203584	2.3111313657	-2.6680323634
C	-.6418655407	2.6688961835	-3.8941490125
C	-.9444301372	1.7110846431	-4.8574365861
C	-.6915414267	.3676229104	-4.5954411833
C	-.1234330829	-.0433298383	-3.3853097955
C	.1804033976	3.3807808164	-1.6110196038
C	-1.1522463815	3.9193840108	-1.0537789638
C	1.0616005918	4.5296248826	-2.1317894470
C	.0684955722	-1.5323640328	-3.1125921379
C	.9540063246	-2.2154415014	-4.1717328866
C	-1.2931015036	-2.2473670410	-2.9959730444
H	-3.3678601276	-.3583442177	.7126475558
H	3.9838874748	-.8980878866	2.2514772891
H	2.7686751468	-2.1334260737	2.6255931170
H	2.6956324330	-.5755390702	3.4338647480
H	3.7471686330	-.0908054980	.2076089539
H	4.0536249813	.6356471148	-1.8211994533
H	2.8566235461	1.7860409373	-2.4559173660
H	2.8240787274	.1154302237	-2.9909518352
H	-1.3690893012	-.1197543577	5.6180158854
H	-1.8829967422	-2.5339952719	5.7221315532
H	-1.1807610513	-4.0293152105	3.8860311665
H	.7058262937	1.4298167923	2.9064145734
H	.7145043318	2.9091621846	4.8493397875
H	1.3413775719	1.3226984867	5.3321214544
H	-.3005860869	1.8068123096	5.7775437101
H	-1.1245508921	3.0991285854	3.1044114446
H	-2.1517762657	1.8951960316	3.9026812150
H	-1.6806373549	1.6785249217	2.2108745111
H	.7834796841	-2.8797549173	.9025093886
H	-.8773374076	-4.4271163081	-.0718193739
H	-1.6658509185	-2.9187612133	.4245746698
H	-1.8372911945	-4.3762080516	1.4159608271
H	1.1749570168	-5.2846551871	1.1925210619
H	.2519413079	-5.3112265857	2.6961747349
H	1.7792549458	-4.4248351132	2.6194017079
H	-.8634477660	3.7137222231	-4.0919816850
H	-1.3882076070	2.0085893704	-5.8031866424
H	-.9496087684	-.3792296440	-5.3408761291
H	.7150545209	2.9088510209	-.7815811192
H	-.9677992396	4.6324865347	-.2419262324
H	-1.7781890709	3.1072070174	-.6741557899
H	-1.7194809536	4.4399326956	-1.8336230615
H	1.2653384286	5.2466642870	-1.3290157692
H	.5735560846	5.0766662015	-2.9455193388

H	2.0220070995	4.1628018168	-2.5087106465
H	.5734247502	-1.6328788821	-2.1474879328
H	1.1183374145	-3.2662689129	-3.9096068659
H	1.9333035155	-1.7320888925	-4.2554375401
H	.4875639682	-2.1930321850	-5.1627952262
H	-1.1475076111	-3.3056291908	-2.7504564485
H	-1.8455295830	-2.1983008001	-3.9413520070
H	-1.9166478673	-1.7942545350	-2.2199323403

20. L¹CuO singlet

Cu	.0592013783	-.3453959403	.7728183253
O	.2361924411	-1.6232906279	1.8878152617
N	1.4960249975	.4987055651	-.1856478126
N	-1.3169940051	.7822669907	.0528702293
C	2.6192300705	2.2525525830	-1.4767249051
C	1.3729932984	1.6308157609	-.8763172087
C	.1569944487	2.2943507896	-1.0946221636
C	-1.1151454924	1.8716050278	-.6792874428
C	-2.3066218711	2.7109810869	-1.0929169212
C	2.7548324974	-.1664535602	-.0403838014
C	3.5562088027	.1080782280	1.0922697764
C	4.7833651153	-.5512125532	1.2053848738
C	5.2040340271	-1.4655641446	.2426791060
C	4.3853473812	-1.7518997258	-.8461681329
C	3.1462210052	-1.1231932971	-1.0066669809
C	3.0814680737	1.0382952854	2.2020723281
C	4.1134857664	2.1238356709	2.5512375653
C	2.6846347571	.2199216706	3.4479275043
C	2.2358290659	-1.5241750297	-2.1625152502
C	1.6914278698	-2.9497708083	-1.9437363191
C	2.9236541037	-1.4025581281	-3.5336963159
C	-2.6182914385	.3191058112	.4155720977
C	-3.1246192044	.6399230120	1.6980787615
C	-4.3837659100	.1464120997	2.0510090679
C	-5.1187133245	-.6494923406	1.1757995805
C	-4.5947087008	-.9769339533	-.0723595947
C	-3.3394859589	-.5122349869	-.4759457165
C	-2.3119934558	1.4556284730	2.6976016937
C	-1.7736841511	.5529466511	3.8265789808
C	-3.0995141209	2.6487886683	3.2647287896
C	-2.7551649979	-.9581752234	-1.8123635442
C	-3.7173957260	-.7357085055	-2.9920392921
C	-2.3100637865	-2.4324544094	-1.7369709802
H	2.3758414922	3.1835817474	-1.9897160033
H	3.0893796607	1.5696695268	-2.1900191575
H	3.3621594679	2.4583860182	-.7007485065
H	.2011637689	3.2102788667	-1.6676982724
H	-1.9832103946	3.6115176726	-1.6162578706
H	-2.8976544438	2.9996475231	-.2187534988
H	-2.9713358759	2.1438239329	-1.7514371288
H	5.4151231753	-.3531527063	2.0658146565
H	6.1619415610	-1.9660427426	.3493506802
H	4.7076792411	-2.4858150395	-1.5788896939
H	2.1810405638	1.5476907157	1.8459800687
H	3.7017301780	2.8072515393	3.3013195535
H	4.3934942485	2.7150846871	1.6726223327
H	5.0302731769	1.6947874956	2.9690609886
H	2.2952800122	.8842609039	4.2280692606
H	3.5534014093	-.3070549384	3.8583206620
H	1.9137775973	-.5205475195	3.2087347128
H	1.3778685946	-.8461732315	-2.1633170881
H	.9855252021	-3.2167188410	-2.7379634513
H	1.1767960155	-3.0319620131	-.9818802320
H	2.5025905915	-3.6858755409	-1.9530249247

H	2.2168722399	-1.6444595774	-4.3345911642
H	3.7707233479	-2.0904505316	-3.6251748939
H	3.2989175360	-.3891396176	-3.7103411525
H	-4.7914918728	.3815160954	3.0293306474
H	-6.0945041164	-1.0241720540	1.4704361780
H	-5.1657020534	-1.6150910928	-.7399878385
H	-1.4459664878	1.8614191843	2.1657817084
H	-1.1594456506	1.1405212907	4.5184239671
H	-1.1587632486	-.2620979689	3.4327104070
H	-2.5978056504	.1142471626	4.4002137195
H	-2.4557466877	3.2489257537	3.9162215760
H	-3.9570590666	2.3234448460	3.8629441028
H	-3.4766571509	3.2992930272	2.4683780505
H	-1.8591987314	-.3608474405	-2.0032782632
H	-3.2247428520	-.9970104069	-3.9344947308
H	-4.0426565148	.3077245619	-3.0586350813
H	-4.6143590246	-1.3581381241	-2.9092341376
H	-1.8393570740	-2.7401259276	-2.6772661812
H	-3.1659681435	-3.0916741834	-1.5560706452
H	-1.5918951715	-2.5880837671	-.9265217899

21. L¹CuO triplet

Cu	.0590465795	-.4036138334	.7453261056
O	.1900136859	-1.7535054522	1.8979134009
N	1.5162875368	.4822497887	-.2109457063
N	-1.3333372762	.7515253511	.0492165323
C	2.6094903273	2.2545453402	-1.5171311279
C	1.3801405623	1.6102340736	-.9060528402
C	.1478276060	2.2549149749	-1.1152267500
C	-1.1250418926	1.8414197175	-.6879111672
C	-2.3093822224	2.6945663410	-1.0964952983
C	2.7891710585	-.1596712666	-.0657982236
C	3.5590256368	.0894533959	1.0937282899
C	4.7793286395	-.5789823936	1.2368583345
C	5.2277703725	-1.4770542123	.2722780927
C	4.4454411582	-1.7315640165	-.8508025736
C	3.2174215686	-1.0898809806	-1.0417210147
C	3.0579325474	1.0106829358	2.2004724635
C	4.0835313965	2.0885510838	2.5898841503
C	2.6248313381	.1875778565	3.4300209295
C	2.3518169504	-1.4508002075	-2.2455947289
C	1.7460502206	-2.8577332319	-2.0710714692
C	3.1082601208	-1.3455212966	-3.5816119579
C	-2.6514400115	.3333311626	.4242640378
C	-3.1531624133	.6946632259	1.6970539806
C	-4.4171370214	.2261055028	2.0692141506
C	-5.1659687636	-.5827560951	1.2186377986
C	-4.6500082090	-.9467855603	-.0221572072
C	-3.3907500890	-.5057733665	-.4426941246
C	-2.3206765157	1.5195699911	2.6723505068
C	-1.7267316174	.6160377922	3.7720987134
C	-3.1026366692	2.6921274652	3.2875840745
C	-2.8190561257	-.9859850107	-1.7730184254
C	-3.7973265466	-.8127711513	-2.9475170744
C	-2.3548040883	-2.4517113274	-1.6590936620
H	2.3531522998	3.1929223103	-2.0105292061
H	3.0743366360	1.5895609455	-2.2508418673
H	3.3650777719	2.4524523781	-.7508322912
H	.1820676066	3.1689985330	-1.6931284705
H	-1.9821124000	3.5832136520	-1.6376557844
H	-2.8845730626	3.0056358240	-.2191498551
H	-2.9940194935	2.1292979808	-1.7363879816
H	5.3830366583	-.3998348695	2.1216309917
H	6.1783583668	-1.9864221310	.4010787466

H	4.7907508781	-2.4494426185	-1.5890881450
H	2.1714425747	1.5286199639	1.8235414885
H	3.6576862149	2.7624538007	3.3410005612
H	4.3826994548	2.6908283480	1.7255930778
H	4.9903338224	1.6505638736	3.0201369513
H	2.1876465584	.8401286432	4.1943417358
H	3.4841134816	-.3248490741	3.8772568606
H	1.8885173698	-.5768461589	3.1610258883
H	1.5191574753	-.7429233584	-2.2835584756
H	1.0732467002	-3.0944618424	-2.9028362648
H	1.1779941841	-2.9317254022	-1.1387321736
H	2.5300876130	-3.6222191563	-2.0425196657
H	2.4292492484	-1.5435165469	-4.4179272839
H	3.9252509701	-2.0717921695	-3.6447150583
H	3.5389883993	-.3492825166	-3.7250688056
H	-4.8183259887	.4920969991	3.0425047413
H	-6.1452929520	-.9374408801	1.5263143646
H	-5.2317803245	-1.5935247369	-.6722769773
H	-1.4835590564	1.9468749382	2.1126593066
H	-1.0708422059	1.1949586464	4.4320862037
H	-1.1485075909	-.2121917642	3.3503427611
H	-2.5227104297	.1796694634	4.3859340713
H	-2.4403121646	3.3002983281	3.9126671071
H	-3.9239522344	2.3463157579	3.9240293973
H	-3.5294398609	3.3404154565	2.5151008264
H	-1.9338116860	-.3832075350	-1.9941691692
H	-3.3102861664	-1.0909973129	-3.8882283321
H	-4.1401644329	.2231585379	-3.0374005632
H	-4.6827558809	-1.4476264452	-2.8387931048
H	-1.8919043579	-2.7849635294	-2.5946401733
H	-3.1995877990	-3.1148222152	-1.4434311033
H	-1.6243812914	-2.5748818602	-.8532378857

22. $L^1\text{CuOH}^+$ singlet

Cu	-.7061093429	.1832933104	.1347841422
O	-2.4894012217	.0683047598	.3319140244
N	.5948988438	-1.2921287128	.2709441372
N	.6464363577	1.5904019795	.0569488085
C	2.7687168546	-2.2921635707	.8797160994
C	1.8902014105	-1.1224792809	.4959811546
C	2.5281322544	.1364163065	.3599186708
C	1.9575540827	1.4039985176	.0910503696
C	2.9103560677	2.5581043992	-.1238858637
C	-.0833425911	-2.5089582193	.5346378556
C	-.2903780781	-2.9595523395	1.8691607693
C	-.9813777960	-4.1588216044	2.0400154946
C	-1.4547432717	-4.8863665458	.9476052429
C	-1.2792185408	-4.4056403001	-.3498116324
C	-.6194841811	-3.2006002251	-.5868080619
C	.0747790450	-2.1112702956	3.0822669212
C	.7756968683	-2.9116717710	4.1933821954
C	-1.1886846023	-1.4058208704	3.6246713424
C	-.4263334989	-2.6868384187	-2.0071762924
C	-1.7358493522	-2.7006113277	-2.8144776758
C	.6840292996	-3.4694697878	-2.7358354951
C	.0266683597	2.7863330768	-.3819067626
C	-.7471493290	3.5026853890	.5769172432
C	-1.3849366444	4.6680287740	.1534106454
C	-1.3057766145	5.0915374698	-1.1721458109
C	-.5848810375	4.3493022632	-2.1091583397
C	.0974603850	3.1887299724	-1.7476822081
C	-.8316642615	3.0686472641	2.0348346701
C	-2.2907812159	2.9058466252	2.4993900250
C	-.0510930600	4.0371046941	2.9464173152

C	.7616279012	2.3354980173	-2.8231455377
C	1.6666717251	3.1508412592	-3.7634570405
C	-.3087418468	1.5649613183	-3.6255864143
H	-3.0621877002	-.0938350012	-.4292525688
H	3.7913554677	-2.1287567372	.5347470348
H	2.3886245701	-3.2248471608	.4594450236
H	2.7986614264	-2.4067048945	1.9681109295
H	3.6057601156	.1253431611	.4698192940
H	3.8206459332	2.4088076675	.4602842296
H	2.4494490398	3.5056725245	.1601947854
H	3.2007863593	2.6295512814	-1.1770148595
H	-1.1696236116	-4.5262925541	3.0429087674
H	-1.9778908087	-5.8234281510	1.1099825901
H	-1.6633154474	-4.9789568552	-1.1866811457
H	.7651038816	-1.3246321115	2.7620461073
H	1.0954699925	-2.2374904065	4.9933982721
H	1.6578822604	-3.4431674313	3.8226506017
H	.1077689657	-3.6521993480	4.6429498998
H	-.9209956603	-.7274196770	4.4412867246
H	-1.9018485687	-2.1383839723	4.0156172898
H	-1.7018648619	-.8321082159	2.8464104884
H	-.0925807945	-1.6454903318	-1.9397686626
H	-1.5779173358	-2.2326504908	-3.7909727377
H	-2.5298827795	-2.1534034240	-2.2963932843
H	-2.0956114516	-3.7176653247	-2.9957267058
H	.8367236957	-3.0678200854	-3.7424288244
H	.4196675372	-4.5273535229	-2.8316238701
H	1.6366144184	-3.4115188597	-2.1995952117
H	-1.9526723323	5.2541438209	.8681994834
H	-1.8169847629	5.9979144359	-1.4810537876
H	-.5677533508	4.6769032520	-3.1428894262
H	-.3480787582	2.0897420500	2.1227779023
H	-2.3111072010	2.5638860933	3.5389409231
H	-2.8172262456	2.1691337062	1.8863264527
H	-2.8377598834	3.8526641027	2.4557192243
H	-.0763394426	3.6832430025	3.9815131173
H	-.4887895697	5.0401379060	2.9247001071
H	.9971036098	4.1237805116	2.6420864147
H	1.3892048432	1.5837155857	-2.3364208981
H	2.1926554590	2.4805453345	-4.4496281346
H	2.4137548809	3.7286844062	-3.2107175899
H	1.0910313285	3.8525114688	-4.3740223982
H	.1664986234	.9160635896	-4.3680794978
H	-.9757236735	2.2529070664	-4.1540039700
H	-.9275164013	.9401239909	-2.9720772846

23. $L^1\text{CuOH}_2^{2+}$ singlet

H	-3.4884255642	.8123443238	-.4028684691
C	-.4572304967	-2.4642688250	.2604098640
C	-.6617515733	-2.8776338166	1.6275534234
C	-1.5400084311	-3.9327184361	1.8452158421
C	-2.2072893088	-4.5605058368	.7872510474
C	-2.0382405861	-4.1254141930	-.5315885959
C	-1.1870496941	-3.0694311459	-.8333888198
C	-.0852031199	-2.1226242185	2.8162838628
C	.6033940231	-3.0522312990	3.8336941273
C	-1.1967944195	-1.2922238537	3.4984561776
C	-.9349020559	-2.6561833022	-2.2749593920
C	-2.2013299345	-2.6832628036	-3.1469267851
C	.1762785063	-3.5357904003	-2.8937227950
C	-.3926433206	2.5596357141	-.5933378461
C	-1.3443370010	3.1481006680	.3237661776
C	-2.1331603995	4.1898811433	-.1493266536
C	-2.0294067877	4.6282969891	-1.4736334714

C	-1.1417239399	4.0189341597	-2.3676124584
C	-.3108142689	2.97744448113	-1.9712851075
C	-1.3883770809	2.7351144872	1.7867035220
C	-2.8055699996	2.7486175929	2.3829144188
C	-.4350042239	3.6252559932	2.6175493321
C	.5178610070	2.2399855393	-3.0131693590
C	1.3918841233	3.1871586588	-3.8570491672
C	-.4085265993	1.3970844501	-3.9195679596
C	2.5173845668	-2.3734465479	.6309967744
C	1.6509128484	-1.2014563090	.2276247929
C	2.2678452045	.0610676892	.1202369712
C	1.6739646251	1.3181078042	-.1165300809
C	2.5951237127	2.4988570258	-.3259729169
H	-3.4518536927	-.7301497674	-.6725079762
H	3.4661290934	-2.3270164888	.0899519559
H	2.0286547993	-3.3240967569	.4146903538
H	2.7488015164	-2.3361216378	1.6999182477
H	3.3454093490	.0670802778	.2367766563
H	3.4003871093	2.4666870186	.4127796595
H	2.0605269607	3.4445404232	-.2307553917
H	3.0590753532	2.4587223352	-1.3162418584
H	-1.7281978636	-4.2698276859	2.8584864614
H	-2.8757063397	-5.3903948909	.9954995117
H	-2.5701277340	-4.6344662612	-1.3269990211
H	.6639063592	-1.4122752364	2.4569675836
H	1.0726499716	-2.4543616280	4.6195788964
H	1.3749376659	-3.6702526162	3.3662345220
H	-.1118915491	-3.7213818651	4.3197321641
H	-.7727584338	-.7016307612	4.3155596786
H	-1.9732171279	-1.9383371373	3.9180943375
H	-1.6815878888	-.6043662968	2.7955653579
H	-.5545009668	-1.6274125395	-2.2681487693
H	-1.9774669753	-2.2662124720	-4.1323203004
H	-3.0156550278	-2.0916024382	-2.7122953591
H	-2.5751639860	-3.6979003951	-3.3075792678
H	.3849220356	-3.2096511978	-3.9164639142
H	-.1329014949	-4.5845562605	-2.9280541960
H	1.1062377208	-3.4758400933	-2.3210163425
H	-2.8300469042	4.6846967697	.5170347494
H	-2.6547219623	5.4467274115	-1.8171214581
H	-1.1167867560	4.3592018067	-3.3968671101
H	-1.0046874007	1.7099520713	1.8588869528
H	-2.7815478126	2.3341481803	3.3941946661
H	-3.5075008264	2.1478259292	1.7934149812
H	-3.2137634212	3.7596593728	2.4629014307
H	-.4393179338	3.3033884697	3.6626574118
H	-.7529473780	4.6713997180	2.5831996656
H	.5935587603	3.5719531418	2.2491970924
H	1.1848268474	1.5385566836	-2.5053319747
H	2.0284018738	2.6020334987	-4.5262416083
H	2.0351325620	3.8138573798	-3.2332151392
H	.7859612129	3.8482327761	-4.4827258899
H	.1890175413	.8220681611	-4.6327183060
H	-1.0919285923	2.0334854340	-4.4891474281
H	-1.0160204069	.6928456032	-3.3385166206
N	.3655344301	-1.3960574311	-.0768742170
N	.3518940014	1.4970153303	-.0938715394
O	-2.9173321239	.0321183099	-.4107708082
Cu	-.8877638247	.0432798091	-.2188211004

24. L¹CuO⁻ doublet

Cu	.0560302397	-.5000102812	.7998240744
O	.2039862811	-1.7264296831	2.0865969330
N	1.5562729108	.4693057835	-.2422658821

N	-1.3730719185	.7251305151	.0237424241
C	2.5993792019	2.2745082768	-1.5565175027
C	1.3904082021	1.5879129525	-.9321706966
C	.1415327158	2.2173138411	-1.1356758200
C	-1.1383877783	1.8104982319	-.7034938897
C	-2.3018402506	2.7058426796	-1.1121926321
C	2.8406237958	-.1160572920	-.0919451083
C	3.5978148616	.1361905558	1.0794968307
C	4.8355957112	-.4974901076	1.2309534689
C	5.3268743950	-1.3747960302	.2674694937
C	4.5579442944	-1.6475811080	-.8612722604
C	3.3146611605	-1.0380066947	-1.0585670269
C	3.0531493215	1.0211935752	2.1956916727
C	4.0396251747	2.1282074475	2.6075470044
C	2.6274984286	.1665814909	3.4073826786
C	2.4430149951	-1.4336580542	-2.2455416532
C	1.7296144707	-2.7680839987	-1.9531473182
C	3.2096370834	-1.4943943863	-3.5767466496
C	-2.6933798812	.3623042094	.3987963126
C	-3.1685998214	.6841699195	1.6948238111
C	-4.4448571110	.2524569562	2.0709516451
C	-5.2456838897	-.4889991475	1.2060183145
C	-4.7588787120	-.8261932716	-.0548717434
C	-3.4895493459	-.4182876958	-.4768683095
C	-2.2901171556	1.4335425466	2.6914703542
C	-1.7628475950	.4818506622	3.7851583162
C	-3.0027033974	2.6521644256	3.3040331496
C	-2.9314174270	-.8893811094	-1.8160730404
C	-3.9526818515	-.8342222265	-2.9634077068
C	-2.3360864793	-2.3035575957	-1.6704599600
H	2.3141784932	3.2032733493	-2.0556031554
H	3.0866469540	1.6216773974	-2.2887150140
H	3.3531657786	2.5020811822	-.7954059653
H	.1690350591	3.1315597055	-1.7170210430
H	-1.9485375615	3.5997595071	-1.6308329700
H	-2.8830771213	3.0136269964	-.2368644043
H	-2.9949978464	2.1741510501	-1.7733479689
H	5.4193044008	-.3093874134	2.1286944596
H	6.2917920149	-1.8567567887	.4041270912
H	4.9251230984	-2.3583416866	-1.5974153062
H	2.1521239409	1.5083226362	1.8132994544
H	3.5836462182	2.7821009064	3.3601954093
H	4.3323111643	2.7487153821	1.7524475196
H	4.9556534745	1.7158787075	3.0470178147
H	2.2343352210	.8127594513	4.2032277078
H	3.4864156108	-.3814235749	3.8161084699
H	1.8440551480	-.5514504146	3.1288267448
H	1.6641645595	-.6733499502	-2.3472356284
H	1.0437579777	-3.0307453852	-2.7684212449
H	1.1550905730	-2.6993658057	-1.0249379517
H	2.4559710513	-3.5823287106	-1.8429090846
H	2.5188651750	-1.6951641460	-4.4041133979
H	3.9615507219	-2.2919629716	-3.5819283009
H	3.7253855678	-.5508672648	-3.7871470567
H	-4.8127889588	.4928438968	3.0653724064
H	-6.2351738606	-.8147403161	1.5170209555
H	-5.3729914795	-1.4292137026	-.7187177370
H	-1.4201001481	1.8025808962	2.1417252662
H	-1.1425365402	1.0382046761	4.4996497792
H	-1.1476644900	-.3170418561	3.3519431623
H	-2.5935300329	.0311080613	4.3433362508
H	-2.3159583215	3.2055867246	3.9551488400
H	-3.8641541840	2.3574261441	3.9149976486
H	-3.3643208748	3.3394736094	2.5304907538

H	-2.1041944973	-.2248996736	-2.0795890459
H	-3.4678004230	-1.0855550255	-3.9138971701
H	-4.3949579614	.1634433768	-3.0612593992
H	-4.7717853740	-1.5483640045	-2.8201893556
H	-1.8766903597	-2.6325372609	-2.6110094176
H	-3.1139481026	-3.0270857336	-1.3984893478
H	-1.5708815747	-2.3189675096	-.8889620718

25. L¹CuOH doublet

Cu	-.7372052051	.1778236694	.3370581029
O	-2.5217072689	.3070121485	.6725892257
N	.5573448863	-1.2626154177	.4636058457
N	.5769014920	1.5631542690	-.0509042632
C	2.7727040322	-2.2924915806	.7169160697
C	1.8769679501	-1.0894429133	.4959921164
C	2.5018849745	.1591372621	.3361433482
C	1.8932920713	1.3940205914	.0506844235
C	2.8076294142	2.5852638341	-.1594535577
C	-.0453866997	-2.5576283242	.5445585239
C	-.5279163829	-3.0194741355	1.7918622801
C	-1.1658839334	-4.2635199106	1.8369497240
C	-1.3343399220	-5.0322048759	.6886839534
C	-.8728125299	-4.5554752229	-.5352970963
C	-.2295507905	-3.3175911654	-.6361425153
C	-.4096214741	-2.1776605985	3.0580184496
C	.2704738609	-2.9389784499	4.2090807860
C	-1.7902142932	-1.6400889048	3.4864261874
C	.2033267289	-2.7998064346	-2.0048906234
C	-1.0249120808	-2.4190150379	-2.8541915486
C	1.0994506836	-3.7951151470	-2.7628502348
C	-.0028878962	2.8162803832	-.4265782055
C	-.4826366448	3.6881177211	.5788880814
C	-1.0920580374	4.8839261812	.1848596324
C	-1.2372381084	5.2141318060	-1.1594700682
C	-.7798148187	4.3365556649	-2.1385855565
C	-.1632597138	3.1275131852	-1.7992346244
C	-.3886517323	3.3374326505	2.0596653953
C	-1.7873848486	3.0581821292	2.6449846151
C	.3497895212	4.4169944764	2.8702684619
C	.2682070396	2.1644893967	-2.9019661523
C	1.1913628944	2.8241796768	-3.9417820283
C	-.9612604254	1.5379294233	-3.5882269612
H	-3.1228382237	.2166414101	-.0776135717
H	3.8199282263	-1.9934698813	.7761063298
H	2.6622144876	-3.0163066092	-.0959736043
H	2.5004955571	-2.8134262252	1.6400222778
H	3.5814656042	.1650297290	.4077074253
H	3.8459904944	2.3195186134	.0427901801
H	2.5204396795	3.4160847893	.4913893731
H	2.7372096534	2.9527612780	-1.1879687518
H	-1.5429768932	-4.6322663799	2.7862291682
H	-1.8323312961	-5.9957641874	.7453239496
H	-1.0217875090	-5.1519753355	-1.4307802568
H	.2194416723	-1.3142033676	2.8227990404
H	.3980775595	-2.2800072135	5.0744114509
H	1.2584783981	-3.3118065308	3.9186339411
H	-.3256600475	-3.7973891593	4.5365449716
H	-1.6890776235	-.9977139696	4.3687542920
H	-2.4637272920	-2.4642851479	3.7486256022
H	-2.2590143201	-1.0588724740	2.6866427720
H	.7843322626	-1.8866694927	-1.8492736968
H	-.7140148956	-1.9915539695	-3.8137843661
H	-1.6475902701	-1.6814506539	-2.3384351524
H	-1.6493696795	-3.2949904418	-3.0606992565

H	1.4423229865	-3.3551218712	-3.7054637825
H	.5643006376	-4.7186014860	-3.0075033827
H	1.9829623550	-4.0696599055	-2.1777022640
H	-1.4654788448	5.5638059773	.9449171507
H	-1.7135044189	6.1479034503	-1.4438810903
H	-.9105000538	4.5912884112	-3.1863914034
H	.1910385268	2.4134005346	2.1435767863
H	-1.7044480010	2.7561596841	3.6953288905
H	-2.2930959750	2.2604730073	2.0926546440
H	-2.4145029515	3.9561735516	2.6047936568
H	.4493080224	4.1041111133	3.9150912590
H	-.1909296971	5.3694094600	2.8624614125
H	1.3545189708	4.6025473966	2.4756421016
H	.8281363104	1.3495720664	-2.4354455551
H	1.5331676970	2.0819442053	-4.6710696725
H	2.0751996788	3.2684590494	-3.4728346819
H	.6778016385	3.6163881587	-4.4964651160
H	-.6519181315	.8057617039	-4.3422645527
H	-1.5670828229	2.3019740358	-4.0873857687
H	-1.6014796449	1.0280934457	-2.8616704124

26. L¹CuOH₂⁺ doublet

H	-3.6656387627	.6758535210	-.3603427033
C	-.4301851627	-2.6211921266	.2207213881
C	-.6944018020	-3.0440518133	1.5531097332
C	-1.4291093947	-4.2185828870	1.7296459659
C	-1.8929565512	-4.9559263192	.6406224673
C	-1.6453420544	-4.5158540670	-.6582203578
C	-.9277825051	-3.3416626019	-.8992719584
C	-.2963478609	-2.2036018467	2.7623484137
C	.3490349871	-3.0309962781	3.8866900621
C	-1.5152697719	-1.4198187573	3.2928160956
C	-.6523985991	-2.8918581989	-2.3297052677
C	-1.9532798822	-2.6752402955	-3.1241143050
C	.2793529687	-3.8790795280	-3.0591863480
C	-.3806482652	2.7246472652	-.5726402908
C	-1.0992670130	3.4970143340	.3811603129
C	-1.7508234353	4.6502159733	-.0629070454
C	-1.7229542706	5.0232277474	-1.4050776252
C	-1.0428403307	4.2373586367	-2.3351157302
C	-.3609713981	3.0808805970	-1.9514741286
C	-1.1310315397	3.1250302265	1.8589524432
C	-2.5704409029	2.8999601646	2.3580342427
C	-.4079920407	4.1791551336	2.7198635953
C	.2784058662	2.1921270232	-3.0141364273
C	1.1512848473	2.9756561196	-4.0098567321
C	-.8076632131	1.3874285271	-3.7583978403
C	2.4433095325	-2.3767604169	.4948929125
C	1.5456280526	-1.1985343898	.1823154527
C	2.1507779244	.0754636464	.1186462021
C	1.5568081929	1.3367587119	-.0834233328
C	2.4843730333	2.5223679287	-.2490653941
H	-3.5315821980	-.8787502654	-.5133999691
H	3.4694097317	-2.1678635738	.1878168607
H	2.0952908822	-3.2824914929	-.0058054366
H	2.4520137674	-2.5776368315	1.5716077206
H	3.2284373772	.0816966112	.2241626800
H	3.4451674211	2.3257158552	.2292666379
H	2.0481291866	3.4271463996	.1795107750
H	2.6738496254	2.7183572576	-1.3096785623
H	-1.6489182818	-4.5631377916	2.7346521612
H	-2.4523144228	-5.8713879970	.8058466362
H	-2.0092826646	-5.1000014375	-1.4977630024
H	.4407860464	-1.4631719553	2.4407453547

H	.7082777464	-2.3682284212	4.6796604243
H	1.1985480410	-3.6155813924	3.5208126133
H	-.3619419442	-3.7265324679	4.3426625227
H	-1.2233378292	-.7735294557	4.1267748282
H	-2.2954445970	-2.1004394883	3.6487638391
H	-1.9579495021	-.7875169643	2.5140985870
H	-.1339536334	-1.9298810694	-2.2807366293
H	-1.7280008276	-2.3087199533	-4.1303606618
H	-2.6002281589	-1.9345818751	-2.6388553420
H	-2.5272092816	-3.6009683839	-3.2300682469
H	.5116712680	-3.5122431933	-4.0638951454
H	-.1853600100	-4.8649425401	-3.1612292267
H	1.2225484720	-4.0098998361	-2.5202118210
H	-2.2809396702	5.2714496773	.6522272873
H	-2.2351000573	5.9238572119	-1.7291050797
H	-1.0492034736	4.5293405199	-3.3801285544
H	-.5898858746	2.1818756808	1.9766652323
H	-2.5663249567	2.5990399687	3.4101537827
H	-3.0728185084	2.1101011197	1.7871959762
H	-3.1765495846	3.8073305468	2.2751972878
H	-.3906885415	3.8667785645	3.7686155307
H	-.9099233916	5.1505861484	2.6684817682
H	.6262715276	4.3211906359	2.3919381205
H	.9254867104	1.4657325061	-2.5153328238
H	1.6658598597	2.2827273403	-4.6823178382
H	1.9082701268	3.5777346497	-3.4981759424
H	.5558094640	3.6503250488	-4.6322947520
H	-.3520113189	.7108825231	-4.4885829499
H	-1.4921671371	2.0526916765	-4.2944554348
H	-1.4055998131	.7839941015	-3.0653883795
N	.2476469717	-1.3985735779	-.0288718144
N	.2378918528	1.5282664369	-.1230737700
O	-3.0512719614	-.0673441738	-.3030642685
Cu	-1.0157590005	.0631083193	-.1475321469

anilido-imine dioxygen activation pathway and Cu/O structures

27. L²Cu

Cu	.1870000000	-1.5450000003	.4890000000
N	-1.3912216707	-.6129595266	.0292797739
N	1.7117222654	-.3912892425	.2862295916
C	-2.3753625473	1.5204258950	-.4726983448
C	-1.2120118932	.7054531990	-.2517642150
C	.0947073340	1.3742845397	-.3594912809
C	1.4449401205	.8123123130	-.1930600763
C	2.6343748162	1.6819167962	-.5893262335
C	-2.6917994379	-1.1927311806	.0747056088
C	-3.2729149974	-1.7280802899	-1.0979604876
C	-4.5234240083	-2.3502744227	-1.0051571516
C	-5.1919684173	-2.4499734977	.2113179818
C	-4.6014990387	-1.9392211611	1.3655707180
C	-3.3534911156	-1.3100828290	1.3218232994
C	-2.5095522482	-1.7209688518	-2.4157949117
C	-3.3657275981	-1.3053388332	-3.6214966089
C	-1.8610062535	-3.1021675215	-2.6381322690
C	-2.6653961147	-.8287328359	2.5934010735
C	-1.7646927776	-1.9484510029	3.1534710002
C	-3.6276586675	-.3208789184	3.6764829856
C	3.0410468704	-.8592587248	.5386662529
C	3.6444108396	-1.7450911800	-.3839001588
C	4.9172234290	-2.2447571249	-.0919733981
C	5.5755718891	-1.8984776543	1.0857107922
C	4.9515475150	-1.0564420453	2.0013663280

C	3.6806531028	-.5243969210	1.7546045985
C	2.8793816116	-2.2096452781	-1.6173672033
C	2.0910120783	-3.4918690618	-1.2798412821
C	3.7582164761	-2.4277539006	-2.8574487101
C	2.974753590	.3072304148	2.8205053636
C	3.8845704172	1.3516167533	3.4863525886
C	2.3416080764	-.6258592020	3.8729166984
C	-2.3206154530	2.8644733684	-.7426845757
C	.0651777747	2.7755842360	-.6446339901
C	-1.0776244483	3.5178637125	-.8242261272
H	-3.3401462878	1.0342608858	-.4052276994
H	2.4797354562	2.1343736090	-1.5702822031
H	3.5457163081	1.0888516048	-.6220964719
H	2.7948324656	2.4939442640	.1285577134
H	-4.9776952812	-2.7691994127	-1.8985468185
H	-6.1650135438	-2.9300771024	.2627206522
H	-5.1220633940	-2.0321225090	2.3135308622
H	-1.7005040842	-.9924068418	-2.3216261991
H	-2.7463194667	-1.2445347989	-4.5230283114
H	-3.8242930486	-.3251061923	-3.4589096134
H	-4.1677170045	-2.0228690661	-3.8261077786
H	-1.2212603237	-3.0998350110	-3.5284491455
H	-2.6250085761	-3.8764150861	-2.7712888867
H	-1.2510000001	-3.3859999999	-1.7730000000
H	-2.0146122720	.0057555804	2.3158294473
H	-1.1938425326	-1.6046230480	4.0231613500
H	-1.0480000001	-2.2910000000	2.3920000000
H	-2.3620584085	-2.8169462909	3.4525314017
H	-3.0620083814	.1166148890	4.5059186996
H	-4.2425499572	-1.1255065562	4.0942338447
H	-4.2997901363	.4471632863	3.2816415122
H	5.4001660582	-2.9173041113	-.7936195659
H	6.5655794124	-2.2934516166	1.2934573910
H	5.4588545673	-.8100539942	2.9290569133
H	2.1498693048	-1.4335127566	-1.8688133120
H	1.4498545122	-3.7970450474	-2.1129888213
H	1.4490000001	-3.3460000000	-.3970000002
H	2.7726754071	-4.3160550215	-1.0430718951
H	3.1310242355	-2.6510248629	-3.7265196898
H	4.4474303907	-3.2693839833	-2.7316708456
H	4.3518922886	-1.5373710138	-3.0863179757
H	2.1558519697	.8494956469	2.3413046676
H	3.2998440071	1.9813451131	4.1648602774
H	4.3582588226	2.0010284408	2.7432736126
H	4.6790437584	.8870796810	4.0797747319
H	1.7714236194	-.0506929245	4.6109090240
H	3.1128740122	-1.1934768825	4.4052348582
H	1.6630000001	-1.3449999998	3.4020000002
H	-3.2450605318	3.4182990987	-.8839534549
H	1.0019916387	3.3107337304	-.6960346824
H	-1.0127025606	4.5831686012	-1.0179214046

28. L²Cu(MeCN)

Cu	-.0025264921	-.8093581571	.2069619034
N	1.5820916918	.3038502117	-.3352056619
N	-1.3269617333	.5912624845	-.0419049494
N	-.0677746858	-2.6717148106	.7224620145
C	-1.0682966344	1.8260319554	-.5237041498
C	.2693003383	2.3033992627	-.8607682483
C	-2.6660938859	.2013377822	.2567960761
C	-3.1594878369	.3338600375	1.5783014931
C	-3.4685633273	-.4086770186	-.7419659724
C	-.1561531919	-3.7950026622	1.0001928628
C	2.8193949773	2.2990602287	-1.0181150882

C	3.4585021493	-.4861726363	1.0438578811
C	-2.9614959331	-.5822921825	-2.1700375772
C	2.9165655345	.2455697336	2.2682900264
C	-4.4329371450	-.1623614430	1.8793978025
C	.3752118407	3.6230577141	-1.3901750554
C	-2.3216544257	.9844920664	2.6731750123
C	1.5189804392	1.5630228595	-.7114347211
C	-2.1517447968	2.7514664532	-.7208019924
C	3.3178019257	-1.1206495971	-1.3298158817
C	-4.7347540436	-.8895321866	-.3916722429
C	2.8172646485	-.4066651147	-.2154626603
C	-1.9787519402	4.0138689157	-1.2326840761
C	4.6050378617	-1.2800370896	1.1592526554
C	-.6945057955	4.4673568830	-1.5870538795
C	-3.0246383453	2.2083657851	3.2863402669
C	-1.9300820350	-.0341327507	3.7597363850
C	4.4652647101	-1.9025826919	-1.1589736006
C	5.1127615952	-1.9843813142	.0712503485
C	2.6099524855	-1.0905309951	-2.6805525935
C	-5.2220116960	-.7721915403	.9079215797
C	3.9483190181	1.2217827298	2.8607037658
C	-2.6804385586	-2.0648920071	-2.4801374250
C	2.4199209296	-.7468437635	3.3367617510
C	-.2697638307	-5.2044831305	1.3452751260
C	3.5533722340	-.7071033924	-3.8328497801
C	-3.9165433449	.0287602371	-3.2094306702
C	1.9107556479	-2.4343684746	-2.9637298402
H	2.8903829041	3.2243595921	-.4416215379
H	2.8774349542	2.5680155593	-2.0783301480
H	3.6825355940	1.6797491407	-.7841872660
H	-2.0109625984	-.0497750221	-2.2461917960
H	2.0531672465	.8346722730	1.9491864845
H	-4.8130309940	-.0678160628	2.8935119071
H	1.3522523825	3.9917248882	-1.6717690307
H	-1.3973903805	1.3345063685	2.2068101784
H	-3.1473678052	2.4162883985	-.4573906376
H	-5.3504463689	-1.3648291939	-1.1511005279
H	-2.8436152015	4.6595468456	-1.3640684317
H	5.1085325492	-1.3447635595	2.1200265346
H	-.5444173184	5.4582344584	-2.0024481396
H	-2.3781157035	2.6921318631	4.0270727553
H	-3.9564793647	1.9299638695	3.7910406694
H	-3.2672796034	2.9453065193	2.5150803008
H	-1.2922590849	.4335991301	4.5186341923
H	-1.3801586062	-.8753672325	3.3250704618
H	-2.8128081560	-.4380755529	4.2679620737
H	4.8598274942	-2.4558795008	-2.0065337801
H	6.0060086879	-2.5923333116	.1805189058
H	1.8287801745	-.3276789671	-2.6315861971
H	-6.2088853260	-1.1499969999	1.1599793583
H	3.5175733691	1.7673993627	3.7070690859
H	4.2743942604	1.9541142342	2.1157236297
H	4.8389818498	.6970057181	3.2230357572
H	-2.2758550315	-2.1812169089	-3.4922306212
H	-3.5943611792	-2.6659849293	-2.4121755734
H	-1.9540634611	-2.4778974765	-1.7728564780
H	1.9862128272	-.2109009959	4.1880798695
H	3.2374630900	-1.3714820193	3.7136783980
H	1.6519217461	-1.4090290969	2.9253444701
H	.3323429124	-5.4207293621	2.2322061964
H	.0895786131	-5.8197690571	.5155926086
H	-1.3134473037	-5.4581477006	1.5515765290
H	2.9929644209	-.6214382167	-4.7698441159
H	4.3359689996	-1.4576834520	-3.9862880748

H	4.0448067702	.2518714625	-3.6413740819
H	-3.4936168692	-.0605330544	-4.2162496196
H	-4.0865618192	1.0902103490	-3.0065935153
H	-4.8901241683	-.4737343087	-3.2153159541
H	1.3686592178	-2.3951725729	-3.9149709767
H	1.1933763987	-2.6741628407	-2.1728028070
H	2.6368815076	-3.2530979417	-3.0215607839

29. L²Cu(THF)

Cu	.0503017423	-.7053854332	.0780574016
N	1.5431745578	.5987985135	.0196623029
N	-1.4162032363	.5143535417	-.1917349852
C	2.5948248150	2.7774231258	-.2550001351
C	1.3610275778	1.8881908937	-.1623643602
C	.0465525742	2.5193336857	-.2720996994
C	-1.2543179110	1.8494434057	-.3015027427
C	-2.4103182318	2.6883519348	-.4617771036
C	2.8243131937	-.0178399204	.1477801184
C	3.3978441635	-.1658495266	1.4365216986
C	4.5817887336	-.9001681460	1.5595070961
C	5.1971434356	-1.4793996949	.4515887866
C	4.6218349371	-1.3273210011	-.8068111193
C	3.4366796877	-.6034352980	-.9866675823
C	2.7038109874	.3894184552	2.6766057477
C	3.6722146897	1.0469627810	3.6728536011
C	1.8752219272	-.7117563131	3.3680906347
C	2.8269914803	-.4871238004	-2.3805437719
C	2.3801685730	-1.8619068221	-2.9134869578
C	3.7833956183	.2024527615	-3.3700485857
C	-2.6960795864	-.1045443959	-.2385952742
C	-3.4271042244	-.3167978907	.9596717417
C	-4.6022663074	-1.0737078917	.9109477604
C	-5.0707256697	-1.6122257742	-.2853740882
C	-4.3552190256	-1.3892895155	-1.4593533983
C	-3.1740477486	-.6384685221	-1.4624549763
C	-2.9162732713	.2131465383	2.2954040246
C	-2.3555001271	-.9313680339	3.1613973553
C	-3.9829970663	1.0112725330	3.0630773656
C	-2.4061364160	-.4366762998	-2.7642969377
C	-3.2592879715	.2655555524	-3.8351722262
C	-1.8369724188	-1.7665026355	-3.2929081372
C	-2.3415608200	4.0569092987	-.5407419960
C	.0399182746	3.9411579362	-.3578902410
C	-1.0964152660	4.7084232193	-.4782484224
C	1.2950634232	-3.5340480574	.6509143478
O	.1544488095	-2.7513503658	.2324736488
C	-.9972411873	-3.6173035587	.3470575523
C	1.0341632789	-4.9393458185	.0834123936
C	-.5016094761	-4.9765999546	-.1631786242
H	2.5701116006	3.4029727260	-1.1503011606
H	3.5003078295	2.1727309379	-.2824020686
H	2.6630294665	3.4436213161	.6113521639
H	-3.3763634520	2.1989186157	-.5036982901
H	5.0310833934	-1.0231271591	2.5403412135
H	6.1177670633	-2.0433614585	.5693552041
H	5.1014769021	-1.7781756524	-1.6714412931
H	2.0007307879	1.1597773128	2.3483108100
H	3.1103234846	1.5278021427	4.4803196821
H	4.2896402109	1.8084588593	3.1864860966
H	4.3439610521	.3170772378	4.1373425671
H	1.3276096848	-.3071820305	4.2264432497
H	2.5240723051	-1.5186049015	3.7282010875
H	1.1449435502	-1.1443614168	2.6766266958
H	1.9305864649	.1334123335	-2.3002949898

H	1.9069434615	-1.7592279343	-3.8961305854
H	1.6551545602	-2.3264967338	-2.2378207062
H	3.2304255142	-2.5447938408	-3.0212275197
H	3.3007880637	.3276079062	-4.3453047810
H	4.6953913964	-.3844905157	-3.5243585260
H	4.0820842013	1.1915650563	-3.0092078622
H	-5.1591721913	-1.2490148570	1.8276514083
H	-5.9859525516	-2.1969796751	-.3027249356
H	-4.7204546806	-1.8065959830	-2.3944503556
H	-2.0879182717	.8923971242	2.0812783914
H	-1.9425010910	-.5455478559	4.1005158467
H	-1.5554218924	-1.4613045061	2.6337410501
H	-3.1354883172	-1.6603108462	3.4103930336
H	-3.5548042438	1.4372346056	3.9771410257
H	-4.8308116819	.3840897697	3.3599372634
H	-4.3698329319	1.8340263535	2.4544744661
H	-1.5561319472	.2121854749	-2.5388359963
H	-2.6644551283	.4561296669	-4.7354325775
H	-3.6353017879	1.2248892702	-3.4673824954
H	-4.1213671408	-.3431094220	-4.1302641569
H	-1.2558247297	-1.6040558325	-4.2079744133
H	-2.6345246151	-2.4809717800	-3.5264085618
H	-1.1750159863	-2.2294899670	-2.5530929451
H	-3.2582468954	4.6320895497	-.6474330273
H	.9835090037	4.4680801372	-.3100625713
H	-1.0251928489	5.7897713866	-.5263493718
H	1.3362573616	-3.5402734998	1.7480066115
H	2.1883143083	-3.0439112269	.2625136781
H	-1.8013471133	-3.1698256623	-.2378535292
H	-1.3027302492	-3.6640125743	1.4007497828
H	1.3634427833	-5.7127917656	.7819973533
H	1.5780486711	-5.0845842216	-.8531971436
H	-.7161414785	-5.0847801560	-1.2292915717
H	-.9913678429	-5.8010574314	.3612204237

30. L²Cu(MeCN)O₂ singlet

Cu	.0664161384	-1.3849030437	.2951073187
O	.8571445857	-3.1047074135	-.0154758819
O	-.4604370885	-3.1120797647	-.2972098135
N	-1.3386739915	-.1508716850	-.0855849914
N	1.5366673411	-.1037131640	.3329900595
N	-.2974860694	-2.1591160288	2.4311208867
C	-.5245134878	-3.2707653614	2.6700665332
C	-.8033455724	-4.6831863958	2.8784692738
C	-2.2590087344	1.9892190709	-.6785752807
C	-1.1463179122	1.1724345308	-.2834963864
C	.1334248750	1.8440589888	-.1313930005
C	1.4072810544	1.1864448157	.1181847270
C	2.6652156427	2.0409373675	.0678583866
C	-2.5993940637	-.7595197348	-.3822035185
C	-2.8621325815	-1.2153560681	-1.6985133079
C	-4.0962906454	-1.8195366444	-1.9609571149
C	-5.0508485209	-1.9805288514	-.9610357388
C	-4.7740663828	-1.5442857978	.3314732241
C	-3.5547928805	-.9354233296	.6495786744
C	-1.8532147518	-1.0536852596	-2.8317055347
C	-2.3457778381	-.0414298104	-3.8833177600
C	-1.5010786121	-2.4015034776	-3.4876744460
C	-3.2909126423	-.4663433652	2.0761101699
C	-3.6971074399	-1.5193010645	3.1220450867
C	-3.9973002934	.8703632044	2.3783183707
C	2.8289953660	-.7410111673	.4410183035
C	3.4270107790	-1.2571205859	-.7330170481
C	4.6644961694	-1.8984070059	-.6138999607

C	5.2907211639	-2.0465137387	.6198742734
C	4.6730114060	-1.5588896184	1.7660268634
C	3.4334373602	-.9095612999	1.7076486714
C	2.7889625913	-1.1177658192	-2.1130585042
C	2.6542789305	-2.4760471902	-2.8258306428
C	3.5657647845	-.1182148875	-2.9919862292
C	2.7969777075	-.3970095006	2.9958393620
C	3.5415622256	.8355758601	3.5452517684
C	2.7199399787	-1.4920633947	4.0743108218
C	-2.1610929656	3.3467865813	-.8563142251
C	.1630002573	3.2573779758	-.3129904125
C	-.9345637532	4.0079010686	-.6588083305
H	.1157411697	-5.2112748953	3.1456700261
H	-1.1896988458	-5.0943095200	1.9414649266
H	-1.5443123107	-4.8190800598	3.6703310990
H	-3.2122694256	1.5003150150	-.8291233456
H	2.7442097656	2.5460458833	-.8984492604
H	3.5575738083	1.4385422941	.2143894890
H	2.6399957093	2.8112310949	.8428670173
H	-4.3121654893	-2.1678283353	-2.9670645638
H	-6.0052231560	-2.4478339012	-1.1867103561
H	-5.5215049905	-1.6750935108	1.1085279439
H	-.9318002870	-.6556076208	-2.3981218711
H	-1.5894703026	.0947956581	-4.6644581692
H	-2.5501844083	.9345365092	-3.4338902541
H	-3.2649649203	-.3901708050	-4.3676551910
H	-.7335545361	-2.2573761914	-4.2568318349
H	-2.3712751624	-2.8551604077	-3.9749153762
H	-1.1163925482	-3.0998971905	-2.7408731744
H	-2.2135599641	-.3082216068	2.1682783742
H	-3.3430859323	-1.2193823474	4.1141812784
H	-3.2704394045	-2.4988296487	2.8879224890
H	-4.7846596361	-1.6354020161	3.1857169840
H	-3.7776184763	1.1955688585	3.4015998569
H	-5.0845840576	.7657277631	2.2849021377
H	-3.6740678254	1.6602565350	1.6965136235
H	5.1439799058	-2.2896158781	-1.5061050798
H	6.2528628243	-2.5459415838	.6878318647
H	5.1613141805	-1.6812901663	2.7282486178
H	1.7764903185	-.7257899406	-1.9793064728
H	2.1254517830	-2.3501631863	-3.7769726898
H	2.0925606637	-3.1756526856	-2.2033506027
H	3.6322502123	-2.9149176165	-3.0513058864
H	3.0667345011	.0077764557	-3.9588754782
H	4.5836807630	-.4747572320	-3.1851499308
H	3.6443889300	.8659862982	-2.5204450789
H	1.7700674873	-.1012922702	2.7639473028
H	3.0485549347	1.2103586383	4.4486975873
H	3.5763970857	1.6503057613	2.8175806171
H	4.5751846750	.5823754896	3.8070177365
H	2.1634400963	-1.1248198950	4.9429690084
H	3.7147534797	-1.7895431315	4.4234202916
H	2.2123537212	-2.3815250363	3.6947083650
H	-3.0450367079	3.9063645263	-1.1503233481
H	1.1002557748	3.7797766257	-.1823866566
H	-.8483710938	5.0813541524	-.7857636486

31. $L^2Cu(MeCN)_2$ triplet

Cu	.2031462931	-1.4112482523	-.4269998704
O	.9587897082	-3.1509331368	-1.3614893361
O	-.3165291403	-3.0439333325	-1.5659363078
N	-1.2694989426	-.1274340556	-.3705452282
N	1.6176241757	-.1517160675	.1097070897
N	-.2803534989	-2.8547805137	1.2966770370

C	- .2165549733	-3.9592649803	1.6414303563
C	- .1641826076	-5.3498617410	2.0721881608
C	-2.1751396425	2.0882377453	- .6492663253
C	-1.0571519762	1.2004465304	- .4703072209
C	.2617678118	1.8202437892	- .4070589417
C	1.4997147897	1.1521587351	- .0281136501
C	2.7169995001	2.0211059294	.2518221096
C	-2.5951789409	- .6516643250	- .2519724067
C	-3.3008104210	-1.0970616155	-1.3991265791
C	-4.5892089625	-1.6210863222	-1.2373217395
C	-5.1836985196	-1.7160730606	.0160468958
C	-4.4795801478	-1.2934895578	1.1393760091
C	-3.1880509497	- .7655319001	1.0352879715
C	-2.7185013074	- .9956654428	-2.8056405976
C	-3.4087743517	.1212336186	-3.6140666387
C	-2.7960378065	-2.3305342190	-3.5692843826
C	-2.4672846719	- .3073988417	2.3006075499
C	-2.5804814346	-1.3250204871	3.4500491906
C	-2.9727992192	1.0706176482	2.7733037558
C	2.7792269539	- .8016969710	.6535306940
C	3.6736068395	-1.4636355682	- .2260192526
C	4.7312778329	-2.1920948974	.3271912645
C	4.9135034727	-2.2774057746	1.7047475284
C	4.0308182102	-1.6211190831	2.5543160599
C	2.9507111020	- .8795782101	2.0582344122
C	3.5341657744	-1.3585601924	-1.7423610435
C	3.8613555778	-2.6694110004	-2.4778602602
C	4.4008789482	- .2122815292	-2.3004324351
C	2.0170719406	- .1890173184	3.0508161413
C	2.7431850351	.9377525933	3.8126639953
C	1.3936773507	-1.1800984595	4.0510307322
C	-2.0329614994	3.4379293620	- .8552184912
C	.3393804046	3.2239725617	- .6492525291
C	- .7532189683	4.0263354609	- .8811672715
H	.8181559055	-5.5742149633	2.4959311752
H	- .3420754243	-6.0063074108	1.2160918025
H	- .9316100938	-5.5353529386	2.8286958449
H	-3.1650291201	1.6496227480	- .6462256620
H	3.0248596759	2.5481733969	- .6560145684
H	3.5567486136	1.4184209179	.5904289033
H	2.4964342832	2.7764875352	1.0099737234
H	-5.1391139072	-1.9536131143	-2.1130198019
H	-6.1875234584	-2.1191577823	.1181043604
H	-4.9438481572	-1.3724189466	2.1180820676
H	-1.6627815485	- .7286023131	-2.7045015066
H	-2.9631638505	.2034922607	-4.6117455055
H	-3.3133805855	1.0912253021	-3.1190679763
H	-4.4767846636	- .0906222847	-3.7409975974
H	-2.2948119487	-2.2388480513	-4.5392008696
H	-3.8332662763	-2.6230883443	-3.7670031493
H	-2.3141626864	-3.1378769278	-3.0133332702
H	-1.4078875760	- .2100688804	2.0477290584
H	-1.9357695846	-1.0249062794	4.2832493546
H	-2.2793111257	-2.3251365562	3.1285775431
H	-3.6021754244	-1.3885656384	3.8405205096
H	-2.4209613799	1.3982512571	3.6620622556
H	-4.0357229049	1.0235287470	3.0378876697
H	-2.8516410006	1.8316089629	1.9988649137
H	5.4245942597	-2.7033405798	- .3324764778
H	5.7415446452	-2.8504079260	2.1120103101
H	4.1764914028	-1.6858216919	3.6288292665
H	2.4896197208	-1.1177831245	-1.9603201459
H	3.6018802880	-2.5722397654	-3.5371365327
H	3.2961036639	-3.5102934425	-2.0701070304

H	4.9286184146	-2.9113570177	-2.4284262603
H	4.2677937457	-.1267801800	-3.3844300018
H	5.4625272126	-.3988771108	-2.1033021054
H	4.1423225691	.7500754181	-1.8517593116
H	1.1950067787	.2619670788	2.4891476054
H	2.0434277611	1.4677597075	4.4677349052
H	3.1892105271	1.6676877445	3.1318354568
H	3.5467995611	.5348371762	4.4388108594
H	.7096587918	-.6539569955	4.7257927562
H	2.1581517107	-1.6625318021	4.6698051743
H	.8288150891	-1.9585860959	3.5352287586
H	-2.9197537573	4.0478885419	-1.0081561785
H	1.3124516047	3.6964239508	-.6514618847
H	-.6288836004	5.0876794747	-1.0663220007

32. L²Cu(THF)O₂ singlet

Cu	.2404810678	-1.1743228183	-.7349623202
O	.3760360841	-1.2526348366	-3.4455406607
O	.0634796497	-2.0065443767	-2.4465011541
N	-1.2577862717	-.0417582183	-.2000475782
N	1.6474128696	.0473337732	.0419890977
C	-2.2906731001	2.1403539804	-.1364461939
C	-1.1216270461	1.3054077988	-.1420465923
C	.1620692785	1.9819948260	-.0134723979
C	1.4537233021	1.3303635432	.2142511130
C	2.6048097774	2.2021071981	.6946856598
C	-2.5567335245	-.6376129469	-.1861857189
C	-3.3342468456	-.7671367148	-1.3643060604
C	-4.5846675115	-1.3908097669	-1.2725291017
C	-5.0675291508	-1.8855897144	-.0655895311
C	-4.2901414408	-1.7668782882	1.0834524366
C	-3.0331214055	-1.1542321214	1.0495569144
C	-2.8583916334	-.2670212804	-2.7258427054
C	-3.7229932989	.8985541789	-3.2433442396
C	-2.8214113065	-1.4047032949	-3.7636325129
C	-2.222392420	-1.0003838630	2.3331407318
C	-2.2572929970	-2.2497940272	3.2286806703
C	-2.6773777905	.2388437485	3.1297650205
C	2.8761208656	-.6157991792	.3631770683
C	3.7583460531	-.9573162016	-.6918803250
C	4.9141041778	-1.6805232290	-.3790196086
C	5.1912681586	-2.0789318353	.9264157999
C	4.3000636115	-1.7578236196	1.9458012685
C	3.1315056240	-1.0291605297	1.6926043121
C	3.4823545157	-.5357222912	-2.1311386592
C	3.7740748687	-1.6513302353	-3.1481810657
C	4.2632803819	.7419786450	-2.4966656029
C	2.1685245764	-.7439031915	2.8409845650
C	2.8281264975	.0950870648	3.9504361450
C	1.5865947511	-2.0506350727	3.4130392436
C	-.7444736989	-4.0737493335	-.1865089571
O	.3886628408	-3.2405448910	.1512402520
C	1.5515083437	-4.0406601599	-.1478117576
C	-.3628748685	-5.4762136259	.3110224621
C	1.1911877689	-5.4536870850	.3377367419
C	-2.2303123517	3.5138749596	-.1053618352
C	.1583307488	3.4029234461	-.0081893355
C	-.9869317971	4.1691828446	-.0699399558
H	-3.2557590349	1.6510876552	-.1602811310
H	2.8999429873	2.9121902244	-.0843713747
H	3.4754634188	1.5972349499	.9384942586
H	2.3174178324	2.7818959850	1.5753837629
H	-5.1895568771	-1.4917103632	-2.1689768499
H	-6.0417738391	-2.3640417929	-.0201414112

H	-4.6699754576	-2.1535708740	2.0240599673
H	-1.8356389048	.1013877156	-2.6115913888
H	-3.3473835581	1.2444564223	-4.2124484531
H	-3.7115284712	1.7475554798	-2.5548764629
H	-4.7647789833	.5878577905	-3.3818962233
H	-2.3635150498	-1.0500539837	-4.6918678370
H	-3.8297579619	-1.7633951172	-3.9989396159
H	-2.2270674374	-2.2451314666	-3.3994688803
H	-1.1833199627	-.8354818784	2.0341125269
H	-1.5880046356	-2.1167628392	4.0846550495
H	-1.9331388496	-3.1436534005	2.6865358338
H	-3.2574688443	-2.4434042424	3.6301087206
H	-2.0559325521	.3731075585	4.0226161469
H	-3.7179115517	.1292389817	3.4565729667
H	-2.6085490032	1.1490045559	2.5281843104
H	5.6066538210	-1.9400321422	-1.1736260091
H	6.0946377347	-2.6404840674	1.1464999505
H	4.5107925591	-2.0808081519	2.9614294054
H	2.4169066549	-.3075670087	-2.2212254497
H	3.4125813183	-1.3505650808	-4.1359066302
H	3.2636189738	-2.5801556587	-2.8770406626
H	4.8455640618	-1.8633143709	-3.2357599934
H	4.0241938825	1.0554271056	-3.5185491529
H	5.3441340468	.5699043755	-2.4379775983
H	4.0223309641	1.5707673244	-1.8245633995
H	1.3300266366	-.1647032093	2.4460310868
H	2.0980898378	.3354461292	4.7306338755
H	3.2280620239	1.0355327360	3.5591170407
H	3.6541101766	-.4456672541	4.4248966639
H	.8756423439	-1.8312269422	4.2167395343
H	2.3738515811	-2.6872625102	3.8319796170
H	1.0637194953	-2.6166117669	2.6372235352
H	-.8840408984	-4.0515523519	-1.2745249709
H	-1.6227412312	-3.6401323940	.2936220342
H	2.4021360388	-3.5891999945	.3632250099
H	1.7256930091	-4.0186008032	-1.2321659808
H	-.7604349238	-6.2518338212	-.3487880058
H	-.7626802775	-5.6545374562	1.3127788056
H	1.5613105782	-5.6172899822	1.3532300273
H	1.6334306704	-6.2192278860	-.3052647790
H	-3.1532374944	4.0879113602	-.1165369448
H	1.1050668038	3.9236347922	.0469371612
H	-.9247651233	5.2520936529	-.0773891691

33. L²Cu(THF)O₂ triplet

Cu	.2184195292	-1.1808654121	-.7377710539
O	.5281150479	-1.0441716160	-3.5556128672
O	.4733226245	-1.8824835390	-2.6162055629
N	-1.2816286962	-.0343499991	-.2055212095
N	1.6739336629	.0265240392	.0133047345
C	-2.2714111773	2.1673084106	-.1575102050
C	-1.1200999030	1.3099594777	-.1367398376
C	.1785954219	1.9645773039	-.0202600546
C	1.4687495593	1.3040968754	.2172371257
C	2.6088272755	2.1653486545	.7446242824
C	-2.5846431195	-.6089314523	-.0864580316
C	-3.3330335176	-.9456083821	-1.2424454596
C	-4.5689191026	-1.5844871569	-1.0860667081
C	-5.0765159113	-1.8914899252	.1725183872
C	-4.3362885695	-1.5592855139	1.3033328618
C	-3.0929021276	-.9244929613	1.2024189261
C	-2.8388086578	-.6156850785	-2.6471229386
C	-3.7031315479	.4756235259	-3.3063301386
C	-2.7734308166	-1.8645117372	-3.5449439823

C	-2.3274977751	-.5764904236	2.4755829350
C	-2.1812456441	-1.7841013390	3.4179879351
C	-2.9770327906	.6089648869	3.2157894219
C	2.9096299022	-.6289183272	.3297739348
C	3.8805186313	-.8112134095	-.6836666684
C	5.0414273712	-1.5288665391	-.3739365230
C	5.2459039186	-2.0708673615	.8918463645
C	4.2712772979	-1.9022172539	1.8706846212
C	3.0915083368	-1.1921161667	1.6168317475
C	3.6969375848	-.2449372967	-2.0881073535
C	3.8725793436	-1.3227200189	-3.1733482056
C	4.6480378531	.9393622498	-2.3459985086
C	2.0547863898	-1.0534103959	2.7287783795
C	2.5866531714	-.2042627985	3.8988015104
C	1.5754361049	-2.4294208123	3.2272863523
C	-.8933640981	-4.0500275736	-.2365647277
O	.3038183909	-3.2557484324	-.0840897556
C	1.4024025681	-4.1227005604	-.4384461889
C	-.5142218285	-5.4322022351	.3161599690
C	1.0325339493	-5.4885847926	.1636367245
C	-2.1867363908	3.5403180839	-.1678682287
C	.1979378907	3.3855212170	-.0466690824
C	-.9321430557	4.1723788039	-.1354858858
H	-3.2449938712	1.6942518862	-.1974819534
H	2.2789073582	2.7865390107	1.5802137833
H	2.9801322626	2.8372220764	-.0365112524
H	3.4436480838	1.5474903178	1.0693824576
H	-5.1471475547	-1.8387913566	-1.9701611185
H	-6.0403771878	-2.3826285651	.2719327092
H	-4.7324243771	-1.7953266860	2.2871981958
H	-1.8245053471	-.2195013186	-2.5573541931
H	-3.3117173475	.7253398257	-4.2987022493
H	-3.7120567595	1.3898773521	-2.7065544675
H	-4.7398054266	.1413213099	-3.4288174215
H	-2.3337317422	-1.6122033149	-4.5153762865
H	-3.7687914418	-2.2835180955	-3.7285612389
H	-2.1572219322	-2.6473686512	-3.0928860673
H	-1.3220509279	-.2709178008	2.1740599875
H	-1.5691774187	-1.5164160420	4.2863708951
H	-1.7002356554	-2.6279723859	2.9136095000
H	-3.1495207476	-2.1275322421	3.7974855404
H	-2.3918457781	.8771183509	4.1028707313
H	-3.9913647899	.3572709954	3.5466334824
H	-3.0409924543	1.4902378439	2.5720662695
H	5.7984276998	-1.6648310050	-1.1407225581
H	6.1554033387	-2.6220243159	1.1123385376
H	4.4265571086	-2.3296323962	2.8572974490
H	2.6724090373	.1285346086	-2.1666727716
H	3.6313091587	-.9099119379	-4.1580041805
H	3.2105014391	-2.1744403975	-2.9963788281
H	4.9020273019	-1.6946567392	-3.2124804700
H	4.4665741905	1.3682139205	-3.3373859547
H	5.6950198261	.6185430085	-2.3046934249
H	4.5162010280	1.7319700235	-1.6035373224
H	1.1837377795	-.5385386356	2.3153544876
H	1.8121236813	-.0779760072	4.6630189194
H	2.8972427273	.7903460221	3.5646907368
H	3.4509676233	-.6798496434	4.3753089541
H	.8223729488	-2.3095207769	4.0124718709
H	2.3996900537	-3.0166771484	3.6464673391
H	1.1262574948	-2.9995316201	2.4095373277
H	-1.1559160889	-4.1001003116	-1.3016755787
H	-1.6931687953	-3.5418791367	.3038400572
H	2.3097951969	-3.6772290689	-.0279797335

H	1.4809378230	-4.1666561290	-1.5326664404
H	-1.0196474611	-6.2311313431	-.2324684597
H	-.8004684724	-5.5184228519	1.3675274763
H	1.5100793605	-5.6211210379	1.1377257119
H	1.3600098235	-6.3078292629	-.4816720025
H	-3.0983125656	4.1308548405	-.2124993733
H	1.1537994114	3.8908908478	-.0028648368
H	-.8485453140	5.2534345344	-.1678265792

34. $L^2Cu(MeCN) + O_2 \rightarrow L^2Cu(MeCN)O_2$ transition state (triplet)

Cu	.4742127008	-.1427789443	1.1360938082
O	2.0591298113	-.3065945495	3.6252311556
O	.8393329787	-.2014421752	3.3548270491
N	-1.2734161845	-.9702294040	1.3069027335
N	.9301121002	-.9606148323	-.6710764867
N	1.5411449948	1.5952739565	1.2619727695
C	2.1341780912	2.5571273549	1.5128273074
C	2.8918939590	3.7562185609	1.8399139804
C	-3.2339863375	-2.1042668770	.4926647421
C	-1.8571555735	-1.7167459655	.3409743709
C	-1.1826584843	-2.1763576060	-.8677149445
C	.1773099399	-1.8448929156	-1.2853370208
C	.7314209237	-2.5377661355	-2.5254558711
C	-1.9781219153	-.6822105970	2.5129460208
C	-2.0008255589	-1.6244631200	3.5735103123
C	-2.6440405124	-1.2780309904	4.7670157304
C	-3.2556343728	-.0390884226	4.9317972960
C	-3.2284917988	.8800150616	3.8865903813
C	-2.5973166229	.5835399012	2.6741169622
C	-1.3593671493	-3.0028287458	3.4463111694
C	-2.4191853634	-4.1202989877	3.4953479890
C	-.2779566177	-3.2426873843	4.5162077773
C	-2.6144521448	1.6117534750	1.5479924657
C	-2.0128124623	2.9598447342	1.9835700348
C	-4.0333509169	1.8014859333	.9791822356
C	2.1773652378	-.5088057321	-1.2029245594
C	3.3859349238	-.9549652716	-.6139173383
C	4.5936827069	-.4464082183	-1.1024953157
C	4.6225673283	.4984967048	-2.1251047291
C	3.4259427604	.9583703364	-2.6656022216
C	2.1892306591	.4740012809	-2.2228189821
C	3.3821487934	-1.9794731750	.5159540835
C	4.4352579399	-1.6847407243	1.5963247858
C	3.5440376531	-3.4150122738	-.0200312604
C	.9057285154	1.0494093632	-2.8167973316
C	.8613382456	.9202204393	-4.3497997395
C	.7058222681	2.5163966908	-2.3899530976
C	-3.9036018525	-2.8842891340	-.4184543829
C	-1.9310751996	-2.9973133470	-1.7612627052
C	-3.2470134702	-3.3538071458	-1.5701526624
H	3.8393366566	3.7609518507	1.2914727812
H	3.0991136027	3.7739871954	2.9150414934
H	2.3152952477	4.6474213265	1.5728455228
H	-3.7579463858	-1.7482485920	1.3705545376
H	.5961662617	-3.6195165780	-2.4573039066
H	1.7931032087	-2.3285838485	-2.6410722661
H	.2221064759	-2.1988441442	-3.4333797534
H	-2.6639707847	-1.9943876346	5.5837292958
H	-3.7516892833	.2077252088	5.8661739102
H	-3.7123787574	1.8451327313	4.0115939523
H	-.8727681383	-3.0508227665	2.4688986524
H	-1.9491550978	-5.0989827945	3.3469604084
H	-3.1734225273	-3.9861320290	2.7151587090
H	-2.9317100067	-4.1404846129	4.4639241430

H	.1753414461	-4.2306013027	4.3813189601
H	-.6986029069	-3.2108300614	5.5267520392
H	.5113574870	-2.4913321759	4.4597408495
H	-1.9903946862	1.2182356694	.7407771857
H	-1.9670697652	3.6504861081	1.1336389114
H	-.9988998661	2.8273120541	2.3739376331
H	-2.6121361162	3.4385009924	2.7658188035
H	-4.0225730522	2.5061834817	.1397677642
H	-4.7172374483	2.1962865523	1.7392855749
H	-4.4414335643	.8523695510	.6198612708
H	5.5278275795	-.7939482388	-.6727377962
H	5.5715088634	.8793691635	-2.4915028451
H	3.4487455399	1.7110865425	-3.4487302207
H	2.3996978784	-1.9266177465	.9985858703
H	4.2718856629	-2.3302126490	2.4644072863
H	4.3771077432	-.6461675554	1.9331835430
H	5.4529592628	-1.8711658831	1.2360726210
H	3.5174565755	-4.1372738668	.8029973810
H	4.5016534892	-3.5292247495	-.5403661341
H	2.7479542264	-3.6759380325	-.7225815702
H	.0611217198	.4846776554	-2.4154244615
H	-.1033798754	1.2683053736	-4.7333588152
H	.9990345523	-.1174799521	-4.6683951665
H	1.6422790757	1.5201981197	-4.8289703690
H	-.2343556969	2.9084146795	-2.7924083386
H	1.5195042527	3.1512472493	-2.7584512516
H	.6727491160	2.6054458283	-1.3006384139
H	-4.9474062017	-3.1316266577	-.2415047856
H	-1.4522778156	-3.3506612141	-2.6640144867
H	-3.7615490295	-3.9718103069	-2.2981250681

35. $L^2Cu(MeCN) \rightarrow L^2Cu(THF)$ transition state

Cu	.1316206521	-1.0080620298	-.2632978640
N	-1.4615040423	.1878605719	-.3723351334
N	1.4397231055	.4197716056	.2911248027
C	-2.5409410682	2.3379594305	-.5731098789
C	-1.3620002606	1.5328163960	-.3672093013
C	-.1123773490	2.2657682564	-.1573823464
C	1.1672644282	1.7041953541	.2735448253
C	2.2324454679	2.6820649646	.7593491363
C	-2.7380206690	-.4374964310	-.4088310829
C	-3.2780145214	-.9025039494	-1.6393113532
C	-4.4938805535	-1.5954255860	-1.6315841709
C	-5.1868959956	-1.8369845110	-.4482630093
C	-4.6590765596	-1.3734511276	.7536765832
C	-3.4471909979	-.6741567468	.8002541081
C	-2.5698157151	-.6300086346	-2.9629805703
C	-3.2091175879	.5547557760	-3.7153425420
C	-2.5269611644	-1.8649480012	-3.8793197830
C	-2.9283346152	-.1681304165	2.1437455987
C	-2.7676736693	-1.3029366766	3.1714421129
C	-3.8252304270	.9514354422	2.7060046302
C	2.6519761871	-.1169900662	.8178153024
C	3.6911302007	-.5031037127	-.0685578169
C	4.8262783076	-1.1235567349	.4616432408
C	4.9449846504	-1.3770444060	1.8263522357
C	3.9111515962	-1.0081441748	2.6824763732
C	2.7545371373	-.3771295056	2.2061873910
C	3.5825850513	-.2395086245	-1.5673982517
C	4.1173331735	-1.4016336864	-2.4208898758
C	4.2883216921	1.0705660391	-1.9679933087
C	1.6486696709	.0077285188	3.1853950027
C	2.1370402045	1.0407832872	4.2180671599
C	1.0545654525	-1.2270748911	3.8878719142

C	-1.0988773824	-3.8545774167	.4951000383
O	-.0169336012	-2.9710980974	.8414664391
C	1.1375256216	-3.8175639446	.9802986002
C	-.9050418055	-5.0753283010	1.4073633749
C	.6224496970	-5.0788193800	1.6992342371
C	.8193847015	-2.6474925698	-3.0764748841
N	.6072325164	-2.2412592912	-2.0115434997
C	1.0846145987	-3.1519552749	-4.4190641453
C	-2.5142347844	3.7054831208	-.6855349475
C	-.1563788119	3.6836675018	-.3019915547
C	-1.2968094203	4.4038860380	-.5737953423
H	-3.4859549528	1.8180912617	-.6722918013
H	2.5793361931	3.3232440546	-.0568179128
H	3.0972733011	2.1509470404	1.1520845901
H	1.8380884777	3.3361306795	1.5409647877
H	-4.9124695981	-1.9464977193	-2.5710331999
H	-6.1313945066	-2.3738921094	-.4641258191
H	-5.2029936736	-1.5525453797	1.6777975044
H	-1.5395353413	-.3546783840	-2.7187763940
H	-2.6717012677	.7555067101	-4.6503858838
H	-3.1889738941	1.4653113169	-3.1130211973
H	-4.2536752875	.3365591223	-3.9682527179
H	-1.9090490906	-1.6569939707	-4.7626754279
H	-3.5223171472	-2.1373231905	-4.2487943761
H	-2.1154413379	-2.7360977125	-3.3594240913
H	-1.9362285085	.2559554968	1.9683234234
H	-2.3805770927	-.9087863785	4.1180236558
H	-2.0654139578	-2.0611245905	2.8131885946
H	-3.7221034793	-1.7965477413	3.3870659136
H	-3.4136938774	1.3401644004	3.6447335323
H	-4.8372209269	.5832434529	2.9122911563
H	-3.9046726717	1.7829592328	2.0003375394
H	5.6331150379	-1.4147294611	-.2043552635
H	5.8354868743	-1.8601046567	2.2178778203
H	4.0020833978	-1.2093585216	3.7465021698
H	2.5183113719	-.1244202181	-1.7932211775
H	3.8892507183	-1.2234974586	-3.4790136517
H	3.6697688896	-2.3536487290	-2.1220864800
H	5.2051353134	-1.5032489708	-2.3446033444
H	4.1587472154	1.2694858035	-3.0381866784
H	5.3630481763	1.0123050034	-1.7624499301
H	3.8898713605	1.9251050321	-1.4174516643
H	.8390723050	.4677124999	2.6132161296
H	1.3130070774	1.3481957415	4.8705416312
H	2.5362607086	1.9360933572	3.7324805792
H	2.9272484069	.6269791085	4.8537638507
H	.2634857923	-.9246703204	4.5817282989
H	1.8132844153	-1.7676135188	4.4640764744
H	.6167110441	-1.9150585899	3.1606323320
H	-1.0130387677	-4.1283355078	-.5665851087
H	-2.0306712619	-3.3089682433	.6460372943
H	1.8944407529	-3.2549768030	1.5288851170
H	1.5254117156	-4.0595302077	-.0193506187
H	-1.2464327390	-5.9963274061	.9259579947
H	-1.4736490050	-4.9526951086	2.3331811927
H	.8113521788	-5.0170639282	2.7744738375
H	1.1190676624	-5.9793871830	1.3261326232
H	.3887504359	-2.6959301564	-5.1298724647
H	.9591081087	-4.2392209310	-4.4442149894
H	2.1088459088	-2.9031249622	-4.7114716024
H	-3.4412825950	4.2432551133	-.8690586064
H	.7639487655	4.2427922397	-.1964661898
H	-1.2547249514	5.4825520234	-.6827210025

36. L²CuO₂ side-on singlet

Cu	- .0095950370	-2.3594091864	.7878255558
O	.7943778168	-3.9656693045	1.3113022804
O	-.5480094464	-4.1016397038	1.1603990307
N	1.3051420403	-.9805065020	.6419985648
N	-1.5047605382	-1.3331491553	.3071816200
C	2.2917132538	1.1723102436	.2298427669
C	1.0695679576	.2700751365	.2901775342
C	-.2509982989	.7809742757	-.0236002730
C	-1.4677398172	-.0154513337	-.0033828567
C	-2.6924750043	.6501523584	-.3403163704
C	2.6431452978	-1.4312510816	.9393067297
C	3.1011236307	-1.3870713043	2.2736433848
C	4.3963554906	-1.8466242823	2.5372089148
C	5.2068391883	-2.3450436355	1.5214851905
C	4.7213458213	-2.4114744963	.2185402475
C	3.4343231020	-1.9653335299	-.1006496973
C	2.2120212434	-.9149944368	3.4200410508
C	2.8778483487	.1687163204	4.2860945270
C	1.7666364109	-2.1158445747	4.2793069179
C	2.9010209221	-2.1245459519	-1.5208980040
C	2.5851917177	-3.6071601382	-1.8060746503
C	3.8473279631	-1.5458108887	-2.5869793512
C	-2.7498578095	-2.0431256647	.3253189907
C	-3.4997764106	-2.1026999482	1.5231266022
C	-4.6961526586	-2.8274427583	1.5225608676
C	-5.1431431379	-3.4820119914	.3779840666
C	-4.3859898840	-3.4280014453	-.7889360891
C	-3.1826935214	-2.7162117610	-.8405286331
C	-3.0069732414	-1.4484561540	2.8088076380
C	-2.5434690168	-2.5212206410	3.8147935838
C	-4.0521722231	-.5097322001	3.4349030708
C	-2.3483928037	-2.7215268449	-2.1160413343
C	-3.1472556118	-2.2639023983	-3.3481744512
C	-1.7176105328	-4.1101989199	-2.3415300953
C	-2.7489875722	1.9828028829	-.6707006492
C	-.3828508284	2.1583033976	-.3743787945
C	-1.5785974078	2.7611121180	-.6900185135
H	2.0820176287	2.1961299783	-.0535750088
H	3.0127901375	.7624198345	-.4820144796
H	2.7887117939	1.1812642265	1.2031739898
H	-3.6026627669	.0659619626	-.3317524655
H	4.7706198828	-1.8208407464	3.5561474849
H	6.2094968187	-2.6956130320	1.7473681778
H	5.3486668720	-2.8248261235	-.5653196237
H	1.3094436941	-.4735633456	2.9871633487
H	2.1805533319	.5180516988	5.0547121579
H	3.1830989612	1.0348666679	3.6894420189
H	3.7674191549	-.2114274154	4.7989070770
H	1.0558426438	-1.7947130639	5.0485501629
H	2.6253114364	-2.5725207432	4.7838767372
H	1.2942319852	-2.8858267152	3.6628959706
H	1.9590628262	-1.5725693702	-1.5919024878
H	2.1126546469	-3.7173795666	-2.7882472640
H	1.9178775231	-4.0219721249	-1.0454571439
H	3.5032221655	-4.2053723739	-1.8043197637
H	3.3885584077	-1.6216216902	-3.5782969987
H	4.7978219912	-2.0879791129	-2.6242238498
H	4.0734785333	-.4907258196	-2.3998929333
H	-5.2816052414	-2.8875555445	2.4354424104
H	-6.0731544982	-4.0428238074	.3990173055
H	-4.7307450164	-3.9541307084	-1.6744001819
H	-2.1352277111	-.8386237410	2.5564304612
H	-2.1125901943	-2.0528632117	4.7070970357

H	-1.7941100099	-3.1807437655	3.3674006459
H	-3.3852064404	-3.1448364818	4.1365541737
H	-3.6358197397	-.0156374489	4.3194494062
H	-4.9481703108	-1.0525977922	3.7544624437
H	-4.3623352382	.2658690609	2.7277327179
H	-1.5307573796	-2.0089272740	-1.9773411160
H	-2.4959313602	-2.2228855657	-4.2279584560
H	-3.5749914268	-1.2680236841	-3.1958756888
H	-3.9678934889	-2.9512596732	-3.5800098249
H	-1.0518486232	-4.0947477021	-3.2119991233
H	-2.4904027925	-4.8655431538	-2.5237848424
H	-1.1439672250	-4.4272640756	-1.4657205971
H	-3.7098247998	2.4272599196	-.9164831495
H	.4958360315	2.7855734892	-.3980671736
H	-1.6083914694	3.8141677340	-.9473550067

37. L²CuO₂ end-on singlet

Cu	-.1568667074	-2.1672920217	.2228548494
O	.4251601368	-4.8184858279	-.2840215265
O	.0938532405	-3.9589322971	.6080268407
N	1.3170901028	-.8793871756	.1298723787
N	-1.5464526550	-.8906393010	-.0031469326
C	2.4379812769	1.2845907290	.0380873471
C	1.1902790125	.4177774735	-.0418988449
C	-.0787861288	1.0719684832	-.3115222327
C	-1.3730122270	.4175088228	-.3034023269
C	-2.5150622060	1.2305135368	-.6105587236
C	2.5761427245	-1.5180336093	.3891058607
C	2.9665534018	-1.7463704244	1.7295114927
C	4.1661629547	-2.4268351158	1.9575843770
C	4.9534327856	-2.8803424695	.9017982991
C	4.5389905403	-2.6664499558	-.4088512803
C	3.3465804023	-1.9917677911	-.6961975539
C	2.0995420971	-1.3138085358	2.9080828594
C	2.8556684457	-.4021651878	3.8907164296
C	1.5095123701	-2.5402793057	3.6324984476
C	2.9052983053	-1.8143921999	-2.1454155085
C	2.5903192830	-3.1738465034	-2.7992634327
C	3.9403029527	-1.0282937104	-2.9710722665
C	-2.8373672484	-1.4962546904	-.0335857035
C	-3.5987073110	-1.5785450502	1.1573303095
C	-4.8290301425	-2.2418642833	1.1149147226
C	-5.2999470688	-2.8178647633	-.0623871575
C	-4.5393409994	-2.7341242159	-1.2267868392
C	-3.3062027422	-2.0749542055	-1.2393251931
C	-3.1044447662	-.9709222377	2.4653035067
C	-2.8760024166	-2.0522813362	3.5378819590
C	-4.0526150622	.1293179585	2.9774978050
C	-2.4608100744	-2.0230046059	-2.5056921823
C	-3.2697372975	-1.6258909073	-3.7512864090
C	-1.7215469755	-3.3588031405	-2.7215078806
C	-2.4161425828	2.5718023388	-.8930647475
C	-.0436351217	2.4640895493	-.6071383681
C	-1.1632009896	3.2112234576	-.8941615962
H	2.2995089924	2.0908510254	.7631310968
H	2.6532037778	1.7429707357	-.9320157296
H	3.3038126827	.6968613890	.3339938906
H	-3.4863655858	.7519414127	-.6106484302
H	4.4853592360	-2.6097157746	2.9793789244
H	5.8815273314	-3.4072962030	1.1012882405
H	5.1477077657	-3.0355507276	-1.2288605375
H	1.2590994916	-.7357561372	2.5137714581
H	2.1878797730	-.0725776356	4.6937402839
H	3.2485103250	.4880873032	3.38911110617

H	3.6995246365	-.9218861227	4.3565188075
H	.8170399193	-2.2231175612	4.4198318947
H	2.2993549877	-3.1382938846	4.1000505258
H	.9690995690	-3.1938020429	2.9408673196
H	1.9794988991	-1.2322633562	-2.1463985159
H	2.2243866371	-3.0282741000	-3.8215674201
H	1.8292948246	-3.7190550061	-2.2334866892
H	3.4845558142	-3.8044153534	-2.8515809553
H	3.5722081881	-.8687110801	-3.9900414062
H	4.8908792329	-1.5673657825	-3.0434123358
H	4.1466303669	-.0488831622	-2.5273843468
H	-5.4267243851	-2.3111137606	2.0195906020
H	-6.2561480970	-3.3328720829	-.0724408773
H	-4.9106709792	-3.1904457521	-2.1392401470
H	-2.1381170113	-.5015236302	2.2623376524
H	-2.4726950784	-1.6054077931	4.4534759803
H	-2.1696105311	-2.8125556022	3.1896093888
H	-3.8095597289	-2.5617536491	3.8000582914
H	-3.6506337237	.5879605459	3.8876202936
H	-5.0432960278	-.2722433881	3.2175271195
H	-4.1810067672	.9175714446	2.2294968097
H	-1.6969991776	-1.2547069631	-2.3592482836
H	-2.6017207665	-1.5062637552	-4.6106899951
H	-3.7961640150	-.6790323087	-3.5956947876
H	-4.0121274264	-2.3845832751	-4.0206140521
H	-1.0806479814	-3.3037090833	-3.6088836781
H	-2.4340112674	-4.1776775668	-2.8719056612
H	-1.0918153115	-3.6325133084	-1.8701725378
H	-3.3174251283	3.1364677051	-1.1181270456
H	.9130118889	2.9691749395	-.6213560247
H	-1.0769849245	4.2685265243	-1.1204094717

38. L²CuO₂ end-on singlet → L²CuO₂ side-on singlet transition state

Cu	.2486644276	-1.6780101631	.9821147244
O	.0036644241	-3.8629600613	2.0272249229
O	.1647311299	-2.6626705112	2.5537294351
N	.4494744492	-1.1486289954	-.8269853798
N	-.2338217187	.0187464855	1.7408026360
C	.5999914630	.2808079245	-2.7634725947
C	.4605195592	.0922564429	-1.2624723483
C	.2553926638	1.2347512172	-.3837147753
C	-.1150929217	1.1630459775	1.0265670703
C	-.3975714522	2.4070259271	1.6856744428
C	.6842465154	-2.3077631218	-1.6448696581
C	2.0107438519	-2.7798635104	-1.7912817527
C	2.2093260548	-3.9698507322	-2.4996626508
C	1.1371923214	-4.6828789838	-3.0316643102
C	-.1620434949	-4.2194620937	-2.8450217808
C	-.4190777555	-3.0351038855	-2.1457392156
C	3.1877833394	-2.0729412499	-1.1263082355
C	4.3777297033	-1.8532275439	-2.0732521371
C	3.6114223793	-2.8345513186	.1474302081
C	-1.8559174651	-2.6034725997	-1.8726970950
C	-2.5220941418	-3.5575846565	-.8595532808
C	-2.6957130052	-2.4862072358	-3.1554060638
C	-.5906712820	.0149674747	3.1166802122
C	.4141907770	.1361310549	4.1103786201
C	.0314167636	.0871824518	5.4552928059
C	-1.2983604606	-.0962499295	5.8225160651
C	-2.2719091082	-.2457428505	4.8373707892
C	-1.9426184931	-.2056845121	3.4798317055
C	1.8849750522	.3213459920	3.7554276032
C	2.7435150967	-.8337856560	4.3040269036
C	2.4189541138	1.6837689791	4.2338595358

C	-3.0305680186	-.4052261169	2.4318641587
C	-4.0578544223	.7414994947	2.4540708690
C	-3.7143779252	-1.7753504659	2.5894462594
C	-.2721609995	3.6268298432	1.0678689739
C	.3742361840	2.5354760421	-.9583893174
C	.1372530800	3.7055323684	-.2762528229
H	-.3818832620	.1493437093	-3.2293373108
H	1.2332881579	-.5098668856	-3.1752389772
H	1.0171073082	1.2348738670	-3.0679872832
H	-.7160902565	2.3603031377	2.7189381311
H	3.2182479182	-4.3518077913	-2.6222738097
H	1.3137106519	-5.6055348492	-3.5766280935
H	-.9955165071	-4.7928531151	-3.2400552084
H	2.8474517587	-1.0857578593	-.8007638934
H	5.1576191297	-1.2715295734	-1.5708178113
H	4.0764211802	-1.3091610669	-2.9740835724
H	4.8282063882	-2.8000275886	-2.3896898497
H	4.3963389252	-2.2870772103	.6811925896
H	3.9956094325	-3.8309357311	-.0986397930
H	2.7691822607	-2.9732214781	.8350819513
H	-1.8241237927	-1.6119397139	-1.4106763925
H	-3.5172266474	-3.1909461957	-.5855791115
H	-1.9324900853	-3.6557692583	.0577576280
H	-2.6368630952	-4.5609756744	-1.2842333737
H	-3.6946459356	-2.1046186511	-2.9198468822
H	-2.8222651718	-3.4569264913	-3.6461630922
H	-2.2335227964	-1.8054478624	-3.8778117550
H	.7897281578	.1863765971	6.2269493803
H	-1.5746309374	-.1324104893	6.8725484500
H	-3.3067435425	-.4018863307	5.1289705074
H	1.9695530260	.2957316424	2.6657449612
H	3.7873855141	-.7135765921	3.9924517799
H	2.3771440576	-1.7954985556	3.9341921708
H	2.7264236504	-.8634585603	5.3989449121
H	3.4626614170	1.8147918538	3.9274200270
H	2.3791659901	1.7664060416	5.3255872151
H	1.8364586201	2.5075536055	3.8118156268
H	-2.5458952120	-.3930717607	1.4519283475
H	-4.8041441915	.6050226591	1.6634867456
H	-3.5716202149	1.7092609942	2.2979439901
H	-4.5897058040	.7826720211	3.4111493078
H	-4.4498982079	-1.9288678559	1.7915101751
H	-4.2452559452	-1.8524598027	3.5446364756
H	-2.9812520888	-2.5861887664	2.5474515358
H	-.4890154048	4.5314495746	1.6298382105
H	.6700855880	2.6219774766	-1.9937923008
H	.2572547643	4.6634717248	-.7704228977

39. L²CuO₂ side-on triplet

Cu	-.0258634515	-2.3647390729	.7984934975
O	.7420104855	-4.1476342353	1.3718247587
O	-.5495097493	-4.2789852001	1.2296193228
N	1.3178105893	-.9619609584	.6409053694
N	-1.5226099929	-1.3074633666	.3037142843
C	2.3008420781	1.1947079797	.2181121529
C	1.0786099299	.2885154784	.2857828206
C	-.2484249059	.7958184499	-.0280419513
C	-1.4747217127	.0061597102	-.0097839561
C	-2.6949645390	.6809401379	-.3518622402
C	2.6511163418	-1.4207929866	.9373364235
C	3.1118770220	-1.3920429079	2.2731351793
C	4.3890002069	-1.8970498423	2.5424941660
C	5.1869718277	-2.4247569453	1.5320132859
C	4.7062223358	-2.4677268116	.2266004437

C	3.4372538379	-1.9757650474	-.0984081333
C	2.2450837140	-.8751703524	3.4181261000
C	2.9416060681	.2260822926	4.2374436408
C	1.7992885204	-2.0346423714	4.3309747782
C	2.9196765788	-2.0972304859	-1.5291249340
C	2.6093578894	-3.5683231699	-1.8706538268
C	3.8824003949	-1.4897241719	-2.5646916948
C	-2.7608720265	-2.0266777847	.3182911783
C	-3.5019648016	-2.1145649653	1.5203342869
C	-4.6635879210	-2.8943567173	1.5332390148
C	-5.0903623839	-3.5746296301	.3958742857
C	-4.3482582773	-3.4852160085	-.7787027848
C	-3.1795329307	-2.7184810838	-.8428944565
C	-3.0368447896	-1.4234405831	2.7977480312
C	-2.5758110809	-2.4551965945	3.8460614108
C	-4.1081950242	-.4854042016	3.3795743552
C	-2.3661152957	-2.6800726810	-2.1323378043
C	-3.1955896128	-2.1949185031	-3.3335866255
C	-1.7246537916	-4.0515722482	-2.4213577368
C	-2.7432649602	2.0109995179	-.6840154920
C	-.3761558972	2.1735169568	-.3818452124
C	-1.5657689656	2.7819319717	-.7009431369
H	2.0962084839	2.2182318704	-.0710925576
H	3.0225334323	.7810637264	-.4913473013
H	2.8004113211	1.2099076904	1.1902238807
H	-3.6057992609	.0962261254	-.3422543938
H	4.7605692743	-1.8813688474	3.5628868204
H	6.1753784880	-2.8110293338	1.7625728867
H	5.3249586260	-2.8967701677	-.5559489142
H	1.3415390681	-.4368171211	2.9849879703
H	2.2645333462	.6108872959	5.0072686571
H	3.2478451325	1.0671751409	3.6069520762
H	3.8358317318	-.1510761988	4.7445200957
H	1.1174068887	-1.6723179495	5.1079658618
H	2.6597477362	-2.4971814499	4.8266582729
H	1.2881669465	-2.8163953609	3.7614359750
H	1.9793983568	-1.5427657575	-1.5958801850
H	2.1650672522	-3.6469079257	-2.8688678887
H	1.9153028360	-4.0086868291	-1.1489067346
H	3.5226772552	-4.1731589909	-1.8585142974
H	3.4394256215	-1.5360825762	-3.5650301561
H	4.8333193541	-2.0312230147	-2.6018518671
H	4.1059912406	-.4410779059	-2.3429202839
H	-5.2386139915	-2.9752542842	2.4514046881
H	-5.9930298427	-4.1778395826	.4269985913
H	-4.6779411873	-4.0256709416	-1.6615883585
H	-2.1706119090	-.8077806353	2.5417181030
H	-2.1750144513	-1.9519357059	4.7333052862
H	-1.7987442227	-3.1118962077	3.4426440857
H	-3.4076996678	-3.0911065637	4.1681706381
H	-3.7191463192	.0360000378	4.2609742347
H	-5.0036891920	-1.0343248266	3.6903253364
H	-4.4120607138	.2678013096	2.6463458644
H	-1.5541190599	-1.9628325154	-1.9865365497
H	-2.5654451962	-2.1227824959	-4.2267930368
H	-3.6264565238	-1.2075845282	-3.1417159280
H	-4.0167101583	-2.8820740931	-3.5646667803
H	-1.0832071155	-3.9989696405	-3.3084234827
H	-2.4884944898	-4.8152698909	-2.6046367460
H	-1.1169438240	-4.3921412328	-1.5772487526
H	-3.6988080898	2.4649281932	-.9340287649
H	.5073469527	2.7938230204	-.4037402364
H	-1.5925428393	3.8346699036	-.9602474231

40. L²CuO₂ end-on triplet

Cu	-.2242866580	-2.1030520427	.3396532168
O	1.1731209421	-4.6269397044	.4422638899
O	.2362691622	-3.8857076859	.8522728952
N	1.3182189773	-.8841848116	.2363532973
N	-1.5950306988	-.8814855152	-.1019657318
C	2.4627336638	1.2450062591	-.0323258464
C	1.1975942807	.3983386792	-.0300068135
C	-.0713804520	1.0591814268	-.3164841170
C	-1.3851251004	.4309303774	-.3549135844
C	-2.5029440411	1.2718653494	-.6712675534
C	2.5680955729	-1.5378213511	.4880991129
C	3.0179158891	-1.6867737739	1.8212411918
C	4.1982434632	-2.4029007479	2.0435008903
C	4.9114952079	-2.9710369715	.9910177534
C	4.4385600981	-2.8385769306	-.3102100548
C	3.2612864210	-2.1349179294	-.5905267698
C	2.2484305224	-1.1122422265	3.0072050526
C	3.0817388616	-.0786393146	3.7867657995
C	1.7450330271	-2.2294840447	3.9411843746
C	2.7681648282	-2.0315069375	-2.0307784472
C	2.4987321427	-3.4189979067	-2.6427636442
C	3.7463434519	-1.2279869268	-2.9081053877
C	-2.8986916314	-1.4634171716	-.1809892055
C	-3.6727424208	-1.5962685827	.9989402427
C	-4.9059254104	-2.2508446554	.9231831287
C	-5.3776248499	-2.7653271193	-.2822274907
C	-4.6081419066	-2.6331901631	-1.4345870121
C	-3.3669619246	-1.9863699521	-1.4108528432
C	-3.1453189816	-1.0992063453	2.3392399726
C	-2.5652433427	-2.2717213704	3.1554271802
C	-4.1969057465	-.3335034663	3.1587372328
C	-2.5311383357	-1.9003002605	-2.6834881115
C	-3.3066460933	-1.2694511525	-3.8529922116
C	-1.9745450598	-3.2847475754	-3.0686812894
C	-2.3764192636	2.6148809896	-.9278041614
C	-.0136748927	2.4572487242	-.5888549812
C	-1.1117974734	3.2298428249	-.8880766553
H	2.3840449165	2.0572990674	.6957269038
H	2.6362460839	1.6925594782	-1.0143415240
H	3.3303038947	.6405745064	.2242653982
H	-3.4827307289	.8110220883	-.6981884468
H	4.5617399683	-2.5213426039	3.0603020742
H	5.8258571169	-3.5233036771	1.1865207102
H	4.9882459511	-3.2960734713	-1.1276676871
H	1.3674792828	-.5944596118	2.6176368525
H	2.4897893583	.3558670565	4.5994003605
H	3.4173909003	.7361084860	3.1375668576
H	3.9713637436	-.5364101299	4.2324168061
H	1.1466270451	-1.8067322310	4.7555931718
H	2.5785282707	-2.7801368286	4.3902084817
H	1.1251510637	-2.9492528539	3.3988255981
H	1.8169626183	-1.4919022580	-2.0217931382
H	2.0801718397	-3.3157112040	-3.6497149268
H	1.7949301144	-3.9901975421	-2.0315648037
H	3.4191533455	-4.0068639758	-2.7245981212
H	3.3513004095	-1.1224001430	-3.9241488885
H	4.7183476173	-1.7280954690	-2.9782057130
H	3.9174432930	-.2252884611	-2.5041471424
H	-5.5058430570	-2.3642513834	1.8213058061
H	-6.3381740576	-3.2709621132	-.3212457235
H	-4.9749340594	-3.0446039328	-2.3708154249
H	-2.3261271125	-.4059323951	2.1305807468

H	-2.1175442446	-1.9145719159	4.0896939872
H	-1.7934159444	-2.8108658882	2.5944592391
H	-3.3479177337	-2.9956050023	3.4085540184
H	-3.7397696243	.0831876184	4.0626381189
H	-5.0199964063	-.9804764217	3.4807844483
H	-4.6240119232	.4928065356	2.5823621268
H	-1.6758086692	-1.2533530681	-2.4724691396
H	-2.6563473924	-1.1635766988	-4.7280873783
H	-3.6802252469	-.2763624639	-3.5859108154
H	-4.1633942934	-1.8828481888	-4.1521501605
H	-1.3444020908	-3.2145754245	-3.9623996125
H	-2.7822348558	-3.9939266368	-3.2802591950
H	-1.3690461703	-3.7061317580	-2.2586292443
H	-3.2630158699	3.1995803831	-1.1595354027
H	.9471537751	2.9524027096	-.5637654280
H	-.9995593581	4.2900459654	-1.0874156166

41. $L^2CuO_2H^+$ side-on singlet (isomer #1)

Cu	-1.0901786001	-.2147796772	.1205544283
O	-2.6594266097	-.3850541526	1.0780078372
O	-3.3718544369	.1497954411	-.0564679484
N	.2140165850	-.6324435580	1.5500355156
N	.1772486616	-.1045463442	-1.2414749257
C	2.3634710910	-1.2927173361	2.4939603376
C	1.5063293151	-.7620975476	1.3582811945
C	2.1931383953	-.3804179264	.1279855033
C	1.5258175745	-.0045151641	-1.0913308605
C	2.3184093914	.3719756439	-2.2144685856
C	-.4669104408	-1.1066493414	2.7107793565
C	-.9435017877	-.1377985350	3.6285012426
C	-1.5893597480	-.5993906592	4.7777900319
C	-1.8004024687	-1.9593282053	4.9871586309
C	-1.3763152921	-2.8920329608	4.0394092842
C	-.7108737459	-2.4962638742	2.8791929142
C	-.7280802682	1.3524409393	3.4104800298
C	.3401436530	1.9066066490	4.3737926721
C	-2.0457473796	2.1398379710	3.5193881729
C	-.3321202845	-3.5351724979	1.8280275392
C	-1.5959141175	-4.0574189018	1.1131893285
C	.4897052247	-4.6997002020	2.4089281538
C	-.5332261083	.5576009409	-2.2596530186
C	-.5566657684	1.9859340194	-2.3619691320
C	-1.3326566609	2.5446165478	-3.3759533694
C	-2.0551907679	1.7461440774	-4.2622663156
C	-2.0392303436	.3546269637	-4.1431193958
C	-1.3013999215	-.2703828441	-3.1432413712
C	.1244392230	2.8988838693	-1.3497643750
C	-.9271390273	3.5988480529	-.4640221870
C	1.0556721792	3.9237922691	-2.0231093201
C	-1.2243657653	-1.7894103097	-3.0565437625
C	-.0779686054	-2.3219541698	-3.9432391598
C	-2.5484697945	-2.4882846043	-3.4019588010
C	3.6957177428	.3680104422	-2.1625523450
C	3.6103894779	-.3665339224	.1267494549
C	4.3549448888	.0008818625	-.9783141186
H	-3.8931990160	-.6157930910	-.3588024959
H	2.9469790878	-2.1562979692	2.1647135379
H	1.7566306880	-1.5817287299	3.3466568827
H	3.0643139251	-.5186889769	2.8200332286
H	1.8084420590	.6106363079	-3.1400270282
H	-1.9389363984	.1161045381	5.5143883646
H	-2.3087691400	-2.2966460265	5.8847998463
H	-1.5734115861	-3.9459540339	4.2058205958
H	-.3501255297	1.4899087972	2.3920353469

H	.5144315351	2.9693969395	4.1788091303
H	1.2944113273	1.3803818231	4.2665573561
H	.0211869160	1.8047944571	5.4158703616
H	-1.8739291405	3.1919111215	3.2707311231
H	-2.4559322473	2.1069854286	4.5334381044
H	-2.7939962509	1.7341213071	2.8336656702
H	.2877222900	-3.0504094985	1.0672120082
H	-1.3206797866	-4.7377920034	.3006408336
H	-2.1854964609	-3.2331283166	.7000721953
H	-2.2396950421	-4.6057779845	1.8080154085
H	.7923614668	-5.3820696899	1.6086806764
H	-.0893202509	-5.2814960748	3.1321363291
H	1.3938432283	-4.3464464057	2.9139066461
H	-1.3873190412	3.6238971546	-3.4705329914
H	-2.6434868029	2.2114374694	-5.0470373682
H	-2.6072530332	-.2437198432	-4.8461957383
H	.7429554306	2.2876196584	-.6883614219
H	-.4302794245	4.2113734830	.2947722689
H	-1.5699746619	2.8747479918	.0479971251
H	-1.5739602605	4.2550308252	-1.0540802803
H	1.5587218316	4.5269209297	-1.2615685313
H	.5026711770	4.6089231896	-2.6725687266
H	1.8229671567	3.4308221542	-2.6266196510
H	-.9707641085	-2.0476263996	-2.0228313500
H	.0009609473	-3.4093126113	-3.8469895289
H	.8855897308	-1.8878057502	-3.6617757841
H	-.2609178100	-2.0877445892	-4.9969463971
H	-2.4694920838	-3.5567842614	-3.1820619102
H	-2.8008114076	-2.3970315712	-4.4626355781
H	-3.3855153930	-2.0839769463	-2.8228664268
H	4.2662982755	.6380962896	-3.0454748342
H	4.1453857037	-.6395203630	1.0253042461
H	5.4377456166	.0008021093	-.9263807359

42. L²CuO₂H⁺ side-on singlet (isomer #2)

Cu	-.0830026754	-1.4029416367	1.3113178021
O	-.2586070404	-2.9285931476	3.1300343225
O	-1.2890730370	-2.3469573423	2.3129993671
N	1.4544224175	-.5658404874	.5913730973
N	-1.3812839141	-.5360775636	.0902519394
C	2.8034862648	.9683440979	-.7385897495
C	1.4841702167	.4872281207	-.1758000955
C	.2671034353	1.2333414185	-.5102021852
C	-1.0793669097	.7419022157	-.3315328820
C	-2.1462406784	1.5587219221	-.8090647286
C	2.5841239908	-1.4229796018	.8491610725
C	3.2439423979	-1.2964703534	2.0961817334
C	4.3053985176	-2.1675782674	2.3570230367
C	4.6873327284	-3.1390760342	1.4353949676
C	4.0091170263	-3.2576399193	.2242422940
C	2.9470685830	-2.4095229117	-.1033354771
C	2.8576922161	-.2381532359	3.1229382677
C	3.9727966224	.8136764849	3.2835821864
C	2.4877556462	-.8674148825	4.4792849818
C	2.2227831531	-2.5938043940	-1.4342603431
C	1.5224499282	-3.9653919169	-1.4994896166
C	3.1725189784	-2.4084177042	-2.6336692861
C	-2.6708851888	-.8921692334	.4746476362
C	-3.4206745441	-.1866610660	1.4767068797
C	-4.7308236345	-.6000242570	1.7065031329
C	-5.2823166501	-1.6836267169	1.0222799754
C	-4.5149154120	-2.4215897818	.1172411558
C	-3.1958443004	-2.0734657733	-.1495224374
C	-2.8163502986	.8941548368	2.3649836459

C	-2.6723865760	.3733524815	3.8121881916
C	-3.6227906617	2.2062571848	2.3397905946
C	-2.3526127410	-2.8584265112	-1.1402936055
C	-2.4684560022	-2.2600825095	-2.5590547661
C	-2.6714564414	-4.3605329108	-1.1524463512
C	-1.9291064110	2.7961096341	-1.3835432567
C	.4342008017	2.5115810619	-1.0870079714
C	-.6281129356	3.2963431681	-1.5050763195
H	-.2477553247	-3.8566654839	2.8330657684
H	2.7390840431	1.1114634115	-1.8197805302
H	3.6002540570	.2613672422	-.5191642786
H	3.0743450345	1.9297636674	-.2903444627
H	-3.1511903854	1.1610296199	-.7629656765
H	4.8421146522	-2.0822393472	3.2961803224
H	5.5136337904	-3.8058312853	1.6606595354
H	4.3134114518	-4.0222289912	-.4834174999
H	1.9686629004	.2839766594	2.7534111416
H	3.6589743968	1.5954190252	3.9820360753
H	4.2221502066	1.2890818275	2.3294489151
H	4.8888167255	.3625309278	3.6779990439
H	2.1580521394	-.0895509215	5.1748662841
H	3.3455104321	-1.3726224580	4.9340761493
H	1.6804426860	-1.5975127620	4.3735786681
H	1.4418542836	-1.8315523424	-1.5139342477
H	.9708037020	-4.0659168816	-2.4394938546
H	.8141449975	-4.0936487547	-.6740499282
H	2.2442352984	-4.7860345623	-1.4476166864
H	2.6166666420	-2.4904329129	-3.5726891708
H	3.9559067823	-3.1723497111	-2.6448713202
H	3.6639157204	-1.4310410967	-2.6146315085
H	-5.3266385416	-.0865965254	2.4535247591
H	-6.3097277563	-1.9750606776	1.2178314816
H	-4.9554407176	-3.2805650402	-.3753562595
H	-1.8090834894	1.1204460558	2.0034951860
H	-2.1534019433	1.1183527851	4.4238427176
H	-2.1111157684	-.5630671181	3.8357488276
H	-3.6524901950	.1951026545	4.2652470925
H	-3.1276333318	2.9562833576	2.9636749852
H	-4.6318877851	2.0641005122	2.7382503431
H	-3.7126606692	2.6124745175	1.3288691487
H	-1.3088139487	-2.7406282436	-.8296932327
H	-1.8167970498	-2.8009928825	-3.2526715141
H	-2.1817122827	-1.2046618067	-2.5771565748
H	-3.4950637842	-2.3387300197	-2.9311921269
H	-1.9318958212	-4.8877737306	-1.7624531812
H	-3.6528444858	-4.5716160854	-1.5883420522
H	-2.6485203640	-4.7854492431	-.1444334734
H	-2.7761389977	3.3723057809	-1.7423025434
H	1.4335025532	2.9083308035	-1.2044870041
H	-.4459167111	4.2755933226	-1.9333290875

43. $L^2CuO_2H^+$ end-on singlet

Cu	-1.3684285321	.1813213255	-.1170406409
O	-3.9028898145	-.7145598096	.2402175091
O	-3.1747104033	.4931198097	.0973048692
N	-.0625727025	-.1428213104	1.2852545773
N	-.0858764036	.2967109338	-1.5053457026
C	2.1172673866	-.1142994504	2.3802114197
C	1.2370666950	-.1680295733	1.1480884966
C	1.8909095846	-.2796738094	-.1561168424
C	1.2069014384	-.1379827977	-1.4147745122
C	1.9547520953	-.3054610246	-2.6157077551
C	-.7294430285	.0132050632	2.5478364969
C	-.8984431431	1.3086259339	3.0974436511

C	-1.5911890461	1.4092206921	4.3054330391
C	-2.0985603794	.2804412276	4.9469238004
C	-1.9346455719	-.9790242848	4.3771392333
C	-1.2648230336	-1.1445343558	3.1615248977
C	-.4088575052	2.5734386844	2.4004700600
C	.5301967441	3.4058463608	3.2925826326
C	-1.6031170609	3.4195914330	1.9129201301
C	-1.1019209262	-2.5361404321	2.5642957545
C	-2.4600014564	-3.2380888485	2.3809917317
C	-.1421164545	-3.3956903504	3.4105895083
C	-.8767824381	.1019449715	-2.6411162938
C	-1.5039927579	1.2698176383	-3.1921246685
C	-2.2855962336	1.1106530584	-4.3313847887
C	-2.4935976790	-.1510147814	-4.8921432732
C	-1.9326160252	-1.2907707184	-4.3109929297
C	-1.1243482272	-1.2060257614	-3.1815352304
C	-1.2919992700	2.6509547440	-2.5919797062
C	-2.6322001962	3.2840922929	-2.1684087569
C	-.5114879459	3.5690645405	-3.5519813730
C	-.6739211105	-2.4826933760	-2.4832322222
C	.1070316188	-3.4235766383	-3.4170535255
C	-1.8902873594	-3.2036037600	-1.8609815301
C	3.3058587986	-.5865190463	-2.5944344117
C	3.2735006158	-.5693561520	-.1883895224
C	3.9764977688	-.7283947203	-1.3712173056
H	-4.7743313138	-.3799966395	.5124641414
H	2.8676912305	.6741639700	2.2814749199
H	2.6449222428	-1.0646308820	2.5072644414
H	1.5274553169	.0681958155	3.2747292868
H	1.4482304830	-.1408346293	-3.5587582945
H	-1.7383315668	2.3868747857	4.7527591614
H	-2.6273277023	.3851505063	5.8889838959
H	-2.3357683639	-1.8503438932	4.8843090186
H	.1649395304	2.2813548265	1.5147230137
H	.8972514004	4.2785497254	2.7436848674
H	1.3959235478	2.8238010440	3.6236013832
H	.0153423036	3.7726118045	4.1856667182
H	-1.2487133751	4.2785710294	1.3340739787
H	-2.1815187604	3.8030184190	2.7594837233
H	-2.2852698239	2.8338014636	1.2885433648
H	-.6558318877	-2.4275444768	1.5701311922
H	-2.3195508251	-4.2024170850	1.8825792650
H	-3.1356609930	-2.6283715606	1.7750313488
H	-2.9456474095	-3.4341543795	3.3419660255
H	.0008602729	-4.3763022784	2.9461474768
H	-.5413227077	-3.5572737065	4.4169402880
H	.8395354431	-2.9227938731	3.5169956350
H	-2.7434275378	1.9801640234	-4.7911570607
H	-3.1132095290	-.2498592245	-5.7780882347
H	-2.1529629293	-2.2641992926	-4.7358780722
H	-.6817390132	2.5300964597	-1.6932491074
H	-2.4484829472	4.2378414513	-1.6641244069
H	-3.1803193714	2.6318363850	-1.4818328311
H	-3.2744853706	3.4864759361	-3.0313192452
H	-.3316633948	4.5390774625	-3.0784289414
H	-1.0687984543	3.7478198342	-4.4770733423
H	.4581256268	3.1381348629	-3.8204319315
H	-.0037406714	-2.2161227427	-1.6623435885
H	.4428251408	-4.3040104490	-2.8613354059
H	.9879107826	-2.9296460940	-3.8365764694
H	-.5114200846	-3.7766881201	-4.2476944674
H	-1.5545400275	-4.0687546044	-1.2804154898
H	-2.5746981661	-3.5652260089	-2.6347481655
H	-2.4605408290	-2.5442712025	-1.1986958655

H	3.8463346064	-.6856341370	-3.5304912269
H	3.8114585476	-.6914264216	.7418438180
H	5.0357170046	-.9581501648	-1.3449640442

44. $L^2CuO_2H^+$ end-on singlet \rightarrow $L^2CuO_2H^+$ side-on singlet (isomer #1) transition state

Cu	-1.3241447461	.2366637761	-.1881886248
O	-3.7677647437	-.4138013191	-.2064045296
O	-2.9465766640	.4703172794	.6427481542
N	-.0439662538	-.1036368464	1.2808959906
N	-.0007167890	.3197599731	-1.4940597905
C	2.1233068969	-.1224202591	2.3960412650
C	1.2583496611	-.1400782183	1.1508672600
C	1.9457232081	-.2529372620	-.1380468226
C	1.2886069643	-.1136096620	-1.4062769436
C	2.0359595051	-.2937562505	-2.5998760622
C	-.7214282515	.0552108119	2.5276860819
C	-.8332444340	1.3407729994	3.1136988828
C	-1.5219272279	1.4337867726	4.3215262526
C	-2.1023763042	.3105581148	4.9141042649
C	-2.0163606409	-.9342043094	4.2921394654
C	-1.3520900206	-1.0877135337	3.0752109321
C	-.2980745552	2.6001413817	2.4424875107
C	.6327687475	3.4131495950	3.3589649277
C	-1.4675883317	3.4670026149	1.9281162661
C	-1.3062639471	-2.4438044277	2.3847168995
C	-2.7217846335	-2.9938871702	2.1259646833
C	-.4479925520	-3.4507501970	3.1742910124
C	-.8768190109	.0589864078	-2.5429285597
C	-1.6280909622	1.1907783524	-3.0379815468
C	-2.5219272279	.9749178567	-4.0829714150
C	-2.7017900727	-.2959308927	-4.6219371810
C	-2.0118695693	-1.4005129343	-4.1068497002
C	-1.1010827205	-1.2713930622	-3.0688196697
C	-1.3911411893	2.6024107763	-2.5271657944
C	-2.6966592670	3.2435340765	-2.0197013116
C	-.7172853577	3.4688357571	-3.6114479336
C	-.5022941468	-2.5273328054	-2.4492392227
C	.2781735466	-3.3700356808	-3.4754434135
C	-1.6115008298	-3.3632517175	-1.7738278201
C	3.3861917596	-.5797130746	-2.5613279592
C	3.3289833501	-.5470397243	-.1526072409
C	4.0418730163	-.7131288420	-1.3282196059
H	-4.6560790814	-.1361116089	.0671721476
H	2.8741465544	.6689619259	2.3286325652
H	2.6492806381	-1.0768888483	2.4956330513
H	1.5237261064	.0309096258	3.2885997927
H	1.5318182884	-.1378164744	-3.5469303510
H	-1.6318559913	2.4015449695	4.8009257261
H	-2.6337840726	.4091293784	5.8553767778
H	-2.4854710780	-1.7964726088	4.7545764678
H	.2890690555	2.3039750941	1.5670258084
H	1.0330640092	4.2758610515	2.8175618003
H	1.4763183749	2.8138426615	3.7152324320
H	.1013801437	3.7948285292	4.2358224989
H	-1.0845723348	4.3251341089	1.3658180087
H	-2.0635018570	3.8520201033	2.7616059588
H	-2.1374393328	2.8901467295	1.2833808739
H	-.8316046010	-2.3059835207	1.4077570302
H	-2.6584088804	-3.9424264868	1.5824053794
H	-3.3117666595	-2.2921925154	1.5303430988
H	-3.2559409155	-3.1879355229	3.0612182160
H	-.3855332519	-4.4018973905	2.6361360855
H	-.8809520289	-3.6524479607	4.1591644691
H	.5707196916	-3.0806224011	3.3300603464

H	-3.0763100306	1.8110502005	-4.4944504170
H	-3.3988128371	-.4381537892	-5.4423455949
H	-2.2142049962	-2.3840567122	-4.5169652936
H	-.6959722571	2.5418003142	-1.6861953795
H	-2.4834236127	4.2348752512	-1.6091762583
H	-3.1551637048	2.6366039451	-1.2336525950
H	-3.4268925202	3.3711065409	-2.8247417932
H	-.5042440379	4.4641812321	-3.2107193417
H	-1.3631643663	3.5916953352	-4.4863317426
H	.2269117874	3.0296520736	-3.9473000435
H	.2029031028	-2.2351857959	-1.6688275864
H	.7178130031	-4.2414524545	-2.9816421087
H	1.0878154459	-2.7966875010	-3.9355300948
H	-.3721914520	-3.7385703228	-4.2744040619
H	-1.1659275426	-4.2112239427	-1.2445715067
H	-2.3127897197	-3.7628682301	-2.5127743034
H	-2.1880265273	-2.7702135017	-1.0573337300
H	3.9383936428	-.6884134651	-3.4894365559
H	3.8588539759	-.6657432241	.7823963217
H	5.1005788193	-.9434943211	-1.2903700250

45. $L^2CuO_2H^+$ end-on singlet \rightarrow $L^2CuO_2H^+$ side-on singlet (isomer #2) transition state

Cu	-1.3408759081	.2013115302	.2067203726
O	-3.8677077646	-.4682013470	.2663793838
O	-3.0767134752	.6152599663	-.2138456910
N	.0884882201	-.0178752101	1.3627505613
N	-.2835613945	.0585870188	-1.3762828007
C	2.2517022378	-.1219014591	2.3786523658
C	1.3800314564	-.0811647949	1.1419853992
C	1.9125091257	-.0817001312	-.1954449056
C	1.0751454678	-.0493899830	-1.3741953869
C	1.7315725396	-.1275722604	-2.6424130703
C	-.6229193693	.0221950189	2.5864136331
C	-.9622759149	1.2978943370	3.1340679013
C	-1.7194627250	1.3123393652	4.3036819777
C	-2.1424749139	.1265542368	4.9043807469
C	-1.8293150043	-1.1102588065	4.3374954944
C	-1.0823074797	-1.2005526459	3.1655010546
C	-.5446460683	2.6036285892	2.4701221974
C	.2797467330	3.4962329446	3.4156531825
C	-1.7764674587	3.3573600293	1.9269326233
C	-.7854698204	-2.5597853365	2.5467761520
C	-2.0888667029	-3.2526250626	2.1003875669
C	.0168697049	-3.4635372043	3.5022341093
C	-1.0657768478	-.0088366055	-2.5419675741
C	-1.4153578945	1.2055943331	-3.2055812705
C	-2.1463232421	1.1129482934	-4.3888111394
C	-2.5578003040	-.1230472000	-4.8894395771
C	-2.2470254675	-1.3007805635	-4.2069806261
C	-1.5115734822	-1.2757960859	-3.0234168293
C	-1.0082869801	2.5678529630	-2.6667474369
C	-2.2479684500	3.3996739743	-2.2798474544
C	-.1118831288	3.3314474110	-3.6608641882
C	-1.1872423507	-2.5767016601	-2.3033334458
C	-.2035227346	-3.4420167442	-3.1151359515
C	-2.4649254244	-3.3636138920	-1.9541391245
C	3.1016675199	-.1806970807	-2.7558140264
C	3.3268704955	-.1293276962	-.3761874733
C	3.9223079766	-.1725750561	-1.6129439464
H	-4.5265707499	-.5575354322	-.4443269728
H	3.3000171105	-.3095276645	2.1743214458
H	1.8855738851	-.8958456281	3.0571517593
H	2.1699464842	.8346977934	2.9048524298
H	1.1177320371	-.1177656418	-3.5333705678

H	-1.9893048189	2.2623171000	4.7524908998
H	-2.7316661939	.1660233308	5.8151686609
H	-2.1818403834	-2.0182640349	4.8150852847
H	.0921185549	2.3624947007	1.6124389175
H	.6127969461	4.3932821420	2.8853887263
H	1.1660659711	2.9781278512	3.7954093287
H	-.3098650248	3.8229084963	4.2774973105
H	-1.4576174739	4.2576673720	1.3927422816
H	-2.4373032342	3.6689157644	2.7419235312
H	-2.3657648780	2.7400168715	1.2420084005
H	-.1767766103	-2.4015005816	1.6511558872
H	-1.8573038461	-4.1924619314	1.5898826368
H	-2.6681363778	-2.6219979573	1.4196418293
H	-2.7261490881	-3.4880810351	2.9584602985
H	.2620801705	-4.4074421747	3.0065107502
H	-.5567250675	-3.7019117387	4.4031009836
H	.9541259188	-2.9956351670	3.8194147732
H	-2.4044215189	2.0182715222	-4.9286357311
H	-3.1315225092	-.1683485365	-5.8101392887
H	-2.5850202615	-2.2514006711	-4.6068082982
H	-.4217404620	2.4043961205	-1.7583981920
H	-1.9378104595	4.3482162531	-1.8298549649
H	-2.8784382807	2.8629793919	-1.5651218293
H	-2.8588530403	3.6338226267	-3.1577117390
H	.2058825006	4.2835797878	-3.2249181876
H	-.6420177221	3.5555347848	-4.5919469544
H	.7850634634	2.7577718157	-3.9124500103
H	-.6987376517	-2.3205523684	-1.3579630845
H	.0494357545	-4.3498010166	-2.5584561238
H	.7238385217	-2.9021164882	-3.3254893430
H	-.6406082971	-3.7480918658	-4.0711764069
H	-2.2115042686	-4.2517813816	-1.3672305573
H	-2.9935808359	-3.7002595038	-2.8511505279
H	-3.1534785361	-2.7518736327	-1.3628720309
H	3.5452655996	-.2259096376	-3.7461339054
H	3.9688801722	-.1273985751	.4930516484
H	5.0016989442	-.2059836981	-1.7032545416

46. $L^2CuO_2H^+$ side-on triplet (isomer #1)

Cu	-1.1095424122	-.0164159528	.3235704586
O	-2.7262029786	-.0040041148	1.2776548086
O	-3.1750136644	.5833888427	.0291302340
N	.2203241150	-.7755727499	1.5846999422
N	.1123936732	.2334758673	-1.1560482556
C	2.3872792364	-1.5250776363	2.4029286485
C	1.4918539819	-.8945600037	1.3571375724
C	2.1317593098	-.4129682504	.0996517671
C	1.4514956204	.0804507235	-1.0913898322
C	2.2434493103	.4657928436	-2.2230371609
C	-.4021019242	-1.1846901543	2.8249909276
C	-.4427668846	-.2734541806	3.9021115392
C	-1.0953128426	-.6878753028	5.0685541537
C	-1.6931826829	-1.9412881598	5.1595474216
C	-1.6733042215	-2.8011593121	4.0653686019
C	-1.0446596502	-2.4393522339	2.8695756194
C	.1191598816	1.1423761718	3.8088101868
C	1.1180040713	1.4562572948	4.9366122503
C	-1.0275496210	2.1740059610	3.7785165435
C	-1.1014210378	-3.3735673755	1.6655314470
C	-2.5572566332	-3.6077506932	1.2183953524
C	-.3806879755	-4.7077840898	1.9305643679
C	-.5533363020	.5663051495	-2.3811582794
C	-1.1187279124	1.8621594468	-2.4962623687
C	-1.8141145684	2.1639757001	-3.6685962568

C	-1.9777765057	1.2155827188	-4.6773639949
C	-1.4449422975	-.0616623328	-4.5272649855
C	-.7193711458	-.4214194647	-3.3865888387
C	-.9099673196	2.9259930871	-1.4240633685
C	-2.1856394196	3.7273526405	-1.1111822994
C	.2517159403	3.8657629407	-1.8081873684
C	-.2315937751	-1.8587919999	-3.2279894827
C	.6498290070	-2.3090764731	-4.4060553789
C	-1.4236993410	-2.8176624412	-3.0310375446
C	3.6208639919	.4025388148	-2.2128201489
C	3.5308860178	-.4468905373	.0525274009
C	4.2752582982	-.0496315334	-1.0622135460
H	-3.7545494379	-.1078156729	-.3412599274
H	3.0245520548	-2.2949243184	1.9636106966
H	1.7898363415	-1.9690072813	3.1943072866
H	3.0364965338	-.7692353254	2.8572200792
H	1.7235430949	.8532806400	-3.0900887493
H	-1.1442980218	-.0111410584	5.9151644216
H	-2.1900926410	-2.2407272695	6.0767536228
H	-2.1635687812	-3.7669191595	4.1352340753
H	.6610394787	1.2373434061	2.8619773358
H	1.5436207385	2.4551863184	4.7983654662
H	1.9410581931	.7347199191	4.9615591362
H	.6342072840	1.4397001276	5.9177474999
H	-.6296827894	3.1824122208	3.6227066781
H	-1.5774453882	2.1746050564	4.7248363945
H	-1.7426486016	1.9482711128	2.9818989658
H	-.5822921282	-2.8858759939	.8323384635
H	-2.5829897870	-4.1972142341	.2959652234
H	-3.0698001592	-2.6559456845	1.0490426977
H	-3.1229284183	-4.1569983953	1.9770277178
H	-.4100908158	-5.3422288335	1.0395428786
H	-.8571401471	-5.2602394149	2.7459342102
H	.6673135865	-4.5530205853	2.2036740529
H	-2.2320199005	3.1563071482	-3.7983189017
H	-2.5269964061	1.4719912524	-5.5778944727
H	-1.6016643438	-.7989378027	-5.3077850589
H	-.6126766816	2.4137442166	-.4979978989
H	-2.0003358535	4.4044635486	-.2725902543
H	-3.0126302340	3.0664956452	-.8393020883
H	-2.4977836124	4.3457637261	-1.9590736371
H	.4290010694	4.5979302504	-1.0153737561
H	.0164031454	4.4149814346	-2.7253201147
H	1.1825384898	3.3159363832	-1.9785869371
H	.3804746916	-1.9214819572	-2.3235915318
H	1.0253195891	-3.3216642296	-4.2295926427
H	1.5101887594	-1.6461552908	-4.5393408508
H	.0913990392	-2.3255031958	-5.3467704732
H	-1.0679631285	-3.8412717967	-2.8775792062
H	-2.0825559923	-2.8185011562	-3.9048950985
H	-2.0261250850	-2.5349405985	-2.1608297566
H	4.1858907391	.7191769786	-3.0830633782
H	4.0828037089	-.7894223026	.9157948078
H	5.3580037802	-.0916992447	-1.0229452616

47. L²CuO₂H⁺ side-on triplet (isomer #2)

Cu	-.1055308583	-1.5893458433	1.1480562621
O	.1551546909	-3.2197009970	2.5745359920
O	-1.1554208120	-2.7909494586	2.1303491880
N	1.4723415699	-.6561693327	.4918821506
N	-1.4239842428	-.3858672728	.2989985403
C	2.8370805912	1.0570709100	-.5734177700
C	1.5050271316	.4539304001	-.1813893523
C	.2685438365	1.1680067735	-.6013486158

C	-1.1080997983	.7356127049	-.3778003847
C	-2.1698751355	1.5300524862	-.9269424821
C	2.6686645203	-1.3882391569	.8657350379
C	3.1883560007	-1.2159451629	2.1656304581
C	4.3000946125	-1.9882121086	2.5239635799
C	4.8573551391	-2.9067812326	1.6411675156
C	4.3071989007	-3.0755924758	.3722979090
C	3.2026959296	-2.3273447643	-.0475240870
C	2.5943651962	-.2290979989	3.1661632723
C	3.5508070421	.9516346529	3.4233072155
C	2.2020539395	-.9182991154	4.4867906572
C	2.5688065459	-2.5797279511	-1.4131597217
C	1.5430468391	-3.7283699563	-1.3195032873
C	3.5948373210	-2.8611641271	-2.5231020966
C	-2.7803854513	-.7332936500	.5970335805
C	-3.4512593032	-.0821706285	1.6616438875
C	-4.7586202817	-.4910531030	1.9411318895
C	-5.3745429904	-1.5024798400	1.2092416318
C	-4.6762933416	-2.1542585759	.1939443824
C	-3.3613635746	-1.8043187066	-.1196213408
C	-2.7540617313	.9225165734	2.5728763247
C	-2.4647759897	.2748984378	3.9442652442
C	-3.5407421025	2.2340637308	2.7293966605
C	-2.6088556569	-2.5346159565	-1.2258842447
C	-3.1791548731	-2.1979933341	-2.6169402707
C	-2.5769951395	-4.0543746479	-.9847054700
C	-1.9339582240	2.7056310914	-1.6084930577
C	.4429252680	2.3701986982	-1.2984860706
C	-.6165368551	3.1387004074	-1.7900403982
H	.2491639680	-4.1027428280	2.1725289701
H	2.9462844890	2.0585706020	-.1472994309
H	2.9237265770	1.1423600201	-1.6604494756
H	3.6564808554	.4414878678	-.2110495236
H	-3.1818720520	1.1683341447	-.7981908649
H	4.7320170353	-1.8661971449	3.5119566130
H	5.7188261166	-3.4950452395	1.9407093927
H	4.7467045358	-3.8002679482	-.3041237666
H	1.6763960159	.1849243355	2.7331164675
H	3.0907642852	1.6742335924	4.1044438846
H	3.8111131924	1.4735703873	2.4969291431
H	4.4834909753	.6083648664	3.8819957549
H	1.7111957846	-.2016968413	5.1526576756
H	3.0803510242	-1.3052626733	5.0125729305
H	1.5176214211	-1.7530390813	4.3130867042
H	2.0200947964	-1.6793752347	-1.7095621592
H	1.0507521909	-3.8920940733	-2.2833489776
H	.7616041090	-3.5167122585	-.5790848470
H	2.0333040543	-4.6619949080	-1.0249017612
H	3.0919691483	-2.9012489726	-3.4938341565
H	4.0982604983	-3.8222265271	-2.3821507028
H	4.3618316133	-2.0824524760	-2.5680532908
H	-5.2961864610	-.0205977194	2.7578261436
H	-6.3935074684	-1.7957244326	1.4405420169
H	-5.1611083086	-2.9498500758	-.3625798235
H	-1.7862454547	1.1769119839	2.1288218024
H	-1.8793391463	.9554111616	4.5713050417
H	-1.9134668497	-.6633398815	3.8309128120
H	-3.3957986016	.0489910902	4.4735121115
H	-2.9792948146	2.9368357092	3.3526712030
H	-4.5084558902	2.0704196913	3.2129916398
H	-3.7259819280	2.7105242801	1.7616166487
H	-1.5702593019	-2.1816630514	-1.2117596676
H	-2.5988720978	-2.6968876809	-3.3995582378
H	-3.1572215249	-1.1208536994	-2.8113058627

H	-4.2179415604	-2.5314060373	-2.7062676296
H	-1.9557923082	-4.5444795293	-1.7414150114
H	-3.5768125820	-4.4942296220	-1.0484080396
H	-2.1725964140	-4.2821372020	.0057259939
H	-2.7647007048	3.2792502339	-2.0054875028
H	1.4419258497	2.7387634108	-1.4810545727
H	-.4049516555	4.0597760014	-2.3221300369

48. L²CuO₂H⁺ end-on triplet

Cu	-1.4415280601	.2752428638	.0466184909
O	-4.0124045946	-.6255827794	-.0690308240
O	-3.2763457207	.5441460854	.1405624558
N	-.0214871582	-.0340250605	1.3740126518
N	-.2383592501	.0836085723	-1.5037070398
C	2.1879533242	-.3732872530	2.3410057113
C	1.2437939818	-.2335675043	1.1659834711
C	1.8202720735	-.3135050290	-.2010077328
C	1.0937180986	-.1606298532	-1.4504626464
C	1.8314537958	-.2071532869	-2.6768937550
C	-.6039469197	.0831250339	2.6920271113
C	-.7732350980	1.3772484989	3.2342683353
C	-1.4305040501	1.4808976466	4.4639278893
C	-1.9081362839	.3528193308	5.1259825371
C	-1.7413934224	-.9076813038	4.5604318484
C	-1.0962518217	-1.0759669549	3.3297791830
C	-.3167388779	2.6347509717	2.4993624326
C	.5172954335	3.5732091733	3.3885772778
C	-1.5238102340	3.3803189146	1.8934699016
C	-.9789705269	-2.4690327897	2.7178632382
C	-2.3674563440	-3.0340012900	2.3572979668
C	-.2104582618	-3.4386377848	3.6344772949
C	-.9704655635	-.0313950470	-2.7106319324
C	-1.6159418691	1.1394240908	-3.2003269928
C	-2.3585991379	1.0324217338	-4.3744322089
C	-2.5019866316	-.1909830846	-5.0298247625
C	-1.9073360306	-1.3376203916	-4.5089912191
C	-1.1314752601	-1.2967142077	-3.3484113797
C	-1.4187517482	2.4932318185	-2.5297877976
C	-2.7283643320	3.2845336401	-2.3855538546
C	-.3423598700	3.3155263442	-3.2680026735
C	-.6263792515	-2.6036337800	-2.7438084792
C	.2172444881	-3.4245959179	-3.7345039253
C	-1.8116653581	-3.4314233366	-2.2036959010
C	3.1916475753	-.4401900245	-2.7099847261
C	3.1982545617	-.5606379881	-.2969840045
C	3.8838286802	-.6330328052	-1.5104652553
H	-4.9282950419	-.3021525719	.0070622208
H	2.9756870330	.3839952564	2.2978469695
H	2.6669760904	-1.3569694106	2.3374104682
H	1.6499112916	-.2576723254	3.2786913328
H	1.2914241109	-.0198593576	-3.5965904638
H	-1.5731796781	2.4605472981	4.9081446513
H	-2.4141940526	.4570311812	6.0803369212
H	-2.1237534258	-1.7805855292	5.0799793391
H	.3277646244	2.3307426827	1.6679824394
H	.8936713906	4.4146844490	2.7987149796
H	1.3746594895	3.0529030331	3.8261910436
H	-.0754967968	3.9892829879	4.2085399726
H	-1.1888008731	4.2485929994	1.3165110772
H	-2.1971973965	3.7371583131	2.6792095721
H	-2.1154669804	2.7364148864	1.2327005745
H	-.4127233436	-2.3869156641	1.7842501600
H	-2.2658142537	-4.0105909221	1.8730295563
H	-2.9081315125	-2.3678133110	1.6777881787

H	-2.9835860487	-3.1687747798	3.2519991593
H	-.0930319110	-4.4106532724	3.1453308936
H	-.7426913815	-3.6060503256	4.5758435713
H	.7858901499	-3.0581563878	3.8803656475
H	-2.8271283126	1.9171487400	-4.7915301126
H	-3.0878877233	-.2512941054	-5.9414736453
H	-2.0642019822	-2.2893958247	-5.0056827094
H	-1.0354643084	2.3103492271	-1.5180428171
H	-2.5456911974	4.2055882346	-1.8237791560
H	-3.4848420026	2.7024903255	-1.8512835719
H	-3.1417634454	3.5752722470	-3.3558433782
H	-.1726181572	4.2687517242	-2.7577279786
H	-.6548718606	3.5323998836	-4.2946130867
H	.6117285154	2.7809620625	-3.3149386942
H	.0139736449	-2.3702098050	-1.8892840216
H	.5961224041	-4.3271731468	-3.2456304729
H	1.0741197926	-2.8525324565	-4.1026661898
H	-.3701697198	-3.7440244788	-4.6005400776
H	-1.4460001968	-4.3342402191	-1.7042221408
H	-2.4778696951	-3.7435612579	-3.0139446744
H	-2.4070988943	-2.8578232845	-1.4862186912
H	3.7150596046	-.4598310838	-3.6601548660
H	3.7759442596	-.7022035632	.6051850498
H	4.9517099742	-.8217926078	-1.5116380972

49. $L^2CuO_2H_2^{2+}$ end-on singlet

H	-3.4011555921	-.6986737003	2.0017213519
C	1.9011550702	-.4175634931	-2.6717713774
C	-.9310716682	-.0562103000	2.3972906585
C	-1.0815700760	1.2666819108	2.8826578989
C	-1.9472462213	1.4599040135	3.9700826900
C	-2.6576887110	.4091891305	4.5369202258
C	-2.5118717146	-.8894722663	4.0316824108
C	-1.6459996574	-1.1581977114	2.9612389198
C	-.4172494237	2.4837597598	2.2472965142
C	.4500347307	3.2633933294	3.2551081349
C	-1.4757980640	3.4099934891	1.6115913744
C	-1.3904086543	-2.5880845961	2.4859102504
C	-2.5850442787	-3.5382544333	2.6645845017
C	-.1485847294	-3.1677140625	3.1999914280
C	-.9924207084	-.0161446836	-2.6389764293
C	-1.7801392296	1.1560361602	-3.0185990018
C	-2.6341190616	1.0335594302	-4.1048427725
C	-2.7578493580	-.1801131516	-4.7866696255
C	-2.0532504559	-1.3241689918	-4.3812033201
C	-1.1659053481	-1.2943991401	-3.3188989990
C	-1.5450028010	2.5011083259	-2.3585601265
C	-2.8183646726	3.3557755812	-2.2545970036
C	-.4248036565	3.2652956223	-3.1078210380
C	-.5875086085	-2.5990936515	-2.7892996890
C	.1323250238	-3.4114336544	-3.8822560041
C	-1.7083565732	-3.4296426908	-2.1235351284
C	3.2580258311	-.6753592684	-2.6300717127
C	3.1796828172	-.6708713352	-.2121213296
C	3.9016557677	-.8163179935	-1.3932652031
C	1.9794289144	-.0541879942	2.3237883777
C	1.1179432678	-.2546260828	1.0971957743
C	1.7997520839	-.3978625736	-.1999358551
C	1.1417784610	-.2719184803	-1.4779547951
H	-4.8368820619	-.3978588352	1.3107515226
H	2.6493805852	.7996208199	2.1922880724
H	2.5994605980	-.9393655971	2.4948933244
H	1.3707367156	.1032806718	3.2109922850
H	1.4062859780	-.2409280719	-3.6200168820

H	-2.0757569993	2.4609835295	4.3674236648
H	-3.3210172020	.5907938983	5.3763853934
H	-3.0479856668	-1.7062285072	4.5020868107
H	.2388454098	2.1431533289	1.4401698190
H	.9576610577	4.0882034137	2.7472540544
H	1.2113392940	2.6309826683	3.7201759041
H	-.1560753131	3.6973810923	4.0553873272
H	-.9840814522	4.2399986868	1.0954770860
H	-2.1347682226	3.8405048441	2.3715305042
H	-2.1035594118	2.8757814413	.8910194980
H	-1.1574331984	-2.5413756641	1.4132104454
H	-2.3524847365	-4.5035812691	2.2082145873
H	-3.4973448347	-3.1638274828	2.1898599109
H	-2.8014406864	-3.7308774133	3.7192819118
H	.0638554706	-4.1733855248	2.8269064751
H	-.3225319770	-3.2359896815	4.2779994220
H	.7418832190	-2.5537755823	3.0438937488
H	-3.2031386638	1.8911034261	-4.4430183454
H	-3.4280054361	-.2456997441	-5.6387628367
H	-2.2331072501	-2.2583355055	-4.9013423804
H	-1.1724973698	2.3151044715	-1.3457995724
H	-2.6055692574	4.2470894348	-1.6581976115
H	-3.6359572884	2.8110208318	-1.7729216485
H	-3.1650486325	3.7049637266	-3.2313079509
H	-.2301624066	4.2159314326	-2.6034317481
H	-.7218385871	3.4837524703	-4.1377478637
H	.5104538148	2.6982840966	-3.1335824320
H	.1496288038	-2.3761370070	-2.0155894734
H	.5764056960	-4.3069227911	-3.4400261596
H	.9312656686	-2.8329309095	-4.3541490835
H	-.5553979056	-3.7407746392	-4.6658774319
H	-1.2866461931	-4.3406939066	-1.6895925548
H	-2.4751099915	-3.7234241351	-2.8458055119
H	-2.2066157807	-2.8690604380	-1.3227318102
H	3.8217404985	-.7518786996	-3.5539460754
H	3.7112606961	-.7890301579	.7221982799
H	4.9641016127	-1.0289592569	-1.3496544693
N	-.1808925945	-.3232266463	1.2084091920
N	-.1451630471	.1744314871	-1.5759010501
O	-3.9507854852	-.7854370771	1.1611706833
O	-3.3687730923	.1153384152	.1233988128
Cu	-1.4931298990	-.1948093776	-.2662502539

50. $L^2CuO_2H_2^{2+}$ end-on triplet

H	-3.3140600776	-.7851908201	2.1258040860
C	1.8806264651	-.1981631427	-2.6956665003
C	-.9407927965	-.0074859813	2.4688661802
C	-1.2267835466	1.2579637123	3.0300984238
C	-2.0685720889	1.2900595963	4.1518970263
C	-2.6401642291	.1336459992	4.6696836191
C	-2.3613189779	-1.1073688588	4.0850014708
C	-1.4995793806	-1.2150873046	2.9796808394
C	-.7012951731	2.5674325083	2.4521479549
C	.1380442973	3.3511525009	3.4795556867
C	-1.8602614896	3.4302785545	1.9111383551
C	-1.0982692595	-2.5867853715	2.4348609425
C	-2.2548056648	-3.5994591917	2.3703939998
C	.0622758692	-3.1658844197	3.2742584604
C	-.9930810207	-.1482637474	-2.8170342032
C	-1.3946382334	1.1169456917	-3.3411939542
C	-2.1813622238	1.1028612274	-4.4922254461
C	-2.5692174955	-.0975028292	-5.0882934580
C	-2.1781035157	-1.3255082858	-4.5435612495

C	-1.3951156239	-1.3907778921	-3.3949430090
C	-.9751631248	2.4359802885	-2.7044037651
C	-2.1939710375	3.3036123759	-2.3369299106
C	.0020685407	3.2077142130	-3.6141647300
C	-1.0189674063	-2.7217668732	-2.7573632425
C	-.7169031285	-3.8259410868	-3.7837772248
C	-2.1276076806	-3.1759638314	-1.7833400782
C	3.2584076944	-.1974359574	-2.6533721432
C	3.1549420994	-.1199796540	-.2223037470
C	3.9048776922	-.1589046238	-1.4102264438
C	1.9509474168	.0216275590	2.3547161510
C	1.0833369059	-.0687660952	1.1202037793
C	1.7598423542	-.1236953974	-.2022232996
C	1.0884181344	-.1650665849	-1.4966032050
H	-4.7740349574	-.4669336089	1.4719481398
H	2.5518204644	.9360098083	2.3322110650
H	2.6357039460	-.8289255067	2.4123309410
H	1.3415607790	.0345920211	3.2553748629
H	1.3552369214	-.2308680789	-3.6432542727
H	-2.2928168670	2.2456676615	4.6137443111
H	-3.2949240275	.1884975707	5.5332709546
H	-2.7847895017	-2.0076901716	4.5173182039
H	-.0478816574	2.3342223526	1.6050951519
H	.5452723943	4.2541972606	3.0163286503
H	.9738743676	2.7575737501	3.8617744763
H	-.4649109000	3.6669459052	4.3357362465
H	-1.4653781014	4.3290216240	1.4287338088
H	-2.5237139369	3.7547482050	2.7184681552
H	-2.4668998495	2.8825947111	1.1828651502
H	-.7282830623	-2.4464653661	1.4117051679
H	-1.9020501014	-4.5262294884	1.9103977692
H	-3.0972115259	-3.2369930760	1.7725348140
H	-2.6275097159	-3.8631175484	3.3641868224
H	.3952724450	-4.1175062313	2.8504991258
H	-.2606449462	-3.3490383078	4.3034469083
H	.9214642861	-2.4912108390	3.3130658892
H	-2.4924775335	2.0426797950	-4.9354220450
H	-3.1805115181	-.0795395816	-5.9847135822
H	-2.4879950033	-2.2425558551	-5.0310289683
H	-.4437026600	2.2126375413	-1.7707831690
H	-1.8639786701	4.2129103986	-1.8268681312
H	-2.8862096864	2.7714470802	-1.6756119990
H	-2.7532722112	3.6110491277	-3.2248511994
H	.3234748319	4.1306733506	-3.1233392394
H	-.4724067539	3.4819149656	-4.5610951539
H	.8935292637	2.6169361331	-3.8463776256
H	-.1062735450	-2.5698484466	-2.1693933679
H	-.3333440287	-4.7113724757	-3.2698855101
H	.0332673776	-3.5050545008	-4.5118722753
H	-1.6124128466	-4.1345458944	-4.3304141779
H	-1.8434260825	-4.1076873028	-1.2855630886
H	-3.0691796805	-3.3445356203	-2.3141925827
H	-2.3243573994	-2.4253676483	-1.0035544517
H	3.8332075753	-.2249563067	-3.5728688927
H	3.7070512372	-.0836942240	.7065010246
H	4.9881613568	-.1555697788	-1.3537733620
N	-.2094432139	-.0860013221	1.2343875031
N	-.2421682820	-.1692019303	-1.6113679878
O	-3.8658685063	-.7775939723	1.2766192490
O	-3.3300429507	.3046875245	.4056243003
Cu	-1.5607234963	-.0862862807	-.2538056973

51. $L^2CuO_2H_2^+$ end-on doublet

H	-3.2008552060	-.5512764041	2.1206130337
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C	1.8819262784	-.2636646938	-2.6370113247
C	-.9350791452	-.0761301935	2.4885949837
C	-1.0992379735	1.2475684391	2.9696341938
C	-1.8834830592	1.4347461499	4.1160737294
C	-2.5076506440	.3711854525	4.7613026365
C	-2.3523833569	-.9243721962	4.2668307941
C	-1.5709736068	-1.1798792536	3.1261177689
C	-.5024667620	2.4657661835	2.2702654178
C	.4545890886	3.2487534698	3.1889540632
C	-1.6146729450	3.3846902697	1.7254652969
C	-1.3265325248	-2.6107714781	2.6487991191
C	-2.5745761594	-3.5065407783	2.7146999063
C	-.1675139179	-3.2449053823	3.4461101886
C	-.9465035237	-.0330562557	-2.8276785630
C	-1.5531476731	1.1599078131	-3.3219488241
C	-2.2662380142	1.0879330073	-4.5188987373
C	-2.4085626500	-.1185776817	-5.2011842696
C	-1.8454475604	-1.2877013406	-4.6863986755
C	-1.1072217874	-1.2806045347	-3.5040325886
C	-1.4024539728	2.4953553259	-2.6038290624
C	-2.7683960363	3.0364139689	-2.1424525625
C	-.6548802595	3.5265887701	-3.4707957619
C	-.6293656853	-2.5913918413	-2.8907467880
C	-.0109792557	-3.5531053583	-3.9183143603
C	-1.7902009249	-3.2652594243	-2.1293721242
C	3.2421134811	-.4783726518	-2.5777634485
C	3.1105748174	-.6082407104	-.1812860816
C	3.8691342119	-.6676958168	-1.3370864341
C	1.9231077467	-.1695716029	2.3548722246
C	1.0440332434	-.2970091146	1.1232859322
C	1.7120755177	-.3885236429	-.1811709474
C	1.0662911583	-.2262823679	-1.4669437369
H	-4.66522020644	-.0008783226	1.7523820997
H	2.6243254578	.6624188590	2.2541309694
H	2.5112697021	-1.0813608239	2.4960042818
H	1.3262397084	-.0175388150	3.2515108189
H	1.4035226742	-.0865454771	-3.5927258462
H	-2.0155456413	2.4404384107	4.5024273636
H	-3.1070366110	.5464263159	5.6489527201
H	-2.8290084554	-1.7534430353	4.7789782914
H	.0768504902	2.1186551904	1.4106516887
H	.9072194351	4.0786266605	2.6379468186
H	1.2611345764	2.6163738735	3.5715398470
H	-.0710711680	3.6748315987	4.0491795755
H	-1.1753964446	4.2126664501	1.1602571460
H	-2.2059226940	3.8179118971	2.5391619633
H	-2.2955125751	2.8395076790	1.0651664869
H	-1.0140857776	-2.5557181385	1.6002737263
H	-2.3508587293	-4.4824634490	2.2748561098
H	-3.4169442114	-3.0801977637	2.1602938267
H	-2.8996849027	-3.6873322007	3.7440186425
H	.0479013782	-4.2497959100	3.0705763588
H	-.4268708967	-3.3273753914	4.5066546391
H	.7481757332	-2.6524540517	3.3734024833
H	-2.7128587995	1.9887536783	-4.9278061347
H	-2.9678450096	-.1528949175	-6.1309140733
H	-1.9958549425	-2.2227434750	-5.2150218170
H	-.7952489480	2.3241835399	-1.7107694021
H	-2.6373990355	3.9746783916	-1.5936247616
H	-3.2796350323	2.3250399650	-1.4842582672
H	-3.4303088995	3.2391118050	-2.9904466979
H	-.5076918429	4.4554012513	-2.9104353950
H	-1.2148240636	3.7720509965	-4.3788667709
H	.3285303154	3.1539129425	-3.7732363872

H	.1481890640	-2.3677033174	-2.1575773131
H	.3981985279	-4.4297882200	-3.4074404056
H	.8013101603	-3.0745907307	-4.4733487678
H	-.7482284033	-3.9143761963	-4.6416795806
H	-1.4486408823	-4.1840285893	-1.6415730080
H	-2.6096079189	-3.5227275615	-2.8078726487
H	-2.2006151060	-2.6028525203	-1.3567797342
H	3.8236189308	-.4930945170	-3.4943012969
H	3.6228670293	-.7503464484	.7602094365
H	4.9365420558	-.8485007638	-1.2772017300
N	-.2569544692	-.3191152790	1.2526129422
N	-.2591700790	.0551398290	-1.5984130989
O	-3.9166622934	-.5286216686	1.4150743620
O	-3.4159554642	.3234084123	.2680535393
Cu	-1.6030876461	-.0966388824	-.2639458705

52. $L^2CuO_2^-$ side-on doublet

Cu	-.0030423404	-2.4153062148	.7951164614
O	.8656741079	-4.0950641917	1.3477432334
O	-.5362196783	-4.2781210532	1.1905310104
N	1.3248562494	-.9093533752	.6224567097
N	-1.5312663299	-1.2704408790	.2873330789
C	2.2958401369	1.2586775523	.2062417806
C	1.0809032024	.3335887070	.2732800636
C	-.2572751203	.8347971077	-.0368652152
C	-1.4886300849	.0353164331	-.0204996770
C	-2.7096967802	.7276570577	-.3602056875
C	2.6540620677	-1.3431836288	.9193798872
C	3.1172618630	-1.3082391072	2.2548614735
C	4.4210496338	-1.7398664435	2.5197320423
C	5.2434582366	-2.2247750397	1.5060681398
C	4.7445374757	-2.3267798900	.2099563919
C	3.4478755513	-1.9078288639	-.1055831336
C	2.1822859396	-.9303133552	3.3978906819
C	2.7992306586	.0650279438	4.3936371136
C	1.7009029044	-2.2144194558	4.1074875636
C	2.8657857856	-2.1703077439	-1.4897486736
C	2.4959271498	-3.6643235012	-1.6130192854
C	3.7836077421	-1.7214608578	-2.6381367826
C	-2.7773566262	-1.9582153319	.2988572877
C	-3.5257781141	-2.0431915565	1.4984341637
C	-4.7351445555	-2.7458630932	1.4938268503
C	-5.2030843739	-3.3749178144	.3427233166
C	-4.4332685642	-3.3342074381	-.8170417501
C	-3.2178387314	-2.6428075339	-.8592227064
C	-2.9706635724	-1.4812492565	2.8010371887
C	-2.4204113975	-2.6351487243	3.6653781231
C	-3.9835013052	-.6234304845	3.5757938832
C	-2.3309538436	-2.7219910232	-2.0944481783
C	-3.0741021413	-2.3975329495	-3.3999232190
C	-1.6526552263	-4.1069122625	-2.1525942187
C	-2.7597024290	2.0595407327	-.6807969139
C	-.3917218697	2.2119582401	-.3773776745
C	-1.5815273929	2.8311062363	-.6916456220
H	2.0919349252	2.2707886589	-.1254695984
H	3.0419747936	.8265599758	-.4663970746
H	2.7679824085	1.3118897054	1.1916572706
H	-3.6232117175	.1466652344	-.3552995817
H	4.7900584346	-1.7143216620	3.5415638155
H	6.2554926321	-2.5515552670	1.7308121086
H	5.3660272761	-2.7587879051	-.5698187133
H	1.3016374051	-.4514052210	2.9615699220
H	2.0611903991	.3449152355	5.1540443323

H	3.1359026562	.9816541117	3.8959086841
H	3.6600101188	-.3640138896	4.9193388489
H	.9195164804	-1.9800771023	4.8407917660
H	2.5340483976	-2.6883969364	4.6421900470
H	1.3104799244	-2.9387649378	3.3827969853
H	1.9374299302	-1.5986854892	-1.5725642631
H	1.9455047478	-3.8491137269	-2.5437447232
H	1.8857588606	-3.9892163596	-.7615664938
H	3.4046120667	-4.2798796707	-1.6308581234
H	3.2863674586	-1.8792378510	-3.6020168876
H	4.7195811065	-2.2914588138	-2.6588138972
H	4.0419290151	-.6590929571	-2.5607591661
H	-5.3111987053	-2.8167142805	2.4131769340
H	-6.1471116150	-3.9141810325	.3567954758
H	-4.7737923924	-3.8639307781	-1.7033298548
H	-2.1271856564	-.8366275952	2.5416490580
H	-1.9016116661	-2.2443742352	4.5501749704
H	-1.7272234215	-3.2569945752	3.0872861627
H	-3.2390549466	-3.2781834700	4.0133787234
H	-3.5145721550	-.1956638789	4.4699872993
H	-4.8465611156	-1.2106036861	3.9114100069
H	-4.3570364679	.2019683178	2.9602378414
H	-1.5413473957	-1.9762518951	-1.9722268000
H	-2.3779609259	-2.4086432592	-4.2470742436
H	-3.5398623594	-1.4071248081	-3.3557120473
H	-3.8607972576	-3.1299957333	-3.6165376718
H	-.9133406585	-4.1438230035	-2.9630578840
H	-2.3969732263	-4.8912376181	-2.3412774869
H	-1.1563671370	-4.3359337544	-1.2024238700
H	-3.7176004696	2.5143495197	-.9260100720
H	.4907911331	2.8354130260	-.3925387255
H	-1.6019037500	3.8878189464	-.9399959335

53. L²CuO₂⁻ end-on doublet

Cu	-.1827871974	-2.2449292934	.2937026394
O	.4411003096	-4.7605631346	-.4155972229
O	.1707301735	-4.0986413294	.7257468075
N	1.3441781086	-.8237144617	.1746265179
N	-1.5495874822	-.8879033501	-.0859828797
C	2.4301849163	1.3678839897	.1054980465
C	1.2033123831	.4638854226	-.0025150212
C	-.0833073169	1.0939898704	-.3096885816
C	-1.3791651677	.4185025977	-.3507579173
C	-2.5166987973	1.2379554985	-.6879784082
C	2.6028082215	-1.4409768073	.4132295358
C	2.9946461315	-1.7438262419	1.7388746467
C	4.2089179092	-2.4060205449	1.9435082198
C	5.0150472889	-2.7911323440	.8755372464
C	4.5888566378	-2.5363022585	-.4255955823
C	3.3860231136	-1.8717015085	-.6840106397
C	2.0871556394	-1.4324521958	2.9233466632
C	2.7717714097	-.5453719355	3.9774450622
C	1.5512658975	-2.7355136472	3.5489525677
C	2.9008503380	-1.7005074078	-2.1198835568
C	2.4577140056	-3.0571016080	-2.7049376055
C	3.9420508521	-1.0126821967	-3.0198689140
C	-2.8469610825	-1.4649551626	-.0930580360
C	-3.6278093490	-1.4764820970	1.0914719853
C	-4.8557462997	-2.1457301592	1.0912162164
C	-5.3270203528	-2.7963712857	-.0462894390
C	-4.5543299347	-2.7842541881	-1.2054483305
C	-3.3211494570	-2.1271270307	-1.2552867897
C	-3.1187296472	-.8260135231	2.3729135393
C	-2.7571249265	-1.8934282529	3.4227243810

C	-4.1083844942	.2057940430	2.9402837933
C	-2.4850575614	-2.1697419313	-2.5294804848
C	-3.2710145736	-1.6761409494	-3.7569572967
C	-1.9004566553	-3.5759828495	-2.7688235284
C	-2.4241565639	2.5801703808	-.9642817649
C	-.0615061460	2.4838988841	-.6042862227
C	-1.1768293834	3.2309271938	-.9258712932
H	2.2542092053	2.1882467999	.8069299665
H	2.6826874544	1.8111193667	-.8639217273
H	3.2923085122	.7988540485	.4488400694
H	-3.4834831150	.7501234311	-.7277228764
H	4.5183480583	-2.6386312181	2.9593910107
H	5.9540712819	-3.3080881014	1.0545566181
H	5.1952663926	-2.8740522993	-1.2619962687
H	1.2245429712	-.8809210490	2.5401612864
H	2.0755143153	-.3109038422	4.7911563034
H	3.1162715882	.3993761390	3.5429316074
H	3.6412512438	-1.0439481081	4.4216508752
H	.8117478510	-2.5100462530	4.3271046871
H	2.3630574044	-3.3077973278	4.0147025992
H	1.0835935968	-3.3707577403	2.7905839211
H	2.0164823205	-1.0586995726	-2.0961822651
H	2.0507586300	-2.9213013953	-3.7149099900
H	1.6929093372	-3.5282253685	-2.0774194649
H	3.3076878735	-3.7466843582	-2.7762688626
H	3.5315738704	-.8521803779	-4.0235040611
H	4.8473596569	-1.6206360600	-3.1302199150
H	4.2422910834	-.0395363429	-2.6157733367
H	-5.4488673518	-2.1658804656	2.0029711102
H	-6.2816851889	-3.3161220824	-.0269066603
H	-4.9124310182	-3.3047033779	-2.0904969689
H	-2.1974144351	-.2955098270	2.1217606419
H	-2.3403950465	-1.4269644898	4.3242222425
H	-2.0152082443	-2.5903814865	3.0216428098
H	-3.6381910705	-2.4740969906	3.7212866980
H	-3.6902317588	.6917268612	3.8300985242
H	-5.0572846124	-.2585627846	3.2340446208
H	-4.3280227359	.9825301791	2.2010460128
H	-1.6438106328	-1.4872991657	-2.3848021314
H	-2.6194819148	-1.6423404271	-4.6381639413
H	-3.6717880649	-.6704900335	-3.5914344265
H	-4.1117530403	-2.3376502237	-3.9976934864
H	-1.3050457402	-3.5863477986	-3.6909598438
H	-2.7015519307	-4.3172311075	-2.8819737720
H	-1.2506816033	-3.8999529240	-1.9482912211
H	-3.3254188471	3.1357476210	-1.2170027971
H	.8902047446	2.9995503670	-.5906914465
H	-1.0867987701	4.2900808033	-1.1470218377

54. $L^2CuO_2^-$ end-on doublet \rightarrow $L^2CuO_2^-$ side-on doublet transition state

Cu	-.1796457832	-2.2280676030	.2412102242
O	-.2668705574	-4.3712470137	-.3471993430
O	.4503403709	-3.9622272848	.7757644973
N	1.3369910046	-.8134475086	.2028552281
N	-1.5537758427	-.8981226378	-.1631034127
C	2.4309078260	1.3656947349	.0158012123
C	1.2000387408	.4632270318	-.0414380799
C	-.0844674284	1.0838292523	-.3783001636
C	-1.3834168641	.4116481420	-.4102582642
C	-2.5232814163	1.2395292018	-.7173966345
C	2.5837510508	-1.4250531295	.5150668115
C	2.9832628970	-1.5580223748	1.8658387922
C	4.1810956066	-2.2232204277	2.1470927195
C	4.9619313966	-2.7712640642	1.1339474527

C	4.5273613638	-2.6811040727	-.1861390105
C	3.3401813245	-2.0233622483	-.5217303669
C	2.1078168568	-1.0583538113	3.0106278491
C	2.8450556631	-.0726413588	3.9348482857
C	1.5276852202	-2.2464070796	3.8043182131
C	2.8445729523	-2.0340176564	-1.9643381163
C	2.3375908750	-3.4365518070	-2.3606787092
C	3.9068683426	-1.5258729198	-2.9546786107
C	-2.8487752006	-1.4840898721	-.1838391468
C	-3.5431480153	-1.6803139231	1.0368251154
C	-4.7708748175	-2.3490699023	1.0225358598
C	-5.3196168007	-2.8301228243	-.1637842884
C	-4.6217940443	-2.6545601727	-1.3561163265
C	-3.3898968823	-1.9932087931	-1.3915967852
C	-2.9255206429	-1.2408037871	2.3586866108
C	-2.4061285886	-2.4648837761	3.1389921818
C	-3.8827049001	-.3934452885	3.2127546007
C	-2.6327905639	-1.8711777238	-2.7087381654
C	-3.4456284662	-1.1210242193	-3.7783929387
C	-2.1710468879	-3.2541170166	-3.2088835132
C	-2.4268613176	2.5782516197	-1.0087641780
C	-.0583502857	2.4686113299	-.6949771479
C	-1.1734825717	3.2186833964	-1.0095538071
H	2.2692854016	2.2175010197	.6828068195
H	2.6687134791	1.7666695630	-.9757453552
H	3.2952045290	.8065265203	.3696540061
H	-3.4956466411	.7614274155	-.7183171276
H	4.4975257532	-2.3263211945	3.1822224854
H	5.8883800818	-3.2868911040	1.3730963731
H	5.1137797892	-3.1461848823	-.9741251591
H	1.2609395526	-.5246028052	2.5712128057
H	2.1719250122	.2968484701	4.7174238763
H	3.2234399781	.7914097278	3.3770090758
H	3.6989145151	-.5470031168	4.4327627432
H	.8288239293	-1.8905667257	4.5714335999
H	2.3226671680	-2.8098298587	4.3079963428
H	.9948126418	-2.9319605252	3.1380605000
H	1.9913193564	-1.3530912515	-2.0268758566
H	1.9773774493	-3.4233572379	-3.3972173760
H	1.5201512031	-3.7793078472	-1.7168554911
H	3.1492441135	-4.1715400653	-2.2987416970
H	3.4908504506	-1.4825562288	-3.9677611484
H	4.7798181889	-2.1881502400	-2.9902637447
H	4.2601118841	-.5235170007	-2.6873171825
H	-5.3000129005	-2.5075040081	1.9593205112
H	-6.2749625126	-3.3489245252	-.1570381297
H	-5.0362841142	-3.0497297951	-2.2808819224
H	-2.0587983811	-.6207926540	2.1182482439
H	-1.9161825382	-2.1522119725	4.0696425048
H	-1.6814742343	-3.0310991240	2.5448011142
H	-3.2286765804	-3.1411892230	3.4015126697
H	-3.3795947474	-.0480512598	4.1240829617
H	-4.7668026072	-.9622500281	3.5236704123
H	-4.2279385631	.4869652975	2.6605007030
H	-1.7308247554	-1.2872007698	-2.5088142536
H	-2.8547608687	-1.0008939937	-4.6944109539
H	-3.7339610809	-.1248001248	-3.4269003329
H	-4.3609046331	-1.6637416899	-4.0458422232
H	-1.6071002529	-3.1539874909	-4.1444084867
H	-3.0254357529	-3.9142553355	-3.4034931242
H	-1.5289891650	-3.7349245647	-2.4652123473
H	-3.3303878745	3.1396781191	-1.2397715992
H	.8963677395	2.9790045170	-.6978466738
H	-1.0796963734	4.2736321973	-1.2481789953

55. L²CuO₂H side-on doublet (isomer #1)

Cu	-1.1008706022	-.0143606977	.3381065527
O	-2.7393740723	-.0390649643	1.2965447393
O	-3.1434725825	.6318627537	.0501328923
N	.2272718213	-.7321048373	1.5936209115
N	.0855087996	.2171524724	-1.1232934406
C	2.4139081045	-1.4039737330	2.4309599922
C	1.5194310354	-.7935806913	1.3631154091
C	2.1427752098	-.3092941650	.1385084220
C	1.4336500280	.1353835652	-1.0481522890
C	2.2273881562	.4862637608	-2.1880850289
C	-.3864419479	-1.2237102029	2.7964878943
C	-.5481186828	-.3534839668	3.8955181201
C	-1.1834902267	-.8509351559	5.0386608212
C	-1.6653256900	-2.1560677591	5.0895849533
C	-1.5425780806	-2.9807791018	3.9748314902
C	-.9185277243	-2.5315573847	2.8062332344
C	-.1271426250	1.1107411392	3.8333746560
C	.8157359755	1.5095596659	4.9809579286
C	-1.3720964925	2.0205400276	3.7893838323
C	-.8885602823	-3.4213586953	1.5679267337
C	-2.3155126257	-3.6162161048	1.0151409955
C	-.2009787457	-4.7737923865	1.8208966393
C	-.5599488752	.5782985596	-2.3505181107
C	-.8811843572	1.9339423743	-2.6091434280
C	-1.5760461048	2.2461864224	-3.7831526286
C	-1.9490846369	1.2586454305	-4.6899129835
C	-1.6303384186	-.0702642503	-4.4265544431
C	-.9386994803	-.4363609283	-3.2663622931
C	-.4919971354	3.0520407309	-1.6494824250
C	-1.7316472530	3.7796291413	-1.0953612789
C	.4891283480	4.0420059242	-2.3037271474
C	-.6167544403	-1.9073749526	-3.0212982485
C	.3398794305	-2.4657855567	-4.0910587507
C	-1.8974615960	-2.7574439031	-2.9293193837
C	3.6019678760	.4671582818	-2.1699720749
C	3.5662449995	-.2958805665	.0970383616
C	4.2953572238	.0839141620	-1.0072433690
H	-3.6691867551	-.0538773244	-.3952712631
H	3.0769216395	-2.1584552520	2.0026240557
H	1.8181560896	-1.8694331797	3.2129394336
H	3.0371859093	-.6327576025	2.8948747474
H	1.7076410355	.7950200240	-3.0867406727
H	-1.3152302870	-.1991056806	5.8969611682
H	-2.1534286183	-2.5227672263	5.9878297868
H	-1.9510624283	-3.9868169288	4.0048624836
H	.4178083262	1.2641700412	2.8974045631
H	1.1400609895	2.5485537359	4.8600022103
H	1.7081852322	.8756971905	5.0078795615
H	.3220361162	1.4316493346	5.9552436708
H	-1.0783282779	3.0658158803	3.6399188281
H	-1.9317320461	1.9604659109	4.7293521896
H	-2.0438682391	1.7189458617	2.9809187912
H	-.3093761212	-2.9042748604	.7979469906
H	-2.2904678149	-4.1581919683	.0633938092
H	-2.8042533204	-2.6489003687	.8638479283
H	-2.9319412491	-4.1928467703	1.7136904181
H	-.1618153519	-5.3600760325	.8964627337
H	-.7423912116	-5.3676784058	2.5648583670
H	.8239686848	-4.6410984521	2.1817323615
H	-1.8281600549	3.2825122700	-3.9897120320
H	-2.4855892668	1.5231443081	-5.5966395347
H	-1.9236953194	-.8399734405	-5.1352648276

H	.0255894813	2.5921396710	-.8029921933
H	-1.4333727050	4.5324801720	-.3572503930
H	-2.4169139571	3.0761919170	-.6137390152
H	-2.2811228596	4.2965483881	-1.8900466259
H	.7938153576	4.8103088656	-1.5848019730
H	.0310641006	4.5499499631	-3.1596954567
H	1.3897506354	3.5309393300	-2.6570350506
H	-.1075305391	-1.9763081278	-2.0566427714
H	.5993622195	-3.5067391449	-3.8691460429
H	1.2664874070	-1.8857142601	-4.1283991388
H	-.1142948529	-2.4409679182	-5.0878759575
H	-1.6510139528	-3.8016673309	-2.7077458747
H	-2.4621162520	-2.7411477680	-3.8677488469
H	-2.5603222879	-2.3939294591	-2.1367224071
H	4.1493940047	.7575802216	-3.0628031793
H	4.1152748631	-.5877779276	.9822472055
H	5.3794007469	.0813308720	-.9779691534

56. L²CuO₂H side-on doublet (isomer #2)

Cu	-.1262706967	-1.5108190740	1.2351249236
O	.2569399027	-3.1283772423	2.6052441672
O	-1.1254335910	-2.7637864717	2.2617339409
N	1.4564719896	-.6709305579	.4958253408
N	-1.4077852528	-.3890648651	.3473721782
C	2.8247665943	.9525290408	-.7031968852
C	1.4749790992	.4019100536	-.2697187382
C	.2754365811	1.0789863912	-.7234479239
C	-1.0897991983	.6747504007	-.4210184676
C	-2.1422907565	1.4749612692	-.9840664673
C	2.6490602569	-1.3761720783	.8864433414
C	3.2141810304	-1.1271843232	2.1574113519
C	4.3226935505	-1.8875414398	2.5472991214
C	4.8502492750	-2.8750455208	1.7217100633
C	4.2672239593	-3.1210363389	.4814240933
C	3.1635918245	-2.3847143860	.0372208470
C	2.6484249083	-.0742437500	3.1044664821
C	3.6528420025	1.0679896722	3.3438443706
C	2.1923687583	-.6990562459	4.4367353819
C	2.5138555807	-2.7201281811	-1.3023250879
C	1.6779147032	-4.0103639020	-1.1910420369
C	3.5318799410	-2.8274417405	-2.4505289908
C	-2.7679971218	-.7457039435	.5978486493
C	-3.4152481593	-.2582510369	1.7573842001
C	-4.7353766947	-.6523424152	2.0011223621
C	-5.4040198930	-1.5136780277	1.1359335151
C	-4.7456807535	-2.0102180596	.0140079618
C	-3.4255195681	-1.6475348352	-.2721195107
C	-2.6997544194	.6483012426	2.7520433593
C	-2.5014482607	-.0664663402	4.1027485855
C	-3.4183255043	1.9976467429	2.9272948111
C	-2.7142656775	-2.2633502077	-1.4715406950
C	-3.4442554276	-1.9837068971	-2.7963655947
C	-2.5005944875	-3.7743858578	-1.2563054973
C	-1.9010771738	2.5696112854	-1.7765230503
C	.4554624283	2.2245761313	-1.5545593116
C	-.5809582586	2.9606482109	-2.0770274887
H	.3760244955	-3.9723685730	2.1387853387
H	2.9380569546	1.9921305514	-.3866584473
H	2.9262474801	.9242250926	-1.7923111539
H	3.6387617266	.3752238833	-.2707548025
H	-3.1619398032	1.1876282786	-.7625484289
H	4.7746574756	-1.7043016181	3.5175770015
H	5.7094026441	-3.4552090737	2.0448114891
H	4.6759202710	-3.9007275474	-.1540813084

H	1.7646570669	.3623255663	2.6299778418
H	3.2121824681	1.8355124417	3.9886501843
H	3.9514581521	1.5437683834	2.4042930323
H	4.5611045426	.7015667406	3.8345439815
H	1.7142553845	.0591729499	5.0660360906
H	3.0398216138	-1.1078877378	4.9976087342
H	1.4776981290	-1.5090561842	4.2677031442
H	1.8233813340	-1.9116045005	-1.5563011369
H	1.1841601204	-4.2368789772	-2.1418458700
H	.8979446687	-3.9135761179	-.4281666361
H	2.3082194697	-4.8653129454	-.9226737198
H	3.0115059395	-2.9723876407	-3.4028301683
H	4.2113721815	-3.6757801859	-2.3183280862
H	4.1405338096	-1.9212767980	-2.5294380749
H	-5.2436320367	-.2837519811	2.8878145055
H	-6.4295191441	-1.8070952681	1.3415058454
H	-5.2624651469	-2.7005895491	-.6470375619
H	-1.7063215672	.8583676350	2.3464249856
H	-1.9159445547	.5606708407	4.7853565486
H	-1.9801338162	-1.0174217019	3.9600175229
H	-3.4619855139	-.2758266202	4.5867415517
H	-2.8571833750	2.6437432613	3.6116249189
H	-4.4228139332	1.8670319011	3.3448427380
H	-3.5165587009	2.5203297015	1.9708058815
H	-1.7258055792	-1.8012882034	-1.5392191168
H	-2.8821892010	-2.4018599798	-3.6389816774
H	-3.5563114634	-.9081628420	-2.9636509593
H	-4.4431728026	-2.4331078548	-2.8104594954
H	-1.9100600276	-4.2030443055	-2.0744862456
H	-3.4557241156	-4.3097024295	-1.2172218028
H	-1.9794519570	-3.9598665421	-.3118227768
H	-2.7413239305	3.1349601397	-2.1710207836
H	1.4617502652	2.5359113657	-1.7998260169
H	-.3824107086	3.8225966237	-2.7046107979

57. L²CuO₂H end-on doublet

Cu	-1.4832745456	.1214907112	-.0146951052
O	-3.9500017438	-.9198181682	.4209809400
O	-3.2929581224	.3437262397	.2505668535
N	-.0787805598	-.0062907360	1.3544755879
N	-.2710466971	.0268232982	-1.4848542890
C	2.1499102576	-.0329099223	2.3494774717
C	1.2190363230	-.0631548166	1.1471089399
C	1.8115754728	-.1612146762	-.1750931884
C	1.0701512722	-.1265053808	-1.4217957245
C	1.8288271998	-.2473747728	-2.6335729889
C	-.6587483398	.0396372292	2.6679186477
C	-1.0143584095	1.2922409959	3.2185608822
C	-1.6369200584	1.3089158127	4.4705010795
C	-1.9132462205	.1292993535	5.1564226824
C	-1.5778922453	-1.0949417506	4.5861908263
C	-.9530736365	-1.1704892084	3.3363080142
C	-.7796321059	2.5984774911	2.4674416024
C	.0694537797	3.5957620070	3.2735206176
C	-2.1202806537	3.2266032850	2.0376656883
C	-.6447378796	-2.5345070269	2.7265234676
C	-1.9420596442	-3.3051141538	2.4128581661
C	.2916853133	-3.3689074924	3.6192130431
C	-.9536621293	.0276764274	-2.7393709905
C	-1.2171002739	1.2587403908	-3.3893154159
C	-1.9383382918	1.2413857633	-4.5871140126
C	-2.3953782493	.0471078096	-5.1384175303
C	-2.1355669463	-1.1559086229	-4.4879358263
C	-1.4171314313	-1.1936730135	-3.2878776757

C	- .7426220486	2.5866125055	-2.8100663315
C	-1.9319562012	3.4890948693	-2.4330180156
C	.2290432840	3.3109583511	-3.7593002330
C	-1.1691155872	-2.5309257089	-2.5983499475
C	-.3323703008	-3.4780940424	-3.4778772438
C	-2.4904313394	-3.1923457281	-2.1608959524
C	3.1953197016	-.3944544445	-2.6405126849
C	3.2261648728	-.3133518319	-.2494787352
C	3.9181904381	-.4319577851	-1.4329387676
H	-4.8492512903	-.6206632656	.6267973212
H	2.8963024100	.7574329612	2.2380109309
H	2.6849648275	-.9823390265	2.4501041540
H	1.5955232881	.1426730004	3.2684184753
H	1.2879868942	-.2191505005	-3.5710849481
H	-1.9144378215	2.2617912464	4.9115997470
H	-2.3966005104	.1639819530	6.1282790005
H	-1.8094004076	-2.0132892608	5.1178530534
H	-.2221129541	2.3648701965	1.5557906872
H	.2573525205	4.4987513792	2.6830231481
H	1.0366178218	3.1644132169	3.5512804297
H	-.4352569469	3.9038638567	4.1952856665
H	-1.9470457165	4.1092544504	1.4122167929
H	-2.7015479686	3.5433087694	2.9109406019
H	-2.7316154080	2.5144016189	1.4750206790
H	-.1297075758	-2.3707636119	1.7760984859
H	-1.7102445705	-4.2505052437	1.9097955912
H	-2.6030751928	-2.7202478801	1.7670210449
H	-2.4916400951	-3.5421251329	3.3306479307
H	.5401377214	-4.3164807463	3.1296008927
H	-.1759860043	-3.6065946603	4.5806021449
H	1.2266419494	-2.8388791271	3.8274372422
H	-2.1459093614	2.1787746798	-5.0958237948
H	-2.9537949284	.0544009285	-6.0700493679
H	-2.4994728560	-2.0851573548	-4.9174522381
H	-.1953697322	2.3645322306	-1.8900190620
H	-1.5785526946	4.4166263722	-1.9685371811
H	-2.6011615412	2.9855567677	-1.7280604715
H	-2.5227134232	3.7622152047	-3.3142254050
H	.5961657161	4.2351176907	-3.2993848605
H	-.2554814550	3.5801589114	-4.7043489454
H	1.0934121328	2.6814432097	-3.9913456167
H	-.5894360062	-2.3318708399	-1.6931550712
H	-.1226876472	-4.4110048602	-2.9430391394
H	.6238628019	-3.0206633284	-3.7493529080
H	-.8574280983	-3.7371586561	-4.4039821824
H	-2.2876559700	-4.1281887299	-1.6277972023
H	-3.1207842854	-3.4325920856	-3.0242231526
H	-3.0614645734	-2.5365813594	-1.4966932979
H	3.7151879661	-.4825029055	-3.5909812989
H	3.7953874500	-.3511493238	.6696425620
H	4.9959679552	-.5534620137	-1.4305964905

58. L^2CuO_2H end-on singlet \rightarrow L^2CuO_2H side-on singlet (isomer #1) transition state

Cu	-1.4648001232	.0890708890	-.0628057794
O	-3.7585360135	-.7151673130	-.0771895485
O	-3.0731201454	.2326845940	.8422091866
N	-.0700252966	.0194195766	1.3476096381
N	-.2460020443	-.0115732729	-1.4875489142
C	2.1497939058	-.0180882865	2.3484921262
C	1.2258621190	-.0391327687	1.1401117704
C	1.8311476951	-.1463803069	-.1800838681
C	1.0973999416	-.1355905847	-1.4291730103
C	1.8542451665	-.2449593347	-2.6394738306
C	-.6581315369	.0841545647	2.6560791545

C	- .9638815434	1.3448854612	3.2135226045
C	-1.5895034635	1.3752482124	4.4645172134
C	-1.9214536489	.2018038066	5.1350907112
C	-1.6432854033	-1.0305006908	4.5499582427
C	-1.0209492269	-1.1182654412	3.3008979699
C	-.6816833433	2.6482421811	2.4732564827
C	.2043686957	3.6063221579	3.2885211162
C	-1.9983287327	3.3302432456	2.0495792108
C	-.8015639014	-2.4824093827	2.6552749444
C	-2.1499840817	-3.1309923412	2.2831536732
C	.0431920158	-3.4177370640	3.5381474871
C	-.9596199548	-.0220800361	-2.7248681684
C	-1.2995999994	1.2098876085	-3.3403443254
C	-2.0559416450	1.1826451607	-4.5162539980
C	-2.4729420620	-.0208579545	-5.0783624601
C	-2.1381108850	-1.2244471988	-4.4628884840
C	-1.3838587954	-1.2547422518	-3.2861086607
C	-.8615777635	2.5462801623	-2.7529197413
C	-2.0718942648	3.3925739857	-2.3158029488
C	.0423095705	3.3265744520	-3.7248079072
C	-1.0454330649	-2.5943111122	-2.6412181778
C	-.1772669532	-3.4664103326	-3.5671401164
C	-2.3165020870	-3.3428528517	-2.1973715625
C	3.2237924897	-.3690692411	-2.6430815223
C	3.2470753239	-.2780029748	-.2501754115
C	3.9428385969	-.3905126912	-1.4334947742
H	-4.6655921361	-.3994712253	.0356142653
H	2.9173859348	.7508969221	2.2360313537
H	2.6607155562	-.9807020240	2.4532943344
H	1.5936244375	.1729707983	3.2627316127
H	1.3114087137	-.2265545833	-3.5767478272
H	-1.8303903044	2.3345486943	4.9130319981
H	-2.4075795994	.2471695725	6.1051653837
H	-1.9258159189	-1.9434752463	5.0658465674
H	-.1354290154	2.4035016038	1.5576302757
H	.4269044891	4.5067239312	2.7060161131
H	1.1544102990	3.1373055130	3.5644631790
H	-.2902327280	3.9251106898	4.2120750369
H	-1.7894343607	4.2214260809	1.4469518054
H	-2.5760623152	3.6458683900	2.9253320879
H	-2.6231259249	2.6478410113	1.4655338319
H	-.2515593320	-2.3296027023	1.7224002980
H	-1.9833982362	-4.0824732091	1.7654455970
H	-2.7355729299	-2.4767007019	1.6311833172
H	-2.7474130067	-3.3370111669	3.1781552829
H	.2277404276	-4.3653888241	3.0210475048
H	-.4646929532	-3.6498858220	4.4802143230
H	1.0119930162	-2.9709545534	3.7846923481
H	-2.3217731932	2.1186995925	-4.9993596944
H	-3.0593730087	-.0211825581	-5.9926565615
H	-2.4702276136	-2.1598670865	-4.9042051308
H	-.2710678989	2.3324583606	-1.8580581340
H	-1.7384651334	4.3287907506	-1.8547320802
H	-2.6873999944	2.8556818212	-1.5866803014
H	-2.7110091940	3.6487399546	-3.1678385810
H	.3893100270	4.2561380925	-3.2605995685
H	-.4895770192	3.5933518551	-4.6446596775
H	.9214256872	2.7375076041	-4.0030100959
H	-.4585546271	-2.3885668064	-1.7420152936
H	.0963097368	-4.4003771740	-3.0643596188
H	.7456761527	-2.9494102701	-3.8462364080
H	-.7098047323	-3.7287894887	-4.4879589216
H	-2.0488869461	-4.2807657445	-1.6979509606
H	-2.9515651834	-3.5941875288	-3.0541690573

H	-2.9080012362	-2.7388797258	-1.5032574636
H	3.7481984924	-.4488555023	-3.5916922556
H	3.8161248223	-.3009773358	.6693089976
H	5.0225252771	-.4927975719	-1.4283939107

59. L²CuO₂H end-on singlet → L²CuO₂H side-on singlet (isomer #2) transition state

Cu	-1.4283784699	.0631261083	.0749388039
O	-3.7301469119	-.7384445857	.4228783032
O	-3.1822101217	.3187678242	-.4714442361
N	-.0223008443	-.0456912287	1.3716094516
N	-.2671666792	.0148692300	-1.4695372537
C	2.2064721942	-.0957483036	2.3519905647
C	1.2725009834	-.1115897609	1.1550072366
C	1.8378757136	-.2002246902	-.1763811102
C	1.0735971555	-.1469954995	-1.4119103297
C	1.8179876032	-.2546897137	-2.6356445444
C	-.6297128446	.0387487917	2.6710296639
C	-1.0130534405	1.3093136008	3.1656060158
C	-1.6875762212	1.3614410896	4.3895461279
C	-1.9863175598	.2024607592	5.0996718853
C	-1.6207462867	-1.0389305960	4.5865878302
C	-.9472573103	-1.1525814175	3.3662169785
C	-.7491028720	2.5954322868	2.3888962307
C	-.0017177038	3.6434549537	3.2304182221
C	-2.0629935020	3.1712558035	1.8222135702
C	-.6201461194	-2.5328393387	2.8060324278
C	-1.9080679186	-3.2858350141	2.4178048775
C	.2378304932	-3.3650976693	3.7759121326
C	-.9621922565	.0392782539	-2.7143439399
C	-1.2441969866	1.2828244117	-3.3271782002
C	-1.9533817348	1.2871204403	-4.5327517373
C	-2.3877079202	.1016878174	-5.1184869398
C	-2.1218841857	-1.1145502669	-4.4942191383
C	-1.4144816119	-1.1733070806	-3.2898932110
C	-.8270485094	2.6025310828	-2.6902566122
C	-2.0624996696	3.4118203682	-2.2512558371
C	.0864307588	3.4298810900	-3.6117431861
C	-1.1846998135	-2.5198262898	-2.6130859095
C	-.4326160879	-3.5068098273	-3.5234049519
C	-2.5141802638	-3.1206516158	-2.1157200160
C	3.1829938138	-.4037422144	-2.6633051433
C	3.2516325356	-.3560553061	-.2734781351
C	3.9255097501	-.4593995233	-1.4672568313
H	-4.5759149763	-.3301763255	.6599013168
H	2.9474334180	.7017217162	2.2545075501
H	2.7476919526	-1.0432147471	2.4349444827
H	1.6505178490	.0598243451	3.2745441420
H	1.2641543642	-.2115226066	-3.5644483847
H	-1.9881736348	2.3254961632	4.7886132608
H	-2.5100700850	.2654571247	6.0488525079
H	-1.8723500778	-1.9398687766	5.1381313481
H	-.1058687197	2.3494495135	1.5391876270
H	.2349914942	4.5198531302	2.6183059253
H	.9360391683	3.2419861704	3.6275194443
H	-.6036140875	3.9877999915	4.0779313358
H	-1.8624008129	4.0769110302	1.2400166275
H	-2.7537161625	3.4382363013	2.6299691993
H	-2.5718333114	2.4533730080	1.1705245303
H	-.0373500725	-2.3964936407	1.8909044334
H	-1.6607214235	-4.2478172962	1.9559498398
H	-2.5100259102	-2.7065388740	1.7117669823
H	-2.5263245521	-3.4874120208	3.2996373982
H	.5022148001	-4.3246329939	3.3194574538
H	-.2982248232	-3.5800284489	4.7063283149

H	1.1654260619	-2.8464191451	4.0385734674
H	-2.1755547131	2.2348298686	-5.0152287869
H	-2.9393848633	.1253834717	-6.0539744647
H	-2.4778847275	-2.0358635423	-4.9464991331
H	-.2530838276	2.3646406152	-1.7905405900
H	-1.7576571574	4.3289464404	-1.7337720467
H	-2.6954552190	2.8250281023	-1.5789745255
H	-2.6722602233	3.7030083933	-3.1136932854
H	.4108258475	4.3461054170	-3.1059665429
H	-.4284557796	3.7254774392	-4.5323505777
H	.9796518639	2.8635819510	-3.8932731683
H	-.5561407705	-2.3457531653	-1.7356624166
H	-.2336987972	-4.4416877436	-2.9879588079
H	.5262859643	-3.0924020415	-3.8498647316
H	-1.0137325293	-3.7572489180	-4.4175909227
H	-2.3309678992	-4.0655225506	-1.5907016113
H	-3.1882520861	-3.3306486865	-2.9537718718
H	-3.0290502724	-2.4381523599	-1.4335895451
H	3.6877609672	-.4800904652	-3.6227906028
H	3.8320346365	-.4062081200	.6382816961
H	5.0028743594	-.5826451736	-1.4835593408

60. L²CuO singlet

Cu	.0362085127	-1.0865171082	.3907560304
O	.2365838130	-2.5011185025	1.3219504913
N	1.4688470977	.0684777517	-.2003229973
N	-1.3260044206	-.0356616652	-.3886973722
C	2.6054889654	2.0096827142	-1.1417828858
C	1.3567128388	1.1776366996	-.8981099722
C	.1071889316	1.6459877932	-1.4608662048
C	-1.1721582330	1.0226136953	-1.2112027177
C	-2.3180488042	1.5959516652	-1.8534604957
C	2.7281757793	-.3979070957	.3207694571
C	3.0933443791	-.0657268640	1.6433201065
C	4.3134609802	-.5507473518	2.1243132634
C	5.1348853742	-1.3521261921	1.3357895332
C	4.7343876772	-1.6986571843	.0486778673
C	3.5237895963	-1.2418814018	-.4832435653
C	2.1795394856	.7400969762	2.5592746483
C	2.8714556599	1.9918235370	3.1260574423
C	1.6225000110	-.1568171092	3.6833913316
C	3.0801532066	-1.7003563092	-1.8679836983
C	2.7444269622	-3.2046386708	-1.8554246981
C	4.1166412907	-1.3666993845	-2.9555962597
C	-2.5950012314	-.6404852498	-.1675778026
C	-3.3603452614	-.2361449293	.9548441853
C	-4.5922300438	-.8583378302	1.1746311861
C	-5.0546317410	-1.8623957018	.3269988280
C	-4.2821316375	-2.2654501059	-.7603215344
C	-3.0455060369	-1.6731206688	-1.0290022593
C	-2.8649521340	.8367302822	1.9168127485
C	-2.6444969118	.2598258170	3.3278256454
C	-3.8047092627	2.0554803506	1.9497547868
C	-2.1892406646	-2.1800496944	-2.1824429745
C	-2.9362285671	-2.1571389697	-3.5264153646
C	-1.6396738826	-3.5874179993	-1.8712820489
C	-2.2251149182	2.6978719570	-2.6701014707
C	.1408626769	2.7856870580	-2.3134704605
C	-.9806043785	3.3112082972	-2.9132081089
H	2.4348411054	3.0464064283	-.8418602595
H	2.8637293333	2.0082364599	-2.2052423111
H	3.4543871474	1.6207120032	-.5858787105
H	-3.2816407465	1.1367875023	-1.6721651531
H	4.6186575573	-.3045536812	3.1367973054

H	6.0788685148	-1.7172712857	1.7290994034
H	5.3667311955	-2.3444936399	-.5530200093
H	1.3256710540	1.0824539364	1.9668208438
H	2.1701031536	2.5675615949	3.7390579810
H	3.2398109925	2.6448525649	2.3278399137
H	3.7240655265	1.7290941892	3.7610434458
H	.9046251846	.4029169601	4.2932445963
H	2.4262679289	-.5011688267	4.3433926532
H	1.1195087813	-1.0365730001	3.2697631738
H	2.1584104398	-1.1689810054	-2.1210472365
H	2.3586505683	-3.5169476015	-2.8321437476
H	1.9909509464	-3.4313746375	-1.0953970825
H	3.6336062249	-3.8060510355	-1.6376112045
H	3.7404681268	-1.6590381200	-3.9415778399
H	5.0591445165	-1.8994090714	-2.7914080039
H	4.3414388484	-.2953715738	-2.9818562153
H	-5.1957852626	-.5570061480	2.0259838905
H	-6.0133468503	-2.3358980557	.5173912686
H	-4.6430520122	-3.0607429355	-1.4057099828
H	-1.8941416302	1.1800038078	1.5496843326
H	-2.2297732157	1.0267758706	3.9915601092
H	-1.9500195289	-.5851593596	3.3034503067
H	-3.5841073853	-.0893401182	3.7696213262
H	-3.3994424637	2.8319276495	2.6077289777
H	-4.7983876522	1.7881092967	2.3256047464
H	-3.9272857218	2.4869165380	.9514931891
H	-1.3315595157	-1.5082132716	-2.2774463046
H	-2.2662039839	-2.4674529162	-4.3353292671
H	-3.3060238513	-1.1534043961	-3.7582404390
H	-3.7916002056	-2.8411519951	-3.5293841801
H	-.9779335610	-3.9240391204	-2.6773168827
H	-2.4547569700	-4.3140134747	-1.7803185977
H	-1.0740298407	-3.5980626787	-.9343933777
H	-3.1265035637	3.0927711339	-3.1310057239
H	1.0919328735	3.2598936993	-2.5159623993
H	-.9029329655	4.1766399922	-3.5620212606

61. L²CuO triplet

Cu	.0454146576	-1.1466845394	.3932990377
O	.2780735233	-2.6060009213	1.3624205331
N	1.4976650428	.0610661832	-.1928561756
N	-1.3278690359	-.0973570462	-.4020801769
C	2.6020477178	2.0290684628	-1.1270380487
C	1.3695960310	1.1719904256	-.8842425476
C	.1035604575	1.6214059446	-1.4392746828
C	-1.1764806693	.9867032294	-1.1998749835
C	-2.3235498246	1.5696058299	-1.8310936570
C	2.7660958454	-.3862982783	.3190468267
C	3.1206509152	-.0719041241	1.6490360947
C	4.3339039804	-.5656599649	2.1399471491
C	5.1643811778	-1.3572478731	1.3516291985
C	4.7812042054	-1.6793775728	.0528836355
C	3.5789113295	-1.2106320029	-.4884836728
C	2.2026600922	.7345230194	2.5617213539
C	2.8914195871	1.9866692051	3.1308734435
C	1.6398347903	-.1549568445	3.6881383792
C	3.1661036663	-1.6297229624	-1.8961484842
C	2.8562507894	-3.1381233480	-1.9502341696
C	4.2161996627	-1.2406550823	-2.9522145721
C	-2.6256150248	-.6540724657	-.1716380152
C	-3.3853572007	-.2090769130	.9366443933
C	-4.6277013824	-.8067227055	1.1752932767
C	-5.1127894358	-1.8190831126	.3518366690
C	-4.3524029444	-2.2509702527	-.7318349346

C	-3.1064784901	-1.6825426850	-1.0165601793
C	-2.8818463432	.8882114273	1.8687440003
C	-2.6932584497	.3635561398	3.3042102070
C	-3.7980229344	2.1252515993	1.8437613167
C	-2.2793157974	-2.2049581242	-2.1853920899
C	-3.0535493268	-2.1801299753	-3.5148512989
C	-1.7358626010	-3.6157613025	-1.8838520878
C	-2.2397495217	2.6803959908	-2.6369870018
C	.12584322611	2.7695087719	-2.2807205516
C	-.9981902176	3.2984402612	-2.8746390233
H	2.4180839605	3.0616167458	-.8199684032
H	2.8629223158	2.0405213523	-2.1899346581
H	3.4573081273	1.6501977506	-.5729690384
H	-3.2857722485	1.1054751411	-1.6562711832
H	4.6267557849	-.3329232725	3.1594741370
H	6.1020276945	-1.7308281337	1.7521358195
H	5.4228343283	-2.3129541584	-.5522338469
H	1.3530984552	1.0783997731	1.9642772987
H	2.1874454567	2.5640163815	3.7396259570
H	3.2622886938	2.6376531589	2.3325007602
H	3.7416964824	1.7250503917	3.7693924291
H	.9130490634	.4025336938	4.2887815655
H	2.4385892512	-.4951082397	4.3563116478
H	1.1479197407	-1.0443080076	3.2813229027
H	2.2412133981	-1.1035110885	-2.1474500157
H	2.4932484810	-3.4189663598	-2.9449444297
H	2.0923550865	-3.4106623702	-1.2155794280
H	3.7493519818	-3.7350102085	-1.73711111752
H	3.8626007382	-1.5009755638	-3.9554756190
H	5.1639582306	-1.7643916062	-2.7899920624
H	4.4237798643	-.1658691257	-2.9338060352
H	-5.2223644934	-.4751268501	2.0217548661
H	-6.0787960505	-2.2721938804	.5550655060
H	-4.7313544319	-3.0470923732	-1.3660335136
H	-1.8999416157	1.2024202216	1.5049498720
H	-2.2816603102	1.1492189285	3.9479129450
H	-2.0098446956	-.4909534025	3.3257950948
H	-3.6440398276	.0404913601	3.7417056158
H	-3.3909624536	2.9159521433	2.4834893875
H	-4.8040535146	1.8885783545	2.2074917491
H	-3.8922852052	2.5247657613	.8294353797
H	-1.4188989453	-1.5401345248	-2.3024491596
H	-2.4020422037	-2.4934801112	-4.3376710227
H	-3.4233624264	-1.1747663624	-3.7393014789
H	-3.9126225066	-2.8592817386	-3.5000193692
H	-1.0950087356	-3.9645106022	-2.7013057437
H	-2.5543519324	-4.3343768362	-1.7665087534
H	-1.1521235715	-3.6283021273	-.9574775765
H	-3.1434345080	3.0773042966	-3.0917980611
H	1.0725512718	3.2530529609	-2.4799382252
H	-.9223952096	4.1715891617	-3.5135062861

62. L²CuOH⁺ singlet

Cu	.1059981468	-.0186741000	1.9496232551
O	.2345055810	-.3235831026	3.7145632271
N	1.4961692573	-.0215815736	.5575776142
N	-1.3465829325	.1251579954	.6448981822
C	2.5957925320	.0966097102	-1.6131291492
C	1.3638353506	.0553960205	-.7336142725
C	.0431532452	.1017921491	-1.3942411336
C	-1.2308054514	.0992582829	-.7104655250
C	-2.4236841850	.1695955530	-1.4942306427
C	2.7694443084	.0439758898	1.2288902068
C	3.3867510897	1.3041226293	1.4194682626

C	4.5818245995	1.3268053464	2.1447734541
C	5.1410631942	.1582994925	2.6573340293
C	4.5011110203	-1.0644406852	2.4688452351
C	3.2950527587	-1.1505313771	1.7678966348
C	2.7678441360	2.6098201344	.9270569562
C	3.7802703824	3.5098357900	.1958091097
C	2.0985555770	3.3664997248	2.0937126903
C	2.5945271992	-2.4950146031	1.6034751352
C	2.2595332140	-3.1273885833	2.9680031719
C	3.4153350288	-3.4554960005	.7219846760
C	-2.5360303213	-.2664580252	1.2838552583
C	-3.1283465391	.6725346762	2.1832522086
C	-4.3042131762	.3039358573	2.8281164951
C	-4.8632396991	-.9623295527	2.6403336244
C	-4.2449158527	-1.8906025714	1.8037322898
C	-3.0778901551	-1.5806310277	1.1064895934
C	-2.5560654576	2.0721303954	2.3489188350
C	-2.5148568581	2.5216634196	3.8173371141
C	-3.3250920412	3.0815287475	1.4725851590
C	-2.3621539310	-2.6818407582	.3297945659
C	-3.2617414172	-3.3291058876	-.7386058136
C	-1.8027094662	-3.7427228101	1.3021932488
C	-2.3919277148	.2186141053	-2.8739690560
C	.0176903418	.1436824521	-2.7993132754
C	-1.1614866510	.1957742705	-3.5383003062
H	.4020009138	.4062432900	4.3253086957
H	2.6330122507	1.0254219911	-2.1897044061
H	2.5830151376	-.7371343566	-2.3206668959
H	3.5001964943	.0243883500	-1.0147937995
H	-3.3695561160	.2356252383	-.9712232352
H	5.0831451328	2.2742870440	2.3123332313
H	6.0741278087	.2024307875	3.2098811867
H	4.9418372279	-1.9676942533	2.8779490031
H	1.9771776442	2.3693579704	.2095845398
H	3.2713823867	4.3831234086	-.2234265447
H	4.2748391810	2.9781496403	-.6229774058
H	4.5582559458	3.8800729826	.8699142443
H	1.6191780059	4.2821151560	1.7325403254
H	2.8338474241	3.6468645618	2.8544947539
H	1.3340848849	2.7531770931	2.5844692768
H	1.6434593664	-2.3175075458	1.0884488983
H	1.6991651132	-4.0567233461	2.8220911832
H	1.6567152373	-2.4487133108	3.5784852870
H	3.1673304320	-3.3759424479	3.5265522325
H	2.8719956264	-4.3937870451	.5725247333
H	4.3750823018	-3.6982873910	1.1888637353
H	3.6256840368	-3.0233662139	-.2619008480
H	-4.7999093668	1.0118144849	3.4832152545
H	-5.7781250435	-1.2302598426	3.1593618489
H	-4.6699906031	-2.8841652371	1.7093903301
H	-1.5248834875	2.0541720851	1.9780503705
H	-1.9993685471	3.4836328521	3.8958938417
H	-1.9856479276	1.7931205304	4.4387184806
H	-3.5171070684	2.6572001203	4.2344236256
H	-2.8823212519	4.0780354920	1.5641162414
H	-4.3737095040	3.1471105488	1.7800454623
H	-3.3018006511	2.7957313954	.4162790973
H	-1.5063228642	-2.2465483944	-.1913943914
H	-2.6935031937	-4.0755206040	-1.3016367734
H	-3.6426554617	-2.5873050661	-1.4465998754
H	-4.1199437094	-3.8401700036	-.2922494824
H	-1.2304075819	-4.4936495962	.7482481394
H	-2.6074114872	-4.2595824587	1.8336592934
H	-1.1442797227	-3.2936742891	2.0525115149

H	-3.3193583887	.2880496765	-3.4328531832
H	.9485678632	.1352539799	-3.3482881227
H	-1.1159361727	.2312450021	-4.6210886962

63. $L^2CuOH_2^{2+}$ singlet

H	1.2939546575	-.7571551043	4.0479751268
C	2.4838934395	.0485404463	1.4178602933
C	2.9877339840	1.3500575380	1.7099120350
C	4.0594147575	1.4283815989	2.6024464293
C	4.6119790066	.2876189557	3.1847808329
C	4.0966451512	-.9783332744	2.8916793919
C	3.0225906037	-1.1323503198	2.0146806982
C	2.3823953626	2.6360396736	1.1553011142
C	3.4281737322	3.5011674041	.4245762030
C	1.6942642579	3.4452960784	2.2743796401
C	2.5156691400	-2.5143365184	1.6170976152
C	2.4920777331	-3.5201791650	2.7794002982
C	3.3450179262	-3.0648920211	.4356949376
C	-2.5590902702	-.0842849308	1.3770279436
C	-3.0472930543	.9093486009	2.3237002126
C	-4.1662571014	.5839133772	3.0774396783
C	-4.7776825581	-.6685440908	2.9509607558
C	-4.2671191280	-1.6460274915	2.0860473086
C	-3.1644578303	-1.4026439069	1.2801509833
C	-2.4549864534	2.3076214486	2.3488237646
C	-2.5425003541	2.9873915725	3.7238873922
C	-3.1250981689	3.1844598187	1.2619012431
C	-2.5430785454	-2.5517394190	.4966392341
C	-3.5535054406	-3.2328968042	-.4466715782
C	-1.9167847171	-3.5742851738	1.4707895765
C	-2.4689843660	.0982841890	-2.8780216586
C	-.0527891776	.1175730849	-2.7793585131
C	-1.2256149178	.0998031208	-3.5268157549
C	2.4838405188	.4015121904	-1.4754528500
C	1.2336734882	.1344054869	-.6670953334
C	-.0533742503	.1233278795	-1.3714840164
C	-1.3365760413	.1128619004	-.7098875409
C	-2.5237403287	.0914825517	-1.4985322516
H	-.1256488314	-.4307479737	4.6367770429
H	2.4092567763	1.3508559143	-2.0124598324
H	2.6215329800	-.3916922986	-2.2166749799
H	3.3646496733	.4231698081	-.8381299589
H	-3.4786336373	.1600298483	-.9905309918
H	4.4715333973	2.4007827913	2.8496830131
H	5.4511910259	.3832798977	3.8662290457
H	4.5545097577	-1.8537068274	3.3382125846
H	1.6050844758	2.3762026249	.4296897371
H	2.9430111583	4.3731242444	-.0231020000
H	3.93444480760	2.9477185448	-.3711222189
H	4.1951704001	3.8708768940	1.1108171724
H	1.2297301273	4.3438393521	1.8577946959
H	2.4124691437	3.7647792954	3.0350442944
H	.9149382032	2.8610218837	2.7775792865
H	1.4843118013	-2.4011445302	1.2579499256
H	2.0322501182	-4.4552600550	2.4484867822
H	1.9138540733	-3.1489621970	3.6325607383
H	3.4967883391	-3.7675818022	3.1321259871
H	2.9512954939	-4.0335796566	.1148569556
H	4.3897943283	-3.2040915465	.7286953609
H	3.3282870490	-2.3890033637	-.4245936063
H	-4.5883433190	1.3126608919	3.7590345061
H	-5.6575511469	-.8942565530	3.5459175147
H	-4.7379609892	-2.6226317642	2.0634584886
H	-1.3970071054	2.2254204472	2.0718582025

H	-1.9706436774	3.9189573919	3.7043297480
H	-2.1362921491	2.3585473301	4.5229182997
H	-3.5694482784	3.2526476971	3.9906655555
H	-2.6683545871	4.1781352262	1.2577994437
H	-4.1937545708	3.3041016339	1.4630166594
H	-3.0103806775	2.7566213743	.2617909767
H	-1.7343373939	-2.1643844394	-.1262157959
H	-3.0481265678	-4.0112823208	-1.0242731054
H	-3.9929457189	-2.5198205689	-1.1494726519
H	-4.3677985260	-3.7113519529	.1042159752
H	-1.4233309909	-4.3696020943	.9049417607
H	-2.6730764692	-4.0372820348	2.1109329647
H	-1.1679084562	-3.1092022645	2.1236579045
H	-3.3881680192	.1203643716	-3.4541382634
H	.8870137098	.1140381490	-3.3142142997
H	-1.1724804225	.0957868296	-4.6099301269
N	1.3280497772	-.1197776837	.6111078574
N	-1.4618416040	.3041995784	.6364305425
O	.3533798514	-.6652599738	3.8304332209
Cu	-.1412141128	-.2369228613	1.9251582123

64. L²CuO⁻ doublet

Cu	.0923564106	-1.2860517116	.2780722177
O	.3914144507	-2.8822315683	1.0044293589
N	1.5225029040	.1346934586	-.2169368004
N	-1.3277451374	-.0945747057	-.4566220644
C	2.5580996823	2.2083764122	-1.0023856170
C	1.3645329921	1.2686642869	-.8459802298
C	.0850742420	1.6865338406	-1.4184394411
C	-1.1920160620	1.0101912745	-1.2066023637
C	-2.3415658941	1.6030563620	-1.8470894250
C	2.7814820033	-.2864607086	.2994423913
C	3.0962518928	-.0567449453	1.6589756215
C	4.3308428040	-.5041526394	2.1418054251
C	5.2239640912	-1.1918362816	1.3245457609
C	4.8655435137	-1.4773835873	.0089831390
C	3.6451471192	-1.0489053160	-.5224047143
C	2.0851981146	.5714401815	2.6104774529
C	2.6492825275	1.7845842679	3.3680982026
C	1.5387396311	-.5001295871	3.5770966467
C	3.1974502982	-1.5102771676	-1.9039847228
C	2.6951321046	-2.9675771404	-1.8173135108
C	4.2773755283	-1.3498956810	-2.9855043269
C	-2.6182091434	-.6173188774	-.1803498702
C	-3.3710076253	-.1074272199	.9081860119
C	-4.6059259442	-.6895032749	1.2134962864
C	-5.1053453747	-1.7598768799	.4759250256
C	-4.3528961106	-2.2666205242	-.5810442097
C	-3.1153584687	-1.7147932250	-.9281670344
C	-2.8328972031	1.0223308453	1.7788621007
C	-2.5355819653	.5244397904	3.2052446090
C	-3.7673691513	2.2445402490	1.7935415247
C	-2.3016631027	-2.3244551744	-2.0633214395
C	-3.0955539656	-2.3868552790	-3.3802784231
C	-1.7490589234	-3.7089546423	-1.6712445721
C	-2.2677512351	2.7289684011	-2.6310785183
C	.0897158567	2.8459962136	-2.2389652172
C	-1.0339457242	3.3737277682	-2.8430423179
H	2.3000860046	3.2237064052	-.6893574768
H	2.8881065990	2.2585537191	-2.0461578082
H	3.3981573511	1.8621109543	-.4027171518
H	-3.2981321776	1.1150124881	-1.7023953996
H	4.5858845422	-.3267328350	3.1835354583
H	6.1795069330	-1.5290981372	1.7180188491

H	5.5386918736	-2.0611457198	-.6130826034
H	1.2413254812	.9217650997	2.0104932641
H	1.8759548521	2.2288614580	4.0053611361
H	3.0070801405	2.5579786497	2.6792090618
H	3.4869051317	1.5035831603	4.0173014892
H	.7534477626	-.0733144557	4.2132550022
H	2.3347930034	-.8756823989	4.2326854079
H	1.1187362028	-1.3459249479	3.0192208036
H	2.3445797346	-.8946454264	-2.2011055610
H	2.2720616510	-3.2863628707	-2.7782380793
H	1.9285357446	-3.0768790166	-1.0416189371
H	3.5237668302	-3.6435558008	-1.5714679411
H	3.8737028439	-1.6253133176	-3.9665455190
H	5.1434732841	-1.9953033274	-2.7991218022
H	4.6373762157	-.3165984210	-3.0437973886
H	-5.1818450815	-.3030186510	2.0517056907
H	-6.0660434966	-2.2019108540	.7290392690
H	-4.7309795768	-3.1149567493	-1.1467822288
H	-1.8822880768	1.3395770176	1.3448579244
H	-2.0941191348	1.3256983671	3.8112876575
H	-1.8336344046	-.3141060778	3.1791306092
H	-3.4481230489	.1859911944	3.7106298752
H	-3.3333390823	3.0557665658	2.3908311225
H	-4.7452103798	2.0021084551	2.2268143197
H	-3.9311967075	2.6205593068	.7788841020
H	-1.4435752758	-1.6676040052	-2.2284650057
H	-2.4594763386	-2.7615737897	-4.1911364717
H	-3.4655557547	-1.3969030164	-3.6685229096
H	-3.9591914249	-3.0587749189	-3.3050567062
H	-1.1672630156	-4.1318143996	-2.5008424890
H	-2.5663357289	-4.4066908357	-1.4473226360
H	-1.0925522357	-3.6378662826	-.7956143290
H	-3.1743337336	3.1156871602	-3.0932752838
H	1.0323045644	3.3484078079	-2.4179290990
H	-.9613783291	4.2596474922	-3.4666162261

65. L²CuOH doublet

Cu	.1153088338	-.5613655119	1.8661217592
O	.2542139214	-1.3348421047	3.5055532563
N	1.5092045510	-.0383572386	.5844990868
N	-1.3014207710	-.1781534489	.6465300914
C	2.6016522113	.4734927630	-1.5386984917
C	1.3640251225	.1916510307	-.7022523942
C	.0734470819	.1921078986	-1.3651981710
C	-1.1957977976	.0352756313	-.6834061440
C	-2.3811529001	.1169280807	-1.4865992229
C	2.7787623326	.0288110610	1.2549962094
C	3.2348413852	1.2708590962	1.7539915741
C	4.4466122194	1.2928785167	2.4532484630
C	5.1817146488	.1299580674	2.6642471883
C	4.7037246698	-1.0856263782	2.1833343259
C	3.4981420155	-1.1664911330	1.4787625271
C	2.4392256679	2.5614199287	1.5818850042
C	3.2439127992	3.6450909978	.8415335106
C	1.9328978693	3.0828930934	2.9400344778
C	2.9856853963	-2.5217155317	1.0048120943
C	2.6563016746	-3.4359909009	2.2012349518
C	3.9666888062	-3.1993506597	.0319369545
C	-2.5717450073	-.2271362413	1.2945661736
C	-3.1703029199	.9732223135	1.7553149701
C	-4.3915478346	.8917921123	2.4319112672
C	-5.0089614908	-.3345920408	2.6645321208
C	-4.4044772247	-1.5068472345	2.2189742436
C	-3.1869194020	-1.4806243104	1.5310775109

C	-2.5196252558	2.3353917962	1.5378190292
C	-2.2052467880	3.0296003807	2.8757406900
C	-3.3780753669	3.2399189610	.6344157682
C	-2.5472730981	-2.7857899258	1.0733685176
C	-3.4641465588	-3.5717861204	.1201668753
C	-2.1136673268	-3.6439962460	2.2777929574
C	-2.3393999079	.3139407058	-2.8463555094
C	.0514900354	.3926781006	-2.7751638594
C	-1.1075386219	.4529748669	-3.5145883940
H	.2277811978	-.7454122218	4.2694515654
H	2.5245117207	1.4472395322	-2.0302401345
H	2.7131468421	-.2836047649	-2.3203199835
H	3.5005291932	.4641115561	-.9271250924
H	-3.3359295245	.0025392091	-.9888305093
H	4.8173152069	2.2371486134	2.8414308618
H	6.1203815605	.1698778504	3.2089193183
H	5.2732791187	-1.9928615196	2.3618137045
H	1.5572214746	2.3374761926	.9760564756
H	2.6275755598	4.5365119008	.6835050458
H	3.5859762904	3.2915564659	-.1361368859
H	4.1275946746	3.9507852297	1.4115743447
H	1.3153571646	3.9768410210	2.8021956930
H	2.7649820840	3.3465841196	3.6013641407
H	1.3279517250	2.3272591513	3.4506944135
H	2.0529664457	-2.3540883919	.4579731040
H	2.2283892695	-4.3802064118	1.8458455317
H	1.9386494544	-2.9578649581	2.8743683686
H	3.5604346794	-3.6754486928	2.7726121581
H	3.5490555105	-4.1444012581	-.3309356206
H	4.9222587226	-3.4252965081	.5171683752
H	4.1763842871	-2.5652033207	-.8359225508
H	-4.8650925336	1.8035329866	2.7855161963
H	-5.9560719214	-.3763543814	3.1947290145
H	-4.8855855284	-2.4620660762	2.4089175510
H	-1.5681396696	2.1675893416	1.0267488102
H	-1.6858919723	3.9787971185	2.7029588625
H	-1.5665042667	2.4021360912	3.5058683018
H	-3.1172703872	3.2482304262	3.4413846347
H	-2.8715087482	4.1947934363	.4551181075
H	-4.3487520661	3.4589343171	1.0928779752
H	-3.5614304275	2.7666671725	-.3345313242
H	-1.6439825822	-2.5273448403	.5130205136
H	-2.9551729627	-4.4725984394	-.2396253978
H	-3.7413718517	-2.9686045591	-.7501717737
H	-4.3871722352	-3.8905292712	.6167667115
H	-1.6161552055	-4.5576064911	1.9323558878
H	-2.9789826893	-3.9442727115	2.8797997837
H	-1.4200808528	-3.0944188826	2.9213062416
H	-3.2707489836	.3567877336	-3.4050389206
H	.9903340185	.5046621700	-3.3010478295
H	-1.0689253262	.6044543646	-4.5878423424

66. $L^2CuOH_2^+$ doublet

H	1.1632943623	-.8221769889	4.2153609610
C	2.6071048820	-.0135563986	1.3131978164
C	3.0232088718	1.2578342092	1.7810870430
C	4.1703764395	1.3113985396	2.5807537780
C	4.8817828927	.1605125552	2.9105631956
C	4.4471297545	-1.0792345328	2.4482115582
C	3.3034243918	-1.1979589101	1.6507747800
C	2.2419775920	2.5372632958	1.4934364120
C	3.1266600987	3.6491766782	.9024785167
C	1.5185791222	3.0322884775	2.7623211100
C	2.8435158474	-2.5722087620	1.1742555674

C	2.4382096748	-3.4710960828	2.3583819751
C	3.9086849426	-3.2594063123	.3000009015
C	-2.6841824469	-.0046171548	1.4039095227
C	-3.2217485594	1.0732521787	2.1733692426
C	-4.3815404214	.8398076803	2.9108635443
C	-4.9856704216	-.4182106275	2.9269599780
C	-4.4294506510	-1.4735800123	2.2060680408
C	-3.2820985930	-1.3016939523	1.4297738345
C	-2.5903945468	2.4578222625	2.1073806153
C	-2.6993097223	3.2432851662	3.4229662780
C	-3.1836156018	3.2724744245	.9379848091
C	-2.6398063783	-2.5107382434	.7577391324
C	-3.6396707794	-3.3340185025	-.0706631986
C	-1.9334181158	-3.3912431448	1.8099121038
C	-2.5216159571	.0866572278	-2.8189082209
C	-.1171891647	.0654915124	-2.7428598933
C	-1.2884703240	.0501412818	-3.4843813482
C	2.4342609904	.4372632280	-1.5225553415
C	1.2197979380	.1192927287	-.6735714136
C	-.0976358175	.0970616181	-1.3308239240
C	-1.3741658487	.1206431220	-.6479322171
C	-2.5601946777	.1184274058	-1.4398476387
H	-.2984393048	-.4358793635	4.6360833994
H	2.2751482541	1.3417073789	-2.1143692328
H	2.6351678869	-.3839644098	-2.2183936195
H	3.3176090824	.5701279571	-.9013166461
H	-3.5122052810	.1797405588	-.9259574794
H	4.5130525283	2.2727183352	2.9503152155
H	5.7734055349	.2304336652	3.5254405415
H	5.0079002241	-1.9722998923	2.7062552340
H	1.4698736488	2.3115026894	.7528120731
H	2.5134476917	4.5154525356	.6357620649
H	3.6472474494	3.3112363433	.0016284363
H	3.8824657995	3.9904061767	1.6163681488
H	.9243868122	3.9250706058	2.5426233626
H	2.2337692722	3.2900891815	3.5502503891
H	.8424048117	2.2687032294	3.1638672058
H	1.9537650626	-2.4318076133	.5529732385
H	2.0696711015	-4.4363858411	1.9979501488
H	1.6415003496	-3.0132518577	2.9552177984
H	3.2869663956	-3.6659133253	3.0217454866
H	3.5304131372	-4.2129024590	-.0814442425
H	4.8215775016	-3.4674462302	.8668819685
H	4.1840753100	-2.6359412429	-.5559589003
H	-4.8272672375	1.6490292097	3.4786238674
H	-5.8872296820	-.5775964884	3.5102361666
H	-4.8945454081	-2.4526901559	2.2566204526
H	-1.5266146089	2.3149764595	1.8885631390
H	-2.1080307480	4.1614097649	3.3562806382
H	-2.3297592102	2.6642497789	4.2760185505
H	-3.7291219038	3.5420891262	3.6419084352
H	-2.6950959764	4.2496491806	.8678884232
H	-4.2554427253	3.4408835529	1.0863082861
H	-3.0517301559	2.7592880838	-.0187360485
H	-1.8722965270	-2.1566392196	.0662589268
H	-3.1190761166	-4.1463901977	-.5865436265
H	-4.1329140617	-2.7146304047	-.8252215073
H	-4.4154833590	-3.7877276677	.5535383303
H	-1.4200043715	-4.2287126733	1.3266997069
H	-2.6499780294	-3.8030725216	2.5279369746
H	-1.1883494334	-2.8211319166	2.3775767832
H	-3.4494830660	.0971193782	-3.3823177962
H	.8199079484	.0347785437	-3.2821976068
H	-1.2442238510	.0150189703	-4.5671909544

N	1.3673180665	-.1350676258	.5967424933
N	-1.4844435315	.2481372561	.7057689031
O	.2679601623	-.6653689951	3.8889736293
Cu	-.0798049704	-.2344904907	1.9294477394

β -diketiminate Cu/O structures in reactions with substrates

67. L¹CuO₂ side-on / methane complex

C	-5.2588092487	-.7784192087	-.2070969614
C	-3.4650081199	.4836192691	3.6144774592
C	3.1686830498	2.3171941456	-3.7356959866
C	2.3695065741	-1.1693752235	2.4891125505
C	2.6818511480	.9470263228	-.3028302054
C	-2.8319566319	.6001518898	-.0483165009
C	-3.8160250432	1.9220286477	-3.3808199138
C	1.0919439846	2.7276809493	.1633190320
C	-1.4385232373	2.5652754838	.2800551742
C	3.3812786933	.4008154748	.7989921470
C	-3.3639645400	-.0127171602	1.1122221012
C	-.2055712900	3.2419002075	.3474066112
C	3.2209261465	.8962821641	-1.6099033396
C	-3.4868566911	.4813629507	-1.2981568950
C	-2.0741299839	-1.4492081070	2.7299372514
C	1.9603165162	.0834075838	-3.6324339924
C	2.2537464785	3.6922177862	.2881743676
C	-2.6972577565	3.3763436329	.5167696591
C	4.6534906016	-.1350700704	.5738064980
C	4.4970643604	.3490772433	-1.7780192008
C	-4.5844733749	-.6882098636	1.0055542022
C	-4.7046779670	-.2059507895	-1.3467577652
C	3.6462183459	.8719666571	3.2967175047
C	5.2158515698	-.1532484784	-.6982345361
C	2.7520084041	.2956527816	2.1860358882
C	2.4143762865	1.3251878917	-2.8327558286
C	-2.3930369302	-.1792712595	-3.4676391515
C	-2.6130898770	-.0314302740	2.4407647714
C	-2.8684550055	1.0004545750	-2.5933297617
C	1.1375780012	-5.4944432604	-1.7003774831
H	-2.4586602859	4.4204507192	.7228280275
H	-.2635904694	4.2995261964	.5678944341
H	1.9050589169	4.7000181855	.5168190033
H	1.7353182811	-1.5826044029	1.7000211709
H	4.0643657941	1.8669573035	-4.1779449668
H	3.4832080537	3.2096172130	-3.1838118971
H	3.2621677366	-1.8003381944	2.5608584901
H	-1.8692716275	.1868456800	-4.3582015594
H	2.8319038080	3.7197858078	-.6407635844
H	2.9402590621	3.3675578544	1.0761978888
H	-1.7187267929	-.8336383734	-2.9084521671
H	-3.3553483475	3.3293044657	-.3566575747
H	5.2051005829	-.5627068371	1.4059764415
H	6.2034790473	-.5789475685	-.8516515600
H	4.9268187964	.2978362861	-2.7742548992
H	-5.0051720676	-1.1667287015	1.8853685753
H	-6.2039359280	-1.3108344712	-.2678623342
H	-5.2188466069	-.3088555429	-2.2981602470
H	-4.3307560032	-.1609281161	3.8014358955
H	-3.8392116744	1.4963095616	3.4301321764
H	-3.2417527140	-.7845408430	-3.8048907373
H	-3.2648075668	2.9696046405	1.3594390457
H	1.8259663912	.8775397350	2.1785844951
H	3.1278549140	.8291968046	4.2607757071
H	1.5112308905	1.8306839987	-2.4772123206

H	1.2997038678	.3761877636	-4.4565477205
H	-1.7488984541	.6331049383	2.3468544737
H	-1.4609137559	-1.4507472487	3.6384198474
H	-1.9841829438	1.5884818181	-2.3306915802
H	-3.3110297740	2.3159046020	-4.2694410316
H	3.9112451718	1.9160626962	3.1015138036
H	4.5778355167	.3070070442	3.4029514858
H	1.8336094472	-1.2384472419	3.4428074435
H	1.4285770400	-.6274010890	-2.9925407276
H	2.8217979692	-.4399508439	-4.0636795308
H	2.5259436495	2.6399591764	-4.5617107852
H	-1.4672741347	-1.8150427949	1.8966232047
H	-2.8962480305	-2.1582105942	2.8810749003
H	-2.8703395084	.5055629901	4.5342282536
H	-4.1490104175	2.7726287352	-2.7773563798
H	-4.7090387311	1.3885942149	-3.7229292629
H	1.0607940556	-4.4200962719	-1.5140438313
H	.2127628535	-5.8533949952	-2.1584615106
H	1.2992703388	-6.0188045822	-.7559871829
H	1.9760645134	-5.6927505037	-2.3729803711
N	-1.5603849691	1.2649687501	.0218147583
N	1.3532517780	1.4528363052	-.1131937248
O	-.6654821391	-1.5329708942	-.5958334239
O	.6911957861	-1.5062456181	-.6731072331
Cu	-.0326982119	.1883832109	-.2870642749

68. L¹CuO₂ side-on / cyclohexane complex

C	2.6109170198	.7882031355	2.4740192132
C	-3.3881034397	1.8999984463	3.5765820692
C	-3.7810987488	3.5656617969	-3.3586864725
C	-1.8278472973	.1243925167	2.6447630186
C	3.1394633459	4.5576377405	-3.6154035250
C	2.7475164761	3.0141854663	-.2472744897
C	1.0055891977	4.6267914232	.2690287184
C	3.4864957211	2.4979133719	.8429337104
C	-2.7268124808	2.1945827309	-.0715704102
C	-2.7695540208	2.6897334149	-2.5992519719
C	-2.4843143017	1.4998970974	2.3966009601
C	-.3320106408	5.0222250789	.4571770535
C	-1.5031052165	4.2488848882	.3487160951
C	3.3001006313	3.0604156824	-1.5492782551
C	-3.2199747097	1.5008197612	1.0593328658
C	-5.0304417750	.6306829215	-.3128990978
C	2.0789649996	5.6817601303	.4452133713
C	-2.8264165664	4.9437293676	.6026308886
C	4.8052600893	2.0927003494	.6137938239
C	4.6232859251	2.6406762643	-1.7219876993
C	-3.3559391640	2.0697092048	-1.3335562851
C	2.1444214996	2.2186926345	-3.6222539477
C	3.6892998835	2.9122387677	3.3571372345
C	5.3773704522	2.1707020994	-.6518271185
C	2.8601040458	2.2912678605	2.2197584417
C	2.4705576049	3.4624426824	-2.7662724782
C	-4.3800339658	.7326589525	.9123427582
C	-4.5124213779	1.2876916041	-1.4241357723
C	-2.1926329415	1.5894569461	-3.5159880187
C	-1.0454778261	-5.8417440286	-2.1007035004
C	-.7671959071	-4.4361136082	-1.5399867458
C	.6072180360	-3.9091429463	-1.9855701133
C	1.7282272598	-4.8963480045	-1.6163701118
C	1.4507444966	-6.3018655874	-2.1769213143
C	.0754859213	-6.8278843661	-1.7341638969
H	-.4803398042	6.0615185668	.7179552748
H	-4.6265597355	2.9783779690	-3.7323455034

H	1.6425124083	6.6454903596	.7090510656
H	2.6608155557	5.7966726340	-.4747688855
H	2.7840738449	5.3865204902	1.2279387729
H	-3.3622426118	4.4631319308	1.4271777436
H	-3.4741824167	4.8719314000	-.2764888582
H	5.3882547638	1.6922540395	1.4375181744
H	6.4018743565	1.8447653330	-.8079593897
H	5.0639440102	2.6651365878	-2.7146468355
H	-4.1847442016	4.3614595045	-2.7237572054
H	-1.4742231861	.9668501219	-2.9752331706
H	-1.6897161054	2.0334619036	-4.3830538620
H	-4.1968511909	1.1775185241	3.7323837787
H	-3.8472619749	2.8823800799	3.4210722991
H	-2.8054170889	1.9427411481	4.5032866290
H	-2.5871390317	-.6578392531	2.7611119309
H	-1.1832478907	-.1585370586	1.8069876462
H	3.3588333233	5.4516915423	-3.0224015588
H	1.8843812805	2.7863361581	2.2208067568
H	3.1692735451	2.7914629186	4.3137297680
H	1.5204302504	3.8664216485	-2.4044158377
H	1.4733215749	2.4835315166	-4.4477845362
H	-4.7703309563	.1909016372	1.7694784483
H	-5.9272502305	.0243701232	-.4059504550
H	-5.0055588915	1.1779664506	-2.3860342564
H	-2.9868931694	.9337424711	-3.8905506965
H	-2.6766674511	5.9964218381	.8456416046
H	4.0802986825	4.2130609979	-4.0576327231
H	2.0180071473	.3446684305	1.6684602274
H	3.5573181508	.2381071807	2.5321521320
H	-3.3018800389	4.0351921655	-4.2247741662
H	-1.9378413263	3.3350865526	-2.3017393774
H	-1.2255207613	.1440643763	3.5603960713
H	3.8584518223	3.9825279494	3.1972890018
H	4.6688038555	2.4322478564	3.4562268179
H	2.0797600166	.6410917158	3.4218043160
H	1.6673450232	1.4394542174	-3.0199490769
H	3.0557220152	1.7912333161	-4.0562850986
H	2.4816829422	4.8526915723	-4.4400560431
H	-1.6788262234	2.2382062558	2.3360812143
H	-1.5584050317	-3.7412785056	-1.8470057330
H	-.7979875464	-4.4759365489	-.4410947834
H	.5998045988	-3.7698401208	-3.0768568407
H	.8057579774	-2.9212053645	-1.5477709203
H	2.6959850110	-4.5281374855	-1.9794477227
H	1.8097308398	-4.9561775367	-.5209437839
H	2.2406538782	-6.9978475299	-1.8683298860
H	1.4823992646	-6.2642338501	-3.2754681846
H	-.1189294098	-7.8107938399	-2.1823151573
H	.0809815771	-6.9788120641	-.6449786996
H	-2.0115530145	-6.2131817934	-1.7371684091
H	-1.1279713506	-5.7836696071	-3.1957306674
N	-1.5141770145	2.9549788231	.0371278882
N	1.3778867025	3.3905648245	-.0526483072
O	-.3769769931	.2566706621	-.6631295271
O	.9713960689	.3986190617	-.7142026716
Cu	.1035463057	2.0211580903	-.2908153144

69. L¹CuO₂ side-on / acetonitrile complex

C	2.2705952470	1.6208713148	-2.8805063327
C	-3.5448658228	1.2074938921	3.6826422291
C	3.0876556050	2.5743216227	-3.7695639723
C	2.1407073949	-.8794767543	2.4671296911
C	2.5121862048	1.2139003932	-.3486992935
C	-3.0109153077	1.3404657603	-.0017650767

C	-3.9480366613	2.7016499684	-3.3436666937
C	1.0850292577	3.1174203824	.1326826700
C	-1.4479392673	3.1853433465	.2956455223
C	3.1912796967	.6303083675	.7483563259
C	-3.5540459934	.7564445986	1.1677137170
C	-.1568070431	3.7465784224	.3369979679
C	3.0452021735	1.1355008845	-1.6582715666
C	-3.6929811068	1.2698009448	-1.2403774270
C	-2.3030647247	-.7865972423	2.7187929604
C	1.7530979503	.4161536908	-3.6961403993
C	2.3297117421	3.9758864454	.2379027388
C	-2.6238166382	4.1039147132	.5568537495
C	4.4362621865	.0336992222	.5176890897
C	4.2937105889	.5276737995	-1.8321975557
C	-4.8192156703	.1660285940	1.0843155677
C	-4.9550244367	.6671918914	-1.2655226458
C	3.5132335006	1.1141970201	3.2360912969
C	-3.0542608590	1.7342646375	-2.5473490355
C	4.9945915429	-.0080586044	-.7561122045
C	2.5777010202	.5655849579	2.1440616399
C	-2.6588572779	.5135141507	-3.4080177843
C	-5.5227008819	.1292492915	-.1151424505
C	-2.7652025789	.6670057949	2.4718866395
C	2.8183638172	-4.6724384176	-1.5484947737
C	3.0080778538	-3.2291193780	-1.4447491471
H	-.1142735237	4.8052770817	.5551870312
H	-2.2898746409	5.1226123065	.7570794625
H	2.0747083913	5.0094169705	.4741508136
H	3.9542373498	2.0738359950	-4.2145697650
H	3.4558826542	3.4388076536	-3.2076395945
H	1.4700634829	-1.2696416811	1.6959363111
H	2.8918159094	3.9560699815	-.7009160567
H	2.9995374539	3.5905926666	1.0127854016
H	-3.2068785528	3.7469189317	1.4115059358
H	-2.0278964826	-.1812201444	-2.8439583250
H	4.9729088215	-.4143648220	1.3491866319
H	5.9646922173	-.4721121042	-.9126773274
H	4.7196597842	.4641588262	-2.8295799533
H	-5.2515116365	-.2917811490	1.9694297330
H	-6.5010846700	-.3407178349	-.1587609916
H	-5.4926300778	.5987102353	-2.2069273280
H	3.0080338067	-1.5470166196	2.5273540802
H	-4.4406607742	.6121046456	3.8879308757
H	-3.8624384041	2.2439077370	3.5293343305
H	-3.5477203310	-.0384117058	-3.7370498200
H	-3.3007661173	4.1150912123	-.3031882651
H	-2.1142728438	.8342380082	-4.3038752941
H	1.6766098259	1.1857019961	2.1423164257
H	3.0064973228	1.1061221484	4.2070968119
H	1.3960136713	2.1734112057	-2.5246670425
H	1.1261505863	.7540442778	-4.5288048275
H	-1.8659609614	1.2810508428	2.3625594545
H	-1.6584536623	-.8408978602	3.6039351158
H	-2.1328464169	2.2704548010	-2.2992458964
H	-3.4261600955	3.0458588086	-4.2431412607
H	3.8230115571	2.1431529150	3.0253503612
H	4.4202462294	.5086056213	3.3380469174
H	1.6229850699	-.9196710978	3.4320580026
H	1.1641377461	-.2596665920	-3.0694235439
H	2.5867315697	-.1567044502	-4.1193176490
H	2.4691386929	2.9456133575	-4.5933992187
H	-1.7512689925	-1.1782869977	1.8591379075
H	-3.1613356090	-1.4467728724	2.8903706747
H	-2.9195337203	1.1743933927	4.5811398501

H	-4.2191093965	3.5829673567	-2.7529889800
H	-4.8771741305	2.2217708589	-3.6701568225
H	3.7417089106	-2.9973331686	-.6644713220
H	2.0686181090	-2.7263725079	-1.1992563883
H	3.3744580633	-2.8269027199	-2.3914405914
N	1.2282411648	1.8220748620	-.1448764090
N	-1.6912669690	1.9028136468	.0423345766
N	2.6758568438	-5.8218608837	-1.6314180002
O	-1.0053008621	-1.0093279495	-.6085579236
O	.3527311036	-1.0045787643	-.6913419628
Cu	-.2886134925	.6982066198	-.2912886979

70. L¹CuO₂ side-on / toluene complex

C	-1.9055207369	-.3029942251	-3.1565747863
C	-3.1157371334	1.3046142352	3.7663110091
C	2.4403135096	1.0125775664	-3.3878391499
C	-3.7428749764	1.4413450997	-3.3220439855
C	-1.3405213745	-.4212316484	3.1991034712
C	2.8317590908	2.4257065123	-.2016376147
C	.8715726801	3.8513878624	-.0237261506
C	3.5792749956	2.1989886036	.9767000971
C	-2.4866865497	.9046073193	.1257598023
C	3.1905720910	3.4056207130	-3.7841120330
C	2.7957129265	.6877022555	2.8303556111
C	-.5128575207	4.0841114763	.0734806539
C	-1.5627584649	3.1469302163	.1138574696
C	3.4284721409	2.3248670987	-1.4800502645
C	-2.8848910991	.4012483740	1.3878169251
C	-2.6121291292	.8714264419	-2.4477110431
C	1.7862093625	5.0595566630	-.0351335386
C	-2.9741189124	3.6871176251	.2401266534
C	4.9445734428	1.9276497891	.8491052946
C	4.7971133211	2.0506107009	-1.5499790368
C	-3.0960481454	.4435968515	-1.0655647693
C	-2.1623084711	.7773651860	2.6787583663
C	-4.5682638030	-.9558062451	.2728606921
C	5.5546780192	1.8621831044	-.3995960771
C	2.9183480897	2.1491448305	2.3515070868
C	2.6074897174	2.4137358653	-2.7629008719
C	-3.9355547450	-.5215845535	1.4330248824
C	-4.1416583513	-.4802924475	-.9619469124
C	3.6386269556	3.0117830610	3.3996344478
C	.9576751196	-7.2574248046	.1714785110
C	2.1092313865	-7.1510329189	-.6049488773
C	2.3672201901	-5.9797875897	-1.3252370226
C	1.4832523804	-4.8950649237	-1.2858112044
C	.3300663704	-5.0153862989	-.4960995534
C	.0680439025	-6.1820125025	.2240908206
C	1.7421825708	-3.6332897100	-2.0786990800
H	-.8103369759	5.1227001255	.1287421882
H	1.2147379580	5.9850714494	.0441722799
H	2.3769524997	5.0866212999	-.9561594015
H	-4.2457652448	2.2843416833	-2.8368491398
H	-3.4522965646	3.3093803501	1.1492400651
H	-3.5913221193	3.3539794733	-.5997617580
H	5.5358274906	1.7457883172	1.7410672331
H	6.6154147487	1.6432161204	-.4767895665
H	5.2740258484	1.9643196567	-2.5220529213
H	-1.0966716301	-.7003730530	-2.5384585862
H	-2.9753162065	4.7774444253	.2683317217
H	2.4988246941	5.0108881936	.7940928968
H	-4.5036028070	.6861187814	-3.5451242431
H	-1.4877268793	.0205692661	-4.1161688533
H	-3.8187865702	.5336853496	4.0992208638

H	1.9036344258	2.5426481289	2.2501363084
H	3.0884848687	2.9924691598	4.3467683525
H	1.6087903015	2.7700365756	-2.4962666837
H	1.7814639286	1.0574604029	-4.2617686501
H	-4.2536960662	-.9174836188	2.3929549199
H	-5.3805897418	-1.6751377613	.3298676891
H	-4.6209760679	-.8435804446	-1.8666526679
H	-3.7037508743	2.1576147159	3.4116492471
H	-2.6073402210	-1.1198219913	-3.3570678512
H	-2.5475549386	1.6286758119	4.6450091883
H	-1.9960940876	-1.2482036623	3.4943124216
H	-.6615822736	-.7953849875	2.4271381624
H	3.7209115712	4.0539647766	3.0774265734
H	4.6495318402	2.6467024575	3.6035494461
H	2.2437508770	.6359931307	3.7758293195
H	2.0179098926	.3059734133	-2.6671934322
H	3.4057469605	.6130796101	-3.7172022581
H	2.5352439175	3.4779831424	-4.6578828354
H	-1.4572668678	1.5809993009	2.4470882045
H	-.7496177283	-.1333544584	4.0763965173
H	-1.8712400574	1.6647845835	-2.3125137183
H	-3.3421543777	1.7926829455	-4.2785738846
H	3.2971706165	4.4079036391	-3.3584518925
H	4.1756194863	3.0907679007	-4.1428167873
H	2.2799226070	.0694874172	2.0916370122
H	3.7842785191	.2471184766	2.9943357394
H	-.3673189742	-4.1831204472	-.4487870646
H	-.8332589539	-6.2527164168	.8270827653
H	.7536741814	-8.1678528662	.7299717176
H	1.7797906716	-2.7434989437	-1.4386704533
H	.9441900030	-3.4614449303	-2.8115359246
H	2.6858057771	-3.6958467983	-2.6286365992
H	3.2675759275	-5.9073952582	-1.9300862453
H	2.8096971238	-7.9802264781	-.6536216760
N	-1.3895454459	1.8282446068	.0498578491
N	1.4181471671	2.6404896876	-.1017935747
O	.0650898639	-.7421792558	-.1912877173
O	1.4000623632	-.4953785600	-.2694984443
Cu	.3585014123	1.0856700464	-.1081499523

71. L¹CuO₂ side-on / phenol complex

C	-2.2904425682	1.1016679016	-3.1393628944
C	-3.4554852591	2.8769786618	3.7578071644
C	-5.1430491087	.9272378628	.1781327261
C	-3.7889092709	3.1398871303	-3.3865701524
C	-1.9664055049	.8901072793	3.2114776339
C	2.7120591200	2.9453367882	-.2318257937
C	1.0554552992	4.7178591963	.0243041485
C	3.4373089836	2.5479258992	.9165590621
C	-2.7768131401	2.4178087921	.1218481601
C	3.1339389415	3.9441671718	-3.7857209373
C	-.2626944118	5.1979931879	.1446292785
C	-1.4655903729	4.4679845654	.1710700594
C	2.4904756419	1.1482606702	2.7823794803
C	3.2380941720	2.7523500305	-1.5324173511
C	-3.2975266853	1.9811305944	1.3663025196
C	2.0317587071	1.6802357072	-3.4648775473
C	2.1785131988	5.7345771419	.0071556299
C	-2.7583148708	5.2491706117	.2957373683
C	4.7214881088	2.0229188813	.7376727093
C	4.5271398607	2.2222728986	-1.6514838812
C	-3.4107451541	2.0662932168	-1.0982146379
C	3.7091560916	3.3037760778	3.3413932983
C	-2.8071887710	2.3919406859	-2.4633157965

C	5.2703429379	1.8693334550	-.5310081595
C	2.8231722649	2.5810848101	2.3132609156
C	2.4179361772	3.0138855547	-2.7914585026
C	-4.4879218500	1.2449514812	1.3651868250
C	-4.5992061039	1.3284748766	-1.0388997168
C	-2.5648879131	2.2162914812	2.6869550692
C	1.6190688954	-4.6465949272	-1.6592362334
C	1.0095596725	-3.4909987452	-1.1480930775
C	-.2848159698	-3.5553587254	-.6166494323
C	-.9541496192	-4.7708819532	-.5960009423
C	-.3486380976	-5.9260509928	-1.0989658786
C	.9404078428	-5.8529277728	-1.6304523911
H	1.7919943693	6.7493331852	.1066542143
H	2.7478060975	5.6615811564	-.9246375231
H	2.8827772132	5.5411478628	.8221123065
H	-3.2999697518	4.9542279115	1.1998085859
H	-3.4194575643	5.0363615106	-.5494765447
H	5.2919048875	1.7061013554	1.6053840599
H	6.2652031502	1.4484643206	-.6475431147
H	4.9457519355	2.0598743138	-2.6402591931
H	-.3648569758	6.2722487882	.2203009399
H	-1.5895774693	.5714841005	-2.4863962272
H	-4.1473279166	4.0698892479	-2.9297845290
H	-4.6659864866	2.5264199353	-3.6262678267
H	-1.7822061983	1.3381954820	-4.0823799088
H	-4.2856084108	2.2249837224	4.0544560910
H	1.8786414290	3.1309392038	2.2523948406
H	3.2008803319	3.3523511006	4.3101264568
H	1.4891933057	3.5086450056	-2.4915741504
H	1.3663794189	1.8592647176	-4.3165884060
H	-4.8996363044	.8990033163	2.3103101647
H	-6.0631933167	.3488793723	.2003657941
H	-5.0966497962	1.0468828683	-1.9641377100
H	-3.8846089450	3.8214244420	3.4014259168
H	-3.1162602345	.4164071725	-3.3690729423
H	-2.5665550600	6.3218638209	.3333958093
H	-2.8714914488	3.0908308930	4.6613535035
H	-2.7581605409	.1770790174	3.4741454356
H	3.9393063943	4.3270672130	3.0287947254
H	4.6596906625	2.7822681801	3.4973222084
H	1.9613697363	1.1703843680	3.7418258669
H	1.5264442078	1.0138336755	-2.7608170615
H	2.9184100561	1.1556772802	-3.8387933287
H	2.4902151936	4.1440680488	-4.6484801977
H	-1.7310950935	2.8987314165	2.4904475468
H	-1.3662459406	1.0682748384	4.1127383926
H	-1.9447977175	3.0473980779	-2.3023657779
H	-3.3014811751	3.3964247940	-4.3350854748
H	-1.3322795327	.4187132574	2.4531141379
H	3.3922315049	4.9041075587	-3.3282144791
H	4.0596437038	3.4973373888	-4.1647460724
H	3.4044501792	.5584260068	2.9169324596
H	1.8673616031	.6275040833	2.0502941766
H	-.7610557661	-2.6559513007	-.2282615013
H	-1.9584344156	-4.8107820123	-.1831071914
H	-.8725292322	-6.8700520178	-1.0784305457
H	1.2314469250	-1.6178134474	-.7684288559
H	1.4237182150	-6.7447151706	-2.0264054502
H	2.6193525266	-4.5777107679	-2.0698623670
N	-1.5351885939	3.1404217661	.0935606762
N	1.3693466467	3.4292471909	-.0767853482
O	.8434065215	.4196663954	-.2580411558
O	-.5187269822	.3315980724	-.1305355203
O	1.7221114918	-2.3362373199	-1.1942121994

Cu .0364469860 2.1064545447 -.0630521008

72. L¹CuO₂ side-on / isopropylbenzene complex

C	2.7331034998	3.3443069697	-2.6755642979
C	-3.4791648701	1.5118872554	4.9384806032
C	-3.9877150445	3.7651163959	-1.8630435140
C	-2.2598266957	-.3750546443	3.7528595835
C	2.2141835165	-.1909732750	3.4368289295
C	2.5109494073	1.9034382640	.6822074993
C	1.1151384779	3.7774923300	1.3428398725
C	3.2618895300	1.3371379590	1.7413950914
C	-2.9959622254	2.0236803324	1.2845276857
C	-3.0845255361	2.7154974285	-1.1931131218
C	-2.7200408114	1.0962153058	3.6668281339
C	-.1125372200	4.3841152024	1.6727695768
C	-1.4044337195	3.8246185741	1.6724770006
C	2.9573950930	1.8057052753	-.6553185708
C	-3.5265735126	1.3237911979	2.3924156580
C	-5.5261476868	.8625328293	1.0878777035
C	2.3625769880	4.6350493988	1.4284426505
C	-2.5599241402	4.7279290252	2.0546720076
C	4.5000132394	.7593398964	1.4434908722
C	4.2086844533	1.2258629777	-.8963301407
C	-3.7043112393	2.1043937260	.0618456565
C	1.7647506020	.9957329254	-2.7214349049
C	3.7158466043	1.6972725617	4.2370956980
C	4.9845740168	.7198081107	.1396396943
C	2.7104704743	1.2470526128	3.1622856339
C	2.0910736199	2.2212342930	-1.8399340419
C	-4.8008769671	.7596829240	2.2696070580
C	-4.9736857109	1.5213748730	-.0062344200
C	-2.6958787392	1.6033625384	-2.1916874412
C	1.9862326871	-3.5044592256	-3.8235568280
C	1.5137926220	-3.5760422552	-2.5110141186
C	1.2776579566	-4.8138500234	-1.8966099718
C	1.5218745866	-5.9781769318	-2.6397632906
C	1.9935991315	-5.9100782656	-3.9502521063
C	2.2294879732	-4.6704483044	-4.5477062896
C	.7698148128	-4.8908007978	-.4632067588
C	-.6273155243	-5.5310321247	-.3887535696
C	1.7614386055	-5.6308432522	.4558209391
H	3.0413325540	4.2520146808	2.1970725863
H	-3.1188402601	4.3022219849	2.8940254041
H	-3.2651924581	4.8237791136	1.2233773241
H	5.0883804757	.3192724351	2.2432942665
H	5.9507738192	.2692175603	-.0711410279
H	4.5701702076	1.1508804582	-1.9182489887
H	-4.9172683647	3.3235684207	-2.2382649546
H	-.0557664547	5.4255927060	1.9598197117
H	2.9136236204	4.6104829370	.4834341489
H	-2.1627772121	2.0264516166	-3.0514296361
H	-2.0568665875	.8524906257	-1.7173629418
H	-4.3752486080	.9019870971	5.0956586896
H	-3.7940662699	2.5593201555	4.8959851944
H	-4.2574644925	4.5690761930	-1.1704009301
H	1.8408949661	1.9082489731	3.2302996002
H	3.2451694293	1.6778198930	5.2259476492
H	1.1460618325	2.6056447895	-1.4439296881
H	1.0282006659	1.2618010212	-3.4881502380
H	-5.2235642989	.2133947265	3.1081085404
H	-6.5105881555	.4096149057	1.0115951872
H	-5.5299098286	1.5660012678	-.9379556783
H	2.1115208545	5.6693075643	1.6669094942
H	-3.5860181383	1.0888492925	-2.5717070434

H	-2.2068709133	5.7219173160	2.3323683640
H	-2.8411504089	1.3860421176	5.8194580476
H	-3.1176520704	-1.0484956191	3.8637866863
H	-1.7195559601	-.6713204213	2.8489251773
H	2.9228693860	4.2383317267	-2.0725991789
H	3.6881833194	3.0267730393	-3.1083837365
H	4.0760039858	2.7160702790	4.0549574938
H	4.5906719102	1.0386843756	4.2820041774
H	1.7374586694	-.2548513218	4.4218139637
H	1.3614647107	.1712643426	-2.1232131872
H	2.6611396330	.6325300014	-3.2369939091
H	2.0754884797	3.6309175842	-3.5035957247
H	-1.8199935955	1.7155775495	3.6053099433
H	-1.6042245135	-.5242897741	4.6181704268
H	-2.1608234840	3.2228540011	-.8994675225
H	-3.4728338744	4.2157515733	-2.7186040456
H	1.4933907802	-.5119084347	2.6778066857
H	3.0495213026	-.9018566224	3.4210746885
H	2.1790984085	-6.8255890836	-4.5059374591
H	2.6007726417	-4.6157103743	-5.5676563282
H	1.3280488009	-2.6562173756	-1.9574460936
H	2.1650277315	-2.5341340335	-4.2790820061
H	1.3449078082	-6.9521622196	-2.1896854404
H	.6800498968	-3.8599537034	-.0962429458
H	1.4161752748	-5.6124157301	1.4955906973
H	2.7539108140	-5.1704197147	.4186673717
H	1.8700805639	-6.6821291406	.1624933295
H	-.9974603435	-5.5319783829	.6417467040
H	-.6064430186	-6.5708600223	-.7348911223
H	-1.3454183573	-4.9861315906	-1.0098397966
N	1.2393875441	2.5073137963	.9647870802
N	-1.6664205194	2.5586634084	1.3561534655
O	-1.0099158126	-.2830535896	.3994845644
O	.3451965811	-.2795676526	.2907074326
Cu	-.2796561710	1.3847943464	.8557004117

73. L¹CuO₂ side-on / cyclohexadiene complex

C	-1.9664793522	1.5130541977	-3.4185102879
C	-3.1827147154	.5364958009	3.6141769028
C	-3.6839385611	3.3236132096	-2.9276430591
C	-1.4973318005	-.9657528217	2.4447437400
C	3.2442017188	4.8448795840	-2.8574336987
C	2.8460598571	2.7700701893	.2382351633
C	.9546027502	4.1261122514	.9440222376
C	3.5914751584	2.1349267000	1.2576930601
C	-2.5346586164	1.4729112091	.0799510187
C	2.7946020879	.1175609720	2.5387971569
C	2.3505087502	2.5022868036	-3.2154750921
C	-.4183949879	4.3689409070	1.1436386217
C	-1.5121518810	3.5265002906	.8652029784
C	3.4307355171	3.0811286588	-1.0157694899
C	-2.9690602745	.5554277834	1.0678036493
C	-4.6975314069	-.2102762304	-.4624496494
C	1.9248802072	5.2244090671	1.3295208246
C	-2.9004167711	4.0510371932	1.1829344113
C	4.9415711691	1.8734999240	1.0194111199
C	4.7846367547	2.7972174502	-1.1997870641
C	-3.1492497724	1.5166801240	-1.1939895660
C	-2.6148083304	2.3908136352	-2.3247456010
C	-2.2446831108	.3867577448	2.4022691155
C	5.5402005318	2.2084924833	-.1916149831
C	2.9427729282	1.6523185552	2.5549963125
C	2.6095792138	3.6214243719	-2.1831395941
C	-4.0589419871	-.2692993865	.7725551570

C	-4.2360178274	.6702442571	-1.4353811163
C	3.6872948587	2.1211445332	3.8193845453
C	.2735406550	-4.9849324232	-.5508520976
C	.9020791947	-4.3444595031	-1.7546682200
C	.1300778703	-4.6179376310	-3.0151184692
C	-.9540918191	-5.3997820421	-3.0705408445
C	-1.5439776520	-6.0943659494	-1.8750431994
C	-.8101498789	-5.7659550741	-.6035290405
H	1.3966554924	6.0909422234	1.7305699053
H	-.6673285670	5.3337204973	1.5658192750
H	-4.1195044628	3.9771988818	-2.1718511276
H	2.5150912115	5.5398188150	.4632295881
H	-2.8528196585	5.0492016216	1.6203803555
H	-3.4149904231	3.3829523872	1.8794277332
H	-3.5147205542	4.0911570596	.2784036986
H	5.5295496953	1.3841370259	1.7897694953
H	6.5894253913	1.9929153817	-.3570033965
H	-1.2069205194	.8521305499	-2.9892543958
H	2.6363851886	4.8630584059	2.0794309558
H	-4.5010554220	2.7696145722	-3.3927452971
H	-1.4958418097	2.1339721356	-4.1876681714
H	-3.9423480321	-.2506593502	3.6391634862
H	-3.7052278582	1.5005413436	3.6076371250
H	-2.6116380588	.4664256399	4.5475928339
H	-2.2024286162	-1.8021008329	2.4305911375
H	1.9374813209	2.0726011498	2.5991403488
H	3.1535851402	1.7950525307	4.7195256087
H	1.6420626404	3.9339867167	-1.7912583208
H	1.6772019407	2.8545521510	-4.0063825935
H	-4.4037962688	-.9806343044	1.5181518721
H	-5.5415238608	-.8615825918	-.6719190006
H	-4.7193149502	.6896442311	-2.4080136442
H	-2.7141719803	.8847953446	-3.9138434304
H	5.2513994757	3.0259054628	-2.1540852116
H	-.8343063003	-1.0752312226	1.5832191521
H	3.4364557680	5.6437306039	-2.1396409622
H	4.1873641274	4.5968505476	-3.3412452012
H	2.2562594121	-.2166752404	1.6461113132
H	3.7750254774	3.2103893142	3.8567866144
H	4.6959422915	1.7067448981	3.8743359136
H	2.2536176745	-.2270283815	3.4276167918
H	1.9064525765	1.6186658425	-2.7418300007
H	3.2860316567	2.1836600144	-3.6904815649
H	2.5821816077	5.2393219410	-3.6352982989
H	-1.4915728237	1.1748632362	2.4742985256
H	-.8998006025	-1.0507344579	3.3598889744
H	-1.8285956320	3.0255588945	-1.9065848379
H	-3.2469589431	3.9513372287	-3.7035146172
H	3.7728095864	-.3685738546	2.5379647377
H	-1.2059365774	-6.1984322454	.3098904572
H	.7487035101	-4.7907090537	.4065651727
H	1.9413855247	-4.7109432100	-1.8697796393
H	1.0115324145	-3.2553023833	-1.6013192391
H	-2.6145503986	-5.8290930115	-1.7725953455
H	.4996015536	-4.1488529205	-3.9219928735
H	-1.4585736950	-5.5591341062	-4.0200673740
H	-1.5473309806	-7.1874173040	-2.0393761213
N	-1.3979874745	2.3071480393	.3461839726
N	1.4443151590	2.9947957971	.4420412044
O	1.3104706494	.1098474687	-.7102792763
O	-.0275098106	-.1230599701	-.7320141354
Cu	.3086989139	1.5810391151	-.0668440576

C	3.3636268782	4.0132825169	-3.5881094508
C	-3.7370992518	2.6414322923	3.4759139991
C	-3.5989410373	4.5129602998	-3.4047369827
C	-2.5539876880	.5972938951	2.5408321017
C	1.9562569791	.3743155412	2.4488130078
C	2.6057759805	2.5643794563	-.2252610182
C	1.2083755577	4.4812769309	.2903976227
C	3.2019943396	1.8923284353	.8685796688
C	-2.9320186039	2.8587543504	-.1517656196
C	-2.8169723620	3.4055329882	-2.6687615660
C	-2.9027525202	2.0835129055	2.3084740271
C	-.0262120014	5.1327458721	.4662098103
C	-1.3262342327	4.6116711548	.3269334083
C	3.1812574585	2.5215168165	-1.5163804671
C	-3.5860109285	2.2608386601	.9538163587
C	-5.5086097731	1.8202715076	-.4731638308
C	2.4654271299	5.3009449134	.5032525442
C	-2.4860317884	5.5566687722	.5708333235
C	4.4165435220	1.2328284847	.6541440786
C	4.3963102952	1.8478325428	-1.6752784805
C	-3.5451681137	2.8933252134	-1.4280763255
C	1.8570069042	1.9598090539	-3.5829164831
C	3.4310960286	2.2173011270	3.3957718921
C	5.0179451464	1.2169903736	-.6013622755
C	2.5166349799	1.7978830409	2.2300775711
C	2.4645815074	3.1002339488	-2.7341389077
C	-4.8781228609	1.7570091787	.7665770124
C	-4.8389880976	2.3761275215	-1.5585090914
C	-2.4876877007	2.2328600297	-3.6199300795
C	.9240984964	-3.2792566586	-1.9358556748
C	-.0170790941	-4.4003722854	-1.5462833443
C	-1.4064642731	-4.2263071143	-1.6090239587
C	-2.2790015921	-5.2737360088	-1.3258469652
C	-1.7649364625	-6.5278165155	-.9721746835
C	-.3919426792	-6.7142639635	-.9022686960
C	.4754161099	-5.6542813946	-1.1905709293
C	1.1806944407	-3.2669551479	-3.4557983096
H	3.0690688116	5.3233962707	-.4092792503
H	3.0902771710	4.8537944354	1.2826499892
H	-3.1202970788	5.1868637456	1.3823366145
H	-3.1217295881	5.6250011308	-.3175299263
H	4.8894378619	.7078130833	1.4795948914
H	5.9594625756	.6948564586	-.7474475789
H	4.8525617722	1.7998063706	-2.6602361067
H	-4.5542924210	4.1452024059	-3.7978117761
H	.0316294956	6.1768501168	.7431531511
H	-3.8161622388	5.3620981318	-2.7458246662
H	-1.8841270031	2.5807466027	-4.4666916270
H	-1.9334992172	1.4467595527	-3.0948644979
H	-4.6799481162	2.0969988966	3.5983620547
H	-3.9819784671	3.6990849182	3.3301157229
H	-3.1831996519	2.5494057648	4.4173040208
H	1.6644684701	2.4840751261	2.2219760506
H	2.8768128810	2.1905813238	4.3406254370
H	1.6332783766	3.7122995098	-2.3709177473
H	1.2658386972	2.3699656372	-4.4106535920
H	-5.3927031146	1.2918215502	1.6029945478
H	-6.5104193864	1.4179709667	-.5979308909
H	-5.3228696912	2.3935597370	-2.5320111789
H	2.2225680833	6.3245934404	.7901412689
H	-3.4030700713	1.7844854861	-4.0260112044
H	-2.1309746422	6.5552037516	.8283769613
H	-3.4621568711	-.0120716193	2.6180416396
H	-1.9575426348	.2017511460	1.7133222559

H	3.7923482112	4.8306003361	-2.9966432990
H	4.1932038658	3.4601775324	-4.0418025579
H	1.3055410705	.0743839438	1.6209349230
H	3.8199597145	3.2330210482	3.2610938965
H	4.2892187060	1.5442743337	3.5032913231
H	1.3809958651	.3255593712	3.3810314094
H	1.2140151626	1.3079653993	-2.9831966274
H	2.6414127130	1.3261694078	-4.0123549006
H	2.7845615290	4.4568993599	-4.4059897615
H	-1.9604991476	2.6393718997	2.2845251813
H	-1.9886465027	.4741333906	3.4727441420
H	-1.8654318331	3.8372979695	-2.3415752128
H	-3.0200805189	4.8875411948	-4.2563760743
H	2.7668294083	-.3609499600	2.5181125883
H	.5378372560	-2.2991791562	-1.6313784335
H	1.8838316409	-3.4093385705	-1.4139352726
H	-1.8290715832	-3.2678514789	-1.8781013012
H	.0016563716	-7.6850666706	-.6224615950
H	1.5476322249	-5.8124265231	-1.1332685389
H	.2222257410	-3.1167568188	-3.9751208674
H	1.5408187540	-4.2673676846	-3.7530479112
H	-4.0529102579	-5.9275006214	-1.1617104699
H	-2.2804927448	-8.3174047210	-.4662982838
H	2.2433493411	-2.1795434145	-4.8392513151
H	2.9945170623	-2.3035260568	-3.3958131691
N	1.3343103404	3.2009935051	-.0512973573
N	-1.5913625249	3.3497635240	-.0015154991
N	2.0799479592	-2.1661591447	-3.8322692275
O	-1.0389540552	.5140693545	-.7242980682
O	.3033459718	.3405721276	-.7840988996
O	-2.7148114533	-7.4981716560	-.7121625733
O	-3.6291731782	-5.0874109802	-1.3931400861
Cu	-.1816762178	2.1145790515	-.3243758718

75. L¹CuO₂ side-on / formylglycine complex

C	2.3410794932	1.6948168922	-2.7037054868
C	-3.6018229288	1.5432108972	3.8250505473
C	3.0988405621	2.5811296363	-3.7081908827
C	2.3338012561	-.3556475207	2.7758332706
C	2.6464738833	1.5352333897	-.1549133107
C	-2.9057502894	1.2995467826	.1687127442
C	-3.7739159787	2.3548523413	-3.2562726851
C	1.0728271785	3.3530640437	.1712332896
C	-1.4668804717	3.2431293112	.3173413442
C	3.3606772670	1.0752522663	.9772792522
C	-3.4765870294	.8270838218	1.3750429918
C	-.2189440345	3.8995361142	.3192459555
C	3.1646566024	1.3669939099	-1.4607875258
C	-3.5388957194	1.0613437685	-1.0746734219
C	-2.2038712946	-.4599575698	3.1258308890
C	1.8473494212	.3945090303	-3.3739849788
C	2.2423823535	4.3194135138	.1896228032
C	-2.7054346471	4.1077551964	.4670090910
C	4.6236273557	.5074062694	.7797470945
C	4.4312967003	.7897806127	-1.6015684853
C	-4.7138935278	.1768162574	1.3173187320
C	-4.7757239400	.4060530080	-1.0750146429
C	3.6569803636	1.7111934990	3.4380988054
C	-2.8875662007	1.4252262186	-2.4059819968
C	5.1638188143	.3723631422	-.4953003516
C	2.7429314752	1.0789966585	2.3737577925
C	-2.5056612412	.1546971338	-3.1925376359
C	-5.3690402078	-.0246292725	.1063777655
C	-2.7407303224	.9266337081	2.7086910993

C	.9719003051	-3.8225344431	-2.2154990556
C	1.8654618769	-4.9673546891	-1.5924358011
C	-1.3929444206	-3.8416155175	-3.0265243517
H	-.2589499324	4.9752460153	.4361417157
H	-2.4420587900	5.1640909673	.5443201695
H	1.9040102374	5.3454536968	.3447782170
H	3.9766086244	2.0703388876	-4.1194242105
H	3.4418798665	3.5151462350	-3.2483907145
H	2.7974787479	4.2683286941	-.7526451773
H	2.9480761406	4.0542373541	.9833283988
H	-3.2723159130	3.8183615436	1.3579958016
H	-3.3755301143	3.9714881370	-.3874690052
H	5.1798004278	.1351821103	1.6358865766
H	6.1377113733	-.0905129519	-.6291476976
H	-1.8676739660	-.5180718721	-2.6153293796
H	-5.1611427311	-.1978267811	2.2342295916
H	-6.3260400530	-.5397497258	.0815123260
H	-5.2683018608	.2081665484	-2.0231557121
H	3.2158948749	-.9970126170	2.8899902017
H	1.6949514615	-.8133164423	2.0143060133
H	-4.4649246815	.9125215880	4.0683755696
H	-3.9818224791	2.5324123596	3.5438853462
H	-3.3921192815	-.4198852915	-3.4834218424
H	4.8370104556	.6350416008	-2.5974795810
H	-1.9708231072	.4181526235	-4.1121122920
H	1.8293797478	1.6802183982	2.3323139476
H	3.1458435483	1.7428122068	4.4077059474
H	1.4566036398	2.2532718055	-2.3819158058
H	1.1905911223	.6223535091	-4.2214793772
H	-1.8757941359	1.5813373417	2.5643327044
H	-1.5999052827	-.3828045455	4.0381070843
H	-1.9634344723	1.9689165698	-2.1869390707
H	-3.2530620445	2.6346381138	-4.1788839341
H	-4.7098876930	1.8639240951	-3.5466628351
H	-4.0335942486	3.2762473678	-2.7218929328
H	-3.0119620189	1.6551801100	4.7425816290
H	3.9401584493	2.7359161874	3.1713282492
H	4.5795741995	1.1359876691	3.5760779650
H	1.7954770290	-.3502742422	3.7318420187
H	1.2953782421	-.2362890320	-2.6713909908
H	2.6894685291	-.1976556933	-3.7503011893
H	2.4480630090	2.8380877785	-4.5516911611
H	-1.5890675892	-.8960061332	2.3329521230
H	-3.0286360067	-1.1543787441	3.3274378672
H	1.3416850743	-3.5416336745	-3.2065579101
H	-2.3084243217	-4.4684456628	-2.9254090011
H	-.4491263296	-5.2018404304	-1.7646605196
H	1.0441653846	-2.9354618840	-1.5676562416
N	1.3214598873	2.0569359914	.0154381794
N	-1.6173586321	1.9279203772	.1954717262
N	-.3866298429	-4.3212426719	-2.2881422557
O	.5793158718	-.9708373637	-.2788554343
O	-.7642307093	-.9595747320	-.1053729282
O	3.0945119078	-4.7575310635	-1.6503500185
O	1.2221540367	-5.9381735934	-1.1096431394
O	-1.3747955991	-2.8463621786	-3.7534032839
Cu	-.0920140189	.7869204767	-.0096973530

76. L¹CuO₂ side-on / methane t.s.

C	-5.3372623022	-.6789000406	-.2453624363
C	-3.3179008186	.1622057923	3.5807662326
C	3.2510137428	2.4049856821	-3.6813533835
C	2.4186668961	-1.1595161024	2.5113170026
C	2.7216887872	.8768491629	-.3297181655

C	-2.8484416698	.5791222113	-.0918703107
C	-3.9238132258	2.2112606103	-3.2544576826
C	1.1269406367	2.6031130194	.2187664527
C	-1.4066764799	2.4642035200	.3371503929
C	3.4441243601	.3464607918	.7644275064
C	-3.3541719206	-.1032469090	1.0385366269
C	-.1623272270	3.1182784376	.4366345115
C	3.2743601965	.8860098423	-1.6316869242
C	-3.5598124988	.5931079684	-1.3133366246
C	-1.9779971951	-1.6704979192	2.4438405492
C	2.0037970691	.1966707619	-3.6980843757
C	2.2880543479	3.5625754067	.3982812488
C	-2.6395190861	3.2865290863	.6641495460
C	4.7295156089	-.1541491553	.5328319739
C	4.5650402223	.3751013893	-1.8102152277
C	-4.6065686830	-.7177436404	.9391695132
C	-4.8081796526	-.0370340592	-1.3613601900
C	3.7729990258	.8509647953	3.2473530689
C	5.2927175028	-.1384815726	-.7403915541
C	2.8402935080	.2814036962	2.1645906519
C	2.4759378590	1.3821718354	-2.8329830535
C	-2.5313217585	.1091914601	-3.5586228546
C	-2.5359500712	-.2382373608	2.3184259655
C	-2.9701885223	1.2134410752	-2.5754940562
C	1.0117176141	-4.1767579446	.1249788076
H	-2.3679527256	4.3065678350	.9387015642
H	-.2061311945	4.1606188469	.7238231149
H	1.9345598805	4.5565703277	.6747471358
H	1.7246803647	-1.5546313518	1.7636168034
H	4.1331610097	1.9591818926	-4.1530004421
H	3.5890622378	3.2543945738	-3.0786129597
H	3.2885386035	-1.8253551026	2.5438190778
H	-2.0272400746	.5468633963	-4.4281585084
H	2.8724681983	3.6415013396	-.5237735180
H	2.9742190054	3.2078473844	1.1731708959
H	-1.8513941775	-.5965249919	-3.0731518667
H	-3.3216648682	3.3217738937	-.1904895856
H	5.2988874793	-.5642256305	1.3618298564
H	6.2933548779	-.5300333592	-.8987916027
H	5.0037268445	.3742142425	-2.8037931119
H	-5.0105310600	-1.2443819047	1.7989690331
H	-6.3086136630	-1.1615392669	-.3030542826
H	-5.3686670935	-.0349274927	-2.2916887292
H	-4.1669512366	-.5050525457	3.7629640729
H	-3.7071941067	1.1828910508	3.5062201509
H	-3.3976236898	-.4553641396	-3.9218204580
H	-3.1970246940	2.8358188549	1.4908295741
H	1.9319003440	.8899788879	2.1623549010
H	3.2648250016	.8607749293	4.2175200213
H	1.5834901542	1.8861492596	-2.4516679314
H	1.3601498160	.5469009639	-4.5126434421
H	-1.6798344444	.4373963712	2.2373231936
H	-1.3027368418	-1.7489096298	3.3038464124
H	-2.0720821436	1.7657382304	-2.2847305768
H	-3.4324488266	2.6783170291	-4.1148260037
H	4.0796157759	1.8759898861	3.0157223290
H	4.6816514661	.2505502909	3.3609151353
H	1.9269356564	-1.1963710895	3.4897359888
H	1.4459152785	-.5353260913	-3.1071544936
H	2.8594248594	-.3228702514	-4.1444657586
H	2.6125133114	2.7915914077	-4.4827436990
H	-1.4359279544	-1.9553780054	1.5373953751
H	-2.7896537293	-2.3930055611	2.5864881615
H	-2.6676885709	.1118354542	4.4609322716

H	-4.2319038164	3.0071571829	-2.5681507793
H	-4.8309755512	1.7205632101	-3.6228434066
H	.7688968170	-2.8155146756	-.5489875236
H	-.0043957560	-4.5524174845	.0392774106
H	1.3453144507	-3.8981914224	1.1203223277
H	1.7558477817	-4.6232429013	-.5284452330
N	-1.5573352673	1.1917732703	-.0201177418
N	1.3785754841	1.3396307112	-.1317216476
O	-.7957821623	-1.6059085792	-.9722300871
O	.5906926213	-1.9139935425	-1.1225733920
Cu	-.0239807202	.0516021415	-.4531265880

77. L¹CuO₂ side-on / cyclohexane t.s.

C	2.2406382857	.4847000687	2.6079016874
C	-3.2859419918	2.3400300160	3.7732359587
C	-4.0104404469	3.3185754189	-3.3465746061
C	-1.8940654356	.4445258318	2.8232264790
C	3.4796733864	3.8634586863	-3.6213870059
C	2.6986071988	2.4587118865	-.28711113695
C	1.1169263739	4.2500087105	.0305775080
C	3.3285153595	1.9594383918	.8779579944
C	-2.8748301580	2.2375636102	.0363483794
C	-3.0443081975	2.4651029061	-2.5083614848
C	-2.5163293951	1.8284464154	2.5436591472
C	-.1689106207	4.7980566272	.1710189401
C	-1.4151942722	4.1425076392	.1628981069
C	3.3400808218	2.3888480296	-1.5448570628
C	-3.3674566549	1.7719698105	1.2784935243
C	-5.3944517209	1.0401310093	.1512723700
C	2.2880034129	5.2055003040	.1629693746
C	-2.6397258574	5.0076352476	.3997461174
C	4.6200608054	1.4336332768	.7639942222
C	4.6308081899	1.8515618026	-1.6058751079
C	-3.6187800244	2.0698457538	-1.1525023802
C	2.2702151917	1.6335072588	-3.6998331824
C	3.4297046335	2.6024865347	3.3461121067
C	5.2743069159	1.3838376298	-.4635853427
C	2.6152588652	1.9308230477	2.2265626153
C	2.6459688526	2.8452388142	-2.8243057084
C	-4.6348446021	1.1815791718	1.3095798191
C	-4.8809528430	1.4721855262	-1.0681031274
C	-2.5974678476	1.2086660133	-3.2835518062
C	-.3000180475	-4.6563897123	-2.2634034892
C	-.4124373405	-3.1651909585	-1.8535987633
C	.8040629669	-2.4041709227	-2.3180269080
C	2.1322278286	-2.9779728710	-1.8872068826
C	2.2335723532	-4.4649453062	-2.3098567168
C	1.0293298403	-5.2651512687	-1.7938791119
H	-.2053432989	5.8663049085	.3393849506
H	-4.9095991858	2.7600527321	-3.6274503573
H	1.9424951964	6.2240083148	.3443238795
H	2.9042422244	5.1996896796	-.7411356431
H	2.9417316280	4.9064918495	.9883177438
H	-3.1764824005	4.6841832365	1.2968464291
H	-3.3441360434	4.9214549716	-.4330853928
H	5.1172971645	1.0498140696	1.6502755243
H	6.2779177445	.9738437094	-.5311320125
H	5.1379919069	1.7950294182	-2.5648460116
H	-4.3307004655	4.2144457341	-2.8042812531
H	-1.9213490134	.5994581995	-2.6767480411
H	-2.0903062788	1.4888629052	-4.2143904177
H	-4.0773550962	1.6475815535	4.0788476036
H	-3.7490772103	3.3143473076	3.5846477055
H	-2.6050327677	2.4487712291	4.6243689585

H	-2.6744241624	-.2831431945	3.0742831799
H	-1.3570016548	.0673386439	1.9483463474
H	3.7347868046	4.7376409848	-3.0136430472
H	1.6827689901	2.4918004504	2.1207528169
H	2.8530567289	2.6182207493	4.2772349563
H	1.7130715806	3.3382782854	-2.5365224158
H	1.7154247114	1.9550240215	-4.5883610175
H	-5.0305891296	.8201949876	2.2539868246
H	-6.3780081846	.5814767581	.1973358977
H	-5.4668938072	1.3364179264	-1.9724171223
H	-3.4624400504	.5883366605	-3.5456299839
H	-2.3608200282	6.0554838677	.5175446873
H	4.4166081112	3.4270324030	-3.9833306845
H	1.6513390487	.0073393195	1.8192563000
H	3.1387230474	-.1229807160	2.7667474033
H	-3.5236115934	3.6405690093	-4.2735419880
H	-2.1519711761	3.0703141836	-2.3243808610
H	-1.1999175104	.4978013074	3.6701563462
H	3.6873434798	3.6358723448	3.0917566773
H	4.3637329032	2.0672829487	3.5477583622
H	1.6558396503	.4692526348	3.5342377202
H	1.6492198551	.9270567249	-3.1408147723
H	3.1654724624	1.0988864329	-4.0366009863
H	2.9199006394	4.2120085717	-4.4958774976
H	-1.6951845800	2.5276535825	2.3618769312
H	-1.3299816922	-2.7209392724	-2.2506286375
H	-.4801315839	-3.1075360137	-.7586654463
H	.7648202329	-2.0386195095	-3.3488071155
H	.6920985229	-1.1743426988	-1.5718102298
H	2.9659007603	-2.4012751353	-2.3017261760
H	2.2131908540	-2.9226523773	-.7926885172
H	3.1721010808	-4.8890824289	-1.9332068629
H	2.2731209905	-4.5269845962	-3.4057946032
H	1.1020107086	-6.3084972638	-2.1238996302
H	1.0516136165	-5.2807766976	-.6950301873
H	-1.1483325181	-5.2124125842	-1.8472345836
H	-.3717337427	-4.7366056972	-3.3565472166
N	-1.5763505187	2.8351858310	-.0260959040
N	1.3562292282	2.9581633299	-.2010021885
O	-.7728502233	-.1066059324	-.5567574976
O	.6146668380	-.3381193183	-.8046589193
Cu	-.0538977809	1.6470891079	-.3833896454

78. L¹CuO₂ side-on / acetonitrile t.s.

C	2.0216752112	1.7717850901	-2.7395194608
C	-3.6975607959	1.2393305738	3.4530551969
C	2.7330740749	2.6022396230	-3.8206883214
C	2.8759840189	-.4599837890	2.8233203044
C	2.6045826086	1.3959324601	-.2685784262
C	-2.9356570304	1.2085625997	-.1474941746
C	-3.7075947469	2.8558351517	-3.3406960279
C	1.0626483463	3.2064100305	.2219565441
C	-1.4727131767	3.0809697409	.2451696007
C	3.4468420965	.8833045425	.7458043069
C	-3.5624590777	.6335355667	.9841341696
C	-.2293942108	3.7357809404	.3692804675
C	2.9624521006	1.2953246912	-1.6362158399
C	-3.5688254666	1.1937766841	-1.4131540439
C	-2.5584057818	-.9031160126	2.7175140461
C	1.2734112913	.5795832263	-3.3681966948
C	2.2261127958	4.1761741499	.2387136162
C	-2.7073070988	3.9466699311	.4202576866
C	4.6555952159	.2877567041	.3643812628
C	4.1802158099	.6897720539	-1.9634602012

C	-4.8418132524	.0882267406	.8309241140
C	-4.8490702024	.6371665209	-1.5103798425
C	4.1038582563	1.7416859981	3.0418379018
C	-2.8931845660	1.7336089747	-2.6701771289
C	5.0259244364	.1902419163	-.9747067468
C	3.0699237245	.9464641916	2.2230155183
C	-2.6158630209	.5957537986	-3.6713853993
C	-5.4895704289	.0954126699	-.4004979129
C	-2.8751378619	.5585729071	2.3440295300
C	1.7986291753	-3.0979783134	-2.1963347945
C	2.4141406846	-2.7508768005	-.9841925151
H	-.2807642952	4.8000828454	.5569007539
H	-2.4312635314	4.9775461837	.6443937888
H	1.8863259193	5.1927752513	.4395048360
H	3.4463417687	2.0032845637	-4.3964055154
H	3.2795188339	3.4450126335	-3.3851359436
H	2.0951611756	-1.0130610446	2.2955245224
H	2.7475102448	4.1675790497	-.7241064566
H	2.9608958582	3.8922715255	.9977896812
H	-3.3337466876	3.5653120333	1.2319542262
H	-2.0100443707	-.1936978992	-3.2176883713
H	5.3156477238	-.1091091737	1.1304820352
H	5.9680415125	-.2760707624	-1.2482276866
H	4.4671622941	.5996028017	-3.0067395521
H	-5.3362821297	-.3531059448	1.6913773836
H	-6.4849015433	-.3284326617	-.4971369645
H	-5.3498102390	.6247442324	-2.4742012815
H	3.8019637117	-1.0439998039	2.7742509592
H	-4.6558952802	.7336139303	3.6119814975
H	-3.9107747786	2.2869615704	3.2161451565
H	-3.5488233212	.1406815456	-4.0209225432
H	-3.3255606009	3.9371656830	-.4812361360
H	-2.0829253752	.9776340161	-4.5492539025
H	2.1114609224	1.4686792397	2.2967991148
H	3.7767966206	1.8310462242	4.0830643036
H	1.2672082614	2.4158765207	-2.2807367374
H	.5741698359	.9251849160	-4.1367817560
H	-1.9253087092	1.0959193384	2.2693619402
H	-2.0135591167	-.9443458985	3.6677036464
H	-1.9279609370	2.1552583174	-2.3758203458
H	-3.1701281840	3.2493011361	-4.2102239417
H	4.2480727500	2.7509863286	2.6436700892
H	5.0798390027	1.2443811288	3.0431644589
H	2.5874751602	-.3862393643	3.8775535055
H	.6951590267	.0216337820	-2.6243105633
H	1.9678262519	-.1252869169	-3.8369019907
H	1.9995432079	3.0024564610	-4.5281871943
H	-1.9529751107	-1.3797414598	1.9422579818
H	-3.4795104702	-1.4845777950	2.8367764314
H	-3.1504202448	1.2126183898	4.4014993680
H	-3.8936173620	3.6896473466	-2.6562641110
H	-4.6798686775	2.4930157856	-3.6904653887
H	2.4857687265	-3.5266848073	-.2257409319
H	1.3560313908	-1.8779200130	-.3045096174
H	3.2275916721	-2.0299807206	-1.0275663279
N	1.3086730403	1.9076713912	.0603160467
N	-1.6267187533	1.7823854300	-.0147302533
N	1.2484523196	-3.3512780179	-3.1997950556
O	.6990701990	-1.3494212755	.3883388258
O	-.6186227081	-1.2749194718	-.1248945105
Cu	-.0784842499	.5797154185	-.0072760196

79. L¹CuO₂ side-on / toluene t.s.

C	-2.7326924679	.9470782770	-3.5596120457
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C	-3.1407042129	.7570846441	3.6204101971
C	2.2435962489	.5979490116	-3.8752748196
C	-3.9908817408	3.0926773526	-3.0526363439
C	-1.9801496665	-1.1385864442	2.3903274775
C	2.7594917522	1.3885508617	-.4016212115
C	1.2132759194	3.1544645947	.1232759236
C	3.4703124721	.9326022872	.7356803936
C	-2.8276652526	1.2435004961	-.0484321374
C	3.3208243385	2.8873996076	-3.6818163044
C	2.0651281146	-.3382780681	2.3976384321
C	-.0538640330	3.6961432057	.3945093073
C	-1.3134447285	3.0679027900	.3499589230
C	3.3207550311	1.3043511395	-1.6947838702
C	-3.3139529589	.5443758103	1.0804316173
C	-3.0525819624	2.0103458081	-2.4900649234
C	2.3990951748	4.0909911027	.2663563452
C	-2.5082663020	3.9210727983	.7372349870
C	4.7516096610	.4060866926	.5506215970
C	4.6076973790	.7673093042	-1.8266993107
C	-3.5993536044	1.3491173615	-1.2287947862
C	-2.4468077537	.3287944871	2.3163405773
C	-5.3858987315	.1241467730	-.1202360057
C	5.3219705512	.3242102112	-.7187192067
C	2.8304190785	.9699516167	2.1210862015
C	2.5650220253	1.7742501464	-2.9334445832
C	-4.6008124925	-.0003555861	1.0228734907
C	-4.8797611723	.7851177136	-1.2360311099
C	3.8279596072	1.2607895409	3.2532542117
C	4.0104237531	-3.8761448007	1.8877495655
C	4.3277110158	-3.5966718269	.5533604355
C	3.3355449732	-3.6077624863	-.4189210822
C	1.9910412883	-3.8927430582	-.0826083136
C	1.6881180455	-4.1569708037	1.2741510059
C	2.6855972602	-4.1568111802	2.2418794583
C	.9443082496	-3.8364234866	-1.0823094599
H	-.0638802117	4.7386758817	.6841173972
H	2.0685908057	5.1028659709	.5041591426
H	2.9849905417	4.1208591728	-.6571424693
H	-4.2177205663	3.8615612217	-2.3065660477
H	-3.0750185001	3.4533907348	1.5476130133
H	-3.1985438055	4.0296394639	-.1045822480
H	5.3137247300	.0536511275	1.4092641555
H	6.3216704625	-.0831514450	-.8410999047
H	5.0555215644	.6999976293	-2.8142884797
H	-2.0520521411	.1895959081	-3.1608022040
H	-2.1900425742	4.9141031510	1.0572877941
H	3.0769784712	3.7521698592	1.0557693019
H	-4.9422871328	2.6694114015	-3.3920139129
H	-2.2703087873	1.4138642036	-4.4371427195
H	-4.0266076871	.1484043500	3.8304812547
H	2.0937525538	1.7784187719	2.1265910293
H	3.2900592791	1.4087362311	4.1954424333
H	1.6123686771	2.1943864957	-2.5982327356
H	1.6569494439	.9462190850	-4.7327022351
H	-4.9908942509	-.5357292307	1.8838617836
H	-6.3844056452	-.3026817529	-.1453787478
H	-5.4872449570	.8597505112	-2.1333976320
H	-3.4586653113	1.8041811770	3.5804336033
H	-3.6462824996	.4406591266	-3.8912900548
H	-2.4566836991	.6444974597	4.4686766383
H	-2.8309537597	-1.8121973602	2.5432468103
H	-1.4836286507	-1.4338414894	1.4610085813
H	4.4154987928	2.1628437624	3.0530533826
H	4.5274679055	.4325574474	3.4083906697

H	1.5430851438	-.2854430304	3.3600451650
H	1.6707430313	-.1757951612	-3.3563772344
H	3.1608673064	.1406710874	-4.2635059264
H	2.7290451238	3.2457041504	-4.5310158249
H	-1.5527486094	.9483259689	2.2046398370
H	-1.2819620460	-1.2811294924	3.2231188909
H	-2.1095552567	2.4977844452	-2.2269816668
H	-3.5261833235	3.5852695200	-3.9135885992
H	3.5285261659	3.7426837068	-3.0304548693
H	4.2790110943	2.5292948399	-4.0737107790
H	1.3216849599	-.5404399122	1.6204057374
H	2.7496394407	-1.1909338857	2.4245880797
H	.6587912962	-4.3654732809	1.5527242654
H	2.4337212463	-4.3704348952	3.2765447340
H	4.7876545157	-3.8695995860	2.6460652042
H	.6306875224	-2.4479849380	-1.1738289896
H	-.0290620513	-4.2469622400	-.8157681057
H	1.2336759538	-3.9991014274	-2.1196599705
H	3.5845874899	-3.3832314505	-1.4522774115
H	5.3515383669	-3.3664068290	.2749542422
N	-1.5104097251	1.8010754126	-.0080917836
N	1.4253498621	1.8860095495	-.2337504829
O	-.8515300931	-.9362176282	-1.2355911610
O	.4877492845	-1.3216478534	-1.4521170396
Cu	-.0176437340	.6314508889	-.5524498869

80. L¹CuO₂ side-on / phenol t.s.

C	-2.5122206080	2.1469298313	-3.6082760647
C	-3.5622954864	2.0047038656	3.5245533028
C	-5.4655650414	1.4556248379	-.4061621272
C	-3.7520667887	4.3385586310	-3.2634713477
C	-2.2321386087	.2019533806	2.3316315816
C	2.6404138356	2.5760462401	-.3950235458
C	1.1541669169	4.3470528351	.3138106304
C	3.3719576279	1.9592177081	.6469778945
C	-2.9099286698	2.5463690803	-.1301539625
C	3.0773114398	4.2690955823	-3.6415708307
C	-.1062523576	4.9095331298	.5805250635
C	-1.3787765996	4.3247548574	.4361170152
C	2.3207252873	.3719586424	2.2901274655
C	3.1358347081	2.5977682169	-1.7199080393
C	-3.5040131617	1.8800318787	.9678795191
C	1.8457493144	2.0529531082	-3.8167050319
C	2.3672032390	5.2253518706	.5490117332
C	-2.5739505230	5.1836824240	.8048308476
C	4.6216804382	1.4087674192	.3439423046
C	4.3915029773	2.0334485561	-1.9702618466
C	-3.5715776413	2.6319171166	-1.3762967478
C	3.7764308063	2.2590388951	3.1541328743
C	-2.8973592178	3.2466823113	-2.5978685253
C	5.1357250229	1.4492419543	-.9497512521
C	2.7972460072	1.8188059833	2.0529817590
C	2.3191547975	3.1746833708	-2.8711526269
C	-4.7879141668	1.3498529423	.8058824096
C	-4.8537443111	2.0830717252	-1.4870265065
C	-2.7435605027	1.6563398481	2.2706500817
C	1.7178723476	-4.3152431871	-.6927916101
C	.9570423066	-3.1025609896	-.5834643465
C	.4996969270	-2.7007415722	.7201774612
C	.8096015260	-3.4638347403	1.8316052126
C	1.5643985836	-4.6406067600	1.7009518964
C	2.0101023524	-5.0596540715	.4314411686
H	2.0694108394	6.2279562062	.8580861125
H	2.9743106737	5.3008590558	-.3581584090

H	3.0127525672	4.7991777615	1.3230970984
H	-3.1606738642	4.7134682099	1.5995803131
H	-3.2452544202	5.3012008261	-.0512942711
H	5.1971145956	.9300156220	1.1308341019
H	6.1082663152	1.0153607764	-1.1633331373
H	4.7870776413	2.0439589898	-2.9818284022
H	-.0980991810	5.9292729112	.9419998898
H	-1.8986457810	1.3767541086	-3.1317231825
H	-4.0137996211	5.1322714112	-2.5557758664
H	-4.6852850527	3.9332546086	-3.6685963784
H	-1.9528630699	2.5748029782	-4.4481664536
H	-4.4248907073	1.3410826704	3.6461269528
H	1.9169846938	2.4646079696	2.1191918650
H	3.2886799484	2.2113405299	4.1336360857
H	1.4261385631	3.6384803859	-2.4434245966
H	1.1845093192	2.4564818996	-4.5915270862
H	-5.2602056635	.8356305713	1.6376852842
H	-6.4621463486	1.0367082119	-.5114475529
H	-5.3760895461	2.1400443136	-2.4375488594
H	-3.9354646042	3.0335967236	3.4914247684
H	-3.4053298736	1.6585421243	-4.0138924331
H	-2.2557532552	6.1712505823	1.1407805986
H	-2.9419275159	1.8987031556	4.4210467556
H	-3.0697164593	-.4996504480	2.4174462776
H	4.1254637312	3.2852164744	2.9994018307
H	4.6582994542	1.6112177088	3.1975084841
H	1.8214256739	.2829202979	3.2618299643
H	1.3049000096	1.2757370830	-3.2687566505
H	2.6957464947	1.5749538872	-4.3162153584
H	2.4421749466	4.6894531551	-4.4287133695
H	-1.8662579963	2.3092461746	2.2611166378
H	-1.5774973428	.0561606655	3.1988836624
H	-1.9707273982	3.7196221835	-2.2608899212
H	-3.2041271106	4.7944748106	-4.0951255307
H	-1.6823646957	-.0499671886	1.4202034292
H	3.3824425612	5.0867895620	-2.9803080747
H	3.9795679484	3.8754769188	-4.1216930736
H	3.1664549010	-.3246262235	2.2797876360
H	1.6246367749	.0534826001	1.5097760535
H	-.1038259101	-1.8040628633	.7953990958
H	.4587698809	-3.1551220543	2.8118771268
H	1.8002891556	-5.2336307348	2.5790337688
H	.5179636674	-1.1272446564	-1.3346446049
H	2.5894144724	-5.9738966368	.3412379724
H	2.0524486173	-4.6085093797	-1.6821259596
N	-1.5900778803	3.0857025873	-.0022837394
N	1.3325292009	3.1028992640	-.1284943880
O	.4613591536	-.0715600301	-1.0482060883
O	-.9362783222	.2324832845	-.9840566837
O	.6853080669	-2.4159107706	-1.6377732158
Cu	-.1206065363	1.8982189847	-.4983744955

81. L¹CuO₂ side-on / isopropylbenzene t.s.

C	3.1952461199	3.4242883778	-2.5861308645
C	-3.4518921894	1.4747913580	4.8224154460
C	-3.8627171853	2.8918704921	-2.2260386738
C	-2.0254442889	-.3802617319	3.8297643526
C	2.4235723527	-.3976068414	3.4869185118
C	2.6585786056	1.7758915509	.7311255564
C	1.1096075728	3.5357916802	1.2785144265
C	3.3929200079	1.1883523565	1.7858101386
C	-2.8937725408	1.5769482942	1.1194360513
C	-2.9425587518	1.9639378127	-1.4151844332
C	-2.6388938882	1.0164210738	3.6010894101

C	- .1635428607	4.0912498701	1.4851114026
C	-1.4194052853	3.4578363731	1.4213955087
C	3.1892697736	1.8420807006	- .5792858677
C	-3.4381861155	1.0286982942	2.3030649938
C	-5.4031130185	.3626866029	1.0367358397
C	2.2925191180	4.4780511471	1.4013665058
C	-2.6383450034	4.3276286240	1.6681759849
C	4.6667958168	.6799493676	1.5079643560
C	4.4658437747	1.3173854161	- .8057591337
C	-3.5773494494	1.4843738269	- .1140930856
C	1.8032577964	1.3066833379	-2.6168865445
C	3.7432381128	1.6266647987	4.2727959501
C	5.2044181066	.7426815696	.2257205049
C	2.8079657083	1.0647102015	3.1883559290
C	2.3864418529	2.4291502129	-1.7367053145
C	-4.7009796464	.4320100735	2.2377165816
C	-4.8376283512	.8769706841	- .1271099348
C	-2.4847073968	.7595847665	-2.2629786490
C	1.4247562009	-2.5981102310	-3.8400392447
C	1.0719976769	-2.5146804537	-2.4923982834
C	.7863556477	-3.6718359776	-1.7547433827
C	.8653539413	-4.9154405451	-2.4040697230
C	1.2239496749	-4.9982516365	-3.7490578731
C	1.5057087433	-3.8380540047	-4.4732511925
C	.4190940072	-3.6183968631	- .2959647947
C	-1.0334761952	-3.8686050751	.0371404190
C	1.4509508939	-4.1809075257	.6594427504
H	2.9985023333	4.1229213355	2.1582210117
H	-3.2076060356	3.9649070437	2.5294507833
H	-3.3160604893	4.2978773218	.8097090175
H	5.2443143547	.2254906329	2.3078316474
H	6.1953365268	.3436910963	.0292773323
H	4.8887198121	1.3568939521	-1.8052773682
H	-4.7614075468	2.3713062546	-2.5736467481
H	- .1833022370	5.1480674830	1.7163337653
H	2.8473524901	4.5372578049	.4600623074
H	-1.9368923354	1.0988790617	-3.1499285372
H	-1.8413861493	.0964632710	-1.6779231202
H	-4.2692427137	.7834659697	5.0534218060
H	-3.8888478076	2.4668032324	4.6662012345
H	-4.1857375370	3.7564982251	-1.6365808008
H	1.8873443069	1.6542581589	3.2146294178
H	3.2569070443	1.5829221851	5.2531884860
H	1.5403192588	2.9755583498	-1.3116457203
H	1.1663910210	1.7231435045	-3.4054396365
H	-5.1370850496	.0069014062	3.1368967412
H	-6.3834916217	- .1039663754	1.0055489556
H	-5.3793027632	.7967019368	-1.0651377034
H	1.9631955242	5.4815326482	1.6736573795
H	-3.3467957663	.1752386894	-2.6048313252
H	-2.3478807877	5.3631357783	1.8504434244
H	-2.8078023129	1.5247072056	5.7070061068
H	-2.8114025759	-1.1184963850	4.0271512013
H	-1.4727392144	- .7135819781	2.9467453098
H	3.6204218360	4.2252846975	-1.9725695640
H	4.0207931302	2.9360412606	-3.1145208402
H	4.0064945718	2.6706816926	4.0730604180
H	4.6758849094	1.0569735587	4.3430980155
H	1.9303393344	- .4757916388	4.4622481942
H	1.2024083042	.6102271426	-2.0245263286
H	2.6039910389	.7303234486	-3.0941506915
H	2.5511082521	3.8844853601	-3.3429901825
H	-1.8075844213	1.7170680994	3.4835923178
H	-1.3496255916	- .3684925898	4.6930797819

H	-2.0487677447	2.5378967654	-1.1546144844
H	-3.3377578720	3.2641698491	-3.1125163060
H	1.7458096910	-.7901399159	2.7224257945
H	3.3122357517	-1.0387713647	3.5058585710
H	1.2826667284	-5.9701679845	-4.2308955396
H	1.7842916262	-3.9015176864	-5.5210805894
H	1.0043603810	-1.5469530198	-2.0084099135
H	1.6379135951	-1.6871086704	-4.3923157614
H	.6496629029	-5.8251429282	-1.8494597067
H	.4612959458	-2.2153676639	.0488288223
H	1.1998569442	-3.9444973797	1.6980223439
H	2.4501135966	-3.7933855312	.4395794050
H	1.5002399818	-5.2773887998	.5709062455
H	-1.2013872095	-3.8618901216	1.1176464192
H	-1.3588021158	-4.8416966246	-.3596567031
H	-1.6740691811	-3.1005382053	-.4106259640
N	1.3284178436	2.2525684468	.9803576463
N	-1.5918241715	2.1650845072	1.1622706111
O	-.9145172834	-.7194552990	.48991111787
O	.4554100303	-1.1026070441	.2943572575
Cu	-.0910175529	.9467332494	.8288014355

82. L¹CuO₂ side-on / cyclohexadiene t.s.

C	-1.9875687575	.6870794210	-3.1871635481
C	-3.3044680042	1.1291143593	3.8589393797
C	-3.6896361847	2.5697929517	-3.1258040709
C	-1.6495612155	-.5875703650	2.9870073953
C	3.5129115822	3.9501882805	-3.0839769453
C	2.8888966734	2.3112509870	.2085203281
C	1.0544509124	3.8172092862	.5742083223
C	3.5757489286	1.8801216214	1.3671068843
C	-2.6177514500	1.3033039773	.2013723566
C	2.6937628622	.1728576781	2.9945800486
C	2.5869051402	1.5885677488	-3.1958035207
C	-.2976275950	4.1782533829	.7010839322
C	-1.4450916124	3.3725422057	.5772877077
C	3.5593740462	2.4297174592	-1.0310187444
C	-3.1130746111	.6540409277	1.3553727174
C	-4.9133790285	-.2743547976	.0076155155
C	2.0729851326	4.9215528009	.7922533133
C	-2.7839513639	4.0521065095	.8008746139
C	4.9418296332	1.5950910775	1.2644723759
C	4.9253200514	2.1315797499	-1.0818281518
C	-3.2467107585	1.1427616229	-1.0538513760
C	-2.6590499826	1.7662191850	-2.3155163313
C	-2.3822850037	.7370166525	2.6920435138
C	5.6182232542	1.7231376610	.0546520139
C	2.8540257390	1.6769216334	2.6957149543
C	2.8149418227	2.8243042269	-2.3024975981
C	-4.2676230729	-.1265034639	1.2323928414
C	-4.3985796244	.3522131662	-1.1247493304
C	3.5385725963	2.4031104850	3.8664601326
C	-.0180803659	-3.6681715378	-.9108119699
C	1.0696151370	-3.0984798636	-1.6983425436
C	.7576348864	-2.7371210091	-3.0831427570
C	-.4885193053	-2.8325331273	-3.5850659233
C	-1.6460153763	-3.3517200827	-2.7835669944
C	-1.2725607834	-3.7787399573	-1.3957087041
H	1.5794652194	5.8650697952	1.0286445089
H	-.4823305672	5.2182763760	.9360795749
H	-4.1619149281	3.3480170528	-2.5172353804
H	2.6926117545	5.0642400021	-.0984002182
H	-2.6523303698	5.1129684002	1.0180707204
H	-3.3210296883	3.5879425640	1.6336055098

H	-3.4245078749	3.9500445978	-.0803718252
H	5.4833662307	1.2656328762	2.1466142956
H	6.6802299288	1.5024560354	-.0032307597
H	-1.2642485090	.1087679496	-2.6056556036
H	2.7554293056	4.6698439836	1.6095277218
H	-4.4850382549	1.9299380555	-3.5227601084
H	-1.4716130721	1.1441531800	-4.0396993466
H	-4.0639204228	.3642711709	4.0532850916
H	-3.8250005336	2.0726177889	3.6636327785
H	-2.7201092257	1.2496393624	4.7776224673
H	-2.3669875520	-1.4028849256	3.1360572619
H	1.8491217760	2.0957465179	2.5944058650
H	2.9457711717	2.2901956677	4.7805759117
H	1.8301495333	3.1961353155	-2.0062287082
H	1.9872677028	1.8511367916	-4.0747533566
H	-4.6624252133	-.6323224131	2.1088507850
H	-5.8109022026	-.8819730401	-.0655762120
H	-4.8970219676	.2223904003	-2.0812689449
H	-2.7348173196	-.0106087139	-3.5839418431
H	5.4546073905	2.2203456312	-2.0261593100
H	-.9968162901	-.8638330436	2.1541157674
H	3.6771475096	4.8324032528	-2.4564713909
H	4.4860087761	3.6352226653	-3.4754037866
H	2.1876912903	-.3405367372	2.1711396549
H	3.6492295880	3.4741065189	3.6669799621
H	4.5356588576	1.9986820886	4.0707176523
H	2.1089694802	.0208832577	3.9087797177
H	2.0679137549	.7968752888	-2.6463850782
H	3.5415804979	1.1805191479	-3.5470666332
H	2.8995314266	4.2538164647	-3.9390970722
H	-1.6197439336	1.5160032800	2.6036924295
H	-1.0469369068	-.4994097513	3.8985466626
H	-1.8752539683	2.4620515522	-2.0039992716
H	-3.2043896158	3.0559650207	-3.9791353089
H	3.6703978909	-.3040043387	3.1356941417
H	-2.0625109769	-4.1858180098	-.7698994787
H	.2000361708	-3.9829309502	.1059867372
H	2.0716065947	-3.4940701332	-1.5123333313
H	1.2003698786	-1.9190269895	-1.0929252252
H	-2.4320058103	-2.5792452803	-2.7275186927
H	1.5649253888	-2.3549734268	-3.7030529639
H	-.6867855700	-2.5314625013	-4.6107572969
H	-2.1315023490	-4.1867764269	-3.3182240129
N	-1.4190706952	2.0758482613	.2842283045
N	1.4828284293	2.5867498899	.2821868419
O	1.0844877489	-.8476226204	-.4376531368
O	-.2984507557	-.6824575510	-.2662824056
Cu	.2654423109	1.1033793381	-.0132983609

83. L¹CuO₂ side-on / dopamine t.s.

C	3.1380884113	4.3430885436	-3.6380818907
C	-3.3438440090	1.3334809646	3.4880683067
C	-3.8514925304	3.0904418370	-3.4671722890
C	-1.7704157796	-.3834331808	2.4742613576
C	2.7468998307	.3853362924	2.3508450504
C	2.7801939113	2.6460222658	-.3227194493
C	.9860718033	4.1392130208	.2300569287
C	3.5472688875	2.1673914939	.7635400968
C	-2.7389842634	1.7107747492	-.1654453405
C	-2.8092139417	2.3089069935	-2.6513742319
C	-2.4620959455	.9809251617	2.2786913032
C	-.3536318817	4.5101154058	.4345254071
C	-1.5167762439	3.7289203573	.3012453776
C	3.3538123114	2.8099261328	-1.6029770776

C	-3.2250276814	1.0028333674	.9579009382
C	-5.0818923871	.2101125191	-.3991809315
C	2.0277838471	5.2207243397	.4531149418
C	-2.8386895626	4.4155904175	.5941194062
C	4.9029372927	1.8947435115	.5495828734
C	4.7127037884	2.5234595668	-1.7673378153
C	-3.3957518331	1.6370324597	-1.4154096305
C	2.1545091617	1.9980230543	-3.6529944477
C	3.6960532657	2.5479071579	3.2862512988
C	5.4884084700	2.0776606912	-.7003814498
C	2.9177557805	1.9014120660	2.1274845765
C	2.4992565362	3.2298538939	-2.7921734881
C	-4.4043686324	.2642518209	.8160255363
C	-4.5714700905	.8853883440	-1.5052141751
C	-2.0828596763	1.2690232347	-3.5284203619
C	.7243811149	-3.1267648890	-1.2918530595
C	-.7252933751	-3.2000395244	-1.2185917570
C	-1.5365103271	-2.5860366625	-2.2017400735
C	-2.9168002883	-2.6022575593	-2.0983068868
C	-3.5226000521	-3.2265952621	-.9937323936
C	-2.7420902038	-3.8137200572	.0026488837
C	-1.3567406910	-3.7941913836	-.1037718231
C	1.4458234617	-3.2949808719	-2.6161354248
H	2.6040597208	5.4022702804	-.4594748134
H	2.7471436635	4.9219305774	1.2213851863
H	-3.3655860663	3.9137831705	1.4113600928
H	-3.4995245255	4.3728048986	-.2771136001
H	5.5084683145	1.5301049233	1.3743337865
H	6.5439232498	1.8655608060	-.8447053438
H	5.1697636661	2.6482732542	-2.7445911891
H	-4.6048632368	2.4298896173	-3.9096155999
H	-.5137660766	5.5370229300	.7357030130
H	-4.3758123643	3.8283761911	-2.8504946903
H	-1.5853690396	1.7599365074	-4.3732723185
H	-1.3387826556	.7210196953	-2.9444278671
H	-4.1281289631	.5863370938	3.6515911619
H	-3.8318999107	2.3058348906	3.3633276504
H	-2.7371871764	1.3744313177	4.3993832293
H	1.9166435596	2.3415750793	2.1211676041
H	3.1661285505	2.3914379621	4.2320909915
H	1.5569145033	3.6210595239	-2.3990168470
H	1.4608975368	2.2686306197	-4.4571807552
H	-4.7938355581	-.2817792111	1.6708913081
H	-5.9969686455	-.3687035635	-.4871679280
H	-5.0897847430	.8225282140	-2.4572889559
H	1.5574545058	6.1556720662	.7603798899
H	-2.7907586890	.5330090789	-3.9245731236
H	-2.6841254935	5.4604336492	.8667887013
H	-2.5115923779	-1.1817514798	2.5974307479
H	-1.1548249081	-.6303800101	1.6052982784
H	3.3827279635	5.2191134871	-3.0281074054
H	4.0594604754	4.0106019732	-4.1278535930
H	2.1689414364	-.0697215535	1.5403149499
H	3.8134446066	3.6268408864	3.1401273804
H	4.6967911258	2.1171333828	3.3974387889
H	2.2303929835	.1908481940	3.2978168141
H	1.6951517694	1.2078426068	-3.0509725275
H	3.0583132046	1.5786795081	-4.1094093614
H	2.4472152792	4.6626067021	-4.4256134451
H	-1.6741791577	1.7366586017	2.2169232787
H	-1.1390447548	-.3699294099	3.3707242730
H	-2.0592473318	3.0278959156	-2.3103578824
H	-3.3628060680	3.6230816436	-4.2900736138
H	3.7211850479	-.1151565179	2.3882234897

H	.8958675344	-1.7643107147	-1.0361646072
H	1.2377942292	-3.6021659182	-.4513813791
H	-1.0952150420	-2.0621097504	-3.0401639136
H	-3.2227370656	-4.2844877395	.8572462902
H	-.7489668155	-4.2406771038	.6769269770
H	1.0596477362	-2.5739000742	-3.3446873451
H	1.2034384137	-4.2991630644	-3.0170779630
H	-4.5984517752	-2.0227719881	-2.7521339364
H	-5.2234419257	-3.5654900516	-.1558723882
H	3.3391398481	-3.0702488823	-3.3686957098
H	3.3060831388	-3.7858356821	-1.9044970866
N	1.3835010417	2.9203429673	-.1441572387
N	-1.5210384976	2.4499967206	-.0611735298
N	2.8808874214	-3.0475492870	-2.4615393236
O	-.5256168315	-.2510216106	-.8318772194
O	.8490713130	-.5709578490	-.9243469236
O	-4.8943085432	-3.1893305692	-.9817003718
O	-3.6802441849	-2.0113028077	-3.0595428188
Cu	.1416604048	1.4715970779	-.4779970938

84. L¹CuO₂ side-on / formylglycine t.s.

C	2.9961154213	1.7177873744	-2.6350705789
C	-2.9312155657	.7907631582	3.7663238048
C	3.8430823917	2.6723145702	-3.4960689370
C	2.4272631327	.0258248648	3.0848390477
C	2.8680013571	1.5991591490	-.0778905993
C	-2.7225365961	1.0690873220	.0578025039
C	-4.1725159781	2.3565328650	-3.1462924256
C	1.1632147472	3.2692655373	.0457061664
C	-1.3706198383	3.0507224165	.2185908945
C	3.4595119192	1.3250129031	1.1799210010
C	-3.1019483214	.4072967698	1.2465553922
C	-.1480536227	3.7587370822	.1854644426
C	3.6201645945	1.4592009238	-1.2676864964
C	-3.4980333253	.9527129957	-1.1195111937
C	-1.4684581875	-.9353540337	2.6106617065
C	2.7287243391	.3950595717	-3.3786033177
C	2.2696331406	4.3108211045	.1343529034
C	-2.6217345125	3.8614393795	.5174418975
C	4.8001435939	.9273134339	1.2203499760
C	4.9562630349	1.0535714647	-1.1743826105
C	-4.2860694254	-.3374434166	1.2487204438
C	-4.6706618161	.1918925001	-1.0701562298
C	3.3306321666	2.3541623094	3.5117912533
C	-3.0446413731	1.6011526215	-2.4245662170
C	5.5511138884	.7933133014	.0565721679
C	2.6669349489	1.4221806612	2.4809349464
C	-2.3921711072	.5610662258	-3.3554924389
C	-5.0707690679	-.4452528351	.1030221851
C	-2.1920921160	.4186904922	2.4697289400
C	-.1683107780	-3.7295365622	-2.1436298714
C	.7251790937	-4.7696097910	-1.3690971685
C	-2.5498139164	-3.0935483669	-2.1875751623
H	-.2303907096	4.8290946411	.3285603773
H	-2.3851426543	4.9185758192	.6527103314
H	1.8523302162	5.3117887176	.2575606056
H	4.8132634028	2.2348639174	-3.7564747047
H	4.0345914918	3.6194629169	-2.9794559183
H	2.8896985136	4.2974601474	-.7679179532
H	2.9409554512	4.1108398851	.9742124904
H	-3.1112369479	3.4914128459	1.4243231430
H	-3.3519633171	3.7659847213	-.2920839618
H	5.2612646956	.7144008456	2.1813407126
H	6.5910876868	.4827174822	.1084153373

H	-1.5927863851	.0247970726	-2.8394390307
H	-4.5866216060	-.8566711787	2.1549100327
H	-5.9838235856	-1.0345872799	.1196879703
H	-5.2719903569	.0831357823	-1.9681212716
H	3.3734580801	-.4550201137	3.3576738408
H	1.9116622907	-.6279594988	2.3762757846
H	-3.6839265574	.0415499216	4.0360959947
H	-3.4398992836	1.7572083049	3.6770887368
H	-3.1130653845	-.1930983289	-3.6838935699
H	5.5407427379	.9378691229	-2.0828230846
H	-1.9783444467	1.0526984226	-4.2452527961
H	1.6874639312	1.8438620523	2.2418741376
H	2.6958902869	2.4519010957	4.3999859121
H	2.0293070099	2.2007742101	-2.4669763842
H	2.2592698269	.5907488270	-4.3499152348
H	-1.4275688556	1.1820519734	2.3010434714
H	-.7258079597	-.8958603457	3.4162633847
H	-2.2704596921	2.3318406048	-2.1742599051
H	-3.7742055938	2.8741129210	-4.0263712914
H	-4.9551962958	1.6763246879	-3.4998333091
H	-4.6456412564	3.1021098367	-2.4972758150
H	-2.2233513554	.8560259814	4.6006652436
H	3.4938650679	3.3575355623	3.1045689599
H	4.3016402679	1.9691949883	3.8427736694
H	1.8147103847	.0996977145	3.9912179507
H	2.0632982216	-.2547038136	-2.8035292600
H	3.6631241514	-.1493430017	-3.5573770872
H	3.3241987506	2.8969334145	-4.4346545148
H	-.9687886523	-1.2104115598	1.6774595727
H	-2.1827778067	-1.7316224216	2.8519171206
H	-.1085193785	-3.6281466088	-3.2266261899
H	-3.3920511569	-3.0366099494	-1.4760476675
H	-1.4203915063	-3.9763430746	-.6402959986
H	.4007010270	-2.5290149300	-1.6875745328
N	1.4904668405	1.9865370852	-.1440927269
N	-1.4730920755	1.7483954992	.0118809967
N	-1.4274239243	-3.6423004362	-1.6117355036
O	.5677765456	-1.4835714712	-1.1905589242
O	-.7197101775	-1.0833411867	-.7540674271
O	1.7097786572	-5.1644956434	-2.0160974292
O	.2743278544	-5.0460938755	-.2328174993
O	-2.6326443168	-2.7396268441	-3.3515171445
Cu	.1159124802	.5916636921	-.4270035484

85. L¹CuO₂ end-on / methane complex

C	-8.1242402536	-4.1453652033	-2.2561706430
C	-5.9840474665	-.8697713260	-.2417957275
C	.2564778210	-4.6493790512	-7.1907381654
C	-.3920165838	-3.6714746662	-.1095394418
C	-.1434953875	-3.7786039253	-3.6256555945
C	-5.6397014540	-3.2141817275	-3.1392254530
C	-6.9002365701	-4.3322597234	-6.4636578656
C	-1.5324953590	-1.9169879101	-4.3358770559
C	-4.0600515667	-1.6665332147	-4.1464776051
C	.5969011695	-3.6312340487	-2.4266907520
C	-6.1015378758	-2.8576173289	-1.8472784966
C	-2.7635318316	-1.2532009519	-4.5119709490
C	.2908981697	-4.6664738720	-4.6408366609
C	-6.4066631162	-4.0635267573	-3.9757269146
C	-4.6362410314	-2.9718035420	.1991238827
C	-1.1064780434	-6.3563393761	-5.9015007220
C	-.2861805751	-1.2064264307	-4.8315111883
C	-5.2096983940	-.7323213983	-4.4715522465
C	1.7909867067	-4.3451300625	-2.2896545941

C	1.4931114374	-5.3567316126	-4.4523979348
C	-7.3501701930	-3.3306913587	-1.4339672919
C	-7.6487277302	-4.5093575944	-3.5124253253
C	1.1329412297	-1.7565060295	-.7789758396
C	2.2452849836	-5.1971281193	-3.2928338901
C	.0895497949	-2.7760825039	-1.2699177197
C	-.5356127697	-4.9224520101	-5.8987162826
C	-5.4409657536	-6.0150041800	-5.2489771961
C	-5.2351603467	-2.0501264727	-.8841549945
C	-5.8836963780	-4.5380954128	-5.3270798513
C	-2.3431731940	-10.6723986488	-2.2386577471
H	-4.8615253202	.1503503716	-5.0095638074
H	-2.7035510465	-.2869861271	-4.9961512463
H	-.5344394027	-.2493411396	-5.2927045343
H	-1.1504508837	-4.3871527035	-.4426555609
H	1.0993100257	-5.3402028246	-7.3034231803
H	.6581092595	-3.6307746507	-7.2124089602
H	.4402442293	-4.2463001393	.3123753216
H	-5.0233741830	-6.3439622737	-6.2073925944
H	.2466573807	-1.8228697276	-5.5620469188
H	.4084550788	-1.0278852480	-4.0042399555
H	-4.6796740964	-6.1745502696	-4.4776563583
H	-5.9603595699	-1.2449025640	-5.0814058173
H	2.3692088041	-4.2436630290	-1.3754643920
H	3.1730248057	-5.7477970738	-3.1632177195
H	1.8385901814	-6.0414528292	-5.2220675609
H	-7.7168431358	-3.0714019710	-.4447846133
H	-9.0889734187	-4.5077280892	-1.9120362947
H	-8.2487958957	-5.1618517069	-4.1405601450
H	-6.7999800729	-1.2052796748	.4074529283
H	-6.4134297793	-.2055049894	-.9991108754
H	-6.2899545788	-6.6663238797	-5.0118327472
H	-5.7164540616	-.4072361422	-3.5564571573
H	-.7767401569	-2.2111615217	-1.6272335595
H	.7004904056	-1.1147855067	-.0034985173
H	-1.3856182803	-4.2341847992	-5.8844838584
H	-1.7549107252	-6.5092490348	-6.7721934439
H	-4.3990086569	-1.6349749356	-1.4541359972
H	-3.9533456072	-2.4121014001	.8484344357
H	-4.9981646589	-3.9431057487	-5.5687799419
H	-6.4512264551	-4.6061540254	-7.4245604032
H	1.4831558279	-1.1137330620	-1.5934644573
H	2.0099415054	-2.2474805380	-.3435779358
H	-.8220121447	-3.0635364954	.6948635960
H	-1.6905340050	-6.5583249172	-4.9980204268
H	-.3034693318	-7.1005927714	-5.9514378697
H	-.3903090694	-4.7758156356	-8.0660158444
H	-4.0783534525	-3.8057192022	-.2399682043
H	-5.4248694746	-3.4002506361	.8278039841
H	-5.2994662360	-.2796265877	.3770273572
H	-7.2279528767	-3.2893674840	-6.5280786597
H	-7.7925432484	-4.9541845008	-6.3326684822
H	-2.2827273567	-9.5847420424	-2.3171436940
H	-3.0783801821	-11.0508342889	-2.9526581989
H	-2.6442294382	-10.9487805938	-1.2257601689
H	-1.3666477205	-11.1113536725	-2.4579843419
N	-4.3282348533	-2.8226799065	-3.5466933983
N	-1.4001895695	-3.1160080652	-3.7720567415
O	-2.7632139442	-5.6335861971	-2.1360156513
O	-2.6559319560	-6.8096672576	-2.6223754486
Cu	-2.9428539743	-4.0565868552	-3.0891356484

86. L¹CuO₂ end-on / cyclohexane complex

C	5.0236654461	4.3577831906	-7.2457230176
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C	-.4751113240	7.4153525917	-1.0111400165
C	5.9960421243	4.8290517774	-8.3438327269
C	4.7774679098	3.8066390336	-1.3222943646
C	5.3147621047	4.6928258927	-4.7057243556
C	-.0892234620	5.9086893189	-4.4258121028
C	-1.1084991519	5.8962877669	-8.0136439994
C	4.2495125525	6.8640304232	-4.9045342844
C	1.7668402368	7.4279122329	-4.8337154792
C	5.9507675376	4.3681448248	-3.4801485949
C	-.6400850761	5.9743057137	-3.1199365803
C	3.1370600049	7.7275388340	-4.9665681279
C	5.7309154515	4.0900854131	-5.9200366803
C	-.8559168792	5.4318516696	-5.5170528846
C	.5955890645	5.1174401832	-1.0970288909
C	4.2380666281	3.1152409013	-7.7127321599
C	5.6216985016	7.4907293796	-5.0750223058
C	.7839826920	8.5772508745	-4.9480477131
C	7.0198288386	3.4677829941	-3.5033841572
C	6.8043732180	3.1933553222	-5.8834057148
C	-1.9724322582	5.5907889409	-2.9430021804
C	-2.1837673083	5.0599948141	-5.2830058410
C	6.5826380977	5.5910743545	-1.3318177305
C	-.2457010826	5.2669006318	-6.9055106812
C	7.4507825991	2.8849761752	-4.6915328260
C	5.4615774631	4.9194430009	-2.1445175925
C	.0346773160	3.7787124960	-7.2089927042
C	-2.7437296290	5.1413237955	-4.0115228964
C	.2058124840	6.3691057103	-1.9112305244
C	4.2516769471	-3.3867317936	-2.0341079398
C	2.9364460186	-4.1815192265	-1.9769929046
C	2.1570303493	-4.0771603425	-3.2985278930
C	1.9178061708	-2.6111955820	-3.6998247781
C	3.2349052381	-1.8196409496	-3.7594179132
C	4.0092219873	-1.9211995790	-2.4348400538
H	6.7214530716	4.0502886923	-8.6040158347
H	6.5599048909	5.7154731371	-8.0347449444
H	6.1522851269	7.0427081460	-5.9205346916
H	6.2371943955	7.3110026732	-4.1873620996
H	.2216410605	8.7008469849	-4.0167034838
H	.0494926359	8.3775596432	-5.7350792872
H	3.3700841236	8.7705767420	-5.1375090277
H	8.2791718199	2.1819894235	-4.6853134574
H	7.1326451067	2.7203505073	-6.8048109208
H	-2.4101814108	5.6297914573	-1.9494729999
H	-3.7756455279	4.8423853667	-3.8501229146
H	.7107957264	3.3276272241	-6.4744950126
H	1.2954564196	9.5141621636	-5.1731632492
H	5.5470773529	8.5668183615	-5.2370168484
H	-1.3823914679	7.0234352343	-.5390636493
H	-.7543314505	8.3117174114	-1.5746666606
H	-.8940984440	3.1965202537	-7.2022233441
H	7.5163789412	3.2079159918	-2.5724781562
H	3.9653073209	3.3336108401	-1.8833072792
H	4.7081776519	5.6841424391	-2.3545918088
H	6.1762498594	6.0269827928	-.4124608415
H	4.2976349900	5.1593909984	-7.0829383006
H	3.6951318517	3.3323947965	-8.6400838893
H	1.1334703550	6.8137756176	-2.2818280112
H	1.2579166167	5.3860428262	-.2660177448
H	.7170436333	5.7868687843	-6.9080396965
H	-.5911302509	5.8324611485	-8.9770793201
H	-2.7865103619	4.6899197770	-6.1074761423
H	5.4929921152	3.0200672475	-1.0562063100
H	.4936280831	3.6672446282	-8.1982123025

H	-2.0698417234	5.3833641967	-8.1264093206
H	-1.3165005006	6.9520868362	-7.8106304600
H	7.0674793872	6.3923556907	-1.8993973461
H	7.3588519850	4.8761530920	-1.0379510401
H	4.3627764622	4.2115581406	-.3921224502
H	3.5146910088	2.7895116641	-6.9588005138
H	4.9125681991	2.2748935908	-7.9111614868
H	5.4449395826	5.0808629446	-9.2565312382
H	1.1139604868	4.3783635016	-1.7171858214
H	-.2911770278	4.6292031309	-.6770177424
H	.2030815976	7.7205189272	-.2065849340
H	3.1368425104	-5.2330914452	-1.7354682170
H	2.3139980390	-3.7882436665	-1.1598548595
H	2.7290775770	-4.5790893157	-4.0928556477
H	1.2024840036	-4.6126533122	-3.2186954594
H	1.4006394856	-2.5621998791	-4.6660465969
H	1.2475303596	-2.1416085709	-2.9649485992
H	3.0447367517	-.7711650021	-4.0193153947
H	3.8597603528	-2.2308361368	-4.5668614563
H	4.9635238326	-1.3854281143	-2.5108874303
H	3.4348737031	-1.4209902264	-1.6412519706
H	4.7684554095	-3.4388937309	-1.0674993413
H	4.9218935140	-3.8549379189	-2.7701674425
N	1.2954531366	6.2027093835	-4.6172550747
N	4.1720926696	5.5508787899	-4.7021837174
O	2.3952120759	2.8985905053	-3.9861249545
O	2.4081758364	1.9429123398	-4.8358045384
Cu	2.4551692602	4.6975206742	-4.4447329826

87. L¹CuO₂ end -on / acetonitrile complex

C	1.4639317947	-1.8508694749	-5.9191800803
C	-3.2605035734	2.4712011778	.0822584624
C	2.0598985319	-1.4221404707	-7.2754290115
C	2.7393652107	-.4266256417	-.3077669764
C	2.3876152474	-.7335874786	-3.7853380860
C	-2.9615360970	.7231508621	-3.1864870174
C	-4.0655247157	.5452790012	-6.7766880934
C	1.3287499166	1.3886685694	-4.2656622861
C	-1.1057018896	2.0894333543	-3.9392278481
C	3.3547399541	-.6583525581	-2.7435216566
C	-3.4923860107	.8577985919	-1.8813292464
C	.2422893813	2.2849164060	-4.3047893492
C	2.4919424763	-1.7256404813	-4.7982191027
C	-3.7588352526	.2397672978	-4.2544064925
C	-2.2908150742	.1291246991	.2200655499
C	.8744167522	-3.2715441923	-6.0044175018
C	2.6491349430	1.8992379344	-4.8168947252
C	-2.0670069215	3.2332443023	-4.1978615182
C	4.4451737024	-1.5282202580	-2.7878460679
C	3.6095626352	-2.5703489531	-4.7920907525
C	-4.8333906873	.5176210613	-1.6727970877
C	-5.0918681030	-.0873751459	-3.9895253621
C	4.4914067579	1.1156130130	-1.2947391953
C	-3.1756356092	-.0010110735	-5.6456160347
C	4.5839987830	-2.4702499239	-3.8081424430
C	3.2071761129	.3154501701	-1.5774799175
C	-2.8800768830	-1.5004894998	-5.8560883153
C	-5.6308952933	.0512602638	-2.7133429257
C	-2.6262810840	1.3142286118	-.7098974714
C	2.8580334527	-5.8063188469	-.3717799518
C	3.0686371645	-4.3975211529	-.6865385230
H	.4703773658	3.2608538366	-4.7135315960
H	-1.5339108757	4.1325589328	-4.5098884169
H	2.5177859397	2.8545999728	-5.3269222498

H	2.8901564356	-2.0741753463	-7.5693547377
H	2.4382571861	-.3948634981	-7.2469669894
H	1.8125360814	-.9788562414	-.4863592106
H	3.0818157342	1.1796069477	-5.5176041022
H	3.3780974553	2.0357471196	-4.0114638897
H	-2.6492320465	3.4596656618	-3.2992770619
H	-2.1986045804	-1.8841839928	-5.0888521926
H	5.2029916855	-1.4720671356	-2.0117149834
H	5.4479666499	-3.1296654661	-3.8270374311
H	3.7131446799	-3.3186935888	-5.5725360541
H	-5.2582827960	.6123294123	-.6775143225
H	-6.6685754224	-.2122626960	-2.5291145466
H	-5.7168245912	-.4671938520	-4.7926477667
H	3.5000377146	-1.1426721769	.0241133256
H	-4.1871174801	2.1672257166	.5806746759
H	-3.4954601211	3.3204104368	-.5679142937
H	-3.7994701299	-2.0947777170	-5.8091992478
H	-2.7849799239	2.9682124590	-4.9807702892
H	-2.4174381912	-1.6713235873	-6.8350853682
H	2.4235876638	1.0329229991	-1.8371510872
H	4.3027865825	1.8714019722	-.5248269547
H	.6420556646	-1.1661628310	-5.6910991388
H	.0913745239	-3.3095456380	-6.7701258875
H	-1.6820698007	1.6827951349	-1.1218463818
H	-1.6334066545	.4508425375	1.0358151042
H	-2.2180417772	.5232827282	-5.7061174207
H	-3.5587059383	.4349559421	-7.7416341048
H	4.8580070034	1.6288323322	-2.1898695999
H	5.3000544770	.4749911596	-.9268917234
H	2.5695304714	.2825958743	.5104783308
H	.4429466394	-3.5684572929	-5.0453142036
H	1.6354525491	-4.0109281518	-6.2782666407
H	1.2995421833	-1.4779847195	-8.0623931047
H	-1.7848612312	-.6783898809	-.3203773355
H	-3.1989614100	-.2921868415	.6657080679
H	-2.5718654143	2.8204050971	.8593379389
H	-4.2925718903	1.6071511073	-6.6343214834
H	-5.0176471119	.0088816683	-6.8478678530
H	3.9354748971	-4.2833883777	-1.3435436806
H	3.2516508855	-3.8336760579	.2334150522
H	2.1924227503	-3.9762116022	-1.1931836908
N	1.2726075617	.1413853058	-3.7974651205
N	-1.5681643295	.9636741679	-3.4018090112
N	2.6961809407	-6.9279862378	-.1202638217
O	.0807518998	-2.0030050081	-2.0542445491
O	.6937210431	-2.9851144081	-2.6199869852
Cu	-.4027047081	-.4756885771	-2.9688042926

88. L¹CuO₂ end-on / toluene complex

C	2.9628869060	1.9758608965	-5.0045806388
C	-3.1958803422	.1302015447	-6.3865160096
C	-2.9317658046	-1.3925290698	-6.3218879406
C	-3.0088726806	3.2485376361	-.8926920801
C	2.3471309391	-.6795716468	-4.1832709470
C	-2.8845207105	1.2163321859	-4.0798111279
C	2.8262809026	-1.0424049590	-7.7893142322
C	1.5335356457	1.5479271626	-4.7212808763
C	-.8700739214	2.4131572672	-4.7615168956
C	3.0121391280	-.8748428080	-2.9450737075
C	-3.3784730681	1.5744468407	-2.7972913410
C	.5260870585	2.5119503263	-4.9326639148
C	2.6282680294	-1.5104274885	-5.2978001048
C	-3.7394156427	.6415371938	-5.0541869693
C	1.9843973730	-.9559659740	-.6338792657

C	3.8804858781	.6641650470	-1.1032101876
C	-4.1117288847	.4756129971	-7.5727629106
C	-1.7053127109	3.6379231842	-5.0807129906
C	3.9883484823	-1.8712955734	-2.8670200466
C	3.6197682659	-2.4892577824	-5.1635915269
C	-4.7395376607	1.3899932131	-2.5367205546
C	-5.0929425435	.4800428102	-4.7399695582
C	-2.1147416751	.8813656545	-.7305224713
C	1.0660359349	-2.6506902350	-6.9357740306
C	4.3015956062	-2.6689963952	-3.9651876053
C	2.6609909998	-.0645152048	-1.6979840246
C	1.8800125767	-1.3799289054	-6.6221194587
C	-5.5952489755	.8578589968	-3.4977654653
C	-2.4505394962	2.0505495459	-1.6817801362
C	-1.6331353161	-8.7829674391	-2.2111866922
C	-.4044921825	-9.0481661347	-1.6049472583
C	.5997408023	-8.0799528666	-1.6046112978
C	.4036776048	-6.8311716887	-2.2103561789
C	-.8388396934	-6.5751569860	-2.8099483169
C	-1.8457935396	-7.5421475753	-2.8132700804
C	1.5113134577	-5.8022437597	-2.2374883314
H	.8796119006	3.4736835611	-5.2818444092
H	3.4120979625	1.3429072657	-5.7752270101
H	3.5795473109	1.8643790602	-4.1072288540
H	3.5494241774	-1.8459475349	-7.9663223092
H	1.0942323625	-1.4470141071	-1.0348701062
H	3.0074094972	3.0150524093	-5.3336624113
H	-2.4810030020	3.3930204658	-5.8133938562
H	4.5080034692	-2.0329013850	-1.9267366755
H	5.0639165993	-3.4382472106	-3.8803156565
H	2.6672335858	-1.7377231602	-.2823151415
H	-5.1346576549	1.6531526549	-1.5592499886
H	-6.6486994669	.7207836415	-3.2708659213
H	-5.7622401593	.0443811560	-5.4756957276
H	-2.2218138911	3.9980738905	-4.1844092855
H	3.3912200474	-.1232024884	-7.6038773277
H	-3.9127878151	2.9858739602	-.3319300698
H	-3.2577081326	4.0869501262	-1.5513956168
H	-3.8536329425	-1.9437466252	-6.1045872046
H	1.9377590960	.7020697349	-1.9926605331
H	3.5751695666	1.2875817607	-.2557821262
H	1.1697315453	-.5532789348	-6.5239790805
H	.4890332774	-2.5136209537	-7.8579709568
H	-1.5110197479	2.3708013858	-2.1394559907
H	-1.4045609521	1.2007133941	.0406685741
H	-2.2322266279	.6186727172	-6.5640650690
H	-3.6305078753	.1897966181	-8.5138659894
H	-2.2115898886	-1.6524512295	-5.5383629339
H	-1.0901277809	4.4475194119	-5.4761897388
H	4.3646994201	1.3119209367	-1.8417582494
H	4.6351371321	-.0393785682	-.7347358302
H	1.6879100818	-.3579226553	.2360334696
H	.3742278553	-2.8837402966	-6.1224547074
H	1.7195965565	-3.5177982707	-7.0820870113
H	2.2535060417	-.9040491842	-8.7129403840
H	-1.6712944380	.0351172900	-1.2667997925
H	-3.0165352036	.5142110503	-.2279661772
H	-2.2683653614	3.5986199777	-.1657552391
H	-4.3281704612	1.5481144618	-7.6144786354
H	-5.0681433529	-.0565485779	-7.5241191697
H	-2.5314424317	-1.7598617198	-7.2740551997
H	3.8491774427	-3.1296600046	-6.0105435447
H	-1.0179737010	-5.6094630463	-3.2783243498
H	-2.8011442860	-7.3243277645	-3.2840285026

H	-2.4184464046	-9.5344340836	-2.2114345018
H	1.1130775426	-4.7898074245	-2.3210249304
H	2.1742193378	-5.9585252195	-3.0983302262
H	2.1328635663	-5.8617948182	-1.3375672110
H	1.5533259389	-8.2943608993	-1.1263948113
H	-.2281706131	-10.0092399236	-1.1283572443
N	1.3219446319	.3046919165	-4.2907138605
N	-1.4808857890	1.3117332668	-4.3354498885
O	-.4840511637	-1.8993098776	-3.0702804509
O	-.2091357039	-2.9579926392	-3.7390520820
Cu	-.4914353681	-.2350545745	-3.8691021541

89. L¹CuO₂ end -on / phenol complex

C	-.3342408187	1.7702673474	-2.2180474575
C	-.2234573437	4.2646093637	-.4467205960
C	-7.5114807092	2.8083996727	-5.6284552440
C	-7.3368162569	6.2590074651	.6200321611
C	-2.1026688798	2.9520700150	-3.3631824619
C	-7.3125886442	4.7568398067	-2.7712320434
C	-2.0200799596	2.6108495755	-6.9929658466
C	-2.9698243610	5.1938285510	-3.7108079330
C	-5.3507947911	6.0478705525	-3.4123843390
C	-1.3101119148	2.7692453621	-2.1998230197
C	-7.7839671004	4.8162751335	-1.4347858559
C	-3.9842939441	6.1743534444	-3.7210675191
C	-1.9381911918	2.1160691598	-4.4983532009
C	-8.1935683580	4.4486805379	-3.8407324370
C	-2.1379093063	2.7284720699	.1907215637
C	-1.5785344345	5.6431253641	-4.1195924812
C	-6.2174859163	7.2861877149	-3.5291727550
C	-3.6462006424	.9558069352	-5.9710905575
C	-6.6310271871	3.8207734323	.5853394233
C	-.9356049167	1.1424049978	-4.4649397976
C	-9.1418939167	4.5763326949	-1.1992629988
C	-9.5413013080	4.2175915615	-3.5474165852
C	-8.5814684087	5.0078281408	-6.3060663924
C	-7.6872468052	4.2996030882	-5.2730824313
C	-.1388558356	.9665962052	-3.3387577060
C	-1.5216814035	3.5916327902	-.9307585877
C	-2.8271322525	2.2413146440	-5.7334448609
C	-10.0166833398	4.2820225890	-2.2402538502
C	-6.8485831809	5.0937720564	-.2603105463
C	-2.4474867623	-2.6675691189	.7827557407
C	-3.1702663601	-1.8643842674	-.1098697726
C	-4.5234912805	-2.1432563464	-.3519351216
C	-5.1388688168	-3.2124487375	.2980608591
C	-4.4239578720	-4.0134817682	1.1894601670
C	-3.0756039551	-3.7319069398	1.4243237850
H	-1.5863724398	6.6746332796	-4.4745137758
H	-3.6649741937	7.1646620198	-4.0185202601
H	-1.1805244738	4.9986586073	-4.9083976632
H	-.8880773381	5.5697561121	-3.2731631948
H	-6.7356753555	7.4822513977	-2.5846880722
H	-6.9919693913	7.1507089962	-4.2910980952
H	.2736956685	1.6039152423	-1.3337347377
H	.6219133325	.1914386414	-3.3248170685
H	-.7914307768	.4978694851	-5.3275806449
H	-8.2841216576	6.0269087810	1.1184317916
H	-11.0667928879	4.0957415868	-2.0326932706
H	-10.2288051659	3.9753601027	-4.3522969401
H	-7.4847172740	7.1714404290	.0328571428
H	-1.4870488873	1.8866283251	.4481649947
H	-8.4696245095	2.2782865126	-5.5865212664
H	-6.8279584407	2.3098308780	-4.9324548637

H	-3.1008588868	2.3095850174	-.1119517586
H	-2.2365388976	4.3880014249	-1.1608895414
H	-.4298535855	4.9115072387	.4129636695
H	-3.5379183785	3.0525307281	-5.5507036655
H	-4.3419421060	1.0953393811	-6.8065783050
H	-5.8772785044	5.3844228704	-.6709580169
H	-5.9291888679	4.0166634405	1.4038588965
H	-6.6976654655	4.7613176492	-5.3299897362
H	-8.1226787214	4.9577151460	-7.2993091539
H	-1.2990862500	1.8273808034	-7.2511328869
H	-5.6219111846	8.1617737441	-3.7913196132
H	.2338151625	4.8788410479	-1.2297815658
H	.5205866353	3.5264836247	-.1286548771
H	-2.2902838575	3.3301801867	1.0942500120
H	-4.2161036753	.6831301365	-5.0788411190
H	-2.9964528374	.1090968208	-6.2201582662
H	-2.6895970169	2.7388539791	-7.8510426358
H	-6.2257355247	2.9967520058	-.0122826424
H	-7.5726046890	3.4745864220	1.0265680221
H	-6.6013203787	6.4761401936	1.4021516330
H	-8.7289388025	6.0634892527	-6.0549186620
H	-9.5703201175	4.5434327544	-6.3825392223
H	-7.1054745445	2.6942771536	-6.6397534366
H	-9.5197088271	4.6153419093	-.1814461061
H	-1.4622093230	3.5436331712	-6.8596041672
H	-5.0786714875	-1.5220119216	-1.0490915047
H	-6.1884871986	-3.4186739604	.1031118587
H	-4.9088335217	-4.8446231308	1.6931707432
H	-3.1242753531	-.3604816846	-1.3125587567
H	-2.5055073281	-4.3484016105	2.1149221980
H	-1.4004188302	-2.4403238540	.9572719372
N	-5.9121881353	4.9041554827	-3.0254265106
N	-3.1457497226	3.9200287019	-3.3692353061
O	-4.6541443506	1.6270878801	-1.9051926216
O	-4.0982331945	.6429832486	-2.5538205006
O	-2.5164299738	-.8372750895	-.7112044007
Cu	-4.8988104356	3.3221383719	-2.7356840426

90. L^1CuO_2 end-on / isopropylbenzene complex

C	4.1604811340	-1.3064478326	-3.1190789962
C	-2.13774817956	.5246228747	-.9368189554
C	1.4230093664	-2.2293867007	-7.2614482981
C	-2.8407853873	-1.3709238701	-6.8097896008
C	2.4581082631	-.2355503834	-4.4653763756
C	-2.9321029490	1.0350632660	-4.2764822219
C	-3.2544692353	2.8000717769	-.9661691387
C	1.4062013525	1.9113503081	-4.9131015997
C	-1.0747212082	2.5025284924	-4.8729742695
C	3.0943246319	-.4074964575	-3.2079156255
C	-3.4568209553	1.2166324340	-2.9706541164
C	.2972316507	2.7718359516	-5.0545947874
C	2.8656275533	-.9944024665	-5.5917498100
C	-3.7171231694	.4523345355	-5.3016282483
C	3.0989681068	-.5110922852	-8.0823649417
C	2.7802811408	2.5023222190	-5.1696003230
C	3.7286069768	1.0996900581	-1.2507314818
C	-2.0508987676	3.6416289786	-5.0886616680
C	-4.0175598052	.6315883968	-7.8301340277
C	3.9394654884	-1.8801656018	-5.4446895843
C	-4.7824756322	.8444266120	-2.7310049887
C	-5.0369391041	.0955792235	-5.0060813386
C	1.9643952695	-.7011955816	-.9712278184
C	-3.1299680021	.1395336303	-6.6742502085
C	4.5896259366	-2.0346819392	-4.2254853346

C	2.6104412504	.3045443452	-1.9478506329
C	2.1489771780	-.9074398375	-6.9366830819
C	-5.5723876573	.2937983098	-3.7369421072
C	-2.5825593882	1.7110044267	-1.8194064020
C	2.8693277123	-9.1023494320	-.3715629693
C	2.4391879022	-7.9094160228	-.9565634317
C	1.5621849669	-7.9095399784	-2.0481537420
C	1.1267343832	-9.1504475558	-2.5387472246
C	1.5524561300	-10.3449656659	-1.9592703193
C	2.4271918298	-10.3263499026	-.8713055846
C	1.0993286412	-6.6033856913	-2.6818885530
C	1.5650360656	-6.4789316865	-4.1441000622
C	-.4243580298	-6.4123994166	-2.5691711834
H	3.4137445247	2.3998286354	-4.2824628401
H	-1.5402918683	4.5429133836	-5.4308007158
H	-2.8103880698	3.3633809234	-5.8263160956
H	4.6568187592	-1.4493492074	-2.1628920082
H	5.4172849043	-2.7325555943	-4.1321325328
H	4.2621421861	-2.4692863758	-6.2987233996
H	-5.2001976566	.9710335073	-1.7363577648
H	-6.5985163234	.0047931626	-3.5266240074
H	-5.6518752406	-.3578438716	-5.7783994942
H	2.7136279963	3.5586863589	-5.4334356153
H	-3.7652090906	-1.9548667864	-6.7310533793
H	.5354593435	3.7879909206	-5.3414062776
H	-3.5851536898	3.6456250690	-1.5782339698
H	2.7005611498	-1.4301773401	-.6133615336
H	1.1526748632	-1.2584401447	-1.4488601752
H	1.8368057509	1.0189680543	-2.2436986408
H	3.3274959364	1.6440498814	-.3887109889
H	1.3863452861	-.1272096186	-6.8587864608
H	.8669492666	-2.1393863077	-8.2019057682
H	-1.6779689078	2.1498856493	-2.2496655498
H	-1.4542134624	.8609611314	-.1486722992
H	-2.1723608863	.6628625777	-6.7522910202
H	-3.5151772968	.4652526520	-8.7891249262
H	3.8668956217	-1.2735595605	-8.2528831661
H	3.6116219847	.4342774966	-7.8757435080
H	3.2856931068	1.9676120419	-5.9798517402
H	-2.1578701140	-1.7310245548	-6.0322911080
H	4.1886943936	1.8285436445	-1.9262338309
H	4.5236264272	.4429028359	-.8808586787
H	1.5574809622	-.1815295354	-.0959069581
H	.7206359799	-2.5050883570	-6.4685839287
H	2.1369247829	-3.0534604480	-7.3756691342
H	2.5396266987	-.3944673016	-9.0171342175
H	-1.6256336029	-.2477448082	-1.5206147296
H	-3.0007429122	.0509339180	-.4550912867
H	-2.5508924806	3.1792903764	-.2169902281
H	-4.2345920287	1.7013065088	-7.7424843696
H	-4.9742482504	.0993704320	-7.8680566461
H	-2.3858364606	-1.5909021467	-7.7824422925
H	-2.5835000659	3.8725459625	-4.1599038848
H	-4.1270783172	2.4184436702	-.4253900688
H	1.2007507878	-11.2932502241	-2.3574157152
H	2.7596968784	-11.2567523033	-.4191009869
H	2.7907281481	-6.9599546011	-.5584771164
H	3.5498786347	-9.0736836507	.4754629653
H	.4455801046	-9.1853346592	-3.3851919603
H	1.5674186072	-5.7800492034	-2.1267956246
H	-.7107743461	-5.4310983308	-2.9617694045
H	-.7547076361	-6.4782100177	-1.5271919859
H	-.9646063311	-7.1776542695	-3.1383428601
H	1.2673258768	-5.5086794580	-4.5548064081

H	1.1203766504	-7.2614404527	-4.7701397476
H	2.6537056621	-6.5691246459	-4.2229924645
N	-1.5511659150	1.3123586716	-4.5194297727
N	1.3254721600	.6274657322	-4.5718484386
O	-.3785019985	-1.8843769262	-3.5142054751
O	-.2366451855	-2.9487949745	-4.2125104148
Cu	-.3956152753	-.1568761837	-4.1904796111

91. L¹CuO₂ end-on / cyclohexadiene complex

C	2.3656435687	-.7213056665	-6.8864346300
C	-3.0680112993	2.3140765922	-.6327127284
C	3.2159362764	-.2439813102	-8.0787825716
C	2.4405315545	-.6797866074	-.9331042371
C	2.7390763707	-.0870640971	-4.4139972403
C	-2.7389437582	.5762566685	-3.9369949049
C	-3.9774819531	.1573745157	-7.4357871169
C	1.4375755962	1.9362085945	-4.7576272059
C	-1.0852750432	2.2399392310	-4.5864182147
C	3.4566920624	-.2202579593	-3.1968902736
C	-3.2120907044	.6872017283	-2.6037267634
C	.2348313287	2.6687674077	-4.8283386738
C	3.1630039951	-.7684162192	-5.5845429601
C	-3.5175194892	-.0597645538	-4.9349287017
C	-1.7905020577	.1225066237	-.6000955790
C	1.7207554026	-2.0897082515	-7.1895126992
C	2.7238993876	2.6820315403	-5.0627251339
C	-2.1943980522	3.2662960528	-4.7231013082
C	4.6139450095	-1.0043240644	-3.1906072240
C	4.3281239422	-1.5398379111	-5.5188724870
C	-4.4817533735	.1830986615	-2.3072637496
C	-4.7802021280	-.5473223391	-4.5818812873
C	4.0420300255	1.2715279488	-1.2100699258
C	-2.9809485224	-.2777817664	-6.3456794633
C	5.0549709185	-1.6558539097	-4.3389782123
C	2.9666127050	.4080079177	-1.8946632966
C	-2.5538498108	-1.7477655049	-6.5453817661
C	-5.2652876909	-.4249146751	-3.2838250921
C	-2.3409728440	1.2598478701	-1.4875323009
C	-.7024449986	-8.5857639430	-1.9183965435
C	.5047354329	-8.8427058220	-1.0547172381
C	1.7155593913	-8.0700390637	-1.5082093143
C	1.7264438763	-7.2745698417	-2.5803626385
C	.5342049053	-7.0582771841	-3.4746994153
C	-.6892699577	-7.7904170864	-2.9905469815
H	4.0267605291	-.9448330432	-8.3057842940
H	3.6685086834	.7345324834	-7.8867946318
H	3.2563555195	2.2123879057	-5.8954451020
H	3.3985550885	2.6508792361	-4.2011079302
H	-2.7135194337	3.4026504166	-3.7685753433
H	-2.9456070789	2.9275212168	-5.4437200495
H	.3417296175	3.7100835210	-5.1031407127
H	5.9542276178	-2.2643693042	-4.3093395376
H	4.6639656202	-2.0696796393	-6.4057739058
H	-1.7977213832	-2.0552086447	-5.8146137920
H	-6.2466257134	-.8153281754	-3.0294763923
H	-5.3892625857	-1.0422292089	-5.3331929660
H	-1.8043921410	4.2315572825	-5.0488422385
H	2.5261011274	3.7246132315	-5.3149419343
H	-3.9071401720	1.8836619461	-.0755046976
H	-3.4609102583	3.1310962043	-1.2467613489
H	-3.4103540954	-2.4233231992	-6.4380269395
H	5.1739630951	-1.1176404883	-2.2663092189
H	1.6559958241	-1.2820996030	-1.4017868513
H	2.1261175412	1.0651921318	-2.1366503004

H	3.6304347865	1.7551775498	-.3172276492
H	1.5525328209	-.0015956358	-6.7541591150
H	1.1027402024	-2.0283944992	-8.0928777338
H	-1.4828208530	1.7538105117	-1.9521251747
H	-1.1136862312	.5206914486	.1647174307
H	-2.0836268284	.3376653886	-6.4572304920
H	-3.5220154337	.0602660531	-8.4273184384
H	-4.8584479580	.2534545158	-1.2907995687
H	3.2439245027	-1.3618772465	-.6320664641
H	-2.1333763844	-1.8948857664	-7.5468008291
H	4.4144668302	2.0561228225	-1.8769751970
H	4.9020201886	.6729221452	-.8903891643
H	2.0287411639	-.2266784978	-.0239430085
H	1.0890326107	-2.4280668989	-6.3621599762
H	2.4839487343	-2.8575166453	-7.3604523927
H	2.5959732855	-.1583438500	-8.9779739076
H	-1.2385379912	-.6195339562	-1.1867130188
H	-2.6042255258	-.4041288272	-.0883598548
H	-2.3793341195	2.7457463464	.1019727501
H	-4.2845890559	1.2003933992	-7.3060928052
H	-4.8836371225	-.4581487082	-7.4315587385
H	-1.6028217381	-7.6534033111	-3.5666222137
H	-1.6254348648	-9.0870610676	-1.6310987527
H	.7316799265	-9.9223461837	-1.0362314946
H	.2740699959	-8.5976134067	-.0046378155
H	.3252707615	-5.9811970903	-3.5767708213
H	2.6196008015	-8.1820946436	-.9117522511
H	2.6402497225	-6.7458227650	-2.8466134832
H	.7782150004	-7.3829842578	-4.5011318557
N	-1.4074988854	.9954716697	-4.2430722600
N	1.5130839174	.6466094116	-4.4391057050
O	.0554536002	-2.0968186109	-3.3837034986
O	.1706392706	-3.1194893369	-4.1427389090
Cu	-.0822987000	-.3574451635	-4.0158475363

92. L¹CuO₂ end -on / dopamine complex

C	-1.9234315047	3.8593599761	-4.7659874322
C	1.5935082553	-1.9501491418	-6.9741027492
C	-2.7028906680	-1.1864270097	-6.3648238006
C	-2.8495395382	3.1634419032	-.6056118917
C	2.7499325886	.1695182070	-4.3296443370
C	-2.6558332752	1.2622347846	-3.8276916663
C	3.1627079848	-.2211400357	-7.9690079465
C	1.5933525220	2.2562486882	-4.7706474366
C	-.8924925799	2.7640431481	-4.5747560365
C	3.4716036721	.0734139265	-3.1128138384
C	-3.1153163471	1.4650126431	-2.5014451555
C	.4509569569	3.0764604308	-4.8601995038
C	3.1157777164	-.6122848201	-5.4537398567
C	-3.4800340607	.6378533472	-4.7962004291
C	2.4313794672	-.1598556534	-.8285000683
C	-1.7146152174	.8973788708	-.4843184001
C	2.9277018506	2.8865950350	-5.1267079420
C	4.1809809274	1.6345433220	-1.2236084063
C	4.5757016065	-.7825735058	-3.0611175065
C	4.2305624644	-1.4512976654	-5.3461803134
C	-4.4151195386	1.0636963427	-2.1805026326
C	-4.7715555559	.2536519791	-4.4203283419
C	-3.9192372308	.8378482496	-7.2993556162
C	-2.9711170708	.3256238054	-6.2004045059
C	4.9614366000	-1.5362450152	-4.1658619183
C	3.0374589626	.8199074521	-1.8544489837
C	2.3048184790	-.5989876843	-6.7469248532
C	-5.2426328437	.4668461569	-3.1282576413

C	-2.2006708492	2.0276849358	-1.4159373714
C	-.7119929074	-7.3392883850	-2.6939802115
C	-1.6993746625	-8.4550330907	-2.4262541757
C	-1.2581747607	-9.6771958477	-1.8964028422
C	-2.1547321688	-10.6987540882	-1.6019927671
C	-3.5259384790	-10.5064316870	-1.8365987278
C	-3.9790464567	-9.3034415573	-2.3628128622
C	-3.0684019735	-8.2834295196	-2.6559687524
C	-.5449619372	-6.3943541441	-1.4901971183
H	3.4165052914	2.3303860925	-5.9322297402
H	3.6069254187	2.8583446931	-4.2684645764
H	-2.4386491091	4.0755939630	-3.8245225985
H	-2.6913734534	3.5429724787	-5.4795568446
H	5.1374143556	-.8714227862	-2.1353150001
H	5.8190733985	-2.1999398282	-4.1009293699
H	4.5228190249	-2.0582875110	-6.1988263034
H	-4.7815538643	1.2067749993	-1.1677617283
H	-6.2474669248	.1564009042	-2.8554370851
H	-5.4155924242	-.2309367151	-5.1490541811
H	.6336932409	4.0911876461	-5.1894595910
H	2.8033416626	3.9241019921	-5.4399443647
H	3.1818269504	-.8776819485	-.4791723852
H	-3.6258718761	-1.7648084919	-6.2418710106
H	-1.9805228491	-1.5585279016	-5.6300197289
H	1.6055582899	-.7321953708	-1.2626674711
H	2.2495562814	1.5236971597	-2.1379266485
H	3.8118402416	2.2091987882	-.3672006617
H	1.5280403818	.1643595947	-6.6446435326
H	.9740132066	-1.9094179229	-7.8778035185
H	-1.3153836080	2.4418071667	-1.9067105118
H	-1.0027540637	1.2831215210	.2544249518
H	-2.0152039473	.8414802433	-6.3288129345
H	-3.4828229576	.6625495453	-8.2885317599
H	3.9494336805	-.9604138111	-8.1550531727
H	-3.7094043771	2.8135191105	-.0242143876
H	-3.1949799741	3.9750893204	-1.2541936920
H	-1.4620565940	4.7781327812	-5.1309538290
H	4.6178036824	2.3384230735	-1.9397298750
H	4.9876306242	.9888145727	-.8601198817
H	2.0530537732	.3822902960	.0456824973
H	.9492300406	-2.2126472035	-6.1286198454
H	2.3195570879	-2.7607192456	-7.1072480505
H	2.5409999439	-.1685975139	-8.8695946447
H	-1.2195966807	.0985524137	-1.0469619998
H	-2.5530669884	.4466546075	.0585285169
H	-2.1268536228	3.5822630507	.1032898388
H	-4.1073412859	1.9118195358	-7.1983212675
H	-4.8878089100	.3268643448	-7.2739945257
H	-2.3049881683	-1.3994951356	-7.3637881996
H	3.6472210262	.7520101501	-7.8371551346
H	.2725923312	-7.7486876783	-2.9444806068
H	-1.0384455853	-6.7518088389	-3.5632214085
H	-.2027173046	-9.8537420769	-1.7099968827
H	-5.0422923922	-9.1629955246	-2.5484369119
H	-3.4325221874	-7.3485891520	-3.0732511441
H	-.2381526468	-6.9908973551	-.6216131546
H	-1.5337059243	-5.9681034558	-1.2393974390
H	-2.4726867186	-12.4543747989	-.9658261455
H	-5.2507253721	-11.3659498216	-1.7122063168
H	.6563006707	-4.8384022001	-.9234876774
H	.2050035808	-4.7517616434	-2.4816331359
N	-1.2986683800	1.5710589296	-4.1492045967
N	1.5748217494	.9782527461	-4.3985290657
N	.5000592246	-5.4037119764	-1.7548219725

O	-.1042290031	-1.5813642972	-3.1618285340
O	-.1954230899	-2.6767923836	-3.8187985832
O	-4.3309437456	-11.5802494852	-1.5144129374
O	-1.7015215234	-11.8815255991	-1.0929355468
Cu	-.0817481738	.1195384668	-3.9004486245

93. L¹CuO₂ end -on / formylglycine complex

C	2.3127232453	-1.8455712513	-4.7128891002
C	-3.1789663016	3.7159668816	-.7498387279
C	3.0602967682	-2.2340991839	-6.0000953054
C	2.7861412114	1.0748234406	.4416598672
C	2.8339409783	-.1107150226	-2.8927024381
C	-2.7077488045	.4587388023	-2.5514442811
C	-3.7464961519	-1.8800655610	-5.2697535598
C	1.3847307034	1.3804126784	-4.1196973881
C	-1.1534390278	1.5764024924	-4.0196130422
C	3.6361745610	.3748413784	-1.8325286971
C	-3.2306623776	1.2734042326	-1.5150662549
C	.1313675788	1.8978471995	-4.5033907268
C	3.2232163296	-1.2514777620	-3.6407706137
C	-3.4355610361	-.6520431188	-3.0418632000
C	-1.8258962817	1.9488545990	.4662690351
C	1.5277364606	-3.0521218356	-4.1556081593
C	2.5985337417	1.8825198778	-4.8834037747
C	-2.3307431612	2.2720806776	-4.6813072334
C	4.8402416105	-.2812681939	-1.5548439909
C	4.4361458421	-1.8693778917	-3.3204057476
C	-4.5026971161	.9815365022	-1.0147803973
C	-4.7067571696	-.8961541775	-2.5083007407
C	4.2496763888	2.6654519824	-.8909638150
C	-2.8360984445	-1.6176807206	-4.0567846929
C	5.2436807021	-1.3908490194	-2.2918633004
C	3.1901552861	1.5516196822	-.9688267584
C	-2.4481736811	-2.9463835142	-3.3723612224
C	-5.2441817942	-.0878752179	-1.5118491112
C	-2.4022807911	2.3957640989	-.8934630363
C	.0958559235	-6.4757919309	-5.0135417791
C	.4234148144	-7.9917827255	-4.7494293225
C	-1.5648240747	-5.3654683747	-6.5144578037
H	.1558977668	2.6240113602	-5.3062329383
H	-1.9982410794	2.9301406616	-5.4861210502
H	2.3273118048	2.6878563638	-5.5685748563
H	3.7631624128	-3.0578277190	-5.8345448105
H	3.6246213816	-1.3902407241	-6.4144497937
H	3.0518421844	1.0711733297	-5.4624854641
H	3.3681245371	2.2461564005	-4.1951381566
H	-2.8953425687	2.8642644631	-3.9536254991
H	-3.0265720491	1.5348798908	-5.0942639545
H	5.4667901504	.0759381186	-.7414212625
H	6.1791329841	-1.8917525659	-2.0562537740
H	-1.7618610873	-2.7873252228	-2.5332777479
H	-4.9161495244	1.5921927225	-.2162608815
H	-6.2311765749	-.3006218231	-1.1088260121
H	-5.2762305084	-1.7467124353	-2.8721600046
H	3.6402886552	.6320274702	.9673885110
H	1.9964107161	.3183560984	.3956986187
H	-4.0111539930	3.6254325972	-.0432535251
H	-3.5916728513	4.0466881047	-1.7090758649
H	-3.3366660451	-3.4569732517	-2.9804617120
H	4.7448525451	-2.7507378071	-3.8746935770
H	-1.9617350381	-3.6028956727	-4.0986763744
H	2.2983717244	1.9806191064	-1.4353737368
H	3.8660105695	3.5195410549	-.3206446694
H	1.5767742359	-1.0851239362	-4.9873053509

H	.7912899810	-3.4068749721	-4.8843076067
H	-1.5535892880	2.5886316664	-1.5552522425
H	-1.1768243158	2.7259837097	.8876871790
H	-1.9147311509	-1.1715602035	-4.4408921449
H	-3.2187769833	-2.5298109998	-5.9746138811
H	-4.6777530514	-2.3821893240	-4.9806583531
H	-4.0174036132	-.9487604748	-5.7821965646
H	-2.5189486971	4.5069391021	-.3751697350
H	4.5294983460	3.0228852500	-1.8877831672
H	5.1640308212	2.3238827174	-.3928764470
H	2.4202350153	1.9148775795	1.0447428189
H	.9959793797	-2.7987731380	-3.2314870507
H	2.2052255165	-3.8805187978	-3.9184599406
H	2.3428117465	-2.5705396016	-6.7553031409
H	-1.2384745408	1.0299379708	.3706105825
H	-2.6295203562	1.7525621031	1.1856930727
H	.9817391762	-5.9751215647	-5.4191760105
H	-2.3824010521	-5.6376009842	-7.2152798590
H	-1.2909515527	-7.4038891558	-6.1645589359
H	-.1551631013	-5.9797611139	-4.0671603346
N	-1.3878159650	.7116454269	-3.0370710511
N	1.5618469385	.4857051751	-3.1518578913
N	-1.0103226003	-6.4375762151	-5.9521745421
O	-.0059072954	-2.5585102050	-.6162177195
O	.1029584414	-1.2813426173	-.6107346589
O	1.3945146801	-8.1948877887	-3.9912880996
O	-.3309085349	-8.8161372493	-5.3326412489
O	-1.2593653312	-4.1800374804	-6.3250772315
Cu	.0567398045	-.2305418185	-2.1495044794

94. L¹CuO₂ end -on / methane t.s.

C	-5.2143708753	.9029978531	1.2898604706
C	-3.1006465167	4.1819903266	3.2680754710
C	3.2493377295	.1639319496	-3.5820694571
C	2.5707411088	1.5582102633	3.4248604929
C	2.8325824910	1.2056815237	-.0508227664
C	-2.6791499282	1.7408700293	.4672053111
C	-3.9374253395	.6724734994	-2.8831160851
C	1.4014521399	2.9805930464	-.8329008010
C	-1.1121904511	3.2322072283	-.6041500171
C	3.5880138352	1.4574041660	1.1182731273
C	-3.1704745062	2.1434192840	1.7322986390
C	.1692267167	3.6351166388	-1.0189904659
C	3.2918903619	.3016403622	-1.0363310149
C	-3.4516234151	.9167653101	-.3883562659
C	-1.7181042224	2.1207605877	3.7944525503
C	1.8814357615	-1.4515983608	-2.1875581889
C	2.6287819686	3.6658032560	-1.4070195303
C	-2.2731044501	4.1391770987	-.9657062032
C	4.8160414056	.8054507962	1.2698693681
C	4.5257490538	-.3265848066	-.8360538429
C	-4.4427829109	1.7111043194	2.1206552878
C	-4.7172158302	.5118645136	.0494561450
C	4.0966514003	3.4326923487	2.6539472133
C	5.2878985216	-.0779183828	.3023315192
C	3.0656149540	2.3778362433	2.2165674383
C	2.4616820803	-.0264194281	-2.2738217255
C	-2.4961695208	-1.0292139249	-1.6957903767
C	-2.3253824730	2.9916925720	2.6772811720
C	-2.9274944288	.4492092844	-1.7442437086
C	.4256319499	-4.1188568060	.5333839879
H	-1.9314090377	5.0078824748	-1.5299164600
H	.2138019480	4.5710053553	-1.5603821474
H	2.3625431998	4.6129940940	-1.8779222103

H	1.8251065764	.8149429760	3.1265484519
H	4.0879920354	-.5362773485	-3.6575762124
H	3.6559553675	1.1771633756	-3.6638750539
H	3.4002798809	1.0207919496	3.8978669227
H	-2.0822225592	-1.3366094284	-2.6632356069
H	3.1187017574	3.0310406392	-2.1513237141
H	3.3683092947	3.8581935723	-.6238291869
H	-1.7405616087	-1.2031563013	-.9267398976
H	-3.0153610391	3.6023848827	-1.5644510430
H	5.4094565148	.9878785444	2.1610875582
H	6.2442201976	-.5748613684	.4375702515
H	4.8939344605	-1.0253226477	-1.5819849693
H	-4.8349460880	2.0096567913	3.0882813914
H	-6.2004470577	.5780440306	1.6087501107
H	-5.3230882105	-.1219507563	-.5911423950
H	-3.9106421519	3.8569653873	3.9294248412
H	-3.5426889000	4.8027935852	2.4817995973
H	-3.3519856355	-1.6770130018	-1.4741945264
H	-2.7897398867	4.4873120855	-.0656863362
H	2.2032861952	2.9159408024	1.8137191854
H	3.64908222798	4.1204979783	3.3794564744
H	1.6142246333	.6641604188	-2.2979130638
H	1.2656678650	-1.6691875966	-3.0676697550
H	-1.4926279342	3.4018737374	2.0990371032
H	-1.0681762135	2.7212702654	4.4409790144
H	-2.0362225150	1.0400044348	-1.9750216079
H	-3.4776082493	.4211085067	-3.8448579200
H	4.4525506796	4.0235594811	1.8035059691
H	4.9706700533	2.9775918777	3.1317667030
H	2.1220108974	2.2161865375	4.1777906325
H	1.2578433213	-1.5705532330	-1.2975205703
H	2.6813900253	-2.1995361296	-2.1441676023
H	2.5979862299	-.0092551792	-4.4454731959
H	-1.1254259295	1.2965203912	3.3854154249
H	-2.5049376213	1.6835352600	4.4192645883
H	-2.4299480381	4.8132258764	3.8606289571
H	-4.2782676331	1.7116774164	-2.9298885785
H	-4.8212592686	.0355829889	-2.7702867069
H	.0753053278	-2.6403236755	.7546418206
H	-.4386361231	-4.3630994850	-.0835047609
H	.4242006552	-4.5286412718	1.5371805601
H	1.3804896823	-4.0706504224	.0221315438
N	-1.3517475678	2.1137032775	.0788992101
N	1.5503956444	1.8211142630	-.1933729431
O	-.4236176497	-1.6793507603	.8728332189
O	.4453369792	-.7559561557	1.4732175479
Cu	.0302386477	.8641629492	.6140876670

95. L¹CuO₂ end -on / cyclohexane t.s.

C	4.4503982828	3.7294476896	-7.2664726772
C	-.4326782019	7.3444491266	-.8856486648
C	5.2179125519	4.1100624093	-8.5457278035
C	5.1741991510	3.9488571731	-1.3504835030
C	5.1662398262	4.3380813399	-4.8707776628
C	-.1614998935	5.7922160340	-4.2830860240
C	-1.1693575223	5.9348180240	-7.8775354807
C	4.1545582229	6.5105214914	-5.1757593577
C	1.7175141885	7.1619641121	-4.8964149420
C	5.9872704452	4.1413283086	-3.7357370948
C	-.7118566571	5.9173589466	-2.9857948095
C	3.0708236719	7.4090498888	-5.1900603444
C	5.3682641897	3.5889963716	-6.0548219554
C	-.9728538343	5.4207454727	-5.3825566964
C	.4826714911	4.9809102317	-.9743264060

C	3.6279872323	2.4449405716	-7.4872794458
C	5.4959887974	7.0448138254	-5.6425522769
C	.7571075329	8.3228177504	-5.0833207299
C	7.0199991576	3.2018788255	-3.8155147510
C	6.4188081786	2.6653999103	-6.0850128039
C	-2.0810599113	5.6868596147	-2.8150463138
C	-2.3372303771	5.2044599462	-5.1595811388
C	6.9860706007	5.6293738575	-1.9237933020
C	-.3872701912	5.2003693215	-6.7742548564
C	7.2432718829	2.4703751994	-4.9801656498
C	5.7348812121	4.8927689905	-2.4324634534
C	-.2889984054	3.6939949728	-7.0860536503
C	-2.8938015488	5.3398892557	-3.8909232139
C	.1687346654	6.2529025272	-1.7871983367
C	3.0299908900	-2.4939995827	-2.0327589248
C	3.5757872767	-3.2083282820	-3.2783355678
C	4.7355817905	-2.4303300059	-3.9184372861
C	4.3144567982	-.9790565395	-4.2545609938
C	3.7554274824	-.3039717991	-3.0229332210
C	2.6121564630	-1.0399954653	-2.3614483479
H	5.9208834607	3.3245709661	-8.8433312307
H	5.7892280597	5.0349963626	-8.4163343273
H	5.8552114062	6.4885804148	-6.5133799322
H	6.2537631162	6.9274990637	-4.8617521334
H	.2175284788	8.5320773590	-4.1540916968
H	.0006908238	8.0934276707	-5.8394392276
H	3.3039797784	8.4173059469	-5.5067489717
H	8.0538576432	1.7486006711	-5.0248710175
H	6.5894393614	2.0856194450	-6.9879408829
H	-2.5184952032	5.7813042877	-1.8256840803
H	-3.9560264582	5.1700368073	-3.7403093776
H	.3099995053	3.1713328215	-6.3340075733
H	1.2899206323	9.2242390981	-5.3890065703
H	5.4259044122	8.1005788832	-5.9078548123
H	-1.3535930287	7.0116825972	-.3953834387
H	-.6672812433	8.2496644201	-1.4554359795
H	-1.2824451736	3.2320843031	-7.1016933297
H	7.6573228452	3.0381771275	-2.9511021963
H	4.2755272986	3.4347834474	-1.7024529230
H	4.9715046583	5.6499674453	-2.6323653063
H	6.7443108820	6.2145812371	-1.0299319304
H	3.7429288393	4.5357211068	-7.0554116405
H	2.9114305437	2.5846444122	-8.3046438149
H	1.1158174853	6.6399544237	-2.1741848418
H	1.1680435983	5.2089584534	-.1501335869
H	.6309710863	5.5981849092	-6.7751053420
H	-.6597576004	5.8223499620	-8.8404953179
H	-2.9733520043	4.9198755196	-5.9927592787
H	5.9130343685	3.1862234439	-1.0778578821
H	.1752235688	3.5315576924	-8.0652157886
H	-2.1824082657	5.5360075887	-7.9958440753
H	-1.2573892278	7.0056239516	-7.6663535176
H	7.3846716271	6.3147999412	-2.6790150500
H	7.7858915880	4.9317051238	-1.6534393365
H	4.9247762220	4.5111177957	-.4431484260
H	3.0788169659	2.1688134085	-6.5829303063
H	4.2776097987	1.6033949990	-7.7536415057
H	4.5198991232	4.2590814820	-9.3768738364
H	.9402285578	4.2027609937	-1.5936948160
H	-.4345371682	4.5614763490	-.5453975292
H	.2766273769	7.6154445271	-.0964435270
H	3.9008174664	-4.2229018626	-3.0181064876
H	2.7663526363	-3.3171667240	-4.0142958120
H	5.5868210330	-2.4061533616	-3.2245787199

H	5.0822978996	-2.9341411374	-4.8288226222
H	5.1583281741	-.4124567030	-4.6615842221
H	3.5407855067	-1.0131088448	-5.0349467481
H	3.1583531077	.8688982784	-3.5136632926
H	4.5083896108	.0951584671	-2.3359312841
H	2.2811630922	-.5201168396	-1.4561818441
H	1.7544237733	-1.0682383830	-3.0478510896
H	2.1724038830	-3.0386332993	-1.6195460670
H	3.8028038329	-2.4783960542	-1.2523083650
N	1.2450346696	5.9890680563	-4.4696461853
N	4.0625470893	5.2405004070	-4.7900962069
O	2.5069567742	2.7997839825	-3.2322144060
O	2.5739911346	1.7146935795	-4.0776922320
Cu	2.4169149218	4.4873173342	-4.0351354840

96. L¹CuO₂ end -on / acetonitrile t.s.

C	3.0053545681	-1.3800567635	-5.7668306912
C	-2.4433708872	3.3778843570	-.7534339398
C	3.9882258899	-.9585099076	-6.8735581204
C	2.0258878555	-.2898292663	.0732936669
C	2.7794060015	-.3053839034	-3.4344489408
C	-2.7082933862	.3821938680	-2.8546554361
C	-4.5930224912	-1.2962170339	-5.6729555091
C	1.3389568928	1.3613854154	-4.4372056111
C	-1.1844510095	1.6129078996	-4.2620861313
C	3.2606826942	-.0924082420	-2.1193674761
C	-2.9622167409	1.0407052990	-1.6247953127
C	.0959910943	1.9605642883	-4.7254947489
C	3.5227547629	-1.0710534860	-4.3650287657
C	-3.6827506472	-.4675451144	-3.4319212327
C	-1.4899914091	1.3442823429	.4083186599
C	2.6655176462	-2.8754914392	-5.9020078423
C	2.5739417546	2.1121594383	-4.8991560992
C	-2.3313561768	2.5226852533	-4.6578587153
C	4.5059711762	-.6232307162	-1.7709441203
C	4.7619564828	-1.5814730561	-3.9632271113
C	-4.2019899908	.8429759228	-1.0062065195
C	-4.9041566261	-.6318661898	-2.7709992970
C	3.1794905635	1.8915722817	-.5283080442
C	-3.3958898056	-1.2475575994	-4.7082143150
C	5.2585141182	-1.3579616862	-2.6827025032
C	2.4427143863	.6548124938	-1.0706395854
C	-2.9338433460	-2.6765932546	-4.3631638155
C	-5.1698964297	.0185117505	-1.5693365414
C	-1.9313390504	1.9371078758	-.9431840143
C	-.8713650452	-5.8512257106	-3.9159798771
C	-.0349903670	-4.9725823292	-4.6333898537
H	.1445597685	2.8607604792	-5.3238101178
H	-1.9861047592	3.3275649571	-5.3076753602
H	2.3010017432	3.0541692067	-5.3757815869
H	4.9240364342	-1.5233795907	-6.8110896059
H	4.2423541668	.1043691485	-6.8187704907
H	1.4698274282	-1.1505634237	-.3103254451
H	3.1540235788	1.5179462655	-5.6089694337
H	3.2323797721	2.3218996261	-4.0507464353
H	-2.8082632272	2.9656744112	-3.7795920767
H	-2.0529334149	-2.6769566226	-3.7125247752
H	4.8873246458	-.4658730995	-.7661713789
H	6.2222430354	-1.7653988492	-2.3918809411
H	5.3452307634	-2.1701164834	-4.6651663718
H	-4.4095681162	1.3439410809	-.0649719924
H	-6.1257490209	-.1204992828	-1.0728761345
H	-5.6609061606	-1.2802601156	-3.2004042808
H	2.9012419938	-.6704484895	.6104478119

H	-3.3050913826	3.4123830310	-.0783546860
H	-2.7477349906	3.8305819436	-1.7020927546
H	-3.7231448250	-3.2219542820	-3.8351333200
H	-3.1074063109	1.9544328850	-5.1808208104
H	-2.6943117657	-3.2341726569	-5.2759107733
H	1.5284913748	1.0116797843	-1.5531805353
H	2.5427570403	2.4346487654	.1785839021
H	2.0748354328	-.8229446426	-5.9104028762
H	2.1826588944	-3.0782864379	-6.8649803111
H	-1.0475432836	1.9839569574	-1.5850134268
H	-.7210321029	1.9737502935	.8694492593
H	-2.5769118647	-.7411662468	-5.2293745982
H	-4.2945774347	-1.7616504880	-6.6178768797
H	3.4524887116	2.5805640638	-1.3344539763
H	4.0985732146	1.6159190304	-.0003740361
H	1.3956231059	.2393205379	.7960317707
H	2.0027022873	-3.1819169060	-5.0926938150
H	3.5694853782	-3.4917921128	-5.8426177179
H	3.5524407111	-1.1514405812	-7.8596376240
H	-1.0814218074	.3367635432	.2874289204
H	-2.3302048647	1.2810848482	1.1080251385
H	-1.6582120354	4.0059234186	-.3191438829
H	-4.9742230000	-.2939522144	-5.8933544970
H	-5.4208700117	-1.8882895203	-5.2695620632
H	-.5386547375	-4.2740951477	-5.2975428177
H	.8967243407	-5.3914865734	-5.0063137912
H	.5273545951	-4.0175167603	-3.5847018962
N	1.4924990061	.2134853783	-3.7792497562
N	-1.4333236116	.5488782018	-3.4951964481
N	-1.5638290955	-6.5549291077	-3.2877158071
O	.3368389984	-2.4204740488	-2.3548877688
O	1.1123643117	-3.4181320768	-2.8771901381
Cu	-.0789570097	-.7853544323	-3.1489236236

97. L¹CuO₂ end -on / toluene t.s.

C	2.6200059320	2.2527153982	-5.4842587431
C	-3.0590045370	-.8064509066	-6.0796707565
C	-2.4972316526	-2.2422552012	-6.1092237665
C	-2.9797887983	2.3373738574	-.6492868735
C	2.8179125168	-.2433081980	-4.1826244279
C	-2.7222763322	.2549975385	-3.7634419301
C	3.4176250831	-1.2200547717	-7.7178923751
C	1.3869250351	1.5361463535	-4.9630456199
C	-1.1365034240	1.7725009692	-4.7735255029
C	3.5143107508	-.0204291087	-2.9719730276
C	-3.1664076394	.5301845967	-2.4477912071
C	.1516753988	2.1880379663	-5.1529080336
C	3.3332565886	-1.1139061436	-5.1708776972
C	-3.5445811995	-.4468733453	-4.6777168180
C	2.5126546747	.0092574205	-.6533736397
C	3.9042429149	1.9801180392	-1.4402927030
C	-4.1367517434	-.6205279952	-7.1607353185
C	-2.2882636666	2.7019262489	-5.1063722743
C	4.7410696726	-.6652842509	-2.7823212727
C	4.5624305785	-1.7367520203	-4.9308878096
C	-4.4429170814	.1014385848	-2.0696323449
C	-4.8135259519	-.8508719830	-4.2500195861
C	-1.6113761226	.2090000674	-.4899439197
C	1.9610340958	-2.8337448318	-6.4150183358
C	5.2673503137	-1.5157169260	-3.7506428518
C	2.9391208794	.8596400354	-1.8662412535
C	2.5632685997	-1.4150759505	-6.4534014240
C	-5.2649482215	-.5819145504	-2.9607245410
C	-2.2604036998	1.2334303759	-1.4422513132

C	-3.7309830495	-6.5006764269	-2.4543077874
C	-2.6097082630	-6.9912502634	-1.7772493468
C	-1.3302730096	-6.7081684997	-2.2440890673
C	-1.1396798552	-5.9371515049	-3.4104655555
C	-2.2850161892	-5.4449281017	-4.0783700408
C	-3.5611775130	-5.7220715937	-3.6042793088
C	.1932457024	-5.5784413697	-3.8772879223
H	.2026977276	3.1415486925	-5.6620741777
H	3.1280387265	1.6500197741	-6.2432236725
H	3.3430386738	2.4181085293	-4.6801235435
H	4.2467725182	-1.9340665159	-7.7624515471
H	1.8130659590	-.7786011168	-.9472402469
H	2.3562737923	3.2159249069	-5.9228406703
H	-3.0118227636	2.2107658758	-5.7643450157
H	5.2876055499	-.5054284812	-1.8571746374
H	6.2202376628	-2.0094554804	-3.5835370033
H	3.3792963783	-.4734780503	-.1880572649
H	-4.7981246826	.3044557626	-1.0639412220
H	-6.2543163792	-.9062398875	-2.6513385155
H	-5.4600326277	-1.3901388327	-4.9352129012
H	-2.8322460630	2.9841885189	-4.1993070655
H	3.8449831232	-.2130890211	-7.7648071914
H	-3.7543163914	1.9331997526	.0109340898
H	-3.4561846679	3.0631741725	-1.3165590654
H	-3.2644621103	-2.9673677073	-5.8113651909
H	2.0387822323	1.3394415620	-2.2597647104
H	3.4296394429	2.6270766081	-.6944505432
H	1.7266210521	-.7133021031	-6.5112047918
H	1.3831713187	-3.0288607680	-7.3259967046
H	-1.4551249540	1.7145430215	-2.0049235760
H	-.9204127798	.7066739093	.1997572680
H	-2.2320662876	-.1342137903	-6.3281652493
H	-3.7003631975	-.7695276508	-8.1538706416
H	-1.6580010096	-2.3586562406	-5.4184363750
H	-1.9312880185	3.6082291755	-5.5971452448
H	4.1956870875	2.6045337292	-2.2912449584
H	4.8202666938	1.5794747825	-.9932872537
H	2.0311912275	.6370262322	.1051677276
H	1.2976395044	-2.9571428917	-5.5551090760
H	2.7486271180	-3.5926516888	-6.3461645249
H	2.8070029955	-1.3709123110	-8.6146238475
H	-1.0508554414	-.5572802082	-1.0356662968
H	-2.3739053094	-.3054288257	.1055026471
H	-2.2639361537	2.8756214593	-.0191378340
H	-4.5729159679	.3832037127	-7.1280493883
H	-4.9532064239	-1.3426822796	-7.0557636034
H	-2.1529337292	-2.5012193928	-7.1171181499
H	4.9713858297	-2.4113954670	-5.6775307355
H	-2.1511586897	-4.7984588691	-4.9410083754
H	-4.4281661042	-5.3236264654	-4.1233334374
H	-4.7288715102	-6.7147490080	-2.0833243741
H	.2320796144	-4.2169155757	-3.5476693145
H	.3279820437	-5.4914142987	-4.9556864626
H	1.0343092306	-6.0498892422	-3.3698565349
H	-.4609549814	-7.0814522650	-1.7096613613
H	-2.7365747766	-7.5908931187	-.8805509980
N	1.5328189479	.3550669417	-4.3670270341
N	-1.3905160785	.6304816922	-4.1334128677
O	.5408458978	-2.2112722497	-2.7724097244
O	-.2509847829	-3.1092215080	-3.4636640079
Cu	-.0143576500	-.6269092367	-3.6324271667

98. L¹CuO₂ end -on/ phenol t.s.

C	4.8542285791	.8015977119	1.2859845787
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C	3.8233725265	1.7305599531	1.1204304536
C	-2.7540076177	3.6990097187	1.6426940546
C	.7679380091	4.3808526610	-1.2210101586
C	3.2573798383	.6447363878	-1.0262218934
C	-3.0633407420	2.1035659278	-.2117623158
C	3.0058477043	2.1561079936	3.4789014754
C	3.1994456008	4.0171512621	-1.6690680208
C	-1.6108239182	5.1171492585	-1.2537566238
C	1.4609852035	-.7361199311	-2.1515585410
C	-1.5673458151	3.9625332622	3.8475715337
C	4.8278285059	3.6219276323	2.4938055927
C	4.3069521720	-.2521869623	-.8113030117
C	-4.0822020067	3.4743712135	2.0170256703
C	-4.3856544087	1.9194386641	.2039539754
C	-3.3495110786	1.5371909151	-2.6767882697
C	-2.5310301133	1.3013015822	-1.3941794711
C	5.0998327592	-.1807068839	.3311762757
C	3.5704204393	2.7878616774	2.1907868894
C	2.3767091691	.4976922999	-2.2635284727
C	-4.8959638583	2.5951681992	1.3074708022
C	-1.8804601068	4.6200577487	2.4882135728
C	-2.4680437094	-.1998137507	-1.0515060620
C	1.8934159784	-3.7700060334	.4884494107
C	.8936013466	-2.8832979672	.9921160040
C	-.3777496927	-3.4363223038	1.3352320995
C	-.6328001830	-4.7844750298	1.1530279305
C	.3528046888	-5.6340954313	.6300708121
C	1.6144079368	-5.1153745273	.3041775711
C	-2.5010684250	6.0161476359	2.6853612216
C	3.0295659189	1.6493630631	-.0510574354
C	-2.2529632341	3.0150738978	.5079032387
C	3.1963247145	.4419767415	-3.5663117001
C	1.9134022490	3.6054151759	-.9826694127
C	-.5402751541	4.1687359051	-.7462471115
H	3.0791987957	4.9747104394	-2.1770506518
H	.8989282124	5.2296837404	-1.8787610098
H	3.5070433225	3.2701704723	-2.4068681325
H	4.0133209554	4.0988189424	-.9422220252
H	-2.0815289404	5.6537878109	-.4253038110
H	-2.4057920422	4.5638531999	-1.7621631496
H	5.4721852027	.8465637670	2.1776390207
H	5.9025886251	-.8962532675	.4813063949
H	4.4985635797	-1.0295792314	-1.5445558084
H	-3.4359524956	5.9667184667	3.2531396212
H	-5.9222257195	2.4282253104	1.6203917802
H	-5.0208745908	1.2252884961	-.3381746607
H	-2.7193288047	6.5036947148	1.7294730814
H	3.7235704559	1.4537445460	3.9169986228
H	-3.4708167384	-.6068933731	-.8813143569
H	-1.8817852942	-.3727988776	-.1444840058
H	2.0774264636	1.6082153617	3.2931524587
H	2.8123048488	3.4748956910	1.8021657633
H	4.5905825001	4.4176167449	3.2078677240
H	1.7272776176	1.3752678512	-2.3226092609
H	.7847139112	-.7848529921	-3.0125077582
H	-.9300803489	4.7553219502	1.9629204505
H	-.8706068202	4.5830174934	4.4225417855
H	-1.5092656091	1.6361081588	-1.5928071057
H	-2.9116107716	.9822274950	-3.5132646600
H	3.8180187864	-.4578939963	-3.6142133372
H	-1.1883210366	5.8437350238	-1.9485814962
H	5.2289621393	4.0874881814	1.5875602001
H	5.6224721954	3.0108896623	2.9343930986
H	2.8014252439	2.9334735596	4.2237701540

H	.8670078115	-.7147933434	-1.2355387263
H	2.0474998700	-1.6604222233	-2.1302933746
H	2.5259459936	.4220516307	-4.4318711356
H	-1.1290995657	2.9693040637	3.7125197523
H	-2.4805008992	3.8459235604	4.4420223382
H	-1.8127459154	6.6599184965	3.2431612605
H	-3.3747719395	2.5969673615	-2.9512269456
H	-4.3847077490	1.1988645621	-2.5628569558
H	-2.0130014514	-.7615207758	-1.8740904432
H	-4.4821738696	3.9875119411	2.8864023785
H	3.8586985010	1.3076112884	-3.6709622411
H	-1.1363417910	-2.7789990088	1.7495539692
H	-1.6069777989	-5.1863207546	1.4186108533
H	.1425531992	-6.6887725412	.4854035552
H	.1779100862	-.8638122212	1.6117234232
H	2.3813240029	-5.7741647979	-.0939434268
H	2.8654271870	-3.3535546576	.2441457048
N	-.8925011325	3.2006891219	.0992634143
N	1.9183840340	2.5353297172	-.1928294006
O	-.1842224643	.9799978248	2.3372806711
O	-.6444053659	-.2878981513	2.0627649264
O	1.1448033603	-1.6109810097	1.1100189480
Cu	.4408172081	1.9858509666	.8771681467

99. L¹CuO₂ end -on / isopropylbenzene t.s.

C	4.6715344391	-1.1340492639	-3.2455598199
C	-1.7863348573	-.2469722529	-.5838837507
C	1.5914829549	-2.1614535797	-7.0883177884
C	-2.7450062851	-2.1705531717	-6.6388954179
C	2.8311998822	-.3276378211	-4.5871283160
C	-2.6417721557	.1735996896	-3.9940082533
C	-2.8039380548	2.0681887140	-.8202526098
C	1.4538791671	1.6073666470	-5.0561192408
C	-1.0541546425	1.8062280732	-4.7728045522
C	3.4854009959	-.3973079521	-3.3350311018
C	-3.0906068552	.3263703555	-2.6613471510
C	.2247591571	2.2834048654	-5.1192566476
C	3.3513947451	-.9904694460	-5.7254074233
C	-3.4691150527	-.4117980814	-4.9811223990
C	3.5014334482	-1.0096285858	-8.2851167464
C	2.7020699375	2.3852150725	-5.4243801254
C	3.9116513896	1.1227969519	-1.3322685540
C	-2.2016865540	2.7910702383	-4.9102977014
C	-3.8973742838	-.0682684348	-7.4729040360
C	4.5451850914	-1.7045872638	-5.5851616906
C	-4.3921783498	-.0793151652	-2.3498015610
C	-4.7624700546	-.7999545155	-4.6175232667
C	2.2510541629	-.7910182172	-1.1687316041
C	-2.9689674016	-.6643824407	-6.3998872792
C	5.2036142527	-1.7781166745	-4.3586053363
C	2.8908279726	.2620929880	-2.0949539112
C	2.5901948780	-.9871367924	-7.0484279638
C	-5.2286385526	-.6302665979	-3.3168684323
C	-2.1824381307	.8740094206	-1.5652930056
C	.6227553912	-5.6830809816	-.2655813359
C	.3709422096	-5.2085936425	-1.5532838359
C	.4364176048	-6.0738748828	-2.6566484301
C	.7487517654	-7.4247000567	-2.4316282142
C	.9986986577	-7.8962588907	-1.1431234368
C	.9361920220	-7.0257557493	-.0537538985
C	.1802161504	-5.5836740209	-4.0566410179
C	1.4238216396	-5.2626663681	-4.8645230789
C	-.9288676022	-6.2881738270	-4.8129869445
H	3.3918560373	2.4257190328	-4.5750027673

H	-1.8486267360	3.7489862638	-5.2943617442
H	-2.9705115708	2.4032018207	-5.5846009526
H	5.1847800906	-1.2036741167	-2.2910775185
H	6.1272813348	-2.3427325744	-4.2712448473
H	4.9664365274	-2.2171767518	-6.4437860565
H	-4.7538288664	.0322518817	-1.3316709677
H	-6.2369557300	-.9370202697	-3.0544367325
H	-5.4119732172	-1.2488713515	-5.3634066245
H	2.4548306506	3.4050707907	-5.7219741506
H	-3.6976987521	-2.7122254243	-6.6195490919
H	.2680009037	3.3112166431	-5.4548835070
H	-3.0746729965	2.8771955868	-1.5069332250
H	3.0065566893	-1.4901399579	-.7928470152
H	1.4863347333	-1.3811235592	-1.6831029532
H	2.0905633703	.9290592580	-2.4282746959
H	3.4226394269	1.6402809509	-.5001421719
H	2.0020727247	-.0649954656	-7.0938169093
H	1.0531385600	-2.1855706199	-8.0423356740
H	-1.2642214159	1.2288013702	-2.0419307702
H	-1.0795374174	.1310029890	.1640225362
H	-1.9990288127	-.1693519404	-6.5004005058
H	-3.4632789437	-.2070100347	-8.4690487248
H	4.0203332576	-1.9676556056	-8.3957041796
H	4.2584013535	-.2198779937	-8.2436297886
H	3.2420065846	1.9017869898	-6.2442035738
H	-2.1031103985	-2.6044760048	-5.8666084171
H	4.3640471036	1.8782771966	-1.9830550850
H	4.7214818405	.5186294745	-.9098095093
H	1.7810813133	-.3061035223	-.3058379868
H	.8504218290	-2.0839992659	-6.2861931364
H	2.1172324015	-3.1132351222	-6.9577871315
H	2.9043102008	-.8611393897	-9.1905891229
H	-1.3225856868	-1.0841291416	-1.1135467008
H	-2.6646698568	-.6290906799	-.0518942653
H	-2.0940970693	2.4698976730	-.0890128009
H	-4.0531275469	1.0049819785	-7.3208274857
H	-4.8810440084	-.5495723772	-7.4731480205
H	-2.2852498886	-2.3379687721	-7.6199436483
H	-2.6879833912	2.9581921105	-3.9446078108
H	-3.7087442585	1.7796551190	-.2749056131
H	1.2408182868	-8.9444669309	-.9916295882
H	1.1286231440	-7.3919588563	.9504902756
H	.1241528797	-4.1635881237	-1.7042226335
H	.5655771344	-4.9975944326	.5753562727
H	.8023227205	-8.1113128986	-3.2725195621
H	-.4102489257	-4.2925479988	-3.9039087648
H	-1.1272771852	-5.7937146951	-5.7691760727
H	-1.8536888297	-6.3069518097	-4.2294408184
H	-.6561667342	-7.3313900610	-5.0325714846
H	1.1670520116	-4.7936052253	-5.8196025886
H	1.9912059653	-6.1824382947	-5.0749341768
H	2.0924146418	-4.5911418005	-4.3168039590
N	-1.3122715510	.5718252584	-4.3407682033
N	1.5703762863	.3382451231	-4.6725310769
O	-.2899354524	-2.3433471412	-3.1681481461
O	-1.0801477250	-3.3797230149	-3.6672983935
Cu	.1065517382	-.7598367066	-4.0595418700

100.L¹CuO₂ end -on / cyclohexadiene t.s.

C	2.7366869866	-1.3353966900	-6.5904578916
C	-2.9840462540	2.5282392518	-.9574951683
C	3.6429187943	-1.1473313876	-7.8183013415
C	2.5362668395	-.0677611503	-.7146440621
C	2.8884448033	-.2455611791	-4.2723471270

C	-2.6817752154	.1554599322	-3.7792023828
C	-4.0366139356	-.9478829088	-7.1284743448
C	1.4063943900	1.4933553819	-5.0697084458
C	-1.1304077051	1.6652976805	-4.8527205677
C	3.5487301462	-.0508927844	-3.0346045549
C	-3.1325355733	.4928906408	-2.4811211335
C	.1473373890	2.0976832251	-5.2624180676
C	3.4560151369	-1.0702748211	-5.2721135759
C	-3.4872261178	-.6175729801	-4.6483137174
C	-1.7639374850	.3879006268	-.3591202645
C	2.1068258942	-2.7400502438	-6.5874640177
C	2.6149315961	2.2441436754	-5.5981788248
C	-2.2996923360	2.5716395829	-5.1928482065
C	4.7767514209	-.6875525102	-2.8249714677
C	4.6845821869	-1.6870550484	-5.0112522195
C	-4.3945640120	.0428385887	-2.0764242472
C	-4.7393812212	-1.0444974007	-4.1957184054
C	3.8774277511	1.9410977534	-1.4878274059
C	-2.9751418774	-1.0389280868	-6.0212115038
C	5.3461016452	-1.5007255628	-3.8004915606
C	2.9410654239	.7990409151	-1.9225643703
C	-2.3785398829	-2.4573602525	-5.9508995959
C	-5.1963673957	-.7185356142	-2.9210082275
C	-2.2640311248	1.2846523982	-1.5081422630
C	-1.2677347479	-6.9153781309	-3.3077753510
C	.0063065633	-7.5953292529	-2.8956666547
C	1.2432654995	-6.8919015938	-3.3782751404
C	1.2037109464	-5.7136803635	-4.0313972799
C	-.0549640741	-5.0011888099	-4.2769079846
C	-1.2843418095	-5.7403244727	-3.9677997731
H	4.4498605863	-1.8870452773	-7.8461945273
H	4.1031772110	-.1542900191	-7.8298991622
H	3.1494455423	1.6504673844	-6.3458450432
H	3.3273516542	2.4454902409	-4.7919843083
H	-2.8040200183	2.9096120224	-4.2820384588
H	-3.0495326095	2.0389904956	-5.7856441552
H	.1667862880	3.0460554312	-5.7836611508
H	6.2987168655	-1.9893690960	-3.6172516091
H	5.1279501256	-2.3305319428	-5.7657963922
H	-1.5951131732	-2.5102528013	-5.1891003186
H	-6.1718007284	-1.0601904816	-2.5871169493
H	-5.3683226491	-1.6422494257	-4.8485208795
H	-1.9683732899	3.4471217279	-5.7526964779
H	2.3218909049	3.1921937920	-6.0508472586
H	-3.8508990908	2.2576349842	-.3455449014
H	-3.3368621181	3.1795750474	-1.7634157764
H	-3.1493772419	-3.1905558420	-5.6881819321
H	5.2912603325	-.5482177039	-1.8782628129
H	1.8350841962	-.8546133872	-1.0058989516
H	2.0304789680	1.2581043284	-2.3168273603
H	3.3862683310	2.5702166576	-.7376307891
H	1.9157509365	-.6178584416	-6.6718202485
H	1.5422150138	-2.9202307154	-7.5092840170
H	-1.3845845862	1.6326049293	-2.0567244144
H	-1.1036061063	.9539247009	.3076023325
H	-2.1588931868	-.3634255156	-6.2919945901
H	-3.5826718557	-1.1569160227	-8.1028478534
H	-4.7510834682	.2893271369	-1.0803528946
H	3.4118652123	-.5464423150	-.2619098367
H	-1.9425914828	-2.7495310374	-6.9129495911
H	4.1551889145	2.5780994440	-2.3339678892
H	4.8022604275	1.5588462074	-1.0423872238
H	2.0588758261	.5500442286	.0543821797
H	1.4247634544	-2.8505572277	-5.7401669363

H	2.8749929610	-3.5168797809	-6.5031858623
H	3.0616728678	-1.2633104192	-8.7392610861
H	-1.2099729219	-.4749262550	-.7389160345
H	-2.6018397792	.0127642171	.2386141219
H	-2.3050177018	3.1101502742	-.3250529021
H	-4.4883065169	.0481782418	-7.1704341846
H	-4.8432477358	-1.6745121877	-6.9848260864
H	-2.2321320302	-5.2887717125	-4.2494562288
H	-2.2016583191	-7.4166625754	-3.0626670369
H	.0050077243	-8.6415881691	-3.2463221198
H	.0388919695	-7.6889383117	-1.7947216947
H	-.0397833620	-4.0494044359	-3.3796126566
H	2.1979388551	-7.3751525220	-3.1839671744
H	2.1264964800	-5.2422508589	-4.3611021026
H	-.0870683222	-4.3901250130	-5.1826441444
N	-1.3640114361	.5344079976	-4.1878883266
N	1.5885299756	.3216556200	-4.4632424739
O	.0953554361	-2.0533473069	-2.4482530352
O	-.0016423992	-3.3714003775	-2.3137523462
Cu	.0944381470	-.6608826452	-3.6814496772

101.L¹CuO₂ end -on / dopamine t.s.

C	-2.5744204848	2.0893692651	-4.8207946568
C	2.6519825410	-2.3327100313	-6.7629022296
C	-1.6523520308	-2.7554231974	-6.3911581278
C	-3.5992236787	1.0878817531	-.6947971844
C	2.8759554842	-.1472062262	-3.9819997065
C	-2.6277932613	-.5910552020	-3.9032644168
C	3.7019222414	-.1755108083	-7.5884090042
C	1.2249494121	1.5179432605	-4.5145358165
C	-1.2966168217	1.3281762460	-4.5257219928
C	3.4860530037	-.0738057489	-2.7067995418
C	-3.2301512153	-.5488465672	-2.6230255026
C	-.0811010972	2.0074624570	-4.7040629032
C	3.5697476113	-.6807459878	-5.0927185613
C	-3.1840807004	-1.3604566348	-4.9518203970
C	2.3761126511	-.7800453626	-.5593774698
C	-1.8154659813	-.7040834857	-.5351615960
C	2.3576579070	2.4973977006	-4.7665828985
C	3.4539655057	1.5153756426	-.7091101865
C	4.8093316385	-.5065449946	-2.5766884064
C	4.8921068946	-1.0992737605	-4.9090065738
C	-4.4051154235	-1.2784227098	-2.4207344014
C	-4.3595452036	-2.0730924379	-4.6966531306
C	-3.4542344272	-1.3540912844	-7.4918618426
C	-2.4852021410	-1.4606369668	-6.3031632880
C	5.5146883151	-1.0081909900	-3.6673615442
C	2.7163645888	.4081681389	-1.4817417072
C	2.9030662032	-.8429101552	-6.4547625546
C	-4.9695177306	-2.0345006506	-3.4454697272
C	-2.5897895438	.2348197859	-1.4809103536
C	-.7589552501	-5.7233234300	-3.7481548281
C	-1.8727812585	-5.3492429786	-2.8722582149
C	-3.2064263335	-5.6226335665	-3.2401081053
C	-4.2525337606	-5.3484037151	-2.3721496954
C	-3.9798013441	-4.8009737268	-1.1048178450
C	-2.6700861776	-4.5325592881	-.7211409702
C	-1.6204488219	-4.8072966965	-1.5936821195
C	.2707038439	-6.7033525702	-3.2178533245
H	3.0161397541	2.1402518546	-5.5633679628
H	2.9797688015	2.6085549937	-3.8732364969
H	-3.2184100098	2.1282845343	-3.9365980981
H	-3.1506111688	1.5900055546	-5.6062741819
H	5.2927050894	-.4550118564	-1.6052849497

H	6.5430677084	-1.3365936652	-3.5474755656
H	5.4407078895	-1.5088629685	-5.7522204297
H	-4.8823062169	-1.2654651149	-1.4451480914
H	-5.8688498888	-2.6149081697	-3.2644693365
H	-4.8009119752	-2.6763648840	-5.4838830985
H	-.1569248862	3.0366344197	-5.0294222363
H	1.9692089871	3.4772875776	-5.0471209032
H	3.2888659032	-1.2199605181	-.1413626197
H	-2.2983407910	-3.6370365952	-6.3135483264
H	-.9078769159	-2.8218864886	-5.5918293040
H	1.8460622014	-1.5673157800	-1.1041287119
H	1.7715176771	.8331797956	-1.8314397680
H	2.8345250257	1.8767562388	.1190472598
H	1.9267383883	-.3527091034	-6.4072090243
H	2.1197897479	-2.4417052334	-7.7148125626
H	-1.8586489366	.91911113656	-1.9198964348
H	-1.2923072868	-.1280726687	.2366463884
H	-1.7851124124	-.6234926134	-6.3760668074
H	-2.8931462778	-1.3207736606	-8.4316216448
H	4.6794467340	-.6490106466	-7.7283253993
H	-4.3279095030	.4707369236	-.1581444065
H	-4.1562063132	1.7607308165	-1.3546911813
H	-2.3578097377	3.1092965712	-5.1412429906
H	3.6865455863	2.3695454342	-1.3537659519
H	4.3957167677	1.1562242743	-.2806569760
H	1.7504639708	-.4490441392	.2779096778
H	2.0574533720	-2.8066365567	-5.9762105112
H	3.5974913838	-2.8806587263	-6.8435179897
H	3.1581497578	-.2589973007	-8.5355049990
H	-1.0779557884	-1.3069896032	-1.0734667403
H	-2.4999872762	-1.3979360376	-.0345219094
H	-3.0781488352	1.6983748095	.0504468745
H	-4.0681461970	-.4495495164	-7.4303527127
H	-4.1304132088	-2.2136840532	-7.5478320363
H	-1.1210644967	-2.8069687016	-7.3480944082
H	3.8746126508	.8878542091	-7.3920061420
H	-1.0136874997	-5.8807444892	-4.7983723830
H	.0391362016	-4.5511167889	-3.8061277467
H	-3.4364035483	-6.0478983398	-4.2115698738
H	-2.4706619184	-4.1035956712	.2580867875
H	-.6056105142	-4.5586452999	-1.3066318980
H	-.2030884452	-7.6964331121	-3.1706991702
H	.5113197419	-6.4353735787	-2.1745675120
H	-6.1094098565	-5.3670282136	-1.9967121497
H	-4.8132491010	-4.1716435546	.5154240881
H	2.0638185453	-7.5069667839	-3.7769047027
H	1.9403331318	-5.9024748434	-4.0483319806
N	-1.3773966888	.0681453191	-4.1051919827
N	1.5169918351	.2747276354	-4.1335995140
N	1.4298408383	-6.7827980756	-4.1067332896
O	.5683632566	-2.7166353222	-2.9346260439
O	.9137189525	-3.7793766595	-3.7784306295
O	-5.0867822192	-4.5597808756	-.3249694214
O	-5.5404322593	-5.6021266844	-2.7448706415
Cu	.1372588798	-1.0600854776	-3.6847801421

102.L¹CuO₂ end -on/ formylglycine t.s.

C	2.4229300774	-1.4862485177	-5.7243418085
C	-2.9593979776	3.3472440413	-.2673850622
C	3.3685608498	-1.3057762410	-6.9251977447
C	2.0384997347	-.3158201835	.0690126814
C	2.6095151469	-.4086132439	-3.4024296626
C	-2.9033572573	.5856873335	-2.7696942471
C	-4.3213050515	-.8112786490	-5.9424179203

C	1.2768639398	1.4274485110	-4.2029992046
C	-1.2297098892	1.8385322708	-3.9406330708
C	3.2464109655	-.2721573627	-2.1465833496
C	-3.3202421390	1.1660303477	-1.5463895550
C	.0701444183	2.1422292181	-4.3844918906
C	3.1315528746	-1.2759326906	-4.3892509549
C	-3.7855725636	-.2363874520	-3.5110878493
C	-1.9000143269	1.1914486830	.5390973221
C	1.7303491993	-2.8598697245	-5.7814802746
C	2.5415007980	2.0862949667	-4.7307769279
C	-2.3173947169	2.8290306959	-4.3289422146
C	4.4195451924	-.9940161201	-1.9080471374
C	4.3042001017	-1.9817877074	-4.0987401583
C	-4.6261234145	.9332452742	-1.1019282894
C	-5.0817429758	-.4382730089	-3.0242703696
C	3.6172548876	1.6001620527	-.4525638514
C	-3.3208599281	-.9398900638	-4.7814259972
C	4.9511037839	-1.8436993994	-2.8739599697
C	2.6296107934	.5771265865	-1.0395978362
C	-3.0001142746	-2.4187654462	-4.4909874587
C	-5.5088130426	.1438150567	-1.8337461438
C	-2.3635423447	1.9932202044	-.6919423328
C	.9986372711	-5.5971611758	-3.1039683087
C	1.4864516033	-6.1586397422	-1.7236026241
C	-.7158014192	-6.2517022491	-4.7771656277
H	.1636047505	3.0702877492	-4.9350668810
H	-1.9093014601	3.6428330189	-4.9308777479
H	2.3267758085	3.0672578599	-5.1588613907
H	4.1495964934	-2.0738118797	-6.9420851213
H	3.8655358222	-.3292652198	-6.9095321086
H	3.0137475077	1.4659836002	-5.4987756647
H	3.2775876546	2.2043639483	-3.9292228425
H	-2.8004923011	3.2581235995	-3.4458226344
H	-3.1060529183	2.3305955011	-4.9023806351
H	4.9103695061	-.9083773293	-.9422440651
H	5.8514512370	-2.4138216100	-2.6644805222
H	-2.2633880662	-2.5311215965	-3.6935867147
H	-4.9551875427	1.3730656569	-.1640621387
H	-6.5202374771	-.0246845690	-1.4736756415
H	-5.7665967058	-1.0689697487	-3.5841028454
H	2.8292343927	-.8666446490	.5907499138
H	1.3475220158	-1.0571894948	-.3411937559
H	-3.8172774445	3.2246194603	.4030772040
H	-3.2958535498	3.9279024583	-1.1328863786
H	-3.9071541895	-2.9546290485	-4.1842511486
H	4.7085582992	-2.6664076462	-4.8390359128
H	-2.5965926946	-2.9164838243	-5.3796236363
H	1.8039066153	1.1419501630	-1.4802492586
H	3.1152359001	2.2323695528	.2892438757
H	1.6398590970	-.7268493884	-5.8056612567
H	1.1926307259	-2.9885060559	-6.7268789094
H	-1.4762018024	2.2005077077	-1.2952708489
H	-1.1766292395	1.7680440623	1.1276314277
H	-2.3905513516	-.4606204410	-5.0988659664
H	-3.9004184342	-1.2565078160	-6.8503699047
H	-5.2621570413	-1.3323074391	-5.7323109212
H	-4.5605293195	.2364684590	-6.1559057841
H	-2.2096696213	3.9416458660	.2670604738
H	4.0275030149	2.2527721800	-1.2309802078
H	4.4593677198	1.1110185592	.0494772121
H	1.5039535334	.2917068412	.8094423798
H	1.0094148111	-2.9844641587	-4.9716972116
H	2.4609829791	-3.6724319838	-5.7022205808
H	2.8089977619	-1.3888370741	-7.8636751793

H	-1.4247689803	.2529379491	.2399576930
H	-2.7471815184	.9459720592	1.1898311628
H	1.7343997906	-5.3059141111	-3.8542568196
H	-1.5860501620	-6.9362474014	-4.8312807352
H	-.4300950671	-6.9342571791	-2.8086269744
H	.4464098559	-4.3404561238	-2.7782170082
N	-1.5589908720	.7649452429	-3.2170935757
N	1.3577483672	.2461868977	-3.6096638428
N	-.0681566098	-6.3593443071	-3.5834966587
O	-.3142454543	-3.4104352512	-2.8196857150
O	.1106971178	-2.3700906771	-2.0634400517
O	2.6240040959	-5.7831062011	-1.3895100982
O	.6505978798	-6.9246926023	-1.1796192661
O	-.4041078374	-5.5144041093	-5.7037358113
Cu	-.2516380655	-.6683311301	-2.8497209146

103.L¹CuO₂H⁺ / methane complex

C	-4.3483569603	-3.1449927979	1.1786165246
C	-2.8058813277	4.5257225210	-2.2188193466
C	-3.1854756194	-4.1481012262	1.3437341526
C	-4.3799535001	2.3051486112	3.3793751490
C	-3.7270100937	-1.0081043866	2.4790152183
C	-3.0332147458	.8908022713	-2.4720037593
C	-1.7067509560	-2.1302458254	-4.2729155166
C	-1.5933788996	-.5729275748	1.4074823002
C	-1.2139375673	.3707003396	-.9216743332
C	-3.8525265262	-.1432974938	3.6115701336
C	-3.6129702426	2.1744119863	-2.7172347424
C	-.8040866060	-.1252399391	.3324451058
C	-4.4575397922	-2.2380500452	2.3961199742
C	-3.0935617606	-.1502343355	-3.4509654215
C	-5.0057778582	3.6911205770	-1.2464455845
C	-5.6581424307	-3.8834719524	.8565067583
C	-.8542179666	-1.0391889438	2.6470529641
C	-.1524353793	.5911367769	-1.9763714526
C	-4.6295021963	-.5848175586	4.6771926034
C	-5.2006401251	-2.6317594341	3.5133061222
C	-4.1990043805	2.4002690473	-3.9636585552
C	-3.7045145093	.1406537578	-4.6688851630
C	-2.5117944340	1.5875527475	4.9368321488
C	-2.6309362175	-1.5775670975	-3.1720592716
C	-5.2808927143	-1.8233311533	4.6414752255
C	-3.2650100621	1.2646021318	3.6340508140
C	-3.8509012419	-2.5026676863	-2.9717762451
C	-4.2450337459	1.4002350482	-4.9315105370
C	-3.5804749441	3.3018788229	-1.6901373249
H	.2661270510	-.2089270107	.4742808591
H	-5.1057398692	2.3033234008	4.1998302232
H	.1605057824	-1.3479271008	2.3895516694
H	.7909129700	.8799034547	-1.5074706678
H	-6.9834581999	-.1751802777	1.4973898822
H	-4.9229785892	2.0977370354	2.4520637893
H	-3.3547384706	-4.8055335535	2.2030709992
H	-2.2258019189	-3.6430546137	1.4903614922
H	-3.5227768301	-3.5146177412	-2.7128316040
H	-1.3731287579	-1.8722243493	3.1250535424
H	-.7823351805	-.2280372998	3.3787014838
H	-4.5072105187	-2.1404760118	-2.1732427626
H	.0273577069	-.3297576269	-2.5409348481
H	-4.7435608131	.0465183439	5.5523641768
H	-5.8709624618	-2.1441264078	5.4950869708
H	-5.7337700427	-3.5754776342	3.4941888619
H	-4.6277737276	3.3729650138	-4.1817875949
H	-4.7143960259	1.5965619031	-5.8909816121

H	-3.7770867434	-.6334016944	-5.4258771585
H	-3.3017737921	4.9707919821	-3.0874997824
H	-1.7862060686	4.2605298725	-2.5160908216
H	-4.4498038635	-2.5674964760	-3.8858126599
H	-.4550922369	1.3655792837	-2.6838245589
H	-2.2375010713	-2.2571457077	-5.2211219684
H	-2.5505338015	1.3552364109	2.8098330612
H	-2.0291203654	2.5663028545	4.8552815018
H	-4.1094955762	-2.5088069339	.3195298305
H	-5.5582512665	-4.4076888507	-.0989850340
H	-3.0453898188	2.9404634437	-.8060471259
H	-4.9606104835	4.4685147614	-.4769209960
H	-2.0676676423	-1.5875717978	-2.2349021459
H	-1.3233391726	-3.1131426868	-3.9820372892
H	-1.7394431650	.8457252560	5.1627603430
H	-3.1880239150	1.6325695186	5.7961887625
H	-3.9510536336	3.3108840343	3.3148327066
H	-6.4970170337	-3.1879042178	.7740557075
H	-5.9048221682	-4.6388311057	1.6097750169
H	-3.1008658732	-4.7779384138	.4523725109
H	-5.5495327262	2.8349947698	-.8342554071
H	-5.5903138982	4.0882291110	-2.0823240059
H	-2.7432958166	5.2960429281	-1.4437117604
H	-.8518486869	-1.4725450269	-4.4579280361
N	-2.9280325855	-.6653460537	1.3753909507
N	-2.4835782970	.6527559167	-1.1875358875
O	-5.6449892334	.6536775881	.5009261453
O	-6.3503497827	-.5117620058	.8367613837
Cu	-3.9026146517	.3451832023	.0119733337
C	-9.0677577726	.8852587070	2.1052246140
H	-9.8188608457	1.5122032856	2.5891685047
H	-9.5162629371	.3779796743	1.2489235892
H	-8.7199807461	.1459880428	2.8342113225
H	-8.2449106514	1.5241691837	1.7698280989

104.L¹CuO₂H⁺ / cyclohexane complex

C	2.8451929543	1.9189299099	4.6523252166
C	3.1632277258	-2.4062315183	-4.3383533221
C	2.3504644928	-1.7028645605	-3.2351082606
C	3.0941894398	4.3266646421	-2.2100868592
C	.7307583863	3.8735600576	-1.3779164212
C	4.1664031937	-1.1868269336	2.6800265198
C	3.5068628451	-.7252240320	1.3946135750
C	4.3570598940	-.4589014103	.3066988852
C	4.0277401662	.0422353814	-.9682116609
C	5.1159608276	.0964419044	-2.0173507030
C	1.3286318375	-.7623980791	2.4675753049
C	1.3108752296	.2291696586	3.4964623581
C	.4763255577	.0111132272	4.5883913137
C	-.3327967622	-1.1276311944	4.6690333422
C	-.3523598284	-2.0558606022	3.6334766659
C	.4442689583	-1.8872494073	2.4972357795
C	2.0734446180	1.5448689399	3.3744339408
C	1.0031083153	-2.4224700483	-3.0021787287
C	1.1012466353	2.6783326642	2.9740757248
C	.4427914150	-2.9263011345	1.3838287275
C	-.9511867330	-3.5131375050	1.1055336117
C	1.4552483202	-4.0544815738	1.6825071132
C	2.3140440486	.7957006134	-2.5464188695
C	1.9283990236	2.1502751443	-2.7907429143
C	1.4098381954	2.4649013043	-4.0472433955
C	1.2348930341	1.4841429385	-5.0205515608
C	1.5731591770	.1562974098	-4.7533499053
C	2.1123398474	-.2244418171	-3.5260929989

C	2.0927078776	3.2505290376	-1.7475410320
C	-6.6386595024	2.1644276310	1.5030472016
C	-6.8957526805	.6498328836	1.5600088090
C	-5.8421859352	-.0692315603	2.4183848254
C	-4.4145250973	.2408683726	1.9346344934
C	-4.1590944438	1.7583805878	1.8797055231
C	-5.2127913962	2.4765958116	1.0195390687
H	3.2314055208	5.0760456532	-1.4241983512
H	.8619676953	4.6218555317	-.5896281983
H	5.1443293643	-1.6231304827	2.4707153482
H	2.6105365562	-2.4575581344	-5.2813781900
H	6.0937974768	.2103326270	-1.5454816220
H	.4404021933	.7437445814	5.3879357723
H	-.9667035737	-1.2762824005	5.5384175602
H	-1.0050965549	-2.9186841799	3.7047654830
H	2.8047195872	1.4496165646	2.5656249052
H	1.1727001852	-3.4715696751	-2.7381294732
H	1.6526982669	3.6106804509	2.8130849831
H	.7752967616	-2.4226289993	.4703994477
H	-.9101157541	-4.1486088788	.2154031702
H	1.4623316375	-4.7822726376	.8645878192
H	1.1334140059	3.4908984605	-4.2677736640
H	.8198534977	1.7502903676	-5.9882523636
H	1.3970617470	-.5970283335	-5.5141413698
H	2.5058714606	2.7979537283	-.8403137104
H	2.9185711623	-1.7882366316	-2.3042675208
H	3.4462579791	2.8166400470	4.4775996325
H	2.1681507003	2.1405249575	5.4826936567
H	4.1098098395	-1.8940265415	-4.5372845193
H	3.3894021368	-3.4344800778	-4.0395573835
H	2.7389451610	4.8474733092	-3.1050548537
H	4.0731802996	3.8948655802	-2.4409650446
H	.0258947337	3.1179116501	-1.0166431015
H	.2739906606	4.3763511575	-2.2362916098
H	3.5472667131	-1.9223080466	3.1974841374
H	4.3134071202	-.3411963671	3.3593779521
H	4.9509435377	.9256035838	-2.7089864219
H	5.1340288701	-.8287080690	-2.6033514533
H	.3819176256	-2.3982983493	-3.9034320383
H	.4294610821	-1.9552555052	-2.1937259830
H	.3662754272	2.8561669975	3.7666809680
H	.5494252372	2.4367081395	2.0601458801
H	-1.6842689520	-2.7236193812	.9244729134
H	-1.3109421918	-4.1395094714	1.9282713616
H	1.1876262127	-4.5863217213	2.6017804322
H	2.4740346891	-3.6722911531	1.8000682686
H	3.5175492584	1.1188797201	4.9778807132
H	-1.8713006861	.3055152337	1.2417056921
H	5.4032312301	-.6877407758	.4649774770
H	-7.8998895810	.4493324826	1.9513870479
H	-6.8720066276	.2397338197	.5400375801
H	-5.9434549172	.2557936758	3.4636641228
H	-6.0168549107	-1.1516253886	2.4100342603
H	-3.6860437184	-.2510034565	2.5966901437
H	-4.2749767985	-.1878504601	.9308390259
H	-3.1537526826	1.9778676426	1.4886351450
H	-4.1847739467	2.1643175411	2.9009384976
H	-5.0344239200	3.5583378298	1.0300092476
H	-5.1058079765	2.1517765315	-.0255878166
H	-7.3726244807	2.6500253849	.8494823610
H	-6.7822629730	2.5942347846	2.5047873252
N	2.1723511950	-.6420498299	1.3482444902
N	2.8094266980	.4817623686	-1.2587294942
O	-1.2419093515	-.1546556428	.6563495637

O	- .3844325071	.8890927445	.2786672992
Cu	1.3352562571	.3606081476	-.0942320259

105.L¹CuO₂H⁺ / acetonitrile complex

C	.5095755705	1.7751106768	.5234786666
C	.6859481607	4.2368751969	-3.77944469516
C	-.0953295294	-4.0758779730	-.1236538484
C	-.5203325208	2.8903575446	.2290987467
C	-.2513143086	-.6630867741	.0056829878
C	.1740778551	1.0467500944	-4.9919115222
C	1.6893813504	-1.3681689956	-7.3837415599
C	1.8225988044	-.5915661767	-1.2393928377
C	2.0510873192	.3531803471	-3.5809638956
C	-.2102739226	.4768393130	.8733116739
C	-.4725208156	2.3228977694	-4.9394171832
C	2.5396652172	-.2148648054	-2.3858691916
C	-1.0786803063	-1.7943259635	.3095736263
C	.1314054996	.2360850172	-6.1678828302
C	-1.7929011943	3.8554148793	-3.3771063688
C	-2.5349255771	-3.6460582346	-.6641868587
C	2.6417618142	-.9304687310	-.0085574263
C	3.0700531052	.7424012737	-4.6299461735
C	-.9499175982	.4230302320	2.0521917957
C	-1.7778036514	-1.7863178553	1.5145250943
C	-1.0848681227	2.7920195278	-6.0993911433
C	-.5209144930	.7577458819	-7.2849169982
C	1.4894863336	2.2305098592	1.6249119467
C	.6807891614	-1.1857563004	-6.2310383764
C	-.4409874977	3.1864766227	-3.6840958376
C	-1.7165890261	-.6939268387	2.3806548993
C	-.4606862827	-2.2181913286	-6.3609652497
C	-1.1287751733	-3.0254791132	-.5857661402
C	-1.1135873836	2.0196257399	-7.2609520553
H	-1.0719647110	3.1610506784	1.1352210640
H	3.6172211240	-.2972254768	-2.3124038880
H	3.5314980345	-1.4912511571	-.3064242855
H	3.9974233793	1.0649048606	-4.1518898415
H	-3.3933032112	-2.1385877814	-3.9253037475
H	-1.2564349872	2.5803131105	-.5171716605
H	-.3069308655	-4.4082974695	.8982772030
H	.9248853929	-3.6797288683	-.1443177255
H	-.0459795437	-3.2315893773	-6.3816746542
H	2.0663951369	-1.5220856504	.7042408162
H	2.9814623894	-.0205117354	.4942806997
H	2.6938940991	1.5435041391	-5.2682929501
H	-1.1627321026	-2.1548751011	-5.5264685916
H	-.9435831488	1.2766952933	2.7218569741
H	-2.2797268046	-.7077881926	3.3093323843
H	-2.3823557648	-2.6441065336	1.7865023329
H	-1.5554961737	3.7689346708	-6.0973061111
H	-1.6112374646	2.3981621173	-8.1489999769
H	-.5805212767	.1624242352	-8.1904996382
H	1.2008793948	-1.2749632396	-8.3588985626
H	.5079353416	4.9276749399	-4.6103407825
H	1.6644246736	3.7708881572	-3.9363022521
H	-1.0195598698	-2.0695998870	-7.2909382854
H	3.3067855011	-.1150078486	-5.2686040149
H	2.4977097588	-.6319886301	-7.3493068744
H	1.0876279939	1.6200425219	-.3921728246
H	2.0538657766	3.1039557816	1.2833767621
H	-.8552465094	-2.7205521117	-1.5997322947
H	-2.5566676243	-4.4087093585	-1.4480429523
H	-.2016098007	2.5343268773	-2.8381658546
H	-1.7295551407	4.3880703316	-2.4234263960

H	1.2011867591	-1.4024099098	-5.2925692376
H	2.1334917056	-2.3673722798	-7.3372764197
H	2.2053128677	1.4500416765	1.8997200267
H	.9603448265	2.5239069014	2.5368482323
H	-.0068310799	3.7899188970	-.1267510404
H	-3.2885732462	-2.8910602137	-.9034958285
H	-2.8257895286	-4.1338369079	.2720792882
H	-.1291109013	-4.9537302333	-.7770079956
H	-2.5972673012	3.1194755431	-3.2924123788
H	-2.0743645162	4.5913701098	-4.1369872331
H	.7352945327	4.8251963938	-2.8575694679
N	.4917225842	-.6937674172	-1.1910457587
N	.7602202742	.5919910721	-3.7890297639
O	-2.4709787808	-2.1337332664	-3.6167690500
O	-2.3207072602	-.7787718092	-3.2251842419
Cu	-.5804617678	-.3156035962	-2.7697285363
C	-4.3487661958	.5738418569	-1.6840404356
C	-5.3695005326	-.2934398109	-2.2622592969
H	-6.2839049354	-.2664186740	-1.6631413290
H	-4.9917255751	-1.3198789456	-2.2895444134
H	-5.6079909172	.0305241169	-3.2790778255
N	-3.5328118199	1.2559448148	-1.2209723520

106.L¹CuO₂H⁺ / toluene complex

C	2.3267778648	1.3521867382	4.9215042989
C	4.8339234148	-2.0426007705	-4.1454513512
C	3.6906662517	-1.5739138572	-3.2246336150
C	3.0538827920	4.4856011694	-2.3225920730
C	.7386115533	3.5792796642	-1.7830719881
C	4.4273733273	-1.0838209283	2.7771590491
C	3.8693827115	-.5842366549	1.4575768748
C	4.7955783381	-.0680913098	.5357312307
C	4.5758709516	.4294219173	-.7659483744
C	5.7950096120	.7212967336	-1.6140787579
C	1.6189059302	-1.1467582576	2.1658729472
C	1.3003179772	-.3571801205	3.3158900033
C	.4032415004	-.8888237163	4.2358712708
C	-.1847204137	-2.1435942948	4.0399181410
C	.0830637628	-2.8783556330	2.8904105040
C	.9557541735	-2.3911373170	1.9124315002
C	1.8202933553	1.0652140441	3.4969592183
C	2.5220010476	-2.5822455988	-3.2504376520
C	.7228255116	2.0763803131	3.0959994105
C	1.2682682816	-3.2126962184	.6711798923
C	.0514017787	-3.9897258509	.1424941235
C	2.4582920860	-4.1642363805	.9278418106
C	3.0282128849	.8636081602	-2.6075289506
C	2.4309681865	2.1121000831	-2.9558745546
C	2.0497225267	2.3099211883	-4.2844856592
C	2.2178412707	1.3115772751	-5.2397491974
C	2.7748553203	.0848286408	-4.8817571208
C	3.1903931963	-.1751692149	-3.5761858372
C	2.2330535382	3.2367402410	-1.9454574341
H	-1.5010370609	-.2280505741	.7806663482
H	2.6032725918	2.8904379857	-.9745122510
H	2.7833893450	2.3458996650	4.9613259292
H	3.0731658464	.6224420700	5.2505476028
H	1.5119531340	1.3427752012	5.6519568057
H	4.4952925415	-2.1758608435	-5.1774401372
H	5.6637201209	-1.3297113281	-4.1609838869
H	5.2206115277	-3.0077067973	-3.8034599181
H	4.0762291421	-1.5636428940	-2.2016325387
H	2.9390669141	5.2576908634	-1.5552205837
H	2.7202060146	4.9127797083	-3.2737599776

H	4.1197698152	4.2548357675	-2.4150864092
H	.6101387357	4.3509059966	-1.0171169383
H	.1549025726	2.7026357533	-1.4861017296
H	.3144066542	3.9651729171	-2.7154621097
H	5.4922163321	-1.3018453240	2.6822591424
H	3.9046196139	-1.9849277602	3.1058483047
H	4.3073695940	-.3289567775	3.5598611802
H	5.8323171967	-.1092295955	.8464043574
H	6.5581784256	1.2129974039	-1.0047343365
H	5.5474917614	1.3613043359	-2.4619650125
H	6.2319023958	-.2060819301	-1.9980305099
H	.1429020241	-.3163634322	5.1199293022
H	-.8723577358	-2.5355875392	4.7835907278
H	-.4029086643	-3.8363103210	2.7438985115
H	2.6596562678	1.2191702339	2.8116426191
H	2.8682786924	-3.5732185107	-2.9393742651
H	2.1004533262	-2.6750046589	-4.2564047278
H	1.7121379669	-2.2759319226	-2.5797392046
H	1.1087682772	3.0990793040	3.1652491812
H	-.1413720386	1.9942986005	3.7637213738
H	.3694717651	1.9040875499	2.0751515972
H	1.5781647915	-2.5121243741	-.1116805793
H	.2961297064	-4.4413482462	-.8239537256
H	-.8097622314	-3.3309196892	.0020890943
H	-.2408546762	-4.8060095767	.8113117881
H	2.6868804831	-4.7363732598	.0227149802
H	2.2240161684	-4.8776399499	1.7250063016
H	3.3624311808	-3.6198495174	1.2180527126
H	1.6122263285	3.2588370566	-4.5768531065
H	1.9058470712	1.4842805462	-6.2654601117
H	2.8745567012	-.6899833156	-5.6351236617
N	2.5592861119	-.7238877626	1.2135372888
N	3.3586028138	.6542863695	-1.2438994461
O	-.7513096617	-.5642735312	.2406712756
O	-.0139721128	.5949907428	-.0128581918
Cu	1.7830846680	.3096386773	-.2656938226
C	-4.1564083496	-.5448212824	2.9406794425
C	-3.8363790580	.6281136876	3.6242948469
C	-3.4189233370	1.7622119695	2.9235616673
C	-3.3159273303	1.7505035429	1.5277697483
C	-3.6386574926	.5604165018	.8496327274
C	-4.0587760593	-.5750608884	1.5477377450
C	-2.8756897843	2.9719588179	.7552767706
H	-3.6009146493	.5396822717	-.2377002827
H	-4.3229867264	-1.4767028377	1.0017706607
H	-4.4932355895	-1.4225012877	3.4843335744
H	-3.6491732375	3.2914558126	.0477875907
H	-1.9700408509	2.7617396051	.1755511443
H	-2.6641908060	3.8117831722	1.4218785777
H	-3.1838678687	2.6742070321	3.4669497273
H	-3.9210117565	.6662649749	4.7068811739

107.L¹CuO₂H⁺ / phenol complex

C	2.9246024950	1.9241826872	4.5973119283
C	4.2217224318	-1.5728588206	-4.5421640618
C	3.2605757549	-1.3284091297	-3.3628722064
C	2.8745351688	4.1355258806	-1.3501143472
C	.3684951750	3.8726182192	-1.1032949465
C	5.0687576105	-.6602269226	2.7077458841
C	4.2768261744	-.4424981835	1.4337998819
C	4.9700624438	.1054962255	.3392066466
C	4.4446949972	.5727943650	-.8801579056
C	5.4222402923	1.0439413176	-1.9350483801
C	2.2104365009	-1.1212865359	2.5206230860

C	1.8797069394	-.1275606262	3.4953219295
C	1.0882716078	-.5171693028	4.5754134181
C	.6226773476	-1.8253877389	4.6959007008
C	.9202718147	-2.7763776558	3.7187303153
C	1.6905585783	-2.4525534639	2.6047101681
C	2.2515754578	1.3429567810	3.3392052913
C	2.2108734946	-2.4591765693	-3.2721960821
C	1.0009702929	2.1713113423	2.9653252898
C	2.0224034850	-3.5040054792	1.5518026185
C	.8943140639	-4.5272505729	1.3396929492
C	3.3480099400	-4.2220620597	1.8866451552
C	2.5157142801	.9393810898	-2.3429230166
C	1.7391880912	2.1441673621	-2.4044029735
C	1.0778476688	2.4274952958	-3.5961335561
C	1.1380210991	1.5529862429	-4.6820014777
C	1.8700999059	.3693756475	-4.5992870211
C	2.5716620441	.0285626537	-3.4441709018
C	1.7068931385	3.1289151038	-1.2414205245
H	-1.1890487461	-2.1018086339	-.3523780034
H	1.8590969073	2.5552454555	-.3195962040
H	3.2513775006	2.9509029232	4.4055527528
H	3.7980584792	1.3410782967	4.9046545146
H	2.2347720038	1.9572132320	5.4463057337
H	3.6847704673	-1.6492278514	-5.4928250461
H	4.9591441874	-.7704453967	-4.6432352548
H	4.7600168797	-2.5146710875	-4.3975760576
H	3.8522265567	-1.3658917238	-2.4431177477
H	2.8633819721	4.8190732994	-.4949287432
H	2.7850473940	4.7367550959	-2.2612031665
H	3.8491553471	3.6380262163	-1.3698276895
H	.3858993161	4.4817093992	-.1939190045
H	-.4708485032	3.1785989690	-1.0220496641
H	.1868255903	4.5555377858	-1.9398630683
H	6.1037671464	-.9118098772	2.4656253208
H	4.6354827565	-1.4566412519	3.3139471372
H	5.0824163633	.2547981822	3.3086451068
H	6.0403050375	.2116986740	.4644584301
H	6.3087915361	1.4757354695	-1.4657595392
H	4.9660088855	1.7849147467	-2.5940388719
H	5.7500688882	.2004308488	-2.5517245289
H	.8130174397	.2153662835	5.3270561476
H	.0088684525	-2.1027705976	5.5481011146
H	.5344806547	-3.7834610278	3.8281766399
H	2.9609468039	1.4402770900	2.5119585268
H	2.7094782185	-3.4266340387	-3.1537856466
H	1.6062844161	-2.5040546150	-4.1839017884
H	1.5245180399	-2.3196351965	-2.4309622952
H	1.2819657141	3.2128908541	2.7775697801
H	.2717604803	2.1655582111	3.7821445080
H	.4913148279	1.7881877430	2.0759626476
H	2.1666825868	-2.9804814638	.6006471819
H	1.1259952355	-5.1546658903	.4737915086
H	-.0591635769	-4.0287663124	1.1489466091
H	.7719355346	-5.1972724652	2.1967444334
H	3.5845021583	-4.9584942159	1.1119226842
H	3.2745520053	-4.7515305018	2.8426407465
H	4.1877195549	-3.5237877024	1.9524007388
H	.4977227050	3.3388920505	-3.6828671368
H	.5996699991	1.7907557061	-5.5948750455
H	1.8788942599	-.3072454935	-5.4474513171
N	2.9959018426	-.8097203710	1.3923139073
N	3.1375341596	.6466883617	-1.1113896703
O	.0225829800	-.6716255522	-.1637777025
O	-.2527767107	-2.0067645148	-.5948655093

Cu	1.8487683268	-.3023826593	-.0798164550
C	-3.4865837059	2.6098182113	1.0542612103
C	-2.8799165991	1.4172968436	.6302959338
C	-3.6648599822	.2758718054	.4057510862
C	-5.0412053659	.3291701386	.6092381989
C	-5.6477594142	1.5133229980	1.0357927400
C	-4.8614629077	2.6495369205	1.2550291395
H	-3.1959818789	-.6445356146	.0645838875
H	-5.6435437675	-.5568040368	.4313980673
H	-6.7208161965	1.5517550653	1.1933478373
H	-1.1910309306	.5452870550	.1773444695
H	-5.3266529983	3.5741373633	1.5839545960
H	-2.8647150985	3.4831496196	1.2210122448
O	-1.5338349933	1.4238852838	.4542161092

108.L¹CuO₂H⁺ / isopropylbenzene complex

C	5.7902845767	.8114139482	5.0095317548
C	7.3119397624	-1.5605834144	-4.5636426634
C	6.3377643766	-1.1252611850	-3.4545625842
C	6.2675151427	4.6822244902	-1.3534327102
C	3.9361832100	3.8009810668	-.8325969789
C	7.5417160999	-1.6151819696	2.5834380995
C	6.9409017008	-.9560469264	1.3561872913
C	7.8463802123	-.4004381926	.4337509414
C	7.5794299093	.3063156111	-.7542427702
C	8.7392243844	.6644004385	-1.6578164790
C	4.7007762379	-1.4244751332	2.1606878554
C	4.5162291032	-.7044709185	3.3825280380
C	3.6364124928	-1.2413281127	4.3167586450
C	2.9471045817	-2.4347537020	4.0681935108
C	3.0858511782	-3.0925770272	2.8512802127
C	3.9302142715	-2.5923373382	1.8551395858
C	5.1336571983	.6708860699	3.6224778546
C	5.0442421414	-1.9707267495	-3.4974780368
C	4.0658620061	1.7687951971	3.4092040195
C	4.1083876857	-3.3319311484	.5371998688
C	2.8121549075	-3.9879808539	.0306929783
C	5.2423523107	-4.3753025743	.6426778029
C	5.9599245787	1.1909539250	-2.3541332452
C	5.4510866922	2.5254365190	-2.4048614444
C	5.0380123994	3.0197139138	-3.6423855980
C	5.0917724029	2.2307266728	-4.7889048419
C	5.5516187462	.9143069389	-4.7201818380
C	5.9871365778	.3590294240	-3.5179221221
C	5.3917113060	3.4256176143	-1.1764861823
H	1.4464731091	-.3569728167	.6680618817
H	5.7963041478	2.8666217683	-.3267151120
H	5.0497703381	.7765496126	5.8141067706
H	6.3027605126	1.7755491286	5.0841419352
H	6.5253729455	.0241610353	5.2034804360
H	6.8602414645	-1.4929257054	-5.5581867831
H	8.2197904862	-.9487419197	-4.5687713233
H	7.6072154845	-2.6035740175	-4.4140759377
H	6.8245788240	-1.3300585684	-2.4965165872
H	6.2568585117	5.2817443954	-.4375670865
H	5.9021304771	5.3172989768	-2.1668832278
H	7.3075629857	4.4221745599	-1.5754240811
H	3.9105016562	4.4088467304	.0776123504
H	3.3189180386	2.9121379994	-.6652608325
H	3.4718467214	4.3855586813	-1.6328755491
H	8.5753683065	-1.9070112515	2.3917172064
H	6.9685433198	-2.4976483242	2.8760242293
H	7.5382085938	-.9227909866	3.4303754637
H	8.8931054922	-.5614255751	.6571289828

H	9.6786763183	.6483837848	-1.1031182052
H	8.5946390756	1.6575149317	-2.0905794028
H	8.8227822857	-.0474527730	-2.4855581622
H	3.4698527357	-.7215102241	5.2542968009
H	2.2832279414	-2.8380461548	4.8273423929
H	2.5232727182	-4.0008933831	2.6686579749
H	5.9146266046	.8359780675	2.8724917393
H	5.2792788283	-3.0352799962	-3.3906442053
H	4.5178831070	-1.8346736567	-4.4483941226
H	4.3499721161	-1.6926456664	-2.6955148796
H	4.5222780366	2.7605643226	3.4987533275
H	3.2760064160	1.6950502841	4.1637409586
H	3.5974413859	1.6905257889	2.4230952064
H	4.4136907724	-2.5925101512	-.2100392958
H	2.9702342282	-4.3740717702	-.9811532637
H	1.9901417700	-3.2684293533	-.0072234288
H	2.5045211682	-4.8364271478	.6502447313
H	5.3779225368	-4.8864569746	-.3159614812
H	5.0066403013	-5.1334404699	1.3970179779
H	6.1983961333	-3.9166171761	.9149475501
H	4.6670140954	4.0371637432	-3.7121084082
H	4.7588052020	2.6347058931	-5.7403650358
H	5.5502127310	.3059187227	-5.6185819101
N	5.6134030306	-.9907269636	1.1845564741
N	6.3533186844	.6945201425	-1.0884631459
O	3.0165866204	.5136782694	.1406704904
O	2.2383272634	-.6544645538	.1820872724
Cu	4.8102613555	.2195509226	-.1208533742
C	-1.9133786372	.7716705030	3.3494616375
C	-1.3420764355	.4497929505	2.1173870119
C	-2.0930535937	.4684501023	.9372869986
C	-3.4474853458	.8188477345	1.0301645255
C	-4.0264011465	1.1419468868	2.2564133037
C	-3.2607507199	1.1203323254	3.4232606081
C	-1.4654950810	.1094311360	-.4035689998
C	-2.0606748072	-1.1877846687	-.9800548561
C	-1.5618672413	1.2680243186	-1.4139611695
H	-5.0778343192	1.4115522368	2.3005418255
H	-3.7102343792	1.3720930721	4.3792565558
H	-.2869575477	.1745678817	2.0882887704
H	-1.3063120510	.7495381313	4.2505289309
H	-4.0613137271	.8414918285	.1333217831
H	-.3946025033	-.0713433631	-.2237772564
H	-1.0473079658	1.0124718350	-2.3459632762
H	-1.1120461507	2.1823437840	-1.0146650275
H	-2.6037693105	1.4936898431	-1.6637594716
H	-1.5616987753	-1.4656147440	-1.9144507996
H	-3.1267000612	-1.0649650298	-1.1960379344
H	-1.9605263128	-2.0199147586	-.2765088953

109.L¹CuO₂H⁺ / cyclohexadiene complex

C	2.9394978789	1.4981007146	4.9525416880
C	3.8194534940	-2.1347200309	-4.3471781230
C	2.9085905258	-1.5334086190	-3.2586989804
C	3.2174898115	4.5261668005	-2.1419243301
C	.8921218804	3.8977898017	-1.3283311485
C	4.4534864188	-1.2430699216	2.6704150143
C	3.8054003144	-.6966513924	1.4126580683
C	4.6723106745	-.2919963428	.3818669627
C	4.3611321564	.2572351622	-.8786024967
C	5.4932352873	.4342786745	-1.8671684343
C	1.6109473414	-.9668636939	2.4039250774
C	1.5278062496	-.1096630653	3.5461568545
C	.6954008294	-.5018328786	4.5897739381

C	-.0474557131	-1.6852363611	4.5233977419
C	-.0090670382	-2.4800509111	3.3838741100
C	.7855413577	-2.1301199427	2.2856923088
C	2.2329806924	1.2424925169	3.6076654382
C	1.6111812920	-2.3583703506	-3.1133329144
C	1.2291169609	2.3774080725	3.3029504605
C	.8458726598	-3.0254190894	1.0539737577
C	-.5148583737	-3.6338611953	.6791107089
C	1.9046813798	-4.1365915514	1.2300364706
C	2.6732782422	.9412486044	-2.5095129245
C	2.2195330227	2.2754621211	-2.7501098970
C	1.7197987318	2.5797887599	-4.0173922587
C	1.6368304659	1.6093162081	-5.0114696963
C	2.0530810018	.3026085410	-4.7545320994
C	2.5745306338	-.0672611363	-3.5154116513
C	2.2967192420	3.3742650907	-1.6934431329
H	-1.5378531524	.1049963912	1.3351608085
H	2.7384256190	2.9453204104	-.7882727785
H	3.5154204020	2.4271989775	4.9011480300
H	3.6259768337	.6889559555	5.2213329799
H	2.2239379824	1.6077562408	5.7735431263
H	3.3103748898	-2.1932063346	-5.3143127394
H	4.7315244840	-1.5473110368	-4.4911166311
H	4.1106476482	-3.1532198160	-4.0716942025
H	3.4375600384	-1.6092503147	-2.3048563712
H	3.3039222123	5.2720811897	-1.3452926358
H	2.8257911649	5.0341211831	-3.0293163808
H	4.2235047868	4.1665589135	-2.3799694311
H	.9654350338	4.6528205430	-.5387288681
H	.2414119019	3.0934341586	-.9713181145
H	.4038319730	4.3664896299	-2.1890354611
H	5.4729977715	-1.5709745764	2.4624238197
H	3.8817595665	-2.0823496814	3.0724911078
H	4.4987997771	-.4735160594	3.4466969781
H	5.7254036860	-.4610872197	.5680415149
H	6.4195875155	.6721960133	-1.3392669307
H	5.2725508292	1.2295465209	-2.5817775851
H	5.6633340971	-.4885114510	-2.4312106501
H	.6145613179	.1240792955	5.4726671130
H	-.6734096232	-1.9737920746	5.3630850009
H	-.6128108511	-3.3793191632	3.3405986667
H	2.9945475751	1.2700401202	2.8218847426
H	1.8480419492	-3.4017495911	-2.8804086418
H	1.0272496541	-2.3458175761	-4.0392940932
H	.9730825396	-1.9655171304	-2.3142725337
H	1.7475189465	3.3416938580	3.2721730459
H	.4633818914	2.4355477266	4.0849042484
H	.7236754665	2.2225648721	2.3452598761
H	1.1662680190	-2.4004906254	.2138148047
H	-.4329873416	-4.1500121163	-.2826723498
H	-1.2813314935	-2.8609677322	.5845631909
H	-.8539527767	-4.3746585445	1.4106809143
H	1.9535498203	-4.7604432306	.3313681747
H	1.6534492223	-4.7861442713	2.0752181874
H	2.9030994461	-3.7254158999	1.4064894226
H	1.3893069338	3.5911551024	-4.2304071612
H	1.2377795511	1.8666457742	-5.9881888366
H	1.9554765439	-.4465477351	-5.5339238157
N	2.4690711224	-.6820521625	1.3271025672
N	3.1293431053	.6313771900	-1.2027096461
O	-.8822496936	-.2881265067	.7079626254
O	-.0985104775	.8115010247	.3686294414
Cu	1.6346601582	.3993356398	-.0750135242
C	-3.0074869095	1.5877938673	2.1462685809

C	-3.5003259295	2.2028592426	.8626726460
C	-4.4533984577	1.3058048843	.1175883171
C	-4.8701668864	.1236473771	.5767489210
C	-4.4381266549	-.4600643514	1.8966899662
C	-3.4192243754	.3955045762	2.6037819983
H	-3.0350679848	.0241279524	3.5527344646
H	-2.2984104568	2.1710175121	2.7315633732
H	-2.6399860554	2.4610952269	.2275344878
H	-3.9818536473	3.1693879504	1.0814197846
H	-5.3123660707	-.5983699812	2.5535766657
H	-4.8151439087	1.6676421933	-.8422113126
H	-5.5669348643	-.4679127517	-.0129726654
H	-4.0444982278	-1.4789479045	1.7540507495

110.L¹CuO₂H⁺ / dopamine complex

C	-.6643286958	-2.5065377578	-.9184760307
C	1.5373306766	3.7883388052	-6.3665580849
C	.2148365650	-3.4566853507	-.0777555772
C	-.3007337325	3.3424681319	-1.4678520191
C	.0754411958	-.0433028627	-.7143862635
C	.9468298519	.2047819550	-5.9740188800
C	1.9191260578	-3.2890035201	-7.0030062778
C	2.2483233564	-.2309356826	-1.7867849242
C	2.6751178425	-.0260742001	-4.2698322391
C	-.0137911641	1.2462920869	-.1104868103
C	.5361084607	1.4567742533	-6.5128939889
C	3.0661929008	-.1927118960	-2.9284502274
C	-.7368006441	-1.1288780023	-.2723741749
C	.8121727273	-1.0046523020	-6.7117423753
C	-.8058067040	3.3315003156	-5.4871226731
C	-2.0538359582	-3.1187603410	-1.1698009923
C	2.9379295695	-.2547177636	-.4370882913
C	3.7498459460	-.0639359157	-5.3347760859
C	-.8801309877	1.3988839094	.9703243574
C	-1.5694202585	-.9138587811	.8268972262
C	.0550116038	1.4758626529	-7.8215403793
C	.3061341471	-.9201018958	-8.0092293365
C	1.4151897359	3.3081914791	.3979179715
C	1.0968600006	-2.3658943570	-6.0872196261
C	.6060852227	2.7512185150	-5.7111471989
C	-1.6424089007	.3323947632	1.4460628033
C	.6993707266	2.4707114249	-.6768016584
C	-.2245766572	-3.0492890474	-5.6680644478
C	-.0591710022	.3042045747	-8.5661752069
H	1.3509688626	-3.6011570288	-7.8845234105
H	4.1304237313	-.2769424516	-2.7508689042
H	3.9291703512	-.7025387877	-.5270887915
H	4.7292945027	.1384338614	-4.8993116913
H	2.8357423720	-2.8036969291	-7.3516405210
H	-3.6485930173	-.3232140426	-3.7736850267
H	-.0188549006	-4.0015476998	-5.1673140759
H	-.8141827300	-2.4243164202	-4.9885953257
H	1.1696492563	4.0970218964	-7.3498131465
H	2.3539772393	-.8139100550	.2963988598
H	3.0644300172	.7637673918	-.0547860934
H	3.5450691708	.6691980435	-6.1185867423
H	3.7860984185	-1.0504160365	-5.8093744446
H	-1.0772508342	3.7435888729	-.8089999748
H	-2.3057359953	.4793552754	2.2934219002
H	-2.1748099872	-1.7308121476	1.2044470675
H	-.2414207038	2.4208617452	-8.2658502966
H	-.4467405789	.3434476625	-9.5796774816
H	.1842675002	-1.8251894358	-8.5942043225
H	1.6020857836	4.6851440623	-5.7430839119

H	-1.2694653634	3.6293945556	-6.4331823032
H	1.2284544181	-3.0641101571	.0528538928
H	-.2153879166	-3.6089925441	.9175195345
H	-.8024093122	2.7713696832	-2.2557531059
H	-.9755837049	2.3701668169	1.4454779843
H	1.4608935710	2.1337670777	-1.3863785363
H	1.9809080267	4.1176325862	-.0728433568
H	-.1795449571	-2.3918517902	-1.8930974596
H	-1.9467673941	-4.0607033528	-1.7170597528
H	1.0237765350	2.5147105305	-4.7285804094
H	-.7524271057	4.2208384051	-4.8508738051
H	1.6812423461	-2.2109905874	-5.1751566357
H	2.2005080350	-4.1979603904	-6.4623927958
H	-1.4648054352	2.6036343065	-5.0032640328
H	.2920778659	-4.4342940258	-.5647714543
H	-.8495958595	-3.2584441837	-6.5428223438
H	2.5501920217	3.3946635000	-6.4982445621
H	2.1132745085	2.7058248316	.9882623633
H	.7080803160	3.7717207263	1.0930987806
H	.2158824768	4.1881310419	-1.9326795005
H	-2.6746050472	-2.4460613343	-1.7673627599
H	-2.5807990609	-3.3453845161	-.2380351164
N	.9169451315	-.2647205062	-1.8297367934
N	1.4149078691	.1851694436	-4.6359162916
O	-1.8667122998	.3108727296	-3.6634256687
O	-2.7144852745	-.7753371319	-3.6919465674
Cu	-.0634009759	.0180737816	-3.4552007804
C	-6.0028320656	.1234665350	-1.7724228108
C	-6.8817902436	.7665139492	-.7204943667
C	-6.3277430650	1.6507830543	.2154155809
C	-7.1275115625	2.2825966507	1.1598318559
C	-8.5119082148	2.0324021453	1.1780939861
C	-9.0722171702	1.1578420141	.2575859751
C	-8.2588193895	.5281375552	-.6882443994
C	-5.8512172124	1.0119062434	-3.0178397547
H	-5.0064653648	-.0935745371	-1.3658041765
H	-6.4402035118	-.8384397017	-2.0727836748
H	-5.2607832271	1.8563191781	.2289592017
H	-10.1419767212	.9616537691	.2807717840
H	-8.7095601512	-.1602697635	-1.3965966157
H	-5.2895107718	1.9160773727	-2.7642979602
H	-6.8431092142	1.3304901953	-3.3672894309
H	-7.2822997496	3.4687350169	2.6273228903
H	-10.1448608328	2.4867641133	2.1077905534
H	-4.9591110814	.9439393214	-4.8745245142
H	-5.6750072388	-.4553343049	-4.4579341786
N	-5.1043723454	.3075098149	-4.0919369164
O	-9.2046226133	2.7033539663	2.1536848187
O	-6.5696236166	3.1322716585	2.0625053157

111.L¹CuO₂H⁺ / formylglycine complex

C	3.0897919795	2.0505986764	4.4892220081
C	3.0870277807	-1.8060586728	-4.6197267503
C	2.2712923725	-1.3247501189	-3.4037191378
C	3.6361941989	4.3996437129	-1.6380374376
C	1.3605091941	4.0366769696	-.5947518802
C	5.1308981415	-1.0261913196	2.5381682146
C	4.2906215263	-.6195555822	1.3431904419
C	4.9662887200	-.1869737749	.1878283819
C	4.4147365071	.3212048954	-1.0017695440
C	5.3629936437	.7521924444	-2.1013612927
C	2.2674580523	-1.0379778650	2.6497837599
C	1.9153362580	-.0073997349	3.5668342882
C	1.1884080886	-.3622393763	4.7059334153

C	.8009637707	-1.6800160185	4.9370442826
C	1.1350455825	-2.6756696408	4.0223522903
C	1.8588521893	-2.3833720071	2.8631650953
C	2.2644635671	1.4588271693	3.3301632814
C	.9250810445	-2.0754349777	-3.3176589933
C	.9933129366	2.2984548513	3.0846586555
C	2.1734730509	-3.5013775817	1.8744348112
C	.8854879452	-4.0914956553	1.2635813117
C	3.0234066832	-4.6139920159	2.5210372772
C	2.4892738978	1.0246046036	-2.3529215995
C	2.2159342770	2.4231310550	-2.3600440681
C	1.5579631589	2.9552347192	-3.4709813526
C	1.1526794166	2.1480653246	-4.5311594697
C	1.4000306969	.7772806513	-4.4991655891
C	2.0602027178	.1856743100	-3.4197768944
C	2.5964286046	3.3449108888	-1.2048055659
H	-1.6343275912	-1.2071431360	.0929199280
H	3.0554937637	2.7326987450	-.4222474597
H	3.3822574664	3.0796459208	4.2552903846
H	4.0019565507	1.4747074437	4.6805126838
H	2.5138933649	2.0789025515	5.4204468022
H	2.5484402990	-1.6366270454	-5.5582929787
H	4.0503716706	-1.2904567912	-4.6935291678
H	3.2828221430	-2.8808995875	-4.5428505637
H	2.8446328648	-1.5746910080	-2.5053449056
H	3.9305845820	5.0127078725	-.7796098101
H	3.2251017051	5.0734252489	-2.3977693149
H	4.5419297177	3.9452791690	-2.0537743537
H	1.6576464165	4.6488823456	.2631761220
H	.5962554474	3.3399698167	-.2428650864
H	.8819524949	4.7066343816	-1.3178650124
H	6.1951580157	-.9677018872	2.3072518630
H	4.8893246447	-2.0467352457	2.8490833832
H	4.9185913829	-.3740535037	3.3910661284
H	6.0464066944	-.2226521992	.2312926369
H	6.4027063339	.6265043124	-1.7970430461
H	5.1949331468	1.8001551228	-2.3652445801
H	5.1861490792	.1623186386	-3.0066020275
H	.9064437862	.4090531629	5.4162037077
H	.2270150851	-1.9288852530	5.8252530958
H	.8164601244	-3.6973881622	4.2065031285
H	2.8814249725	1.5181625069	2.4278862921
H	1.0966977100	-3.1566582248	-3.2688880191
H	.3072705919	-1.8776745303	-4.2006076773
H	.3493587052	-1.7828429413	-2.4348849381
H	1.2518089922	3.3414650074	2.8772695251
H	.3365765045	2.2915412817	3.9611599993
H	.4035043180	1.9400714996	2.2369327914
H	2.7585788023	-3.0710569526	1.0557023144
H	1.1354334245	-4.8612626718	.5247223215
H	.2881252210	-3.3207660422	.7693546175
H	.2608670731	-4.5612896808	2.0313886184
H	3.2862159256	-5.3725966673	1.7759811686
H	2.4773395224	-5.1180118132	3.3258909190
H	3.9533592328	-4.2236089207	2.9477117750
H	1.3428524679	4.0191480821	-3.4985256445
H	.6300683369	2.5863758366	-5.3768030660
H	1.0630968731	.1548055244	-5.3226296028
N	2.9678083407	-.6965135847	1.4563626104
N	3.1098100775	.4436639757	-1.2112426832
O	-.0177338984	-.2271032004	.1502722167
O	-.6793601231	-1.3629982432	-.2533486434
Cu	1.8128428217	-.1739619949	.0199978360
C	-2.5803063460	1.7381362389	.4844355015

C	-2.4657311505	3.0840421655	1.3146475794
C	-3.8408014516	-.3196943506	1.0806009416
H	-1.6613439002	1.1631020379	.5799513814
H	-4.7497367677	-.6404573768	1.6143591881
H	-4.3420873991	1.6154397853	1.5230041810
H	-2.7173548987	2.0165058782	-.5680059704
N	-3.7265057300	1.0002048969	.9856538674
O	-1.3587585896	3.6510351909	1.1747556883
O	-3.4879829085	3.3847563452	1.9615460334
O	-3.0652019221	-1.1815295703	.6264569777

112.L¹CuO₂H⁺ / methane t.s.

C	-3.8000438286	-3.4756770954	1.7859404308
C	-2.6811262017	4.5625402060	-1.7195700480
C	-3.0229907853	-4.7186241714	2.2597721101
C	-4.0341355252	2.2374567968	3.1077861882
C	-3.3117081064	-1.1136725794	2.6832251581
C	-3.4569575694	1.0582646725	-2.2556341232
C	-2.9051853935	-1.9487947085	-4.5035963893
C	-1.4051344362	-.7343779594	1.2239616357
C	-1.4660552073	.3770099343	-1.0440384644
C	-3.3864365672	-.1197223051	3.6954159557
C	-3.8802795262	2.4100874935	-2.3216052135
C	-.8230181104	-.2259261041	.0508543550
C	-3.8713525932	-2.4040059883	2.8674139451
C	-3.7698786310	.1301887929	-3.2855265095
C	-4.8545974626	3.9446492405	-.5605674331
C	-5.2059703295	-3.8635378495	1.2904644133
C	-.4758647474	-1.2411332775	2.3060761723
C	-.6081870199	.7869964576	-2.2230444840
C	-4.0097054807	-.4560309551	4.8982083056
C	-4.4752253524	-2.6868039159	4.0959859776
C	-4.5928491182	2.8211660235	-3.4527783236
C	-4.4895619688	.5953942229	-4.3892208562
C	-2.0596022435	1.8467869775	4.6494629146
C	-3.3882604638	-1.3439195840	-3.1754325557
C	-4.5453405776	-1.7272934682	5.1038993289
C	-2.8675356377	1.2940321517	3.4623475891
C	-4.5579712625	-2.1673475706	-2.5988023193
C	-4.8940017790	1.9290766118	-4.4800536550
C	-3.5663868846	3.4082339824	-1.2135889932
H	.2540856101	-.3012344609	-.0146970909
H	-4.7318504182	2.3257395249	3.9470553362
H	.5440226297	-1.3326866118	1.9315414868
H	.4511708136	.7130596561	-1.9762467009
H	-7.5431127994	-.4979961420	.3040265269
H	-4.6070143785	1.8744247898	2.2461472400
H	-3.5262448255	-5.2143123035	3.0959158971
H	-2.0125760562	-4.4579218553	2.5895067625
H	-4.2697923028	-3.2169205342	-2.4808981781
H	-.8072670678	-2.2120828545	2.6831289583
H	-.4678312450	-.5524218484	3.1570184193
H	-4.8663486778	-1.7962761146	-1.6152542921
H	-.8042645684	.1450164931	-3.0877575843
H	-4.0793170873	.2839217645	5.6887108043
H	-5.0174664383	-1.9686761067	6.0511968562
H	-4.8909836264	-3.6744267129	4.2703971083
H	-4.9086342326	3.8566952835	-3.5345273693
H	-5.4387001457	2.2714752340	-5.3548408378
H	-4.7317350448	-.0880743953	-5.1964147383
H	-3.1927841200	5.1573643831	-2.4830611832
H	-1.7477525201	4.1932990596	-2.1559109858
H	-5.4278998997	-2.1295439910	-3.2642376020
H	-.8326168652	1.8125821892	-2.5279017470

H	-3.7130703515	-2.0292680423	-5.2376929706
H	-2.1991668814	1.2735929928	2.5966435953
H	-1.6228392349	2.8147345345	4.3853652499
H	-3.2570579107	-3.0537533031	.9352120871
H	-5.1374013876	-4.6064085447	.4892925584
H	-3.0031753513	2.8775262646	-.4409890257
H	-4.6076363053	4.6061265189	.2759887314
H	-2.5644486811	-1.4285540209	-2.4615944070
H	-2.5214787070	-2.9593611459	-4.3345704688
H	-1.2441196770	1.1734529727	4.9313824591
H	-2.6837424679	2.0032707717	5.5345598239
H	-3.6605895988	3.2386821252	2.8701170892
H	-5.7433006441	-2.9917691635	.9001265143
H	-5.8100456135	-4.2954247489	2.0948384797
H	-2.9349494754	-5.4455480306	1.4462261184
H	-5.4760123764	3.1277689548	-.1801479484
H	-5.4537646588	4.5227325172	-1.2720861047
H	-2.4249838387	5.2329508376	-.8932395811
H	-2.1043564020	-1.3523463643	-4.9507644727
N	-2.7227218776	-.7933859447	1.4264361647
N	-2.7767560177	.6148934663	-1.0874158394
O	-5.9209915127	.5560372847	.2667668976
O	-6.8031815226	-.4592797001	-.3354438076
Cu	-4.0241551515	.0250282802	.2819247857
C	-7.8858085257	.4879373169	-2.5472557843
H	-6.9698550297	.9171549358	-2.9500523279
H	-8.2539106424	-.4304324560	-2.9983984265
H	-8.6264687284	1.1747812544	-2.1446667498
H	-7.2288051361	-.0442150156	-1.2784115435

113.L¹CuO₂H⁺ / cyclohexane t.s.

C	2.9330889524	1.6303938013	4.8072344675
C	1.9655339930	-1.9642085311	-4.5421050314
C	1.5108134403	-1.2162284520	-3.2775862172
C	3.5419263181	4.5328831976	-1.8367503062
C	1.4248359185	3.9951126979	-.5446799654
C	4.2436982410	-1.5672417375	2.4157303162
C	3.5344145332	-.8668571409	1.2761213573
C	4.2856304744	-.5650169446	.1279710181
C	3.8435500880	.0649112406	-1.0461528940
C	4.8310040129	.2342495267	-2.1800255864
C	1.4600662683	-.8990975560	2.5583914293
C	1.3410759187	.0500231342	3.6070419472
C	.5203723694	-.2666707302	4.6938636426
C	-.1668664443	-1.4776264071	4.7542110641
C	-.0446900976	-2.3982578739	3.7153548905
C	.7623136800	-2.1376148874	2.6014894331
C	2.0559882056	1.3963260711	3.5626667671
C	.0930173102	-1.6573221191	-2.8611486043
C	1.0519596674	2.5522652785	3.3833966813
C	.8722224749	-3.1837165890	1.4941179100
C	-.4736380181	-3.4052780974	.7779444029
C	1.4206905668	-4.5227116328	2.0251678696
C	2.1026635664	1.1223688787	-2.3947398502
C	2.0876125552	2.5387247289	-2.4895339472
C	1.5546717214	3.1100448708	-3.6472725044
C	1.0437152969	2.3166825903	-4.6731615635
C	1.0500396389	.9267317603	-4.5565498562
C	1.5697437250	.2997043423	-3.4228487787
C	2.6027715747	3.4145767385	-1.3538263340
C	-6.1993900465	.0342710331	-.0330238350
C	-6.5941019622	.4404381175	1.3909095036
C	-5.7337158750	1.5936264532	1.9180079771
C	-4.2157016089	1.2311189707	1.8468464535

C	-3.8951187756	.8384766285	.4287350983
C	-4.6801116113	-.3272093102	-.1107502475
H	3.9589268074	5.0681975715	-.9781660990
H	1.7932065921	4.5722230301	.3098175039
H	5.2921094317	-1.7422392650	2.1739676648
H	1.2778433438	-1.8110789801	-5.3795625266
H	5.8094548675	-.1628497858	-1.9096929608
H	.4212756419	.4434808104	5.5087247137
H	-.7921559655	-1.7059380203	5.6119667142
H	-.5778734243	-3.3423768832	3.7745145083
H	2.7214715127	1.3937254068	2.6941435132
H	.0572530665	-2.7399335924	-2.7011414589
H	1.5826587606	3.5044631803	3.2820752667
H	1.5846999571	-2.8121239836	.7523739192
H	-.3587657947	-4.1345036281	-.0301881817
H	1.5584265082	-5.2281363372	1.1998088842
H	1.5389038272	4.1900394268	-3.7508730653
H	.6363153090	2.7821234352	-5.5653312405
H	.6420792609	.3239650667	-5.3613178906
H	3.1784678247	2.7767504823	-.6760171097
H	2.1879080639	-1.5027627397	-2.4675439024
H	3.4876212662	2.5682797308	4.7045404446
H	2.3329419284	1.7017024173	5.7196861263
H	2.9607150397	-1.6425778730	-4.8642338061
H	2.0049494201	-3.0402226803	-4.3464054836
H	3.0194274404	5.2682972543	-2.4562986506
H	4.3745502296	4.1322716784	-2.4231867328
H	.7625636870	3.2082898059	-.1655361960
H	.8147594199	4.6602218175	-1.1648777580
H	3.7693209648	-2.5278738845	2.6360161613
H	4.1900213651	-.9681102027	3.3296516194
H	4.9372584897	1.2915952250	-2.4420414594
H	4.4803968042	-.2829185482	-3.0783906200
H	-.6376231537	-1.4048631559	-3.6368856122
H	-.2239612368	-1.1653119985	-1.9349749630
H	.3912305043	2.6319802882	4.2536001978
H	.4248924236	2.4073040592	2.4987836958
H	-.8531136003	-2.4783604724	.3386236688
H	-1.2314703668	-3.7930907720	1.4674993635
H	.7349836738	-4.9834590699	2.7432808275
H	2.3857650195	-4.3961258492	2.5247838347
H	3.6589045318	.8234639791	4.9492323147
H	-1.4718489733	-.2226109371	1.5263788414
H	5.3245231636	-.8646016008	.1458537711
H	-7.6503889734	.7337604638	1.4092632849
H	-6.4973627114	-.4248371760	2.0603584884
H	-5.9086625284	2.4986502950	1.3240250030
H	-5.9828410371	1.8353850990	2.9568182195
H	-3.6096620986	2.0797395797	2.1788606932
H	-4.0360822314	.3898073530	2.5303270789
H	-2.6176129838	.4406280402	.4421935224
H	-3.7904214697	1.6828863602	-.2635166072
H	-4.4011568404	-.5604133562	-1.1425584990
H	-4.5091483704	-1.2227334904	.5006755436
H	-6.7756941659	-.8319714973	-.3752119946
H	-6.4034847225	.8558352199	-.7300273597
N	2.2400940944	-.5764083452	1.4112926576
N	2.6040212439	.5255626312	-1.2063706396
O	-1.4348523518	.0081414923	.5764318246
O	-.5250091932	1.1446997448	.5500791047
Cu	1.2528120543	.4769903557	.1268019482

114.L¹CuO₂H⁺ / acetonitrile t.s.

C	.2394518984	1.1873831271	1.0858794527
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C	.7824520610	4.6435998873	-4.4702823607
C	1.0607386671	-4.6418092658	-.4835927065
C	-1.0426017047	2.0311696199	.9262419551
C	.1586236910	-1.2102577750	.1308115794
C	-.0657559996	1.1100252267	-4.6977165559
C	.4432975209	-1.9975818996	-6.7628967162
C	2.0766361659	-.5916283606	-1.2413898173
C	1.9670090350	.4981629949	-3.5143440252
C	-.1001606893	-.2956107978	1.1902933219
C	-.4670561227	2.4666473486	-4.8304406168
C	2.6400436648	-.0466571654	-2.4092437624
C	-.2315132603	-2.5761472978	.2148048786
C	-.4443666390	.1242497776	-5.6550548742
C	-1.2888501429	4.1253077703	-3.0982764001
C	-1.2580458769	-4.2227896342	-1.4162211511
C	3.0172685923	-1.0184428841	-.1370925200
C	2.7912104161	.8634640853	-4.7308668662
C	-.7291434940	-.7862278640	2.3360057668
C	-.8401580757	-3.0092776106	1.3942715913
C	-1.2272706626	2.8156218899	-5.9495948042
C	-1.2218122027	.5292366127	-6.7419149545
C	1.0707000822	1.6882902460	2.2807325111
C	-.0813140664	-1.3446442111	-5.4722556681
C	-.0620262155	3.5327215733	-3.8182990828
C	-1.0896508969	-2.1284145587	2.4456587877
C	-1.2818349467	-2.1355272772	-4.9115009085
C	.0404807861	-3.5676073130	-.9105553404
C	-1.6089320858	1.8600997164	-6.8954965005
H	-1.6824851313	1.9406634978	1.8101442886
H	3.7198388181	-.0625840722	-2.4692579361
H	4.0506219987	-1.0232831674	-.4842027731
H	3.8547432012	.8710297266	-4.4909971655
H	-4.03329278149	-.1558003032	-2.1378919600
H	-1.6333418999	1.7170187918	.0588128929
H	.6786838706	-5.2493378374	.3428327809
H	2.0060796928	-4.1970284620	-.1582729044
H	-1.0042251304	-3.1799835912	-4.7387136313
H	2.7584524850	-2.0104853418	.2403547058
H	2.9438661710	-.3243402871	.7066920101
H	2.5039370896	1.8431476544	-5.1202866023
H	-1.6327505192	-1.7190238371	-3.9599112965
H	-.9410032541	-.1102767343	3.1580699072
H	-1.5666212276	-2.4882082850	3.3519294965
H	-1.1202982810	-4.0529252074	1.4963552145
H	-1.5161673777	3.8522088300	-6.0950117069
H	-2.2079378616	2.1522550442	-7.7521497027
H	-1.5325763175	-.2018644659	-7.4804702952
H	-.3346292571	-2.0770125424	-7.5280498915
H	.2072293187	5.2006061096	-5.2167949407
H	1.6687693631	4.2384744664	-4.9680801903
H	-2.1245112972	-2.1184243210	-5.6101226081
H	2.6271548524	.1350393779	-5.5321401135
H	1.2767765908	-1.4323273286	-7.1908230247
H	.8419452696	1.3373705735	.1842785639
H	1.3586890536	2.7324959330	2.1258024961
H	.4767221945	-3.0126901148	-1.7462091377
H	-1.0431190843	-4.8867596049	-2.2593972314
H	.5572150787	3.0479393736	-3.0584564498
H	-.9713243086	4.8612258823	-2.3529318970
H	.7168479839	-1.4079762843	-4.7274635217
H	.7950682220	-3.0115221558	-6.5502918707
H	1.9842983278	1.1012048478	2.4155842222
H	.5047843949	1.6401012727	3.2160060937
H	-.7888193151	3.0889244457	.8029014837

H	-1.9810498693	-3.4717459128	-1.7517479665
H	-1.7377137191	-4.8237816294	-.6374711137
H	1.2765509247	-5.3136015882	-1.3202448129
H	-1.8600855707	3.3451947120	-2.5858281696
H	-1.952940977	4.6397562435	-3.7998089940
H	1.1171423787	5.3572179755	-3.7113523639
N	.7660455395	-.7549000052	-1.0728902677
N	.6532385424	.7267553253	-3.5391791738
O	-3.3998174500	.0757549175	-2.8465822951
O	-2.3598600428	.8349533345	-2.1178907787
Cu	-.5653549727	.0776651926	-2.1532930098
C	-4.8905355214	1.3649841070	-5.4983111574
C	-4.3394560949	2.0151642743	-4.3933533349
H	-3.3298212721	2.4099009451	-4.5018205500
H	-3.8730685997	.8447742796	-3.4985224312
H	-5.0218848221	2.5575678326	-3.7406843221
N	-5.3365461635	.7608899759	-6.4026182970

115.L¹CuO₂H⁺ / toluene t.s.

C	3.5693221271	1.8024289051	4.8292437680
C	2.8315507548	-2.0641852173	-4.4401185715
C	2.2971230181	-1.2986646954	-3.2170888843
C	4.0612593355	4.5884441116	-2.0082722053
C	1.9425664953	4.0426043704	-.7256955894
C	5.0892464992	-1.3837604765	2.4308894369
C	4.3375781012	-.7296717722	1.2915708510
C	5.0601067939	-.4111907073	.1275399775
C	4.5730985478	.1721676639	-1.0557462649
C	5.5405307703	.3596419907	-2.2040489213
C	2.2757087491	-.8460522380	2.5882533709
C	2.1062723128	.0956404043	3.6363100918
C	1.3131496811	-.2699581481	4.7283436950
C	.7006347353	-1.5196366491	4.7925469475
C	.8676465872	-2.4299380053	3.7511971003
C	1.6486249206	-2.1211433783	2.6320569668
C	2.7255344445	1.4877405729	3.5808650587
C	.8875570942	-1.7958650477	-2.8379350314
C	1.6410824735	2.5641748962	3.3723863567
C	1.7947817136	-3.1507507493	1.5137636018
C	.4522761172	-3.4102577700	.8031635710
C	2.3939967616	-4.4757396456	2.0238129022
C	2.7811203608	1.1001255385	-2.4209809197
C	2.6975584299	2.5087226917	-2.5756732691
C	2.1425488016	3.0060058857	-3.7576161992
C	1.6736588761	2.1489969728	-4.7509671403
C	1.7443464087	.7678022968	-4.5751198665
C	2.2900968994	.2130109358	-3.4155908152
C	3.1570540213	3.4621239405	-1.4793915741
H	-.6871835974	-.2516128994	1.5292208540
H	3.7465632869	2.8849981266	-.7604956194
H	4.0567289314	2.7758698950	4.7175024811
H	4.3486967541	1.0510235965	4.9907595796
H	2.952954600	1.8446242451	5.7342514996
H	2.1690831679	-1.9673060731	-5.3058844831
H	3.8229521860	-1.7088549949	-4.7376285042
H	2.9104762425	-3.1310914415	-4.2090583981
H	2.9585535821	-1.5253735899	-2.3758028958
H	4.4383642418	5.1888524060	-1.1746524559
H	3.5226982830	5.2644333835	-2.6796086867
H	4.9215783594	4.1896843750	-2.5547401360
H	2.2729977073	4.6760213679	.1040684273
H	1.2969962637	3.2552427945	-.3211261140
H	1.3271728572	4.6548225375	-1.3935126931
H	6.1424481190	-1.5118722880	2.1809103810

H	4.6624475421	-2.3634105489	2.6648672444
H	5.0141896680	-.7788221718	3.3393672384
H	6.1114418243	-.6644066308	.1357631882
H	6.5388871798	.0148004366	-1.9347727109
H	5.5944370988	1.4140923110	-2.4919701130
H	5.2066056207	-.1941870667	-3.0866131852
H	1.1744759028	.4336143666	5.5431016884
H	.0948236849	-1.7846749659	5.6536650467
H	.3878818823	-3.4021723249	3.8110687260
H	3.3984495419	1.5208809550	2.7185967356
H	.8996677382	-2.8727217839	-2.6398527590
H	.1783747207	-1.6102933229	-3.6519215620
H	.5093540894	-1.2880696828	-1.9444309001
H	2.1009080778	3.5516011280	3.2612774871
H	.9658578306	2.6068823188	4.2340601414
H	1.0368945511	2.3598283323	2.4834719467
H	2.4875346722	-2.7446048314	.7712118882
H	.5863925906	-4.1268764780	-.0135172402
H	.0389715233	-2.4913021609	.3777616867
H	-.2878071830	-3.8293083679	1.4935347251
H	2.5541707633	-5.1636105601	1.1876741739
H	1.7281135341	-4.9721239898	2.7368280921
H	3.3557663993	-4.3213261899	2.5221038334
H	2.0756862526	4.0789738086	-3.9052936614
H	1.2486254041	2.5574328362	-5.6626805351
H	1.3670004689	.1126890314	-5.3537112275
N	3.0364868617	-.4868814650	1.4368166332
N	3.3117606191	.5693895341	-1.2094568266
O	-.6495761708	-.0611053674	.5726564472
O	.1926771032	1.1337992630	.5329309524
Cu	1.9867381112	.5218496460	.1691618519
C	-6.0022945582	-1.8137769697	.3255372225
C	-5.8511400589	-.8981562253	1.3810937203
C	-4.8478876643	.0540427002	1.3332622292
C	-3.9732673223	.1295313862	.2136775702
C	-4.1501761836	-.8056026752	-.8478262695
C	-5.1459138052	-1.7627925872	-.7880929189
C	-2.9274894657	1.1219569608	.1413881811
H	-3.4885845824	-.7536574756	-1.7077441551
H	-5.2727147195	-2.4702719679	-1.6009176205
H	-6.7858881930	-2.5635051122	.3695701158
H	-2.6958486319	1.4972064151	-.8608504745
H	-1.8015638941	.5398272251	.3503916859
H	-2.9683302514	1.9185082400	.8858458168
H	-4.7266642315	.7665002571	2.1437041726
H	-6.5252453558	-.9369301588	2.2303121987

116.L¹CuO₂H⁺ / phenol t.s.

C	2.7205687298	1.7937838784	4.7423866783
C	6.0434489332	.4737974813	-1.5024685522
C	1.9499378738	-1.0195709448	2.5343460001
C	1.5095406759	-.0334734672	3.4569746966
C	.5504253076	-.3989856853	4.4085620583
C	.0194980761	-1.6873080368	4.4500025925
C	.4406404771	-2.6400801626	3.5240950418
C	1.4065312120	-2.3362970346	2.5537119478
C	2.0243811765	1.4017810209	3.4259131843
C	1.7853071219	-1.9159559694	-2.9708479128
C	.8890162350	2.3894951617	3.0964941931
C	3.9052073072	-2.0286323965	-4.3558369295
C	1.8684847349	-3.4277732713	1.5888106333
C	.7209701483	-3.9419320388	.6982273096
C	2.5228462313	-4.6021436375	2.3413867906
C	3.3313879630	1.0709255398	-2.2742252923

C	3.1589221318	2.4742165291	-2.4072146262
C	2.7932378412	2.9733264382	-3.6596023684
C	2.5867571220	2.1212368632	-4.7424903103
C	2.7379017084	.7438296602	-4.5900159471
C	3.1075786985	.1881570344	-3.3632991986
C	3.3195046203	3.4116946694	-1.2162453556
C	3.1933105634	-1.3236903931	-3.1901849654
C	4.1360359974	4.6730499406	-1.5442971446
C	1.9369287427	3.7902423038	-.6452300317
C	4.7636578428	-1.2794261508	2.9657468844
C	4.2051866020	-.7454032211	1.6624535768
C	-5.0282939599	.0907442880	1.0029191856
C	-3.6442552741	-.1129822079	1.3593037271
C	-3.2966152398	-.3484344916	2.7399189588
C	5.1309962663	-.3647541397	.6757764305
C	-4.2869886199	-.3768997880	3.6907616146
C	-5.6393580114	-.1805703701	3.3204991092
C	-5.9987830233	.0514030879	1.9746119048
C	4.8729246348	.2078782904	-.5828293893
H	-.1155025326	-1.0506011782	1.3892231803
H	3.8592619101	2.8686380978	-.4344910109
H	3.1235078754	2.8080276153	4.6679313398
H	3.5482715631	1.1213265966	4.9834884197
H	2.0231255821	1.7778908018	5.5856259989
H	3.3302412307	-1.9664894438	-5.2849636663
H	4.8929616651	-1.5968786889	-4.5445383331
H	4.0374707971	-3.0904609388	-4.1268478522
H	3.7714262752	-1.5268988912	-2.2835559323
H	4.3088191834	5.2538656727	-.6330220584
H	3.6158822175	5.3270049645	-2.2511969906
H	5.1100980568	4.4203855318	-1.9745551498
H	2.0458699417	4.4198041874	.2439920485
H	1.3532118446	2.9051300649	-.3649701573
H	1.3478107335	4.3448142789	-1.3832013752
H	5.8534758714	-1.2898708366	2.9473193503
H	4.4077787690	-2.2959088898	3.1550023414
H	4.4358941145	-.6645080942	3.8090693978
H	6.1727127091	-.5321296192	.9142514200
H	6.9900832680	.2647146559	-1.0036346068
H	6.0408055920	1.5143129778	-1.8407500089
H	5.9771521717	-.1528171896	-2.3980088287
H	.2157182122	.3397585668	5.1306413437
H	-.7083757079	-1.9526618658	5.2107483556
H	.0299129576	-3.6440746088	3.5637506479
H	2.7653173896	1.4733895528	2.6252254856
H	1.8440448166	-2.9955019301	-2.7973417282
H	1.1485118494	-1.7454487401	-3.8452266603
H	1.2847411230	-1.4603902781	-2.1085527293
H	1.2875090012	3.4034026561	2.9953874606
H	.1398571385	2.4112794103	3.8949652686
H	.3887514933	2.1162985357	2.1638079673
H	2.6228015964	-2.9887284078	.9311622729
H	1.0917310596	-4.7134452671	.0163085233
H	.2863561617	-3.1412813567	.0938867478
H	-.0792297068	-4.3917639591	1.2958134602
H	2.9318179422	-5.3241515404	1.6279467645
H	1.7969333189	-5.1306240711	2.9672932453
H	3.3378454216	-4.2704557575	2.9907235835
H	2.6653902677	4.0426574385	-3.7921541349
H	2.3018407125	2.5308999912	-5.7065570115
H	2.5621232281	.0936079480	-5.4402559469
H	-2.2536320409	-.4865032241	3.0051158291
H	-4.0370120194	-.5446281524	4.7324336852
H	-6.4115354678	-.2077958991	4.0822518102

H	-1.6086426836	-.4058461355	.5805202595
H	-7.0409785323	.1983437188	1.7138339619
H	-5.2533327737	.2657521954	-.0426764291
N	2.8795896929	-.6718763982	1.5093502785
N	3.6510499398	.5421222616	-.9889571512
O	.2014308283	.5250635865	.2661416937
O	-.4788237025	-.7565926308	.5251433294
O	-2.7680503643	-.0686733394	.4302058311
Cu	2.0586321252	.2504519406	-.0265258487

117.L¹CuO₂H⁺ / isopropylbenzene t.s.

C	5.5992119970	1.4936445860	4.8314647804
C	5.9679702319	-1.7615540621	-4.6772315718
C	5.3211668574	-1.0610703227	-3.4701497852
C	7.0526255379	4.6783589360	-1.6227241237
C	4.8043003377	4.0675446228	-.6230768928
C	7.3210052918	-1.5802545283	2.5082660979
C	6.7516781390	-.8468006339	1.3125457133
C	7.6375825533	-.4906201928	.2817469120
C	7.3390818190	.1734967036	-.9190328200
C	8.4606004414	.3973653566	-1.9094968426
C	4.5204825475	-.9660226050	2.3022203392
C	4.2305554823	-.0633671767	3.3595328311
C	3.2688015893	-.4388315076	4.3025133216
C	2.6065642214	-1.6621698916	4.2137470154
C	2.8971601285	-2.5364809176	3.1675190622
C	3.8513195286	-2.2162563645	2.1928308455
C	4.9114386938	1.2964413497	3.4677501078
C	3.8625888569	-1.5273613681	-3.2851428079
C	3.9155899239	2.4421066251	3.1971402228
C	4.1484029112	-3.2154975360	1.0767010784
C	2.9301946060	-3.4401623284	.1604306558
C	4.6471514557	-4.5618413964	1.6378314498
C	5.7655420237	1.2551713023	-2.4457102744
C	5.7379280090	2.6748622211	-2.5032085973
C	5.3514086600	3.2744148126	-3.7039024250
C	4.9915185701	2.5067340935	-4.8100404852
C	5.0034113410	1.1145158148	-4.7321427585
C	5.3803634609	.4592192542	-3.5585890015
C	6.0865772739	3.5285944613	-1.2900357172
H	1.8812398135	-.4008664076	1.1241713878
H	6.5896687160	2.8842031316	-.5626178613
H	4.8745537545	1.5172216218	5.6513294096
H	6.1400253604	2.4449301764	4.8437812721
H	6.3164523519	.6946389279	5.0437949831
H	5.4101893652	-1.5840297847	-5.6018801066
H	6.9959069104	-1.4218571914	-4.8370890848
H	5.9910092218	-2.8434518000	-4.5141608813
H	5.8746024151	-1.3683046269	-2.5778901303
H	7.3472271639	5.1969171247	-.7052548582
H	6.5946432096	5.4211529398	-2.2831512948
H	7.9604790548	4.3108671285	-2.1108575482
H	5.0491234431	4.6298193574	.2838499450
H	4.1157249925	3.2597897738	-.3479194938
H	4.2631740957	4.7363324925	-1.3007682501
H	8.3955893405	-1.7275898243	2.4005665633
H	6.8433048784	-2.5570330069	2.6270256955
H	7.1340514152	-1.0192889815	3.4288399186
H	8.6710785202	-.7751840170	.4241001837
H	9.4036780229	.0049862223	-1.5291829348
H	8.5793863925	1.4648892424	-2.1196776417
H	8.2377579685	-.0919774215	-2.8626096276
H	3.0356160266	.2351724128	5.1206424495
H	1.8700964778	-1.9359642079	4.9631580873

H	2.3827588557	-3.4910571280	3.1107732950
H	5.6911147767	1.3420877621	2.7019318156
H	3.8172692756	-2.6146174661	-3.1644451204
H	3.2531628704	-1.2570012515	-4.1539021516
H	3.4043753882	-1.0669585794	-2.4026223511
H	4.4344474356	3.4060669803	3.2078895894
H	3.1397657014	2.4747443537	3.9699034863
H	3.4192710507	2.3242029163	2.2299582808
H	4.9517839516	-2.8000054062	.4618318796
H	3.1838989201	-4.1419875890	-.6402087487
H	2.5991156649	-2.5085439200	-.3061495257
H	2.0849958130	-3.8621030444	.7148395919
H	4.9262451158	-5.2307105051	.8178869163
H	3.8731143648	-5.0648467616	2.2260383787
H	5.5219160344	-4.4348161848	2.2824850489
H	5.3323017082	4.3566571969	-3.7786585633
H	4.6968273672	2.9939460374	-5.7344036555
H	4.7115172785	.5315184758	-5.5995612381
N	5.4457368731	-.5790090230	1.2916555668
N	6.1224222707	.6227874933	-1.2231747007
O	2.7793879879	1.0617800597	.2217991283
O	1.9690463183	-.1360995912	.1850598257
Cu	4.6214557373	.5145428026	-.0695402794
C	-1.3147134044	-1.9935425386	2.7932452088
C	-.6056334473	-1.2100030121	1.8832475429
C	-1.2586338793	-.5553942480	.8281974858
C	-2.6493621684	-.7321387579	.7004424450
C	-3.3589445075	-1.5076678364	1.6140609342
C	-2.6947991758	-2.1423090747	2.6656568684
C	-.5505554321	.3175388502	-.1708282046
C	-.7029398962	-.0720936748	-1.6270260007
C	-.5686665175	1.8107506466	.1264574955
H	-4.4331316348	-1.6163660504	1.5017494483
H	-3.2472499247	-2.7504693906	3.3744150679
H	.4724946656	-1.1506296878	2.0248045685
H	-.7820196900	-2.4900309162	3.5981375280
H	-3.1806828449	-.2415341364	-.1094782669
H	.7486209539	.1419055431	.0143550122
H	.0930952791	2.3669399228	-.5430294795
H	-.3035005234	2.0266172462	1.1647205253
H	-1.5927656708	2.1834429931	-.0298911085
H	-.0659056318	.5377969790	-2.2740100039
H	-1.7418911902	.0927430656	-1.9489535446
H	-.4815685848	-1.1303310946	-1.7881354000

118.L¹CuO₂H⁺ / cyclohexadiene t.s.

C	3.7639972743	1.5476910546	4.2858959041
C	4.6179414892	.7708280015	-2.9399115584
C	2.4813213150	-1.2382048840	2.2010396974
C	2.3876526806	-.3616767356	3.3138588220
C	1.9414896084	-.8866208937	4.5295982746
C	1.6006326607	-2.2317579650	4.6551800181
C	1.6931096363	-3.0782540687	3.5531030595
C	2.1238672560	-2.6079719871	2.3091030805
C	2.7495890001	1.1160385605	3.2115811544
C	.3373899675	-2.1663393214	-2.6830409854
C	1.4860070995	1.9967774732	3.2664693987
C	2.0363177103	-2.2270107296	-4.5632824562
C	2.2207711811	-3.5738226401	1.1330237511
C	.8328904309	-4.1122531729	.7380166491
C	3.1884174172	-4.7388476273	1.4205774205
C	1.7928716102	.9996004359	-2.6817153630
C	1.4748479633	2.3688558865	-2.8592143888
C	.6793832063	2.7174738172	-3.9562219137

C	.1995419983	1.7497155635	-4.8386797818
C	.4929027640	.4027970313	-4.6276071894
C	1.2876284337	-.0006783797	-3.5517586490
C	1.9639710635	3.4401810412	-1.8906822765
C	1.5706970782	-1.4787145516	-3.3034793491
C	2.7138529348	4.5801334906	-2.6011432274
C	.7980964916	3.9913043623	-1.0448007201
C	5.2455430692	-1.2312700527	1.5523841335
C	4.2070384533	-.6893923577	.5921636180
C	-4.2789298330	1.6808648846	-.6014120159
C	-3.0184833239	2.1004021900	-1.1700134500
C	-2.7778068150	1.8801894439	-2.5706342565
C	4.6685269020	-.1723173541	-.6295301339
C	-3.6673086828	1.1822149571	-3.3320293000
C	-4.9473264544	.6471916517	-2.7743803551
C	-5.1907798767	.9947197778	-1.3403659110
C	3.9036808017	.3869429038	-1.6613121545
H	-1.9023929869	.0212177656	.7029662955
H	2.6661297811	2.9629298536	-1.2011189439
H	4.0573349403	2.5904106729	4.1293619686
H	4.6700363198	.9342491293	4.2567841317
H	3.3457312935	1.4732500208	5.2945027694
H	1.2479180683	-2.2888234362	-5.3200309220
H	2.9025697158	-1.7409852766	-5.0224283170
H	2.3218414763	-3.2516883987	-4.3057832029
H	2.3752023291	-1.5477120646	-2.5666878704
H	3.1146322953	5.2819993773	-1.8633027353
H	2.0558369823	5.1462010179	-3.2682719949
H	3.5499239377	4.2035706866	-3.1985263767
H	1.1677520334	4.7240186388	-.3198383285
H	.2971140203	3.1890446621	-.4944397456
H	.0579370106	4.4955102848	-1.6770092909
H	6.2463106973	-1.1519636694	1.1275590594
H	5.0466720626	-2.2793666740	1.7918670008
H	5.2229418925	-.6804960322	2.4972993023
H	5.7350879667	-.2264631116	-.7991892644
H	5.6935231062	.6222607476	-2.8428170610
H	4.4266532172	1.8175569833	-3.1929192391
H	4.2578686478	.1684037407	-3.7798525497
H	1.8691535338	-.2366011998	5.3957930799
H	1.2675043057	-2.6208356942	5.6125059903
H	1.4333615103	-4.1266424123	3.6640184731
H	3.2201223864	1.2802377059	2.2373767088
H	.5579358853	-3.2124535194	-2.4471896180
H	-.5122162553	-2.1478571964	-3.3741065386
H	.0204211606	-1.6706223137	-1.7581015757
H	1.7510875280	3.0514065193	3.1375420127
H	.9801966304	1.8937185483	4.2327574790
H	.7683026903	1.7255565349	2.4853631976
H	2.6161137998	-3.0211638245	.2759359356
H	.9121014521	-4.7704966569	-.1333720142
H	.1454514847	-3.2974102771	.4874135539
H	.3837141403	-4.6904134432	1.5519483677
H	3.2877215613	-5.3768395134	.5365970417
H	2.8311625592	-5.3667581147	2.2429780036
H	4.1870266208	-4.3813751579	1.6896339642
H	.4409616566	3.7627104740	-4.1292278859
H	-.4009727290	2.0463261010	-5.6937930139
H	.1080295982	-.3427439326	-5.3162192404
H	-6.1317619956	.6820021750	-.8970606473
H	-4.4951355007	1.9321020879	.4337278875
H	-2.1076764169	1.0723215138	-.6246933123
H	-2.4624614034	2.8959582820	-.6698922368
H	-5.7982597314	.9856053428	-3.3915558648

H	-1.8605038095	2.2573073038	-3.0094431948
H	-3.4603969683	1.0051038467	-4.3832688033
H	-4.9790998800	-.4519025091	-2.9015177544
N	2.9202739729	-.7345525972	.9392548057
N	2.5899846413	.6039189402	-1.5719451728
O	-1.4333644665	.2303962321	-.1281531023
O	-.2324269419	.9119129890	.4037315568
Cu	1.5011084662	.1387393597	-.0493934776

119.L¹CuO₂H⁺ / dopamine t.s.

C	.4295938923	-3.4413952252	-1.1953666142
C	.3830763599	4.5071777112	-4.9597543787
C	1.3947516323	-4.5692063893	-.7851332011
C	-1.1714027335	1.9952525028	.5085849429
C	.3701370696	-1.0746196814	-.1714846894
C	-.1723402517	.8420726075	-5.1793018155
C	.4209530739	-2.2901693122	-7.1614213428
C	2.1812894630	-.4517344178	-1.6748450699
C	1.9216443364	.4401039064	-4.0111837888
C	.0367181137	-.1798836682	.8750535689
C	-.5889304493	2.1858058752	-5.3504880111
C	2.6711537739	.0240979188	-2.9011920175
C	.1447998605	-2.4713268647	-.0531295682
C	-.5380188665	-.1679164397	-6.1073730490
C	-1.5224659463	3.6548116076	-3.5246475108
C	-.8824023662	-4.0270848348	-1.7542208794
C	3.1898989280	-.8753975588	-.6285032819
C	2.6766750105	.8692127999	-5.2519415954
C	-.4888163266	-.7123992372	2.0546957987
C	-.3811620981	-2.9488515164	1.1504397924
C	-1.3583419672	2.4979322087	-6.4754989840
C	-1.3096865100	.2010438080	-7.2128449895
C	.9721017401	1.9735517075	1.8707983972
C	-.1533551074	-1.6289323141	-5.8957796060
C	-.2631167964	3.2639508498	-4.3241025822
C	-.6907225606	-2.0841240993	2.1984130097
C	.2024128119	1.3248013124	.7085343410
C	-1.3570212101	-2.4339464578	-5.3663506753
C	-1.7147912547	1.5208434825	-7.4019948747
H	-.3302881721	-2.3878032845	-7.9514194223
H	3.7466076404	.0558205110	-3.0087649830
H	4.2084887993	-.7208502994	-.9847821618
H	3.7532663748	.7991544130	-5.0958082336
H	1.2612560140	-1.7194293035	-7.5686771746
H	-3.5608156870	-.3495404875	-3.5462652024
H	-1.0708484445	-3.4719396011	-5.1684049838
H	-1.7477980565	-2.0111091026	-4.4346840654
H	-.3072652099	5.0257145267	-5.6329636393
H	3.0653667193	-1.9316469665	-.3732002705
H	3.0481571557	-.3064609863	.2954620068
H	2.4251802665	1.8994522902	-5.5215026890
H	2.4053768115	.2423127569	-6.1068488220
H	-1.7890951721	1.8829661709	1.4070567933
H	-1.0931750999	-2.4795274810	3.1261096625
H	-.5528947036	-4.0141947839	1.2696551786
H	-1.6820342955	3.5225059650	-6.6311273864
H	-2.3086733637	1.7861625266	-8.2714504291
H	-1.5953404122	-.5528456235	-7.9395203924
H	.6773046863	5.2180262204	-4.1810038526
H	-2.2667593397	4.1174389797	-4.1837573550
H	2.3395502023	-4.1754306647	-.3977847084
H	.9616603136	-5.2110238849	-.0113995677
H	-1.7196463848	1.5548955616	-.3294449717
H	-.7427529878	-.0468173346	2.8737439869

H	.7814887105	1.4973833896	-.2036576303
H	1.1336594199	3.0371197858	1.6682544439
H	.9060343100	-2.8789421949	-2.0035088788
H	-.6756969021	-4.6728825535	-2.6141866917
H	.4619096189	2.8458322413	-3.6196539572
H	-1.2682511223	4.3788018777	-2.7426878006
H	.6259024583	-1.6640190038	-5.1292573884
H	.7789445270	-3.2976194444	-6.9274783936
H	-1.9913810976	2.7843383221	-3.0570797546
H	1.6233456689	-5.2027360629	-1.6481036274
H	-2.1714884261	-2.4438748752	-6.0991390464
H	1.2771222792	4.2478020033	-5.5351048574
H	1.9503863558	1.5048480007	2.0158713848
H	.4236979259	1.8993128370	2.8152128887
H	-1.0481780326	3.0671915984	.3179899967
H	-1.5704441473	-3.2379671007	-2.0734884849
H	-1.3984720301	-4.6305792024	-1.0002976104
N	.8836623915	-.5419383199	-1.3880209172
N	.5887975841	.4809581757	-4.0295359691
O	-2.3873923080	.5575386768	-2.3593274128
O	-3.2319060008	-.5841530905	-2.6592079889
Cu	-.5298969662	.0924739545	-2.5127813555
C	-5.2728173871	.2936342296	-1.2818022205
C	-5.5070925634	1.5457146382	-1.9971365495
C	-5.8415784290	1.5508391838	-3.3708854978
C	-5.9690542774	2.7370358364	-4.0658997531
C	-5.7347366026	3.9736787980	-3.3905212474
C	-5.3566756024	3.9883898912	-2.0443784005
C	-5.2203253441	2.7895703442	-1.3654779221
C	-6.3621961144	-.7874025846	-1.3113419102
H	-4.3144059738	-.1972643895	-1.8793793317
H	-4.8865652896	.4616196174	-.2706549168
H	-6.0318756560	.6255917294	-3.9058980511
H	-5.1584541618	4.9340953423	-1.5480265440
H	-4.8951497826	2.7897901873	-.3309075491
H	-6.6580661350	-1.0033961280	-2.3449238705
H	-7.2558362421	-.3556662279	-.8216142860
H	-6.3309513322	3.6419865404	-5.6999080462
H	-5.7095667541	5.8825158819	-3.6724357447
H	-6.5737229301	-2.7684122053	-.8282096527
H	-5.7381328484	-1.9134816526	.2883160560
N	-5.8910091817	-2.0253393876	-.7109282814
O	-5.8867675904	5.0685284622	-4.1651620384
O	-6.2922860397	2.7298730105	-5.3717352054

120.L¹CuO₂H⁺ / formylglycine t.s.

C	2.6545188961	2.2375767385	4.4175606126
C	-.3963166018	-1.7969742904	-3.0238120960
C	.3241110830	2.7198739100	3.5193313796
C	1.6225312708	-2.0101094544	-4.5461004080
C	1.2489683475	-3.2152444957	2.1776124240
C	.1371373869	-3.2880732342	1.1112882177
C	1.4286858970	-4.5841133630	2.8564542628
C	1.7486248260	.9412726513	-2.3157933354
C	1.7640691398	2.3614508144	-2.3605414970
C	1.1672612035	2.9934196853	-3.4544969192
C	.5711390264	2.2595773103	-4.4766949001
C	4.4930303788	.0987354248	-2.1567526129
C	.5573350755	.8688152657	-4.4176539836
C	1.1364836607	.1824677219	-3.3451256854
C	2.3549729319	3.1974832610	-1.2270383028
C	1.0531960227	-1.3390819234	-3.2826570620
C	3.3635334419	4.2472397985	-1.7286604640
C	1.2365981481	3.8629000721	-.3964731305

C	4.2309999216	-1.2250106131	2.6201836705
C	3.3943256397	-.7152995897	1.4589610936
C	-3.7673848346	.7831735766	1.4578578797
C	-4.5067320238	2.1359647310	1.3766789109
C	1.4285291732	-.7439033985	2.8871664323
C	-4.2928277947	-1.5635724263	1.1032993022
C	4.0599211380	-.5272423638	.2284979360
C	3.5426909180	-.0499601196	-.9866783598
C	1.1272132839	.3226089229	3.7688549287
C	.4398358275	.0291428626	4.9524007534
C	.0287640378	-1.2663618625	5.2425656028
C	.3064324252	-2.3020632866	4.3512983434
C	1.0027691464	-2.0722959465	3.1633280377
C	1.5323956966	1.7636359015	3.4726087444
H	-2.0940125487	-.8541370515	.5165631346
H	2.8971062084	2.5232692849	-.5580044412
H	2.9486096990	3.2662024882	4.1807640298
H	3.5458013391	1.6057355666	4.3413495214
H	2.3238872082	2.2204098768	5.4622478151
H	1.0346732353	-1.7645261831	-5.4369696829
H	2.6559529755	-1.7016505035	-4.7355556777
H	1.6094796892	-3.0997208765	-4.4355605209
H	1.6583163928	-1.6709159147	-2.4336223679
H	3.8232903888	4.7635490384	-.8790860323
H	2.8854705195	5.0092501659	-2.3531732043
H	4.1645204331	3.7883894315	-2.3178376365
H	1.6640677444	4.4301587632	.4379405429
H	.5418363859	3.1247033568	.0189761806
H	.6496514894	4.5573568998	-1.0074320626
H	5.2848018618	-1.2869733488	2.3449128257
H	3.8966849668	-2.2165462843	2.9397321916
H	4.1280595255	-.5629537204	3.4847648866
H	5.1140852162	-.7717218397	.2261486286
H	5.5072133653	-.1948481334	-1.8826230376
H	4.5118680987	1.1341464883	-2.5113770552
H	4.1626144332	-.5182755012	-2.9989921286
H	.2120674919	.8312857814	5.6479250964
H	-.5147797807	-1.4727180963	6.1604299011
H	-.0308538783	-3.3053657853	4.5884345447
H	1.9273135744	1.7924046532	2.4522278537
H	-.4413398556	-2.8846638577	-2.9013569363
H	-1.0515115361	-1.5242110409	-3.8585047579
H	-.8066974213	-1.3349093250	-2.1203969664
H	.6261987262	3.7222919954	3.1960462288
H	-.0791191563	2.8150221603	4.5334600397
H	-.4830822866	2.3784526092	2.8653093508
H	2.1821460862	-3.0037675223	1.6462047210
H	.3467060671	-4.0928721903	.3969288300
H	.0747775305	-2.3554752999	.5418413711
H	-.8448992905	-3.4646096496	1.5592068712
H	1.7330768490	-5.3297016996	2.1143710999
H	.4985703104	-4.9453106319	3.3077027398
H	2.1925229889	-4.5530950563	3.6405642694
H	1.1583046362	4.0784586367	-3.5026201669
H	.1065464052	2.7735544420	-5.3133615733
H	.0785471077	.3062771817	-5.2138155035
H	-3.0615170554	.6031651321	2.2746090071
H	-5.1187415679	-2.2789801301	.9937496957
H	-5.5864311247	.0688504289	.9437650838
H	-2.7014238824	.6545258717	.4585165673
N	2.1063869841	-.4599882168	1.6650784245
N	2.2648604000	.2821018533	-1.1561962598
N	-4.6636097228	-.2794891454	1.2314760259
O	-.7161149257	.4874970071	1.0120213196

O	-1.7677436776	.0306619890	.0965964944
O	-3.9228695967	3.0204901867	2.0454589721
O	-5.5806614173	2.1031415211	.7463382427
O	-3.1048384697	-1.9452277503	1.0915796047
Cu	.9594160230	.1942917062	.2005739159

121.L¹CuO / methane complex

C	-1.9214724994	-4.8499299528	3.4770033775
C	.2721059927	-.0656474039	-.1010442229
C	1.0263505484	.2620468839	1.0504368269
C	2.2618780917	-.3678749014	1.2286680199
C	2.7330092960	-1.3075580165	.3169715153
C	1.9552939553	-1.6544364218	-.7835907737
C	.7118249047	-1.0566652553	-1.0107782998
C	.4840449459	1.1860053260	2.1356232266
C	1.4767247456	2.2885086270	2.5430088902
C	.0421347048	.3489409398	3.3561930408
C	-.1715580286	-1.5527129781	-2.1509584264
C	-.7394150935	-2.9451889624	-1.7988106424
C	.5476187712	-1.5684478278	-3.5107583708
C	-5.1222525932	.4315967600	.3425173763
C	-5.5792288186	.8100708779	1.6310494445
C	-6.8160966794	.3228227374	2.0621697398
C	-7.5760363455	-.5274046597	1.2642039905
C	-7.0991610396	-.9187562179	.0164442134
C	-5.8695242714	-.4620043524	-.4666218433
C	-4.7323076176	1.6662371251	2.5684675071
C	-4.1894567545	.8119639275	3.7339474567
C	-5.4880389537	2.8994324731	3.0937943356
C	-5.3361287615	-.9854302689	-1.7965846844
C	-6.3288974546	-.7870979691	-2.9555927486
C	-4.9280877490	-2.4684342808	-1.6659410856
C	.1314531650	2.3385650765	-1.5583978399
C	-1.1259950919	1.7025340095	-.9939674031
C	-2.3420520599	2.3639013740	-1.2302689763
C	-3.6241844021	1.9680380234	-.8087993632
C	-4.8042334550	2.8372375444	-1.1897482646
H	-1.9775487919	-3.9401659077	2.8767441649
H	-2.8934792631	-5.3489492984	3.4881390022
H	-.1103932650	3.2427289658	-2.1185158595
H	.6554426797	1.6405559980	-2.2177252963
H	.8276314950	2.5956797030	-.7542070885
H	-2.2843455609	3.2799758838	-1.8027460204
H	-4.4793474743	3.7243773986	-1.7352149340
H	-5.3554953945	3.1511569518	-.2979982559
H	-1.6334819648	-4.5986928806	4.5007784719
H	-5.5069238658	2.2770976336	-1.8152051579
H	2.8567524217	-.1329391373	2.1066065620
H	3.6944581824	-1.7877344860	.4773599338
H	2.3120096608	-2.4176340620	-1.4694640378
H	-.4089640901	1.6790440579	1.7399791714
H	1.0184788695	2.9559811417	3.2808852700
H	1.7844424020	2.8956655877	1.6847032322
H	2.3828753864	1.8742561737	2.9981507362
H	-.4385821104	.9881432858	4.1061625105
H	.9047997716	-.1329874020	3.8307434922
H	-1.1753682747	-5.5246273152	3.0498276215
H	-.6622954078	-.4349701562	3.0593591393
H	-1.0212353114	-.8688553225	-2.2369955536
H	-1.4483676834	-3.2761279062	-2.5668516035
H	-1.2537845401	-2.9250025883	-.8325832277
H	.0625302280	-3.6901129481	-1.7405850449
H	-.1434612452	-1.8825841906	-4.3006988411
H	1.3905705157	-2.2679238277	-3.5192221823

H	.9349883151	-.5787361446	-3.7762602792
H	-7.1840794699	.6008108975	3.0456589576
H	-8.5328096449	-.8980390695	1.6215307480
H	-7.6864785625	-1.6048624973	-.5872604143
H	-3.8694822428	2.0281986780	2.0015944596
H	-3.5331576263	1.4114663848	4.3750189988
H	-3.6172127311	-.0461652024	3.3676583786
H	-5.0068363843	.4298313853	4.3559031499
H	-4.8213670059	3.5199153618	3.7022953911
H	-6.3385296622	2.6187951702	3.7243965643
H	-5.8713145061	3.5180619553	2.2753632743
H	-4.4312428110	-.4206555431	-2.0395220523
H	-5.8781615564	-1.1120771590	-3.8995100359
H	-6.6190054097	.2633517956	-3.0640769947
H	-7.2444895475	-1.3711834093	-2.8130795730
H	-4.4906804649	-2.8294186998	-2.6037338822
H	-5.7962223651	-3.0972710373	-1.4369968916
H	-4.1922666313	-2.6115771978	-.8682313413
N	-.9983280106	.5615703414	-.3170713232
N	-3.8362692235	.8705836359	-.0963680820
O	-2.0983448818	-1.7544093351	1.3255855016
Cu	-2.4811930267	-.3342364067	.4690881217

122.L¹CuO / cyclohexane complex

C	-3.0256522008	-5.4628326759	4.0298939083
C	-.5311560547	-.1045185903	.2077318671
C	.1491181163	.3816682066	1.3487765204
C	1.3232951183	-.2683644944	1.7409219108
C	1.8025096643	-1.3760125884	1.0476038393
C	1.0939653290	-1.8692377709	-.0440310223
C	-.0858623355	-1.2580651965	-.4795938091
C	-.4147334109	1.5122884723	2.2034186829
C	.6115784311	2.6207964124	2.4953115347
C	-1.0033646130	.9328152146	3.5084427770
C	-.9005533995	-1.8896795519	-1.6034005988
C	-1.9726841531	-4.6528696474	3.2532577488
C	-1.6012318089	-3.1649111508	-1.0859217195
C	-.0677786776	-2.1807215777	-2.8638376383
C	-5.9049971250	.8189369950	.0538931424
C	-6.4194227168	1.3837590043	1.2480657917
C	-7.7232207795	1.0510304661	1.6272324186
C	-8.4966509109	.1769052848	.8686687034
C	-7.9687332326	-.3939727769	-.2864179762
C	-6.6704480838	-.0971701722	-.7122590879
C	-5.5743933822	2.2850317142	2.1440201349
C	-5.2024082652	1.5562271185	3.4525815269
C	-.6787903604	-4.4910685337	4.0694461487
C	-6.2564805231	3.6338471778	2.4363747000
C	-6.0886228038	-.8094230064	-1.9294473879
C	-6.9955471614	-.7136580355	-3.1690710452
C	-5.7718558665	-2.2810732323	-1.5893024566
C	-.9550310605	-3.8822959486	5.4546366936
C	-.3725717599	2.0113995296	-1.6302289659
C	-2.0065484428	-4.6954140471	6.2279221003
C	-3.3021211563	-4.8533949272	5.4147684879
C	-1.7164818841	1.5672407260	-1.0804275039
C	-2.8490007108	2.2699059622	-1.5215511055
C	-4.1903498506	2.0459617476	-1.1624886396
C	-5.2528822635	2.9366404766	-1.7710981559
H	-1.7527793819	-5.1458275175	2.2975085313
H	-2.3761762178	-3.6613312038	3.0024572626
H	-.2057769986	-5.4766314259	4.2004136351
H	.0387858681	-3.8696447482	3.5197020601
H	-.0254895213	-3.8160595720	6.0350053959

H	-1.3192024451	-2.8528982472	5.3266812383
H	-2.2188235675	-4.2224842189	7.1954656731
H	-1.5982715367	-5.6923544906	6.4525121052
H	-4.0234547473	-5.4702247489	5.9664310990
H	-.4978381318	2.8268182637	-2.3437166879
H	.1355067650	1.1793615971	-2.1266006963
H	.2853958420	2.3455551079	-.8224539527
H	-2.6671846116	3.0756970998	-2.2199096320
H	-4.8065149981	3.7055190436	-2.4033088934
H	-5.8430175450	3.4211269965	-.9869083124
H	-5.9509657069	2.3470273216	-2.3742036511
H	1.8617537228	.0871431683	2.6147505265
H	2.7150230373	-1.8686113247	1.3722068554
H	1.4550202318	-2.7557744337	-.5574143362
H	-1.2413543099	1.9693352587	1.6511306254
H	.1402847957	3.4338347933	3.0584506739
H	1.0244272719	3.0453893148	1.5735713457
H	1.4505041086	2.2535347107	3.0962208218
H	-1.4932980361	1.7213716557	4.0920514060
H	-.2141442005	.4963848851	4.1316422684
H	-1.7362767036	.1489593986	3.2913854387
H	-1.6846027583	-1.1805851783	-1.8855212536
H	-2.2623771212	-3.5791447176	-1.8564041133
H	-2.1951806508	-2.9499108402	-.1916922520
H	-.8656360094	-3.9352837991	-.8265813144
H	-.7101707850	-2.5765276989	-3.6581490728
H	.7122305794	-2.9263654231	-2.6755071234
H	.4212777436	-1.2774786732	-3.2449484795
H	-8.1353344788	1.4724155825	2.5396948074
H	-9.5054478333	-.0720442789	1.1862259070
H	-8.5699103386	-1.0949947326	-.8580441529
H	-4.6406122094	2.4990729337	1.6152956493
H	-4.5567154036	2.1892829982	4.0719025750
H	-4.6703564354	.6208665478	3.2516341870
H	-6.0970443544	1.3164910882	4.0383835820
H	-5.5893019170	4.2765656745	3.0209913885
H	-7.1780133680	3.5075506451	3.0149009868
H	-6.5139626098	4.1649327190	1.5137647227
H	-5.1402752268	-.3250228648	-2.1800433216
H	-6.5001357624	-1.1662874199	-4.0348045067
H	-3.7682658096	-3.8660129832	5.2857319561
H	-7.2300196719	.3263849278	-3.4197189507
H	-7.9439691731	-1.2420532530	-3.0241005923
H	-5.3075472440	-2.7820632064	-2.4463336292
H	-6.6845511299	-2.8307018325	-1.3321959573
H	-5.0874578579	-2.3557180003	-.7381717349
H	-3.9565145242	-5.5270579438	3.4526142152
H	-2.6672389292	-6.4955525610	4.1596427865
N	-1.7327059337	.5450661631	-.2243764732
N	-4.5535416158	1.0908551685	-.3190871185
O	-3.1007007192	-1.3487952546	1.6748586592
Cu	-3.3495344226	-.0898541142	.5568973069

123.L¹CuO / acetonitrile complex

C	2.7752600989	.0514084404	-3.2780357325
C	3.4836701673	.4015840832	-2.1023399962
C	4.7271294426	-.1975724466	-1.8793648005
C	5.2474480402	-1.1355686533	-2.7657506920
C	4.5138219578	-1.5086136270	-3.8880281116
C	3.2668885378	-.9403005222	-4.1624209698
C	2.8931870639	1.3231812637	-1.0404469763
C	3.8254997122	2.4917901164	-.6755137578
C	2.5155040649	.5018789629	.2123962296
C	2.4391089305	-1.4634278856	-5.3309253971

C	.8969290205	-5.0282596903	.3201547249
C	1.8937027010	-2.8685712406	-4.9940105886
C	3.2114305357	-1.4693044242	-6.6618319982
C	-2.5927451147	.4636895877	-2.7671817627
C	-3.0079705987	.9221773529	-1.4898329852
C	-4.2218092634	.4515008888	-.9820922925
C	-4.9981988976	-.4595553501	-1.6932124480
C	-4.5596570046	-.9311676273	-2.9275816254
C	-3.3528223764	-.4963331140	-3.4837301149
C	-2.1361407658	1.8380350586	-.6348629113
C	-1.5610213240	1.0606995172	.5680783749
C	-.2219369166	-4.6006829904	-.5123456500
C	-2.8770754164	3.1022325278	-.1638960272
C	-2.8492302617	-1.1208854084	-4.7813701434
C	-3.8643059989	-1.0082770834	-5.9313943546
C	-2.4450143598	-2.5932055014	-4.5425160324
C	2.5943123978	2.4425799026	-4.7847092126
C	1.3520163370	1.7810482082	-4.2198491990
C	.1165122893	2.4064920497	-4.4580501604
C	-1.1482542704	1.9911332612	-4.0073103634
C	-2.3519355730	2.8366681308	-4.3661952221
H	2.3354880611	3.3415977015	-5.3453373723
H	3.1307435879	1.7534548440	-5.4440345895
H	3.2857256162	2.7130912209	-3.9806279244
H	.1443582072	3.3150280378	-5.0443820888
H	-2.0586436773	3.7088079634	-4.9519058525
H	-2.8692562121	3.1740558938	-3.4628641103
H	.0040715190	-3.6385194638	-1.0014299146
H	-3.0725522504	2.2478671182	-4.9433797703
H	5.2875394596	.0569577633	-.9844927084
H	6.2116068356	-1.5958076716	-2.5677138048
H	4.9093554753	-2.2709146028	-4.5528163527
H	1.9700506970	1.7520440452	-1.4420050498
H	3.3358471992	3.1567322920	.0442837173
H	4.0942259967	3.0861612466	-1.5554379394
H	4.7554828032	2.1424726825	-.2144348793
H	2.0210675325	1.1386028832	.9550394316
H	3.4066599887	.0702788117	.6816635894
H	-1.1196418271	-4.4874988327	.1042893841
H	1.8417289921	-.3228346339	-.0404679671
H	1.5773603795	-.8003489829	-5.4543844983
H	1.2350181357	-3.2250166302	-5.7950784484
H	1.3265579541	-2.8578498007	-4.0571456209
H	2.7130394030	-3.5886477882	-4.8878899905
H	2.5559289493	-1.7945390053	-7.4770455069
H	4.0634377599	-2.1572174441	-6.6365441950
H	3.5950289058	-.4746150334	-6.9138178586
H	-4.5564149968	.7887031871	-.0051230452
H	-5.9346022431	-.8182926775	-1.2747578466
H	-.4223838350	-5.3535934619	-1.2813543670
H	-5.1561062090	-1.6665077192	-3.4591049096
H	-1.2893621297	2.1628955683	-1.2463295270
H	-.8856487692	1.6983820678	1.1495845565
H	-1.0020690132	.1774960912	.2439992488
H	-2.3607015433	.7233549400	1.2371914380
H	-2.1941386003	3.7559877371	.3893846979
H	-3.7101273799	2.8610424786	.5050899532
H	-3.2819593745	3.6729233621	-1.0062802342
H	-1.9489792048	-.5779770396	-5.0864609432
H	-3.4276447359	-1.3956435390	-6.8581233530
H	-4.1646852941	.0302771933	-6.1065554125
H	-4.7719246451	-1.5885145951	-5.7332260827
H	-2.0326402660	-3.0281345525	-5.4604615891
H	-3.3151897201	-3.1922930754	-4.2500665612

H	-1.6902466474	-2.6821142076	-3.7539896676
N	1.7857698395	-5.3710839357	.9842335594
N	1.5020417160	.6488748949	-3.5376837723
N	-1.3338766013	.8946842354	-3.2844340842
O	.2119188964	-1.8369565342	-2.0383811076
Cu	.0398102633	-.3166456228	-2.8035283527

124.L¹CuO / toluene complex

C	-1.8097477989	-7.8319123248	3.8534052695
C	-.7980894298	-.1295704755	-.2974810104
C	-.0075314844	.0433090894	.8639029651
C	1.1987257258	-.6587689276	.9495468441
C	1.6061872148	-1.5233206405	-.0620688830
C	.7932195394	-1.7190351132	-1.1741998234
C	-.4225448963	-1.0426632510	-1.3126760226
C	-.4816218964	.8812156466	2.0466935765
C	.5749302371	1.8849445986	2.5393194378
C	-.9450557517	-.0496094297	3.1887849703
C	-1.3440869750	-1.3743347385	-2.4814765174
C	-3.2012013068	-7.8985473790	3.7923587242
C	-1.9782113578	-2.7655750542	-2.2627475222
C	-.6423526997	-1.2882264888	-3.8477104625
C	-6.1695975077	.5566201159	.2659644865
C	-6.5877299138	.7898858952	1.6019624709
C	-7.8370372028	.3043458972	1.9967094138
C	-8.6473701554	-.4071159160	1.1160503687
C	-8.2106636709	-.6579308222	-.1817530246
C	-6.9697903678	-.1955005331	-.6313672819
C	-5.6874096171	1.4856060311	2.6199389895
C	-5.1597191858	.4712290763	3.6569987983
C	-3.9503693418	-6.7382226253	3.5878028736
C	-6.3779658583	2.6738056061	3.3122730554
C	-6.4840047201	-.5660144436	-2.0291556835
C	-7.4915785694	-.1847306910	-3.1281133167
C	-6.1339362564	-2.0674672395	-2.0970805907
C	-3.3302826141	-5.4903403563	3.4430534750
C	-.8461268292	2.4109223671	-1.5025584465
C	-1.9295200252	-5.4407011915	3.5024538620
C	-2.1236365412	1.7820530302	-.9768753184
C	-1.1765665890	-6.5961514344	3.7057745170
C	-4.1375724548	-4.2284603287	3.2513942093
C	-3.3104866908	2.5182239789	-1.1247078789
C	-4.6076961837	2.1398480631	-.7332475848
C	-5.7463364377	3.1003243161	-1.0047304703
H	-1.4285779078	-4.4829607279	3.3831109437
H	-.0919800760	-6.5333703281	3.7462651989
H	-1.2235416348	-8.7333072411	4.0114370375
H	-3.7147157598	-3.5863210090	2.4681404415
H	-4.1562938080	-3.6346007863	4.1749117677
H	-5.1754967534	-4.4575631931	2.9897052626
H	-1.0486183672	3.3872275196	-1.9447684290
H	-.3836820752	1.7678776047	-2.2575076052
H	-.1136381153	2.5307884090	-.6985801743
H	-3.2154987012	3.4851935558	-1.6001431237
H	-5.3836994181	4.0203746626	-1.4653146572
H	-6.2661477485	3.3506277238	-.0744263694
H	-6.4865351374	2.6420030269	-1.6683637108
H	1.8215418487	-.5401725199	1.8315414802
H	2.5457343450	-2.0619698285	.0271801527
H	1.0997818226	-2.4246686849	-1.9411288670
H	-1.3540549158	1.4564142837	1.7221610558
H	.1643231697	2.5008850638	3.3468172470
H	.9034569239	2.5554558032	1.7375881772
H	1.4633480080	1.3814113765	2.9355861725

H	-1.3674514626	.5358175554	4.0141161049
H	-.1018278846	-.6272885941	3.5859049007
H	-1.7037239567	-.7561837258	2.8361774337
H	-2.1575104264	-.6428361388	-2.4846430555
H	-2.7121486018	-2.9804681967	-3.0484629895
H	-2.4794509746	-2.8206022390	-1.2908907846
H	-1.2148590145	-3.5517039917	-2.2944483458
H	-1.3588685705	-1.4817670053	-4.6536875986
H	.1601794819	-2.0278903061	-3.9427944100
H	-.2038348237	-.2986543626	-4.0169611158
H	-8.1749216777	.4711354310	3.0155847281
H	-9.6121593524	-.7811866679	1.4473624907
H	-8.8377784977	-1.2378354385	-.8526873621
H	-4.8198941735	1.8805015437	2.0830494935
H	-4.4676225703	.9601141628	4.3521932319
H	-4.6296479006	-.3554271875	3.1735630353
H	-5.9806520397	.0467209448	4.2459669613
H	-5.6743461619	3.1827344679	3.9801147359
H	-7.2305945427	2.3527564885	3.9203769265
H	-6.7448793726	3.4072981484	2.5863846278
H	-5.5618727299	-.0097171681	-2.2216108617
H	-7.0723719259	-.3988603807	-4.1171872434
H	-7.7460905512	.8798446172	-3.0920478451
H	-8.4246494027	-.7516937849	-3.0394872973
H	-5.7307455102	-2.3236632337	-3.0834537643
H	-7.0216205912	-2.6871418681	-1.9271062811
H	-5.3884437298	-2.3370747470	-1.3425589474
H	-5.0354109851	-6.8005898062	3.5416240123
H	-3.7063296021	-8.8549355342	3.9028924318
N	-2.0395432767	.5749769566	-.4196059567
N	-4.8676745902	.9868820963	-.1340516074
O	-3.2374835056	-1.8264856919	1.0252712134
Cu	-3.5591315001	-.3194030287	.2986866475

125.L¹CuO / phenol complex

C	-3.6399405826	-5.2503763118	3.1513304880
C	-.3855813555	.1646612603	.3196909916
C	.4178623936	.9188837873	1.2116749006
C	1.6394188634	.3746543814	1.6175961797
C	2.0590944289	-.8768790023	1.1749496821
C	1.2492011396	-1.6166504155	.3187372147
C	.0149960799	-1.1239774907	-.1174821666
C	-.0355482724	2.2592081512	1.7823549072
C	.9935981092	3.3809691128	1.5503034214
C	-.3710943899	2.1196601584	3.2821397965
C	-.8583059937	-1.9841377439	-1.0277439020
C	-3.1584330112	-3.9421835556	3.3008547961
C	-1.3156111141	-3.2723742066	-.3134908061
C	-.1482733824	-2.3183531528	-2.3545561885
C	-5.7923835808	.4760345288	.5637077284
C	-6.3382795633	1.1488669399	1.6903929663
C	-7.5376573233	.6734690831	2.2267962032
C	-8.1811689786	-.4358942565	1.6856041022
C	-7.6228853342	-1.1008122451	.5974859531
C	-6.4229371168	-.6758018081	.0211036253
C	-5.6381939253	2.3396039329	2.3410640623
C	-5.0822053773	1.9629167898	3.7308484141
C	-2.2025151692	-3.6654141826	4.2906459478
C	-6.5505725373	3.5768347893	2.4310257702
C	-5.8085438067	-1.4871486400	-1.1170936128
C	-6.7382304416	-1.5712698277	-2.3433017361
C	-5.4169054908	-2.9017887452	-.6385504303
C	-1.7419112926	-4.6908158832	5.1149417394
C	-2.2186326481	-5.9949671286	4.9697077967

C	-.6204798001	1.8775840370	-1.9424645946
C	-3.1698665075	-6.2640905634	3.9825639735
C	-1.8366657367	1.4575066592	-1.1384400916
C	-3.0904784807	1.9377457118	-1.5682539926
C	-4.3556909960	1.6531782566	-1.0293448054
C	-5.5735247247	2.2374698580	-1.7144433617
H	-1.8329859092	-2.6497012443	4.4002825638
H	-1.0012498342	-4.4652661469	5.8784301584
H	-1.8549171748	-6.7892691324	5.6150739536
H	-.9108879196	2.4703903790	-2.8109927078
H	-.0617735514	1.0006758367	-2.2822491915
H	.0634659043	2.4692642616	-1.3262144840
H	-3.0777692844	2.5826385736	-2.4370034772
H	-5.2861436481	2.8813289769	-2.5468726695
H	-6.1656796507	2.8218997139	-1.0024594639
H	-6.2253291991	1.4449926979	-2.0936890378
H	2.2683649079	.9350589354	2.3035076864
H	3.0110518411	-1.2805706572	1.5085905806
H	1.5738308584	-2.6004594119	-.0075902469
H	-.9581191737	2.5475722583	1.2686902118
H	.6000731374	4.3368388924	1.9130643796
H	1.2390313691	3.4985248728	.4893515418
H	1.9295974300	3.1890839922	2.0860514221
H	-.7723538715	3.0621707180	3.6730968310
H	.5259199873	1.8738358045	3.8620368952
H	-1.1075201666	1.3269835122	3.4436630136
H	-1.7553547453	-1.4081427289	-1.2726678364
H	-1.9510163219	-3.8676406135	-.9792966440
H	-1.8881084276	-3.0578177296	.5929615550
H	-.4590296923	-3.8938811044	-.0306189962
H	-.8189903576	-2.8796806347	-3.0143197318
H	.7428154782	-2.9343323712	-2.1906760031
H	.1678946490	-1.4142340023	-2.8859825000
H	-7.9702283320	1.1733218122	3.0886464590
H	-9.1093214142	-.7930078559	2.1227594236
H	-8.1188594897	-1.9815828839	.2002320353
H	-4.7865364767	2.6110615883	1.7097111647
H	-4.5459465024	2.8115646835	4.1708048307
H	-4.3863757877	1.1182871874	3.6740964088
H	-5.8890952469	1.6833934473	4.4174146493
H	-5.9932629861	4.4298714552	2.8330103804
H	-7.4068423556	3.4043528236	3.0918605414
H	-6.9410607309	3.8608367275	1.4481484123
H	-4.8903950655	-.9827505234	-1.4327995726
H	-6.2421025466	-2.1095516205	-3.1581492406
H	-3.2369654667	-2.0878519268	2.6625213263
H	-7.0193594303	-.5810901043	-2.7171444500
H	-7.6629227224	-2.1101613984	-2.1095802540
H	-4.8935140049	-3.4387182622	-1.4381275611
H	-6.3055431178	-3.4875422229	-.3761768723
H	-4.7691898844	-2.8760946010	.2421327545
H	-3.5508444219	-7.2747979959	3.8573639659
H	-4.3799227128	-5.4488843176	2.3820987561
N	-1.6613618947	.6598142215	-.0905584419
N	-4.5290200457	.9053889284	.0558338696
O	-3.6389568144	-2.9837639183	2.4701427487
O	-2.6098637211	-.5679436496	2.7030294845
Cu	-3.1246898029	.2067715499	1.1175019836

126.L¹CuO / isopropylbenzene complex

C	-1.9879992929	-2.5924619319	5.8943290403
C	-.5442634248	.2155110628	.0544878731
C	.1836375570	.7758856208	1.1296284601
C	1.4566648664	.2636487506	1.3983897851

C	1.9897910386	-.7785213163	.6463914522
C	1.2430697633	-1.3429734607	-.3834018371
C	-.0349786556	-.8711602053	-.6957090250
C	-.4157660721	1.8412741747	2.0416011036
C	.5128257083	3.0501919369	2.2497984385
C	-.8202932869	1.2015782196	3.3875393766
C	-.8715177660	-1.5849048440	-1.7532387535
C	-2.3866261808	-2.9992579977	4.6186819015
C	-1.3631406474	-2.9408978287	-1.2020824049
C	-.1337933432	-1.7591021392	-3.0924447931
C	-5.9753207252	.4989534539	.4670068015
C	-6.4412050887	1.0892786727	1.6709231279
C	-7.6404799278	.6216395312	2.2147553810
C	-8.3577034733	-.4048893663	1.6071273087
C	-7.8764930580	-.9911563395	.4401039249
C	-6.6827700586	-.5641776875	-.1489405059
C	-5.6440408511	2.1632526796	2.4071862250
C	-5.0541999784	1.6018439079	3.7176356333
C	-2.7752335534	-4.3242377729	4.3785243824
C	-6.4713057877	3.4336531014	2.6768399118
C	-6.1518504679	-1.2785408054	-1.3880316893
C	-7.1742266666	-1.2991640500	-2.5392186242
C	-5.6885147542	-2.7070901470	-1.0351176534
C	-2.7519633071	-5.2282622050	5.4513160038
C	-.8297728866	2.3073733649	-1.7884880270
C	-2.3544147744	-4.8239051567	6.7250380017
C	-2.0504800011	1.7103592618	-1.1105203941
C	-1.9701768994	-3.5011053236	6.9519974545
C	-3.2983960795	2.2548000924	-1.4524083373
C	-3.2117801152	-4.7507802813	2.9820122236
C	-4.5604280441	1.8770101787	-.9602441187
C	-2.2773596130	-5.8263621534	2.3972023279
C	-5.7795126001	2.6146008254	-1.4714901513
C	-4.6763994725	-5.2260870505	2.9653845873
H	-2.3442453020	-5.5419216439	7.5415372134
H	-1.6594340463	-3.1843564762	7.9443245669
H	-2.3951887045	-2.2894136711	3.7923264542
H	-1.6881549388	-1.5604594596	6.0597433766
H	-3.0471952793	-6.2625792958	5.2930962854
H	-3.1424089786	-3.8595237458	2.3432389993
H	-4.9939517135	-5.4724771724	1.9453725426
H	-5.3464357972	-4.4516954632	3.3526320781
H	-4.8144549890	-6.1236925668	3.5800661326
H	-2.5733124922	-6.0832546971	1.3735055583
H	-2.3047347705	-6.7479478174	2.9909256572
H	-1.2408234612	-5.4756620041	2.3734315725
H	-1.1202930076	3.1081177843	-2.4695887345
H	-.2869493695	1.5421227073	-2.3512198381
H	-.1320834835	2.7075660368	-1.0468531808
H	-3.2851915211	3.0580437409	-2.1765181449
H	-5.4992360517	3.3877903959	-2.1881728651
H	-6.3219687729	3.0807118960	-.6431489820
H	-6.4750336694	1.9210849797	-1.9548780970
H	2.0331957135	.6754794745	2.2217563635
H	2.9787199861	-1.1654554344	.8765233081
H	1.6541887481	-2.1777950278	-.9436672783
H	-1.3314767960	2.2084569027	1.5679814123
H	.0137276984	3.8099986165	2.8611679424
H	.7943140187	3.5148965346	1.2985290572
H	1.4362472114	2.7716744907	2.7690629905
H	-1.3447510586	1.9296948641	4.0177742293
H	.0629340987	.8561071731	3.9368655458
H	-1.4753656076	.3400963723	3.2223606919
H	-1.7582224834	-.9736918586	-1.9459717422

H	-2.0401003988	-3.4239438393	-1.9168494897
H	-1.8915834250	-2.8055925578	-.2530909823
H	-.5206321514	-3.6201262322	-1.0275336986
H	-.7957496694	-2.2245233552	-3.8310668364
H	.7460424445	-2.4039580349	-2.9936798401
H	.2022026466	-.7990785555	-3.4995906352
H	-8.0119680880	1.0580620792	3.1376143320
H	-9.2841971664	-.7579258333	2.0512807187
H	-8.4321128205	-1.8061514116	-.0147285698
H	-4.8022490129	2.4504658795	1.7702949799
H	-4.4328278185	2.3571889116	4.2122144785
H	-4.4335975568	.7200533980	3.5297788003
H	-5.8467241361	1.3115930896	4.4163558590
H	-5.8441669165	4.2013420048	3.1431342213
H	-7.3080434271	3.2380419059	3.3559910640
H	-6.8848819368	3.8516958953	1.7529288727
H	-5.2725357297	-.7301243679	-1.7394282818
H	-6.7311119265	-1.7538822962	-3.4318046254
H	-7.5062080729	-.2895991017	-2.8037279135
H	-8.0641947923	-1.8835666952	-2.2817703456
H	-5.2590791504	-3.1993068271	-1.9150383913
H	-6.5268342126	-3.3195841365	-.6847720928
H	-4.9294334708	-2.6954256348	-.2464425417
N	-1.8539722095	.7166962885	-.2425706074
N	-4.7154788511	.9104305930	-.0676270938
O	-2.7550748966	-1.3611900252	1.6990685750
Cu	-3.3006260335	-.1198188799	.6723836341

127.L¹CuO / cyclohexadiene complex

C	-.8570000000	-3.6000000000	4.9260000000
C	2.6510000000	.7310000000	1.9060000000
C	2.2030000000	-1.0120000000	-3.7060000000
C	.4620000000	-3.7530000000	5.6350000000
C	1.6580000000	-2.4380000000	-3.4860000000
C	2.8910000000	-.8920000000	-5.0760000000
C	-2.6520000000	.8300000000	-1.1260000000
C	-3.1590000000	1.1510000000	.1560000000
C	-4.4180000000	.6570000000	.5080000000
C	-5.1520000000	-.1380000000	-.3660000000
C	-4.6280000000	-.4660000000	-1.6140000000
C	2.7220000000	.3450000000	-1.5820000000
C	-3.3720000000	-.0010000000	-2.0180000000
C	-2.3450000000	1.9670000000	1.1560000000
C	-1.8080000000	1.0640000000	2.2850000000
C	1.6170000000	-3.9360000000	4.6860000000
C	-3.1330000000	3.1600000000	1.7230000000
C	-2.7880000000	-.4470000000	-3.3540000000
C	-3.7500000000	-.2250000000	-4.5340000000
C	-2.3430000000	-1.9200000000	-3.2790000000
C	1.4860000000	-3.9580000000	3.3590000000
C	.1670000000	-3.8030000000	2.6490000000
C	3.5220000000	.6190000000	-.4500000000
C	2.5860000000	2.7640000000	-3.0190000000
C	-.9890000000	-3.6220000000	3.5980000000
C	1.3400000000	2.1430000000	-2.4190000000
C	.1240000000	2.8050000000	-2.6370000000
C	-1.1490000000	2.3830000000	-2.2210000000
C	-2.3400000000	3.2230000000	-2.6350000000
C	4.7500000000	-.0400000000	-.3380000000
C	5.1710000000	-.9540000000	-1.2990000000
C	4.3510000000	-1.2400000000	-2.3890000000
C	3.1130000000	-.6120000000	-2.5490000000
C	3.0480000000	1.5490000000	.6600000000
C	4.0800000000	2.6350000000	1.0080000000

H	-1.9740000000	-3.5060000000	3.1510000000
H	-1.7370000000	-3.4670000000	5.5510000000
H	.4150000000	-4.6030000000	6.3340000000
H	.6420000000	-2.8780000000	6.2800000000
H	.2150000000	-2.9510000000	1.9520000000
H	2.3430000000	3.6960000000	-3.5330000000
H	3.0560000000	2.0820000000	-3.7320000000
H	3.3290000000	2.9690000000	-2.2430000000
H	.1680000000	3.7220000000	-3.2110000000
H	-2.0160000000	4.1230000000	-3.1590000000
H	-2.9310000000	3.5110000000	-1.7610000000
H	-3.0040000000	2.6550000000	-3.2930000000
H	5.3820000000	.1580000000	.5230000000
H	6.1290000000	-1.4540000000	-1.1930000000
H	4.6750000000	-1.9740000000	-3.1210000000
H	2.1470000000	2.0590000000	.3040000000
H	3.6690000000	3.3180000000	1.7580000000
H	4.3600000000	3.2260000000	.1310000000
H	4.9970000000	2.2070000000	1.4260000000
H	2.2610000000	1.3950000000	2.6850000000
H	3.5200000000	.2040000000	2.3150000000
H	1.8810000000	-.0100000000	1.6670000000
H	1.3450000000	-.3350000000	-3.7060000000
H	.9530000000	-2.7060000000	-4.2800000000
H	1.1440000000	-2.5200000000	-2.5240000000
H	2.4700000000	-3.1750000000	-3.4950000000
H	2.1840000000	-1.1330000000	-5.8770000000
H	3.7380000000	-1.5790000000	-5.1670000000
H	3.2660000000	.1220000000	-5.2520000000
H	-4.8250000000	.8930000000	1.4870000000
H	-6.1280000000	-.5130000000	-.0720000000
H	-5.1990000000	-1.1040000000	-2.2820000000
H	-1.4790000000	2.3730000000	.6240000000
H	-1.1920000000	1.6530000000	2.9750000000
H	-1.1920000000	.2490000000	1.8900000000
H	-2.6310000000	.6250000000	2.8580000000
H	-2.4890000000	3.7600000000	2.3730000000
H	-3.9900000000	2.8340000000	2.3210000000
H	-3.5100000000	3.8100000000	.9260000000
H	-1.8920000000	.1500000000	-3.5460000000
H	-3.2580000000	-.4860000000	-5.4760000000
H	2.6030000000	-4.0540000000	5.1320000000
H	-4.0760000000	.8190000000	-4.6010000000
H	-4.6470000000	-.8470000000	-4.4510000000
H	-1.8720000000	-2.2290000000	-4.2190000000
H	-3.1990000000	-2.5800000000	-3.0980000000
H	-1.6250000000	-2.0760000000	-2.4690000000
H	2.3660000000	-4.0950000000	2.7320000000
H	-.0140000000	-4.6760000000	2.0020000000
N	1.4630000000	1.0100000000	-1.7280000000
N	-1.3510000000	1.2930000000	-1.4890000000
O	.2030000000	-1.1120000000	.3460000000
Cu	.0260000000	.1660000000	-.7690000000

128.L¹CuO / dopamine complex

C	-.4434463901	-4.2847404362	.0534934515
C	2.7118107294	-.0301759985	-3.7217726879
C	3.3657440777	.2357741526	-2.4894872415
C	4.4837607672	-.5335995770	-2.1514110573
C	4.9477644179	-1.5446049981	-2.9890479103
C	4.2801271290	-1.8148905822	-4.1801967619
C	3.1515074157	-1.0836303929	-4.5637363874
C	2.8431490623	1.2804588606	-1.5059767694
C	3.9241130926	2.2931896130	-1.0867100353

C	2.2182334225	.5975258212	-.2703303410
C	2.4022649583	-1.4652243656	-5.8369269376
C	-.7369673732	-4.6621844561	1.4907753640
C	1.8000029042	-2.8800191723	-5.7136362627
C	3.2870469927	-1.3554854527	-7.0924910738
C	-2.6800710692	.8532802067	-3.5779694423
C	-3.2432629032	1.3275686739	-2.3688270247
C	-4.5668766643	.9840688244	-2.0763426988
C	-5.3130314647	.1806886438	-2.9339145318
C	-4.7313104155	-.3160127082	-4.0968397454
C	-3.4107261838	-.0034459458	-4.4367043888
C	-2.4193075409	2.1131842623	-1.3535714529
C	-2.0935526745	1.2142156625	-.1417800245
C	-.1621679099	-5.8120846847	2.0537720008
C	-3.0936121597	3.4245380399	-.9144572397
C	-2.7589947134	-.6711291649	-5.6437039642
C	-3.5897623543	-.5392228896	-6.9315831449
C	-2.4598431764	-2.1519777293	-5.3231048202
C	-.3963730913	-6.1572573386	3.3808991811
C	-1.2206648711	-5.3424191380	4.1738354773
C	2.8188845098	2.3871957148	-5.2613523149
C	1.5095721519	1.8184275604	-4.7518032684
C	-1.7963476178	-4.2007740424	3.6321755951
C	.3282197349	2.5260667050	-5.0411959945
C	-1.5546161843	-3.8632756878	2.2969350799
C	-.9882436515	2.2067643844	-4.6604578762
C	.7993243179	-3.3895617075	-.0903845039
C	-2.0954283135	3.1145850026	-5.1648594888
H	-.2938885721	-5.1844470372	-.5540000582
H	-1.2927114387	-3.7431122410	-.3782407146
H	.4742128213	-6.4637540284	1.4618900100
H	-2.4387335423	-3.5760731996	4.2501481987
H	-2.0148935112	-2.9704574184	1.8848526871
H	1.6760740097	-3.9050514073	.3278247581
H	.6573705116	-2.4792747881	.5155253910
H	-.1225383463	-7.3492185619	4.8273532543
H	-1.9836485435	-5.1675754155	5.9393028280
H	1.8955842588	-2.5296356427	-1.6039597377
H	.2508515947	-2.6274918215	-1.9736235761
H	2.6514284546	3.2691325174	-5.8814924966
H	3.3666442306	1.6422640158	-5.8459680156
H	3.4645306483	2.6672884654	-4.4219878283
H	.4439608463	3.4203938904	-5.6393497558
H	-1.6833030922	3.9802017213	-5.6854770695
H	-2.7202683596	3.4619081296	-4.3369208545
H	-2.7540135049	2.5724640598	-5.8512336405
H	4.9945252323	-.3440425230	-1.2113540908
H	5.8185896282	-2.1296138686	-2.7065275114
H	4.6323736168	-2.6213779566	-4.8172361430
H	2.0466375534	1.8402504047	-2.0050362512
H	3.4897395308	3.0649077885	-.4418601036
H	4.3712569547	2.7901605863	-1.9540712422
H	4.7338952233	1.8159253486	-.5240001138
H	1.8024958189	1.3473972520	.4123407372
H	2.9705317159	.0244354697	.2845631540
H	1.4118023805	-.0851883965	-.5572718306
H	1.5691216892	-.7662949548	-5.9533750190
H	1.1908555947	-3.1145995581	-6.5939850626
H	1.1662321983	-2.9684529706	-4.8258835816
H	2.5835707448	-3.6423893173	-5.6385619463
H	2.7052374278	-1.5901334566	-7.9906610114
H	4.1294552872	-2.0550663567	-7.0545925587
H	3.6989287398	-.3478312180	-7.2112913804
H	-5.0163384863	1.3385456115	-1.1527724660

H	-6.3391651086	-.0760445701	-2.6847358847
H	-5.3061211472	-.9741448169	-4.7420940896
H	-1.4689253860	2.3749905822	-1.8278864091
H	-1.4410185900	1.7424580617	.5638809519
H	-1.5900596398	.2964195980	-.4626831978
H	-3.0082368893	.9339440451	.3941113866
H	-2.4361919701	3.9795109980	-.2359954519
H	-4.0329092797	3.2421893295	-.3808071811
H	-3.3178445228	4.0712334620	-1.7697089157
H	-1.7988183189	-.1781630032	-5.8217557207
H	-3.0491435894	-.9770418384	-7.7778661251
H	-3.7995182864	.5088258321	-7.1711679870
H	-4.5499151605	-1.0607284349	-6.8546506203
H	-1.9172669133	-2.6240399027	-6.1506278793
H	-3.3881677258	-2.7135767279	-5.1660318389
H	-1.8567676059	-2.2466941770	-4.4140204822
N	1.0646842492	-3.1069087803	-1.4936984240
N	1.5249663739	.6887909119	-4.0551242875
N	-1.3215369577	1.1749408298	-3.8892545679
O	-1.3946070544	-5.7737311511	5.4736308717
O	-.4832932314	-1.3112438572	-2.0819073553
O	.1689326948	-7.2835913215	3.9054467045
Cu	-.0240554061	-.0607924301	-3.2022928715

129.L¹CuO / formylglycine complex

C	3.1421746353	1.2353480317	-1.0928940623
C	2.7718765057	.6767188012	-3.5699833122
C	-1.4565504153	-1.8164096027	6.4194180666
C	2.4121868836	-.8097695038	-3.7842785034
C	3.3845839211	1.2947004484	-4.8382908697
C	-2.2462260736	.7406322169	-.1835782226
C	-2.5858025844	.6975045092	1.1931062520
C	-3.6596020342	-.1091276469	1.5871286058
C	-4.3785580075	-.8462620957	.6486201992
C	-4.0306577485	-.8034792763	-.6992633392
C	-2.9551186601	-.0273001573	-1.1413967710
C	3.9252430789	1.1783255482	.0826739214
C	-1.7633208955	1.4381191154	2.2433736075
C	-.8300703493	.4551857673	2.9836379587
C	-.8349901093	-2.5911486674	7.6412656828
C	-2.6358192733	2.2091198020	3.2526310563
C	-2.5341338218	-.0712319958	-2.6080678520
C	-3.6945587551	.2506335357	-3.5669246422
C	-1.8922206633	-1.4311174363	-2.9538352297
C	2.5420827253	3.9315420485	-1.5605090208
C	-3.7902598788	-1.7161073150	5.5359179004
C	1.4367180151	2.9433036993	-1.2262442050
C	5.2581652771	.7681191889	-.0321888488
C	.1289357653	3.4514802249	-1.1693308459
C	-1.0590366048	2.7580429648	-.8542655129
C	-2.3537820749	3.5436171313	-.8099090316
C	5.8008980289	.4017414808	-1.2595519411
C	5.0006058346	.4103522535	-2.3982535919
C	3.6619932720	.8115509597	-2.3388025612
C	3.3307877669	1.4484694044	1.4610063083
C	4.1429890871	2.4650358179	2.2820489032
C	3.1610997285	.1168709406	2.2237777907
H	-.8825640351	-2.0481320207	5.5139935262
H	-4.7769187828	-2.1998734743	5.6971796024
H	2.1377270347	4.9380065713	-1.6804971215
H	3.0560697886	3.6441266243	-2.4829570523
H	3.2989134563	3.9448093122	-.7704662891
H	.0228696719	4.5089366577	-1.3737410108
H	-2.2015498231	4.5751690790	-1.1327405353

H	-2.7625577497	3.5499273400	.2058026034
H	-3.1073125994	3.0755491868	-1.4513078172
H	5.8750530353	.7170887099	.8607564649
H	6.8388359424	.0847735204	-1.3241159642
H	5.4164000350	.0803660244	-3.3463528200
H	2.3312982638	1.8683749678	1.3156540504
H	3.6431083665	2.6637532004	3.2361953980
H	4.2539369266	3.4189770265	1.7533674495
H	5.1477374388	2.0940235317	2.5136551614
H	2.6536653742	.2824648912	3.1806607889
H	4.1357424217	-.3392932548	2.4347623887
H	2.5725174636	-.5927146288	1.6337452460
H	1.8376614287	1.2080367464	-3.3656170898
H	1.6936393862	-.9181013577	-4.6065856119
H	1.9772989487	-1.2352726860	-2.8734897050
H	3.3064574141	-1.3911273367	-4.0400984973
H	2.6760175722	1.2286878014	-5.6719134250
H	4.2976251070	.7735508098	-5.1475289014
H	3.6381235703	2.3511089384	-4.6942807272
H	-3.9031857795	-.1998881003	2.6423531927
H	-5.2027684071	-1.4745968804	.9767349138
H	-4.5863034322	-1.4026114574	-1.4160941879
H	-1.1320856752	2.1664027745	1.7243991246
H	-.1755810498	1.0006143981	3.6741339961
H	-.1969115917	-.1032110690	2.2859176676
H	-1.4195675815	-.2553612119	3.5701799772
H	-1.9980289376	2.8253138078	3.8971262669
H	-3.1920073178	1.5255441415	3.8998486088
H	-3.3481339239	2.8743302229	2.7490628389
H	-1.7671336580	.6952969511	-2.7560667511
H	-3.3376563611	.2772144030	-4.6032487095
H	-4.1464635243	1.2220461197	-3.3390607779
H	-4.4872533910	-.5039306408	-3.5130471758
H	-1.5538274337	-1.4436333356	-3.9971837236
H	-2.6108631447	-2.2483700792	-2.8235181444
H	-1.0286884628	-1.6378612708	-2.3135230320
H	-3.0182581194	-2.9610860281	7.0191293610
H	-1.3889812838	-.7351127380	6.5817682086
N	-2.8388713379	-2.2469648844	6.3003746724
N	1.7801873496	1.6731940141	-1.0065073642
N	-1.0823351650	1.4624677126	-.5972818656
O	1.2298699590	-1.1731648684	-.5198341399
O	.3505321790	-2.2988849173	7.9016668332
O	-1.6062938754	-3.4137864052	8.2043399550
O	-3.6587366668	-.7968794854	4.7166741765
Cu	.4605987195	.3422843830	-.6120946229

130.L¹CuO / methane t.s.

C	-3.0965556063	-3.7722507043	1.6668916750
C	.3208195952	-.0738076737	-.1145906459
C	1.1065120671	.3010356346	1.0016131148
C	2.3454723828	-.3225151928	1.1803306332
C	2.7969891413	-1.2983855441	.2962093628
C	1.9995329027	-1.6788867482	-.7795558854
C	.7525317433	-1.0866474105	-1.0040917381
C	.6042790090	1.3078121721	2.0298572430
C	1.6218638996	2.4253947275	2.3150728343
C	.1922042989	.5865674987	3.3288061084
C	-.1246026981	-1.5786942616	-2.1509516014
C	-.6778850860	-2.9834091950	-1.8410034242
C	.6007036399	-1.5665363520	-3.5079143141
C	-5.1000986042	.3057782762	.4252397278
C	-5.5736207310	.6841535128	1.7036766420
C	-6.8007746284	.1695963449	2.1349912338

C	-7.5415033026	-.6972711757	1.3366952951
C	-7.0592275785	-1.0671140380	.0834883513
C	-5.8392874634	-.5811475203	-.3973087815
C	-4.7591297504	1.5885807011	2.6217423857
C	-4.1674161772	.7881868187	3.7990908514
C	-5.5672342495	2.7976734240	3.1236243807
C	-5.3183486392	-1.0445531955	-1.7551262913
C	-6.3703883927	-.9249914495	-2.8714499187
C	-4.7762587143	-2.4840629149	-1.6717218598
C	.0631147722	2.2061456029	-1.7599200702
C	-1.1420536315	1.5903351595	-1.0759737849
C	-2.3895103737	2.1977360471	-1.3028575737
C	-3.6416647582	1.7915383487	-.8128153433
C	-4.8532556634	2.5967968305	-1.2386687713
H	-2.5998357253	-2.6391514506	1.9525145605
H	-4.1779764776	-3.6635034397	1.7423603632
H	-.2238673629	3.0852808534	-2.3381704476
H	.5397932453	1.4861404321	-2.4315659332
H	.8191524518	2.4970611448	-1.0241828265
H	-2.3870269110	3.0679197951	-1.9457433655
H	-4.5567778098	3.4643047592	-1.8296727856
H	-5.4171361547	2.9375137358	-.3652414824
H	-2.6838465564	-4.4283092848	2.4340649077
H	-5.5370806463	1.9868702334	-1.8371598274
H	2.9616458099	-.0461916021	2.0307244868
H	3.7624332145	-1.7708270826	.4523749062
H	2.3477645408	-2.4569541050	-1.4526889620
H	-.2905038818	1.7835674251	1.6186298951
H	1.1912169020	3.1614386219	3.0022738732
H	1.9141011448	2.9488836698	1.3984379766
H	2.5332903936	2.0369683255	2.7817809008
H	-.2403731855	1.3001389370	4.0397166518
H	1.0642165274	.1244624223	3.8060759775
H	-2.7649977008	-4.0391152706	.6643717843
H	-.5412426957	-.2038061730	3.1372517166
H	-.9811928113	-.9033666959	-2.2292911934
H	-1.3677220306	-3.3098831307	-2.6271857712
H	-1.2130512833	-2.9923268777	-.8869788246
H	.1312584028	-3.7189246601	-1.7739694083
H	-.0861412584	-1.8645814022	-4.3073487431
H	1.4442973991	-2.2645242303	-3.5240980327
H	.9891761354	-.5719386967	-3.7497070414
H	-7.1780473768	.4476713528	3.1145976857
H	-8.4904982227	-1.0884153393	1.6917174807
H	-7.6387878435	-1.7509987344	-.5294834481
H	-3.9213601302	1.9808221752	2.0371075957
H	-3.5334730482	1.4350872802	4.4163272059
H	-3.5645634361	-.0557287135	3.4499583110
H	-4.9650477937	.3933898561	4.4392125252
H	-4.9258857304	3.4608709838	3.7137325762
H	-6.4002672265	2.4920115815	3.7654821629
H	-5.9823201660	3.3784976177	2.2931219638
H	-4.4775281904	-.4022992295	-2.0294851672
H	-5.9242157266	-1.1801877366	-3.8384771673
H	-6.7722886474	.0909828879	-2.9407847599
H	-7.2136875603	-1.6051589532	-2.7126559880
H	-4.3627066901	-2.7975483262	-2.6367845833
H	-5.5692741166	-3.1885522038	-1.3977084671
H	-3.9860578959	-2.5641765915	-.9204136018
N	-.9662640544	.5256357130	-.2970152028
N	-3.8098625860	.7513397794	-.0001054973
O	-2.1768241095	-1.4962097337	2.1234813108
Cu	-2.3750173565	-.3081139150	.7605188454

131.L¹CuO / cyclohexane t.s.

C	-4.4747236177	-4.0467594517	2.7813305931
C	-.2750414728	.0325345808	.0100905057
C	.4806629622	.5666999997	1.0792051949
C	1.7400744967	.0176524171	1.3390443697
C	2.2376401618	-1.0379029181	.5792097187
C	1.4674093543	-1.5728559813	-.4500442768
C	.2015729860	-1.0598745846	-.7511048909
C	-.0768081839	1.6668556943	1.9756597216
C	.8867210819	2.8558176639	2.1300769934
C	-.4724212628	1.0897377454	3.3494816951
C	-.6398145937	-1.7039139290	-1.8485390110
C	-3.0330357860	-3.7930465255	2.3492167908
C	-1.1496730156	-3.0865909903	-1.3986660778
C	.1076272038	-1.8073709626	-3.1894780365
C	-5.7022419337	.3610354441	.5495260372
C	-6.1652256957	.9311043838	1.7594873782
C	-7.3859265733	.4857407564	2.2766032301
C	-8.1266080931	-.5007541533	1.6312505350
C	-7.6469310118	-1.0680632098	.4532285740
C	-6.4324774288	-.6585647334	-.1069755835
C	-5.3414793562	1.9630992947	2.5225942794
C	-4.6958031318	1.3290612574	3.7714010272
C	-1.9975523716	-4.2579563661	3.3714145893
C	-6.1541698668	3.2146183555	2.8953939381
C	-5.9017511794	-1.3386314117	-1.3654746496
C	-6.9467977588	-1.4137143513	-2.4916763591
C	-5.3526400059	-2.7404011717	-1.0367378046
C	-2.2896941481	-3.6776630087	4.7643867355
C	-.5946777973	2.1058944203	-1.8801339254
C	-3.7295644369	-3.9777388210	5.2087832378
C	-4.7511114673	-3.4708727013	4.1790190392
C	-1.7823602506	1.5336440082	-1.1298453098
C	-3.0449280390	2.0787501697	-1.4217782837
C	-4.2860815800	1.6990389363	-.8852935933
C	-5.5194547091	2.4131588174	-1.4010752829
H	-2.8242041547	-4.1682407850	1.3410562040
H	-2.8922281039	-2.6166254346	2.3058796300
H	-2.0139572337	-5.3593163353	3.4206522588
H	-.9914470843	-3.9736647487	3.0420206043
H	-1.5733060503	-4.0717498905	5.4955975237
H	-2.1454953357	-2.5912389095	4.7220370610
H	-3.9242183020	-3.5233609360	6.1881282443
H	-3.8519508762	-5.0635539973	5.3380710374
H	-5.7711650736	-3.7207755121	4.4954485909
H	-.9074511371	2.9077922367	-2.5501683120
H	-.0973452986	1.3306330272	-2.4706085141
H	.1528681348	2.4982311831	-1.1841181705
H	-3.0642725998	2.8716545639	-2.1577231181
H	-5.2476569270	3.2092813355	-2.0955101934
H	-6.0940728342	2.8436289460	-.5755493859
H	-6.1848818554	1.7135046161	-1.9167949087
H	2.3356339851	.4163773069	2.1549534437
H	3.2186374659	-1.4505447963	.7962008369
H	1.8528686449	-2.4101052934	-1.0246901632
H	-.9878088204	2.0480290899	1.5055225153
H	.4159924927	3.6482697542	2.7216641303
H	1.1652599257	3.2789520476	1.1589912735
H	1.8095702033	2.5685217945	2.6449667901
H	-.9434013865	1.8632457075	3.9670717222
H	.4121203189	.7258001836	3.8848784341
H	-1.1688145027	.2514812696	3.2452384678
H	-1.5180386460	-1.0723576102	-2.0086283081
H	-1.8054520395	-3.5236288366	-2.1600159587

H	-1.7112498925	-3.0114007507	-.4631705950
H	-.3170261604	-3.7788144374	-1.2319884423
H	-.5538687444	-2.2143241014	-3.9618194378
H	.9764875029	-2.4701891793	-3.1199244481
H	.4632889440	-.8294998759	-3.5300173140
H	-7.7576097709	.9118717063	3.2036802995
H	-9.0716976881	-.8338475599	2.0501893028
H	-8.2218387303	-1.8498785641	-.0342338055
H	-4.5310637026	2.2905444413	1.8646669161
H	-4.0555404558	2.0584379919	4.2807392723
H	-4.0885067926	.4551251630	3.5145736147
H	-5.4651511877	1.0048274142	4.4816366767
H	-5.5040697056	3.9590600717	3.3671656941
H	-6.9555236867	2.9846945538	3.6055179211
H	-6.6121365517	3.6751645968	2.0135992764
H	-5.0623459008	-.7443226818	-1.7368155202
H	-6.4959867388	-1.8325859059	-3.3975968722
H	-4.6902925658	-2.3771833499	4.1202722485
H	-7.3460713152	-.4244051783	-2.7377812179
H	-7.7920905781	-2.0553027021	-2.2217836272
H	-4.9223618387	-3.2065613635	-1.9301898398
H	-6.1470885193	-3.3955591934	-.6626079951
H	-4.5738749537	-2.6900058595	-.2700778745
H	-5.1721410694	-3.6222838370	2.0503179276
H	-4.6548660375	-5.1345042967	2.7913700601
N	-1.5804491126	.5565264434	-.2476952034
N	-4.4247614019	.7517479469	.0389953595
O	-2.7500867190	-1.2367696714	2.3593200971
Cu	-2.9738540108	-.2063804683	.8906992341

132.L¹CuO / acetonitrile t.s.

C	2.9545386110	.0532351419	-3.3736945678
C	3.7435028979	.4403131574	-2.2629473145
C	5.0164652081	-.1215954554	-2.1277256563
C	5.4993239906	-1.0451199741	-3.0513254698
C	4.7017211803	-1.4340525795	-4.1238373946
C	3.4192419376	-.9058229924	-4.3052829048
C	3.2187147916	1.4141747489	-1.2135369479
C	4.2157460948	2.5408020912	-.8923693926
C	2.8009557042	.6579626745	.0634055600
C	2.5536224740	-1.4011108211	-5.4584433352
C	-1.3379953489	-4.3236605806	-.6825057317
C	2.1182683697	-2.8604114382	-5.2208997552
C	3.2474415308	-1.2544378469	-6.8247452669
C	-2.4328967152	.2269901342	-2.5874540276
C	-2.9176414454	.6248807354	-1.3185559439
C	-4.1150903581	.0610408837	-.8642244120
C	-4.8115575780	-.8713483974	-1.6285440697
C	-4.3136637209	-1.2630224750	-2.8700017794
C	-3.1202815402	-.7330193669	-3.3717877544
C	-2.1518688370	1.6048570003	-.4353074231
C	-1.5446443383	.8909761575	.7894901786
C	-1.7196822171	-2.9360283123	-.6772031871
C	-3.0173288152	2.8013708021	-.0027985311
C	-2.5638920916	-1.2205781796	-4.7075353919
C	-3.6222473559	-1.2483478164	-5.8230161050
C	-1.8976154145	-2.6027688721	-4.5553211504
C	2.5492097788	2.3594766714	-4.9623005126
C	1.3968792196	1.6819755410	-4.2480900608
C	.1198716633	2.2444520380	-4.4066881926
C	-1.0893014959	1.7804714236	-3.8643946926
C	-2.3536423118	2.5278542332	-4.2400628331
H	2.2082429249	3.2488194004	-5.4935315475
H	3.0168184251	1.6802709080	-5.6811943570

H	3.3283118599	2.6496894733	-4.2508927166
H	.0576234617	3.1232527174	-5.0342890289
H	-2.1228699885	3.3966688439	-4.8575273758
H	-2.8889273629	2.8608190384	-3.3460715008
H	-.7281932322	-2.2580447885	-.7628802065
H	-3.0375355063	1.8771109582	-4.7939286237
H	5.6382900097	.1651683816	-1.2852995388
H	6.4920817644	-1.4683813101	-2.9298449918
H	5.0785802452	-2.1684285756	-4.8294933622
H	2.3185376702	1.8860720823	-1.6184977629
H	3.7632784686	3.2574195927	-.1990556397
H	4.5138804164	3.0842553535	-1.7951350569
H	5.1256645465	2.1592534414	-.4176842539
H	2.3841946334	1.3545907693	.7995917156
H	3.6643009499	.1612068957	.5199930191
H	-2.1630655357	-2.6316952429	.2738082362
H	2.0482621295	-.1106897895	-.1414069392
H	1.6471989489	-.7893537232	-5.4825745282
H	1.4475201367	-3.1964295078	-6.0191510602
H	1.5962015848	-2.9687427428	-4.2656234908
H	2.9833486774	-3.5319350417	-5.2035866858
H	2.5705802934	-1.5627026341	-7.6285432437
H	4.1439867622	-1.8792807012	-6.8931557227
H	3.5499943921	-.2198703743	-7.0169490149
H	-4.5028624894	.3513536433	.1077408919
H	-5.7366163035	-1.2999549171	-1.2544976602
H	-2.3805199825	-2.6847860505	-1.5056178222
H	-4.8569839232	-2.0000190060	-3.4533636993
H	-1.3205857632	1.9997026763	-1.0269330139
H	-.9585128449	1.5986954705	1.3867792609
H	-.8884576884	.0717795004	.4813085816
H	-2.3307515537	.4828405528	1.4351090286
H	-2.4132385540	3.5170217993	.5647080111
H	-3.8464687832	2.4896993534	.6411261810
H	-3.4439130143	3.3260973569	-.8640561449
H	-1.7817450375	-.5221733332	-5.0171612671
H	-3.1531031944	-1.5058284131	-6.7782223629
H	-4.1146122816	-.2772402647	-5.9368097403
H	-4.3987867914	-1.9960419987	-5.6313849046
H	-1.4580639572	-2.9243447260	-5.5056054975
H	-2.6257956440	-3.3614065791	-4.2480769754
H	-1.0999425594	-2.5837277366	-3.8064177513
N	-1.0148544394	-5.4418040612	-.6951485730
N	1.6388960242	.6008377360	-3.5094163740
N	-1.1820261063	.7286116873	-3.0544071787
O	.2974863799	-1.4357531607	-.9695174541
Cu	.3443505791	-.2901174054	-2.3857946373

133.L¹CuO / toluene t.s.

C	.4133915199	-4.7961866370	-.2878466741
C	2.4265944375	2.6479985600	3.1805849002
C	2.1039363753	-.0337327584	-2.1586291859
C	-.9338492535	-4.4763374319	-.1051720593
C	1.5434915898	-1.4210357521	-1.7966417689
C	2.8717618130	-.0888635733	-3.4913627397
C	-2.9395383640	2.0562497216	.3768276433
C	-3.3566553462	2.6713617756	1.5806326453
C	-4.5795410185	2.2779670645	2.1335917793
C	-5.3698250751	1.3079366032	1.5221932822
C	-4.9449549438	.7136647837	.3361752014
C	2.4893927420	1.5927735612	-.2067099775
C	-3.7311789078	1.0714956490	-.2598154285
C	-2.4894601048	3.7074099037	2.2889758103
C	-1.8641570853	3.1231706823	3.5709074985

C	-1.3089637441	-3.5580209310	.8746379364
C	-3.2551478358	5.0081636548	2.5901204595
C	-3.2686288835	.3824299947	-1.5396254808
C	-4.3557180994	.3533265338	-2.6275835209
C	-2.7541939976	-1.0375249883	-1.2399760858
C	-.3475918131	-2.9436622289	1.6950315101
C	2.2054089342	3.7089557931	-2.0390507581
C	3.2665077248	2.0818642503	.8688066330
C	1.0057511829	-3.2781236636	1.4992574942
C	1.0056599420	3.1388427075	-1.3057742079
C	1.3822324484	-4.1928740722	.5205474109
C	-.7328211864	-1.9679154030	2.7378132513
C	-.2455174244	3.7092582356	-1.5956269483
C	-1.4937593339	3.3492773339	-1.0636860350
C	-2.7075209019	4.1072129476	-1.5646868226
C	4.5138884964	1.4951213630	1.1048154035
C	4.9827681899	.4509746981	.3120589346
C	4.2007280884	-.0258119194	-.7367147221
C	2.9475759008	.5281963156	-1.0180289235
C	2.7643620523	3.1966331562	1.7802608580
C	3.7519545385	4.3740059901	1.8665844797
H	1.7606908108	-2.8062730657	2.1223926620
H	2.4322092028	-4.4362137133	.3854073251
H	.7072501698	-5.5097077444	-1.0519256706
H	-.3883248038	-.8525567125	2.4439557355
H	-.2034027457	-2.1050192291	3.6852452671
H	-1.8099515230	-1.9076194520	2.9084932237
H	1.9070232560	4.5329355233	-2.6885370096
H	2.6911842155	2.9419212733	-2.6490140278
H	2.9579385639	4.0712022424	-1.3323870248
H	-.2484934684	4.5112308869	-2.3217944261
H	-2.4126666951	4.9101215463	-2.2416795672
H	-3.2722781226	4.5363854440	-.7321709667
H	-3.3904103596	3.4368749139	-2.0964537898
H	5.1241233262	1.8580561336	1.9267431139
H	5.9535254152	.0071814548	.5133855027
H	4.5686196838	-.8457478603	-1.3467341398
H	1.8364596611	3.5835185822	1.3493820614
H	3.3250521483	5.1823479144	2.4699820719
H	3.9847948786	4.7797305622	.8761502499
H	4.6970063630	4.0786601330	2.3345889174
H	2.0087909587	3.4429123215	3.8092386521
H	3.3262367640	2.2663516233	3.6770217234
H	1.6987291045	1.8319625275	3.1201752724
H	1.2481931962	.6319775683	-2.3001787107
H	.8974953742	-1.7977533591	-2.5976020924
H	.9586341605	-1.3872569174	-.8737924220
H	2.3503966657	-2.1457848724	-1.6461454985
H	2.2093297216	-.4268548115	-4.2954550684
H	3.7137869272	-.7875302992	-3.4457094729
H	3.2706811337	.8915083357	-3.7718127902
H	-4.9146168470	2.7346926608	3.0602276364
H	-6.3142463060	1.0135017934	1.9706246069
H	-5.5653775818	-.0448380889	-.1319352869
H	-1.6670276835	3.9646725918	1.6150161941
H	-1.1971411043	3.8585527646	4.0353220108
H	-1.2876553981	2.2167988549	3.3608638366
H	-2.6414203412	2.8700007105	4.3012037656
H	-2.5769691831	5.7540914845	3.0182322610
H	-4.0633608481	4.8483569507	3.3116390365
H	-3.6976900151	5.4349677932	1.6838236949
H	-2.4234123170	.9510713528	-1.9369721615
H	-3.9512049986	-.0698243108	-3.5531389068
H	-4.7321570787	1.3573074139	-2.8492060229

H	-5.2107128594	-.2644722577	-2.3335776575
H	-2.3777786774	-1.5146611195	-2.1515618173
H	-3.5540658440	-1.6676469678	-.8349362540
H	-1.9424388656	-1.0228887338	-.5072772256
H	-2.3578687516	-3.3104199611	1.0134238891
H	-1.6935234348	-4.9435117017	-.7252755373
N	1.1890003804	2.1435778578	-.4401479800
N	-1.6557655907	2.3868342384	-.1586873072
O	.0241790314	.3900765548	2.1743398051
Cu	-.2267277087	1.3629033048	.6710185778

134.L¹CuO / phenol t.s.

C	-2.5199314400	-5.1175886451	4.6497746131
C	-.4050871172	.0174382611	.0944847661
C	.3831269751	.4443619897	1.1884881410
C	1.5908048334	-.2175078572	1.4311230393
C	2.0046600497	-1.2810407040	.6333740308
C	1.1972957994	-1.7151796329	-.4143977157
C	-.0200945680	-1.0885900656	-.6990372684
C	-.0917156548	1.5394604168	2.1371062102
C	.9561547239	2.6444538838	2.3517492650
C	-.5292979903	.9235890085	3.4816771796
C	-.9312705030	-1.6514461115	-1.7842799177
C	-2.7951879124	-3.8822842235	4.0109474249
C	-1.5190914344	-3.0046140572	-1.3349578254
C	-.2291074839	-1.7797890594	-3.1466891426
C	-5.8232412190	.4719733573	.3734413701
C	-6.3176930196	.9760030510	1.5997021111
C	-7.5767080750	.5496133839	2.0326850564
C	-8.3264838280	-.3557413597	1.2859844555
C	-7.8140629614	-.8633426464	.0953758334
C	-6.5581145580	-.4721981250	-.3806851384
C	-5.4807671910	1.9109229508	2.4659730163
C	-4.8986371634	1.1430754119	3.6696709301
C	-2.7762003995	-2.6915604062	4.7851235111
C	-6.2558790441	3.1557860699	2.9286753989
C	-5.9823625913	-1.1196033859	-1.6351511063
C	-6.9422093279	-1.0581647346	-2.8357023757
C	-5.5633875382	-2.5740376613	-1.3391720620
C	-2.4735011421	-2.7473386667	6.1381080240
C	-2.2021139101	-3.9725445451	6.7610592103
C	-.5440290680	2.2800510204	-1.6139495734
C	-2.2316215752	-5.1540923954	6.0054591788
C	-1.7861094064	1.7004162211	-.9665837738
C	-3.0199554289	2.3024297477	-1.2741390037
C	-4.2984634909	1.8999128493	-.8517200553
C	-5.4861820685	2.6931122976	-1.3586902814
H	-3.0175784996	-1.7546652759	4.2951098929
H	-2.4638752909	-1.8305089708	6.7212964028
H	-1.9812368042	-4.0081699844	7.8232645660
H	-.7932694664	3.1399873561	-2.2368279143
H	-.0465168322	1.5277350817	-2.2337323336
H	.1806423794	2.5917122639	-.8560532661
H	-2.9810571170	3.1605501519	-1.9319791405
H	-5.1603406620	3.5463803852	-1.9548086878
H	-6.0974248573	3.0553331856	-.5268997169
H	-6.1350917779	2.0623681618	-1.9745456230
H	2.2103257745	.0960524210	2.2660858839
H	2.9459385450	-1.7820881012	.8391056090
H	1.5103773785	-2.5652414001	-1.0134039154
H	-.9748370841	2.0061241486	1.6910072849
H	.5443414342	3.4388512458	2.9832534953
H	1.2691229950	3.0940514290	1.4036381817
H	1.8530799185	2.2621141324	2.8501507480

H	-.9417083068	1.6946220180	4.1424410581
H	.3203547989	.4594968857	3.9943786498
H	-1.2875037035	.1496025135	3.3313032323
H	-1.7671851119	-.9581967691	-1.9115677024
H	-2.2300221767	-3.3805888560	-2.0790754163
H	-2.0378600936	-2.9152215315	-.3754243776
H	-.7292725967	-3.7542969374	-1.2153259996
H	-.9359300097	-2.1328785665	-3.9051643471
H	.5980930912	-2.4965361391	-3.1107804039
H	.1766164924	-.8199041262	-3.4830723842
H	-7.9727176529	.9243384291	2.9717393875
H	-9.3028529551	-.6752910451	1.6381468391
H	-8.3943428578	-1.5871886174	-.4689911856
H	-4.6356927140	2.2568801811	1.8645106236
H	-4.2431339832	1.7918691051	4.2614936943
H	-4.3208500690	.2729834864	3.3421927177
H	-5.6982025029	.7807670686	4.3252358217
H	-5.5930659559	3.8296526880	3.4816992373
H	-7.0857457649	2.8955588400	3.5939232479
H	-6.6705556745	3.7095238883	2.0799901664
H	-5.0780841364	-.5684710070	-1.9094922498
H	-6.4569979240	-1.4670703797	-3.7282628770
H	-3.0922797281	-2.8762625047	2.3180117628
H	-7.2469406645	-.0299269701	-3.0570627873
H	-7.8508032610	-1.6437499949	-2.6608276868
H	-5.0947887220	-3.0259823607	-2.2205324925
H	-6.4327685327	-3.1837418408	-1.0696767677
H	-4.8535271391	-2.6228579341	-.5081899063
H	-2.0230372020	-6.1064726837	6.4848217517
H	-2.5335515224	-6.0176771182	4.0441258263
N	-1.6624644927	.6524912409	-.1583449266
N	-4.5123797833	.8574603209	-.0528134378
O	-3.0512873873	-3.8804709004	2.7160773383
O	-3.0794673344	-1.6449023237	1.8076088261
Cu	-3.1341713433	-.2388929294	.7425251643

135.L¹CuO / isopropylbenzene t.s.

C	1.7113823724	-1.9038937731	4.1475223324
C	2.4195366896	2.3395475477	1.3730966116
C	2.3356059708	-.6845659854	-3.7612602697
C	1.0297237607	-1.6855223445	2.9493470075
C	1.8824159029	-2.0945623839	-3.3380617453
C	3.1091880195	-.7364332521	-5.0909789961
C	-2.8108464052	1.3280764490	-1.4797186232
C	-3.2436295954	1.8247331076	-.2269641651
C	-4.4422214094	1.3339945013	.3004086929
C	-5.1915538723	.3767832341	-.3779464446
C	-4.7486976939	-.1073013907	-1.6071703411
C	2.6283693068	1.0844040399	-1.9210878726
C	-3.5577434799	.3499612663	-2.1805081521
C	-2.4298030790	2.8523340109	.5535917780
C	-1.8508087170	2.2414165685	1.8450497148
C	.2224012187	-2.6869624288	2.3925874216
C	-3.2415595663	4.1243586751	.8569188006
C	-3.0707527958	-.2326837395	-3.5034737192
C	-4.1566982325	-.2293417934	-4.5927339130
C	-2.5024088038	-1.6505375495	-3.3014598926
C	.1127282709	-3.9110235711	3.0713040870
C	2.3080994030	3.1360147660	-3.8307761224
C	3.3709313891	1.6685107463	-.8665769483
C	.7926289175	-4.1283848689	4.2696175865
C	1.1143994430	2.5497780137	-3.1005051525
C	1.5966415840	-3.1242855335	4.8130448238
C	-.1473505784	3.0887816182	-3.4093658589

C	- .5316385148	-2.4541901737	1.0956312252
C	-1.3944829276	2.7046557447	-2.8902123210
C	- .1720805025	-3.4521049336	- .0024713210
C	-2.6210228757	3.4363793846	-3.3969106706
C	-2.0383066669	-2.2981074268	1.2997619074
C	4.6219509065	1.1260562265	- .5572296668
C	5.1372870233	.0452666525	-1.2674842717
C	4.3960215182	- .5157899217	-2.3031132151
C	3.1362923867	- .0155101393	-2.6490130451
C	2.8201585313	2.8227615389	- .0343411433
C	3.7973263273	4.0092542884	.0461065076
H	.6939163158	-5.0832274388	4.7788044012
H	2.1282234323	-3.2936301257	5.7451613068
H	1.1177014217	- .7419409860	2.4231712457
H	2.3354112207	-1.1151571525	4.5593434052
H	- .5103568876	-4.7018052393	2.6612720098
H	- .1576574335	-1.3831978511	.7031877145
H	-2.5427661213	-2.0568244910	.3589753291
H	-2.2566054695	-1.5057631759	2.0206802773
H	-2.4714155517	-3.2307080191	1.6864513475
H	- .7212144257	-3.2368614140	- .9246111816
H	- .4311812185	-4.4753208746	.3004161375
H	.8999560195	-3.4325447948	- .2183587176
H	2.0002125412	3.9502714939	-4.4879942338
H	2.8105118930	2.3715741483	-4.4310312110
H	3.0497080049	3.5163265251	-3.1224354828
H	- .1593105570	3.8840860766	-4.1428925349
H	-2.3411850571	4.2445431821	-4.0740227198
H	-3.1932253922	3.8547145203	-2.5632908806
H	-3.2909908032	2.7541264989	-3.9290923260
H	5.1993722581	1.5536466403	.2571921520
H	6.1108680191	- .3618831506	-1.0105455319
H	4.7999503196	-1.3631495037	-2.8496780459
H	1.9121266969	3.1846880176	- .5254234215
H	3.3404350312	4.8380282855	.5974524004
H	4.0729939572	4.3752209219	- .9486559977
H	4.7214488311	3.7401900470	.5684740788
H	1.9935342848	3.1659549724	1.9537609749
H	3.2936657799	1.9652553811	1.9181390358
H	1.6855384981	1.5297803207	1.3177453627
H	1.4322118856	- .0907113136	-3.9260782510
H	1.2593179052	-2.5496726275	-4.1161176466
H	1.3036693101	-2.0580149788	-2.4109935912
H	2.7418573493	-2.7520776095	-3.1673816211
H	2.4838950701	-1.1704395707	-5.8786046620
H	4.0101829122	-1.3535471617	-5.0093613147
H	3.4208972764	.2610266882	-5.4174484138
H	-4.7896726077	1.7037777364	1.2607398851
H	-6.1174607875	.0053380014	.0513030639
H	-5.3359305570	- .8589667275	-2.1264375187
H	-1.5833817034	3.1489524339	- .0728578327
H	-1.2383209383	2.9824160897	2.3715714060
H	-1.2257444596	1.3699042983	1.6284855988
H	-2.6523983896	1.9311697311	2.5251080348
H	-2.6089080499	4.8670393340	1.3547254983
H	-4.0879919514	3.9154160827	1.5198046384
H	-3.6391941213	4.5771027641	- .0575995240
H	-2.2465654106	.3903502101	-3.8600235762
H	-3.7374694217	- .5719268179	-5.5446570521
H	-4.5716270407	.7722648452	-4.7452572579
H	-4.9872324521	- .8976166849	-4.3426106553
H	-2.1193641477	-2.0519428069	-4.2462411564
H	-3.2720559634	-2.3354532109	-2.9290198277
H	-1.6811250816	-1.6440579558	-2.5781887103

N	1.3151471641	1.5765939057	-2.2134396884
N	-1.5407045501	1.7412164223	-1.9851470397
O	.2529714149	-.1376568978	.4014854665
Cu	-.0987228474	.8038084002	-1.1012480546

136.L¹CuO / cyclohexadiene t.s.

C	-2.0186863995	-2.7294765697	3.7451554395
C	2.4653248631	2.2862686875	2.1534734952
C	2.1994314930	-.4822187541	-3.0444922643
C	-.9341535504	-3.6811450589	4.1632282132
C	1.7727543340	-1.8868790868	-2.5758324057
C	2.8852859234	-.5454890122	-4.4202059494
C	-2.8275573396	1.4326739416	-.4709306815
C	-3.2085587124	1.9511396026	.7907770035
C	-4.3862100702	1.4705560614	1.3723763229
C	-5.1617987128	.5024726327	.7383625261
C	-4.7614355577	-.0097633452	-.4944177042
C	2.5771444518	1.2551304790	-1.1959950765
C	-3.5914379192	.4355390328	-1.1189523409
C	-2.3500999535	2.9763576743	1.5238874106
C	-1.6498124981	2.3436171566	2.7415600630
C	.0722139505	-3.9539898649	3.0819146534
C	-3.1504204637	4.2262988198	1.9293230817
C	-3.1439237426	-.1674395168	-2.4460591609
C	-4.2713214189	-.2248220817	-3.4895759465
C	-2.5203309615	-1.5603378980	-2.2337183981
C	.0247515028	-3.3680295289	1.8758248799
C	-1.0330201008	-2.4040755908	1.4947724500
C	3.3558401161	1.8078511712	-.1514621898
C	2.1481416154	3.3504496019	-3.0288942398
C	-2.0692135445	-2.1686554033	2.5270714739
C	.9986200525	2.7362375591	-2.2520703662
C	-.2844249368	3.2580425249	-2.4938243833
C	-1.4994413440	2.8331764693	-1.9316932055
C	-2.7635389689	3.5363582064	-2.3846384055
C	4.6458561310	1.3088604954	.0514711654
C	5.1542586700	.2825272142	-.7407841479
C	4.3625648209	-.2743425354	-1.7413896108
C	3.0654664319	.1900331797	-1.9851163056
C	2.7962083705	2.8846200261	.7720913129
C	3.7247489822	4.1042785772	.9018013492
H	-2.8822890197	-1.4944533832	2.2697717217
H	-2.7944746174	-2.5112750671	4.4758496428
H	-1.3794431853	-4.6289458028	4.5099087713
H	-.4175411997	-3.2871246965	5.0554129374
H	-.4821857666	-1.3468973636	1.3383588018
H	1.7961156638	4.1609919733	-3.6685392980
H	2.6412216499	2.5995733971	-3.6537472466
H	2.9115672381	3.7438855981	-2.3509175871
H	-.3438799144	4.0684270539	-3.2085105183
H	-2.5295483362	4.3670457691	-3.0519427072
H	-3.3240716068	3.9193609901	-1.5264973453
H	-3.4274834485	2.8437352003	-2.9114831538
H	5.2579792492	1.7246072124	.8464740371
H	6.1600460825	-.0907954982	-.5706179726
H	4.7572357003	-1.0906038728	-2.3397739087
H	1.8564682218	3.2377484452	.3389661669
H	3.2462469046	4.8799716933	1.5094188882
H	3.9606646131	4.5385712959	-.0756723647
H	4.6715519257	3.8471609254	1.3885910880
H	1.9958749599	3.0426900335	2.7931136140
H	3.3770970202	1.9420609286	2.6551297360
H	1.7865549004	1.4316338129	2.0696954312
H	1.2888636355	.1129563872	-3.1562111181

H	1.0956013792	-2.3490871530	-3.3029081644
H	1.2607462691	-1.8375712437	-1.6097587723
H	2.6420382312	-2.5433558735	-2.4583447791
H	2.2078269008	-.9777420174	-5.1644725412
H	3.7869509888	-1.1664863538	-4.3961441104
H	3.1783689329	.4502841344	-4.7687117257
H	-4.6971976317	1.8566448428	2.3390619900
H	-6.0740464813	.1431276217	1.2060582303
H	-5.3645430924	-.7752104200	-.9741386273
H	-1.5678859394	3.3045507411	.8338969105
H	-1.0002763034	3.0821742102	3.2261114248
H	-1.0426206770	1.4802375859	2.4543434374
H	-2.3854815398	2.0119250583	3.4837546267
H	-2.4832925763	4.9712489205	2.3764180179
H	-3.9229865460	3.9928086791	2.6699922188
H	-3.6437686436	4.6880679472	1.0673811095
H	-2.3536482165	.4707501815	-2.8498948933
H	-3.8794763192	-.5795549318	-4.4487101797
H	.8723821101	-4.6531770352	3.3144266390
H	-4.7219310449	.7600654963	-3.6496274205
H	-5.0702973040	-.9111757069	-3.1899673071
H	-2.1660938565	-1.9745200986	-3.1844212623
H	-3.2486257998	-2.2594020000	-1.8075461979
H	-1.6657246990	-1.5056574086	-1.5527433843
H	.7809801996	-3.5998928864	1.1296296032
H	-1.4564966252	-2.5935586412	.5012300162
N	1.2477587390	1.7431977801	-1.3999704609
N	-1.5862293465	1.8522037389	-1.0383633747
O	.1435063370	-.1198392932	1.2184013362
Cu	-.0868456933	.9160748256	-.2351805004

137.L¹CuO / dopamine t.s.

C	.8458619516	-3.6109331765	-.2286181378
C	2.7797977701	-.1038005901	-3.6107734156
C	3.5932517916	.2826620160	-2.5191485933
C	4.8127076443	-.3791151158	-2.3354362170
C	5.2169730605	-1.4017441368	-3.1909309106
C	4.3894949680	-1.7911211297	-4.2401130892
C	3.1592459661	-1.1643312906	-4.4657111928
C	3.1436512631	1.3496336363	-1.5255460802
C	4.2113725587	2.4280069283	-1.2781165895
C	2.6935476753	.6979961942	-.2013099561
C	2.2316969848	-1.6761134819	-5.5622185424
C	-.3105825031	-3.8377903601	.6887293656
C	1.6641832248	-3.0583179014	-5.1790978062
C	2.9076553916	-1.7213568150	-6.9428159936
C	-2.6796801132	.4032755354	-3.1800773002
C	-3.1778679633	.7897668237	-1.9127727943
C	-4.4487771689	.3458439335	-1.5330577150
C	-5.2098100569	-.4655056636	-2.3694491403
C	-4.6971176006	-.8574843827	-3.6028376085
C	-3.4312286857	-.4423196940	-4.0298899613
C	-2.3415817061	1.6147296067	-.9396927681
C	-1.8301886116	.7075484038	.1969363485
C	-.5861693741	-5.1263930485	1.1788589368
C	-3.0907079248	2.8396706858	-.3906677286
C	-2.8647598595	-.9658187551	-5.3453197626
C	-3.8246280777	-.7704430628	-6.5311982415
C	-2.4633485828	-2.4477557685	-5.2009751573
C	-1.6189176189	-5.3364241486	2.0852644933
C	-2.3994485785	-4.2476756196	2.5134047840
C	2.5997138671	2.2463583055	-5.1789612395
C	1.3726189093	1.6352087617	-4.5304140034
C	-2.1417660783	-2.9703927453	2.0295026924

C	.1399101109	2.2778851353	-4.7521535915
C	-1.1005821379	-2.7642251747	1.1238001572
C	-1.1370573787	1.8826531356	-4.3149112047
C	2.1423852784	-3.1793987216	.4461447090
C	-2.3150207889	2.7358004365	-4.7421911259
H	1.0194890420	-4.4351934934	-.9264209767
H	.5653967001	-2.6439344428	-.9164538621
H	.0018734093	-5.9815585057	.8603079659
H	-2.7569396206	-2.1345666208	2.3567174829
H	-.9086044737	-1.7695402276	.7384010207
H	2.4417053463	-3.9772924530	1.1428670375
H	1.9399135314	-2.2873287125	1.0658941980
H	-2.6279010137	-6.5268674283	3.1589278464
H	-3.9101775227	-3.7698309941	3.6125007782
H	4.0736416866	-2.7593697453	-.0919647544
H	2.9648826181	-2.2431574394	-1.1720071830
H	2.3398108754	3.1507814990	-5.7303704964
H	3.0666525584	1.5353345868	-5.8677906864
H	3.3543293749	2.4975863896	-4.4279053400
H	.1753414048	3.1741285635	-5.3573795413
H	-1.9795178341	3.6202622790	-5.2851907115
H	-2.8999099593	3.0535714338	-3.8737232528
H	-2.9930045259	2.1677391014	-5.3868792649
H	5.4523840856	-.0937639678	-1.5051477164
H	6.1670499374	-1.9031046048	-3.0315453388
H	4.6968069725	-2.6072867669	-4.8872713562
H	2.2653259712	1.8457021659	-1.9480313353
H	3.8152693139	3.2070864459	-.6181851580
H	4.5300256741	2.9032553660	-2.2115783284
H	5.1029554813	2.0144649504	-.7949440379
H	2.3281849685	1.4609979292	.4957583550
H	3.5258334377	.1731741000	.2817923886
H	1.8916607822	-.0266625453	-.3729954158
H	1.3863180540	-.9858582640	-5.6300409175
H	.9453047439	-3.4003527790	-5.9320961522
H	1.1583493849	-3.0215737907	-4.2095590831
H	2.4618663717	-3.8061072616	-5.1105524901
H	2.1882512859	-2.0371051991	-7.7060025725
H	3.7407028327	-2.4320315640	-6.9636090224
H	3.2991475688	-.7404909701	-7.2320099090
H	-4.8452630307	.6344745286	-.5638483346
H	-6.1945748114	-.8005713020	-2.0567250593
H	-5.2860929470	-1.5092285115	-4.2413565899
H	-1.4659010478	1.9825780031	-1.4820340517
H	-1.1968422603	1.2729093529	.8904757705
H	-1.2435892421	-.1208583060	-.2164360017
H	-2.6666562811	.2873232633	.7667295097
H	-2.4254516160	3.4372565197	.2417076508
H	-3.9515636245	2.5506915229	.2217668719
H	-3.4576150024	3.4814518116	-1.1983112012
H	-1.9519796472	-.4042310558	-5.5633789894
H	-3.3447594559	-1.0894706987	-7.4624645737
H	-4.1191810594	.2780966682	-6.6438691926
H	-4.7392578865	-1.3615503154	-6.4160531169
H	-2.0053303895	-2.8150974890	-6.1261687117
H	-3.3377585186	-3.0717467664	-4.9856760503
H	-1.7472691961	-2.5865287583	-4.3854397987
N	3.1998839783	-3.0114766491	-.5467465729
N	1.5123235343	.5300445827	-3.8036383293
N	-1.3598003190	.8058254161	-3.5645659444
O	-3.3988884060	-4.5622490610	3.4079229963
O	.2099531232	-1.5994877173	-1.6374140421
O	-1.8723987393	-6.5916330697	2.5559771106
Cu	.0398425788	-.3224698636	-2.8506831137

138.L¹CuO / formylglycine t.s.

C	2.8378167134	1.1023479650	-.4849797434
C	2.3725670815	-.2069087713	-2.6377032419
C	-.3767464553	-2.4424979947	3.5018451189
C	1.8672192053	-1.6476695625	-2.4233233492
C	3.0384180539	-.0533060406	-4.0158949528
C	-2.6619295433	1.3425236964	.2384910070
C	-3.1248360041	1.6974690308	1.5270684294
C	-4.3358660646	1.1592541319	1.9735092840
C	-5.0776996070	.2906986865	1.1770154056
C	-4.6009879996	-.0665628644	-.0817107563
C	-3.3908789550	.4388427090	-.5690728553
C	3.6421432044	1.3694413949	.6487353905
C	-2.2934756515	2.5979703272	2.4350421469
C	-1.5518073507	1.7609994537	3.4966769249
C	.5930308317	-3.7024833926	3.2708509112
C	-3.1234543701	3.7128142065	3.0932849650
C	-2.8292542789	-.0564752688	-1.8976239000
C	-3.8480511824	.0066772945	-3.0475726969
C	-2.2613456441	-1.4812010007	-1.7354867550
C	2.4573651848	3.5203362330	-1.8659868076
C	-2.8323214248	-2.2416065830	3.8457924439
C	1.2933053326	2.7890479198	-1.2152072073
C	4.9075415729	.7787252898	.7271858536
C	.0207741553	3.3794243835	-1.3601183725
C	-1.2271059434	2.9083371276	-.9010015148
C	-2.4503145177	3.7347491580	-1.2633890868
C	5.3735199041	-.0689745966	-.2741695311
C	4.5567496701	-.3565682931	-1.3638596281
C	3.2822438026	.2074225719	-1.4859755603
C	3.1160366977	2.2136499941	1.8044348464
C	4.1059391574	3.3013427220	2.2544730139
C	2.7086528545	1.3070086447	2.9838048692
H	-.0603069791	-1.7597653167	2.6048121748
H	-3.7560733825	-2.7752281007	3.5425965778
H	2.1253125002	4.4477613352	-2.3364538644
H	2.9361273929	2.8952665135	-2.6265029224
H	3.2300521453	3.7568034596	-1.1273178293
H	-.0041558181	4.3089081945	-1.9157191691
H	-2.1669178689	4.6508402167	-1.7852920608
H	-3.0198132045	4.0009314965	-.3674102984
H	-3.1283708870	3.1622927562	-1.9054532013
H	5.5310918504	.9721448461	1.5956951629
H	6.3582729920	-.5213502639	-.1938742507
H	4.9072410989	-1.0478241599	-2.1258221605
H	2.2113316955	2.7191146784	1.4558497321
H	3.6535507935	3.9256547589	3.0332990125
H	4.3950842004	3.9533072300	1.4224450506
H	5.0223085473	2.8713820853	2.6743664377
H	2.2731569869	1.9050247523	3.7935284876
H	3.5802614469	.7772102783	3.3856019878
H	1.9733089572	.5581082119	2.6744808752
H	1.4971423817	.4476154524	-2.6182050517
H	1.1562019591	-1.9296506118	-3.2092010478
H	1.3686225710	-1.7464742598	-1.4547462926
H	2.6979513102	-2.3623121723	-2.4459057181
H	2.3280184011	-.3035957911	-4.8121770628
H	3.9016508040	-.7190074660	-4.1272384200
H	3.3866633202	.9718399041	-4.1832627761
H	-4.6936058751	1.4086965775	2.9677430633
H	-6.0148074838	-.1199640110	1.5433137311
H	-5.1689412264	-.7659345848	-.6898154518
H	-1.5322943421	3.0775376911	1.8129024932

H	- .9312978836	2.4122409239	4.1259421594
H	- .9059807687	1.0113042428	3.0310981344
H	-2.2519134235	1.2212626757	4.1405479713
H	-2.4689725883	4.3851625745	3.6596410621
H	-3.8598973115	3.3098194354	3.7970928588
H	-3.6633008283	4.3101927235	2.3496182643
H	-1.9914969077	.5936316931	-2.1641441600
H	-3.3733749209	-.2841019421	-3.9917715289
H	-4.2551753255	1.0164634711	-3.1692287456
H	-4.6911465501	-.6739814665	-2.8841834543
H	-1.7944179893	-1.8215680696	-2.6676875971
H	-3.0562619600	-2.1904631793	-1.4766804659
H	-1.5108565314	-1.5178585626	-.9401241394
H	-1.7945514487	-3.7367880459	2.8512804299
H	-.1874864853	-1.8968739992	4.4288551190
N	-1.7174209099	-2.8962783373	3.4247607235
N	1.5236097795	1.6551066410	-.5604939348
N	-1.3811767457	1.7993246137	-.1912722257
O	.1595651612	-.8159839219	1.4172304604
O	1.7006270894	-3.5280412657	3.8081623595
O	.0765136026	-4.6271477459	2.6210508538
O	-2.8611302349	-1.2113136877	4.5040922146
Cu	.1134974091	.6412502117	.4243091498

139.L¹CuOH⁺ / methane complex

C	-5.3479621173	-.5625133858	1.0280629429
C	.6340318626	-3.2487522075	-.1119610498
C	.5101606574	-3.6849548825	1.2410869000
C	-.2088640718	-4.8566246087	1.4775699129
C	-.7924620385	-5.5745767870	.4338568362
C	-.6968972978	-5.1121816756	-.8778857000
C	-.0127011275	-3.9360063344	-1.1811998968
C	.9859496530	-2.8443768207	2.4221080738
C	1.7367465659	-3.6652274384	3.4856628630
C	-.2160779177	-2.1004228616	3.0477213790
C	.0551872241	-3.4487587149	-2.6246646145
C	-1.3527298707	-3.2672531739	-3.2259541087
C	.9122448895	-4.3861761375	-3.4992310211
C	.7284995818	2.0457962230	-1.0363858579
C	-.0527328577	2.7460505607	-.0680118026
C	-.7164861041	3.9020518700	-.4786612429
C	-.6599417524	4.3352651835	-1.8009951791
C	.0622243811	3.6100682644	-2.7494367086
C	.7686150013	2.4595821581	-2.4044549151
C	-.1431680623	2.3051365323	1.3879917768
C	-1.6053772496	2.0730650686	1.8178954372
C	.5633623299	3.3121737110	2.3190498964
C	1.4157027743	1.6248807398	-3.5071678932
C	2.3104399868	2.4574759760	-4.4434476528
C	.3284527232	.8773113882	-4.3116149167
C	3.5233435194	-3.0625335537	.0382905682
C	2.6289742998	-1.8835924873	-.2781635184
C	3.2589107213	-.6219752721	-.4320155781
C	2.6838637137	.6548897302	-.6495479634
C	3.6393828822	1.8048268268	-.8819289847
H	-5.4512149693	.4776894500	1.3440207923
H	-6.0871444915	-.7802606155	.2540681087
H	-2.3114316694	-.6522842425	-1.1358073798
H	4.5104104255	-2.9196609102	-.4067070467
H	3.0911986887	-3.9936877839	-.3328126814
H	3.6584180142	-3.1647811494	1.1202300266
H	4.3413959504	-.6363968691	-.3790894720
H	4.5092820046	1.7013871921	-.2281700168
H	-5.5172272334	-1.2185863273	1.8842364452

H	3.1581042063	2.7646598104	-.6902603800
H	4.0033897777	1.8058057640	-1.9144691788
H	-.3356602892	-5.2069805365	2.4964465218
H	-1.3409447877	-6.4873213768	.6467430755
H	-1.1692731456	-5.6750049661	-1.6767112687
H	1.6756058462	-2.0787367679	2.0543901749
H	2.1347984762	-3.0002678584	4.2582125064
H	2.5723284749	-4.2265688602	3.0557830338
H	1.0787739713	-4.3821703861	3.9859190090
H	.1243425824	-1.4370772938	3.8496188619
H	-4.3419553897	-.7292694899	.6379479864
H	-.9307341217	-2.8095598729	3.4777812580
H	-.7566777654	-1.5011436501	2.3070814761
H	.5441719858	-2.4687953180	-2.6263349266
H	-1.2818241186	-2.8322919655	-4.2282126388
H	-1.9684277643	-2.6068646611	-2.6070163548
H	-1.8821960884	-4.2205609264	-3.3198406122
H	.9773570421	-3.9993244682	-4.5212540846
H	.4758205167	-5.3892201907	-3.5505342203
H	1.9300296529	-4.4853113759	-3.1084922779
H	-1.2905384306	4.4707582392	.2453352832
H	-1.1927093798	5.2329397271	-2.0999836467
H	.0575445866	3.9416026701	-3.7824426588
H	.3854611033	1.3507193617	1.4863962560
H	-1.6339981171	1.7234449867	2.8552171355
H	-2.0871038395	1.3175582518	1.1907932509
H	-2.1925361255	2.9957810192	1.7681418762
H	.5304296442	2.9562739441	3.3537851229
H	.0741726585	4.2914088529	2.2895828145
H	1.6129263131	3.4546187668	2.0414685919
H	2.0478571063	.8601718806	-3.0481298775
H	2.8230230879	1.8003897221	-5.1527124335
H	3.0688472498	3.0192320029	-3.8897338848
H	1.7295631549	3.1752563682	-5.0305309727
H	.7885613523	.2406265405	-5.0744113784
H	-.3416026904	1.5794950636	-4.8180121544
H	-.2865497114	.2421794415	-3.6638834363
N	1.3223634112	-2.0503392910	-.4333733220
N	1.3743001107	.8577287675	-.6147560052
O	-1.7423223783	-.5942490155	-.3574251473
Cu	.0530128770	-.5667488095	-.5214564548

140.L¹CuOH⁺ / cyclohexane complex

C	-6.7812885699	-7.0109765786	-1.0244110979
C	1.4981530211	-8.3582450317	-2.2691814367
C	1.4346515887	-8.7588046375	-.9017964180
C	.7141911922	-9.9145170237	-.6007376429
C	.0728787297	-10.6528666263	-1.5946937986
C	.1094457544	-10.2262621117	-2.9214720935
C	.7909177925	-9.0649605836	-3.2860682879
C	1.9786367772	-7.8948001502	.2319514697
C	2.7685316293	-8.6977904132	1.2801029695
C	.8181654665	-7.1161970483	.8942683009
C	.8104884785	-8.6231671979	-4.7429139488
C	-5.3305007324	-6.8680060209	-1.5156493331
C	-.6114591612	-8.5002070170	-5.3232359742
C	1.6802374731	-9.5662785143	-5.5998956150
C	1.6690559213	-3.0865514934	-3.2908522863
C	.9623356869	-2.3510610668	-2.2898218683
C	.2879107378	-1.1968460561	-2.6854216748
C	.2654283318	-.7949144637	-4.0188946168
C	.9178907279	-1.5516560988	-4.9936025147
C	1.6285825054	-2.7043946847	-4.6663014869
C	.9757305311	-2.7488579050	-.8176447096

C	-.4519066486	-2.9276041200	-.2635849835
C	-4.5087615579	-5.9538192066	-.5919037615
C	1.7848986660	-1.7379581065	.0215444467
C	2.1970589554	-3.5709557221	-5.7863865983
C	3.0571906833	-2.7708264436	-6.7817038175
C	1.0546240877	-4.3094396820	-6.5196779428
C	-5.1826362632	-4.5812656844	-.4181160654
C	4.3823955770	-8.2467771502	-2.2888252833
C	-6.6336562836	-4.7226093953	.0738621120
C	3.5061420160	-7.0458709638	-2.5739656901
C	-7.4550352779	-5.6396394476	-.8471252375
C	4.1640324761	-5.8065507078	-2.7865264498
C	3.6137476383	-4.5183551894	-2.9970421375
C	4.5817454214	-3.4005383460	-3.3143720254
H	-4.8575299593	-7.8555133779	-1.5945703859
H	-5.3363355056	-6.4430472789	-2.5308975540
H	-4.4168094392	-6.4343414803	.3930453934
H	-3.4868810960	-5.8302873755	-.9745197925
H	-4.6056132164	-3.9588173081	.2773242159
H	-5.1811587777	-4.0542512639	-1.3839886002
H	-7.1078763128	-3.7363651677	.1495586931
H	-6.6293122289	-5.1433738899	1.0897971643
H	-8.4700314019	-5.7638280197	-.4511182392
H	-1.4461850782	-5.8612789760	-3.0710399466
H	5.3496355881	-8.1367593435	-2.7840514456
H	3.9063698938	-9.1690353306	-2.6267787721
H	4.5678561250	-8.3421284612	-1.2134589499
H	5.2468753594	-5.8531405768	-2.7994894696
H	5.4821984271	-3.5068206425	-2.7038026256
H	4.1336411276	-2.4240420807	-3.1265035654
H	4.8905241047	-3.4389312388	-4.3638132765
H	.6333072217	-10.2369049183	.4322164599
H	-.4729579384	-11.5538319380	-1.3303271625
H	-.4049579574	-10.8050884057	-3.6817655850
H	2.6605099426	-7.1496203392	-.1894273940
H	3.2100306354	-8.0186486303	2.0159108565
H	3.5766433313	-9.2801636722	.8263970894
H	2.1262537730	-9.3936720162	1.8287118055
H	1.2076925609	-6.4302015083	1.6538096670
H	.1205891761	-7.8016994708	1.3859454309
H	.2435952006	-6.5370911285	.1632674355
H	1.2710514183	-7.6307240827	-4.7832981906
H	-.5700377830	-8.0891410491	-6.3370136516
H	-1.2372122391	-7.8413508015	-4.7124841362
H	-1.1150886123	-9.4697592325	-5.3853275207
H	1.7118922660	-9.2189691988	-6.6374669828
H	1.2765022100	-10.5844058459	-5.6000436077
H	2.7087591137	-9.6168394521	-5.2278412198
H	-.2309175689	-.6027955479	-1.9403577747
H	-.2741800686	.1031048898	-4.3042959377
H	.8540490376	-1.2442616280	-6.0321888161
H	1.4847665191	-3.7149540327	-.7314396493
H	-.4052141578	-3.2535878758	.7808948900
H	-1.0038567611	-3.6809630335	-.8330106704
H	-1.0165960553	-1.9903652431	-.2876033442
H	1.8264534247	-2.0622302275	1.0661760989
H	1.3226785279	-.7456993732	-.0004210797
H	2.8119094234	-1.6360491998	-.3443049502
H	2.8367511887	-4.3411887554	-5.3466882976
H	-7.5624505484	-5.1602156977	-1.8311679229
H	3.5134039421	-3.4479734149	-7.5103097673
H	3.8586481337	-2.2209458853	-6.2790030568
H	2.4601452693	-2.0456017453	-7.3428403040
H	1.4616202292	-4.9701055296	-7.2922752934

H	.3743797926	-3.6025526303	-7.0053297718
H	.4605467634	-4.9185077988	-5.8289698932
H	-7.3587234892	-7.6312041536	-1.7207131695
H	-6.7838943839	-7.5406489403	-.0607055035
N	2.1890576148	-7.1782621578	-2.6505425980
N	2.3149633427	-4.2798184611	-2.8851112688
O	-.8193163830	-5.7117569181	-2.3512790050
Cu	.9560578086	-5.6484161527	-2.6653846055

141.L¹CuOH⁺ / acetonitrile complex

C	1.6140172155	-2.8478220757	.8751702920
C	1.6716377680	-3.4048573946	2.1842245932
C	.9193407886	-4.5551923310	2.4279910686
C	.1296193623	-5.1314309389	1.4358617651
C	.0418946362	-4.5406791846	.1762304359
C	.7498312045	-3.3790011174	-.1256800863
C	2.3806175118	-2.7140272329	3.3457534314
C	3.2843110375	-3.6652495586	4.1512032721
C	1.3379499031	-2.0333420622	4.2625622776
C	.6454819289	-2.7368602103	-1.5037797214
C	-4.2051960607	-1.0712426032	.5544819727
C	-.7796582795	-2.7795209461	-2.0795936436
C	1.6557194626	-3.3630897207	-2.4874644572
C	1.8382390044	2.4028892698	-.2690313690
C	1.2281539088	3.2393877531	.7145462498
C	.5288034505	4.3614103316	.2705938070
C	.3977045031	4.6423126871	-1.0878718325
C	.9714369070	3.7978821248	-2.0374242319
C	1.7015949912	2.6688626362	-1.6642842755
C	1.3995227338	3.0004985626	2.2124625840
C	.0594757609	3.0230938284	2.9713801714
C	-5.6477631433	-1.2794826615	.5322196835
C	2.4021459552	4.0107176472	2.8098245518
C	2.2112593922	1.7272370173	-2.7534989536
C	3.1047901816	2.4451781556	-3.7844050236
C	1.0278836739	1.0214761250	-3.4522469617
C	4.5199627957	-2.7961620455	.6399247822
C	3.6402136357	-1.5728905143	.4991220909
C	4.3078401677	-.3387127442	.2608316293
C	3.7713513933	.9529139280	.0148559885
C	4.7478479979	2.0141005866	-.4437113895
H	-1.2177101311	-.4115340576	1.2457675948
H	5.3499499705	-2.7448712464	-.0689644188
H	3.9573367232	-3.7134717752	.4684709208
H	4.9487348990	-2.8456428786	1.6461555266
H	5.3885196814	-.4082324841	.1918460301
H	5.6395349418	1.9876538091	.1913664689
H	-6.0950940192	-.9921701901	1.4874461581
H	4.3062996027	3.0104050867	-.3927059910
H	5.0715275940	1.8306070841	-1.4737578801
H	.9319051176	-4.9979354972	3.4185625000
H	-.4379595623	-6.0318510775	1.6513753461
H	-.5958521514	-4.9892057137	-.5771930260
H	3.0170627769	-1.9188596472	2.9449426820
H	3.8328645934	-3.1046589621	4.9145996740
H	4.0125156484	-4.1770386479	3.5148969937
H	2.7030542649	-4.4328193849	4.6713102768
H	1.8423727479	-1.4678665439	5.0535815693
H	-5.8675906503	-2.3331696729	.3401033444
H	.6981854262	-2.7811149130	4.7432333947
H	.6902497731	-1.3509188141	3.7025855279
H	.9183340689	-1.6795051564	-1.3897045288
H	-.8241661173	-2.1799755762	-2.9950192989
H	-1.5091450502	-2.3758155118	-1.3719108566

H	-1.0864270743	-3.7960922400	-2.3489076753
H	1.6024261641	-2.8646452581	-3.4607824998
H	1.4388807163	-4.4259616771	-2.6415542546
H	2.6843690760	-3.2818172893	-2.1228394883
H	.0813576236	5.0301391552	.9989770404
H	-6.1023938022	-.6746093499	-.2577616885
H	-.1576658220	5.5186519226	-1.4092810196
H	.8365992033	4.0170588999	-3.0921834333
H	1.8319741366	2.0029347772	2.3511193748
H	.2350171542	2.8225094579	4.0337946279
H	-.6164519110	2.2522071163	2.5920079885
H	-.4376173987	3.9961108346	2.9007881551
H	2.5607472526	3.8029955031	3.8731707089
H	2.0273589230	5.0357393931	2.7201655729
H	3.3740898996	3.9658626976	2.3061494122
H	2.8127187446	.9414847952	-2.2872723051
H	3.520554416	1.7213312984	-4.4933402149
H	3.9377810549	2.9717483515	-3.3072947723
H	2.5392535556	3.1808226046	-4.3649124344
H	1.3972667040	.2997977634	-4.1891409246
H	.3902493404	1.7393166060	-3.9784563059
H	.3987115106	.4862766033	-2.7325074291
N	-3.0555697109	-.9122047418	.5489199213
N	2.3197513482	-1.6605015096	.5466119918
N	2.4877744454	1.2269179892	.1879548100
O	-.3924639957	-.1428840968	1.6948743699
Cu	1.1778242322	-.0699347962	.8357245974

142.L¹CuOH⁺ / toluene complex

C	-6.4979155975	-6.1809035863	-2.9748962062
C	2.6456109026	-9.1329331809	-2.9412196304
C	2.4532616785	-9.5544566818	-1.5909277995
C	1.7354171512	-10.7316125382	-1.3760170305
C	1.2130674407	-11.4663520321	-2.4397510596
C	1.3708076240	-11.0164822257	-3.7501029255
C	2.0601759217	-9.8387738565	-4.0324939523
C	2.8506150724	-8.6880065359	-.3989912282
C	3.5325680045	-9.4813392214	.7289850963
C	1.6069463849	-7.9364807852	.1302846204
C	2.2120166649	-9.3739681577	-5.4762206120
C	-5.2959453534	-5.7777864377	-3.5586961532
C	.8528078650	-9.2815469242	-6.1958409596
C	3.1896241495	-10.2784203843	-6.2554816764
C	2.7698971774	-3.8764974889	-3.9999410430
C	1.9103950939	-3.1769723153	-3.0987849316
C	1.2490014407	-2.0463364665	-3.5764056884
C	1.3833095525	-1.6380161483	-4.9015706289
C	2.1833283328	-2.3649757764	-5.7847959789
C	2.8904610069	-3.4913660456	-5.3688803895
C	1.7362381162	-3.5928038651	-1.6422830262
C	.2529583753	-3.8230160549	-1.2893983901
C	-4.0798909359	-6.1392334218	-2.9778523703
C	2.3893049075	-2.5694834164	-.6915091410
C	3.6270480987	-4.3345708754	-6.4060227107
C	4.5710076398	-3.5052650242	-7.2946050658
C	2.6137249277	-5.1207673246	-7.2670989501
C	-4.0378820061	-6.9056286055	-1.8055871165
C	5.5169553024	-8.9373426341	-2.6500292036
C	-5.2546877109	-7.3048141733	-1.2318452839
C	4.6400070748	-7.7631623903	-3.0293533856
C	-6.4714987259	-6.9471020609	-1.8071247198
C	5.2782942290	-6.5052515261	-3.1777696753
C	-2.7234630749	-7.2802038516	-1.1627317414
C	4.7161879258	-5.2351179272	-3.4578042511

C	5.6767614367	-4.0836591340	-3.6542893706
H	-5.2457465856	-7.9021974362	-.3227970456
H	-7.4017410946	-7.2663735172	-1.3457111348
H	-7.4464051353	-5.9017635826	-3.4245713223
H	-2.6911691431	-8.3490791561	-.9212195506
H	-2.5783614492	-6.7379712227	-.2195490869
H	-1.8727651284	-7.0524484570	-1.8106776739
H	-.2250230758	-6.7455626976	-4.1688981299
H	6.5260505419	-8.7993415932	-3.0442143081
H	5.1044064095	-9.8730459092	-3.0319846039
H	5.5943046566	-9.0270879324	-1.5611030360
H	6.3558765444	-6.5178553080	-3.0613770792
H	6.5090572264	-4.1707498650	-2.9512583826
H	5.1786136358	-3.1247789120	-3.5049883705
H	6.0980009486	-4.0948484381	-4.6648508796
H	1.5594671658	-11.0706859466	-.3606401557
H	.6630705977	-12.3824345734	-2.2452706591
H	.9442321928	-11.5932654115	-4.5644450548
H	3.5599173374	-7.9266023408	-.7371375916
H	3.8760847626	-8.7981965899	1.5118138713
H	4.3972720865	-10.0463324864	.3666566806
H	2.8462892287	-10.1915523817	1.2002285114
H	1.8926537953	-7.2484101970	.9328463163
H	.8710213457	-8.6390378680	.5345261405
H	1.1103760851	-7.3626864091	-.6595218132
H	2.6451308484	-8.3675774653	-5.4608419958
H	.9821397393	-8.8403760169	-7.1894500713
H	.1448990346	-8.6625239525	-5.6355502295
H	.3928874555	-10.2646101985	-6.3347357271
H	3.3143724567	-9.9130115770	-7.2799299534
H	2.8155078033	-11.3063056923	-6.3102384740
H	4.1769586357	-10.3082303710	-5.7832136673
H	.6149060419	-1.4777719213	-2.9039235628
H	.8512523007	-.7593492259	-5.2539245104
H	2.2398599444	-2.0553911112	-6.8230630851
H	2.2594317115	-4.5441272038	-1.4967633692
H	.1690307913	-4.1675322740	-.2534016272
H	-.1936610663	-4.5814222144	-1.9383996444
H	-.3316324634	-2.9012179314	-1.3740102512
H	2.2961102561	-2.9045998487	.3464109506
H	1.9033204300	-1.5915982684	-.7700725039
H	3.4533092185	-2.4327973185	-.9105762967
H	4.2391864442	-5.0770429104	-5.8867542308
H	5.1439753333	-4.1677095732	-7.9506654827
H	5.2782662101	-2.9177394486	-6.7012459879
H	4.0205101134	-2.8115617741	-7.9373929874
H	3.1380390277	-5.7643108226	-7.9812015148
H	1.9680940371	-4.4430402119	-7.8350760730
H	1.9662753844	-5.7540559711	-6.6498001160
H	-3.1461930640	-5.8174321162	-3.4348476728
H	-5.3068110550	-5.1821024249	-4.4674041972
N	3.3428311385	-7.9369402563	-3.2417302404
N	3.4066904604	-5.0426160508	-3.5130500986
O	.2819287714	-6.5829283405	-3.3626859556
Cu	2.0836054009	-6.4522215148	-3.4463778145

143.L¹CuOH⁺ / isopropylbenzene complex

C	-13.1124417341	1.0010104671	.3075473588
C	1.6589834404	-2.7787872892	-3.5692076395
C	1.4639624198	-3.1587199676	-2.2080283496
C	1.1637210331	-4.4960261094	-1.9475422790
C	1.0514116747	-5.4306487872	-2.9758014744
C	1.2115756156	-5.0368495843	-4.3025325638
C	1.4923182227	-3.7119665727	-4.6349033229

C	1.4261701437	-2.1477196331	-1.0662808145
C	2.2430117980	-2.5984333787	.1586721008
C	-.0389788099	-1.8518061585	-.6739743492
C	1.6502933221	-3.3189770850	-6.1002759329
C	-11.7538816536	1.1785137756	.5660295871
C	.3926322767	-3.6700500945	-6.9207950271
C	2.9127958413	-3.9514550193	-6.7200239686
C	-.0648350250	2.0715683633	-5.2036297805
C	-1.2489226238	2.4500859938	-4.5037678859
C	-2.1631530071	3.2685805034	-5.1678128736
C	-1.9600791863	3.6604243159	-6.4883111889
C	-.8307452870	3.2276271184	-7.1821298973
C	.1379605310	2.4322361257	-6.5715828733
C	-1.5192626073	2.0467291964	-3.0586252558
C	-2.9024526266	1.3792545221	-2.9104939857
C	-10.9563402615	1.9819069034	-.2620831611
C	-1.3695399462	3.2542283494	-2.1114819608
C	1.2746237588	1.8683306171	-7.4212988195
C	1.9738450118	2.9379062205	-8.2793650688
C	.7452260465	.7191659724	-8.3087180307
C	-11.5667259269	2.6052686244	-1.3644427291
C	4.1951095405	-1.4338300701	-3.0070904730
C	-12.9221584123	2.4306388273	-1.6281681133
C	2.9850190967	-.7389031860	-3.5902705879
C	-13.7029155039	1.6270313794	-.7924967284
C	3.0812694132	.6642295224	-3.7846555776
C	-9.4773268589	2.1822649026	.0381939001
C	-8.5837254877	1.7047096537	-1.1243422000
C	2.1132993168	1.5845633749	-4.2618693115
C	-9.1756711714	3.6493577117	.4002525682
C	2.5637184214	3.0188834865	-4.4422378605
H	-13.3739166502	2.9202705941	-2.4862738937
H	-14.7608540408	1.4906876166	-.9969995621
H	-11.3030325636	.6888718731	1.4259504372
H	-13.7108776928	.3754668825	.9641371988
H	-10.9753365946	3.2362232955	-2.0221669868
H	-9.2402836165	1.5686495295	.9177088410
H	-8.1225621064	3.7709636527	.6771879860
H	-9.7909867852	3.9842698017	1.2409623221
H	-9.3768040642	4.3164676752	-.4449024278
H	-7.5216394245	1.8578927030	-.8936394940
H	-8.7994693741	2.2623399088	-2.0428821588
H	-8.7431886839	.6429578741	-1.3376972981
H	-1.7642771198	-1.2821793031	-5.7234469698
H	5.1097495055	-.9900389306	-3.4081021294
H	4.1844439664	-2.5012440056	-3.2319569150
H	4.2217599676	-1.3174910522	-1.9185262134
H	4.0440613913	1.0972983778	-3.5387584814
H	3.2956177964	3.2804234727	-3.6746887051
H	1.7185132292	3.7067795798	-4.3836566009
H	3.0429972636	3.1572087560	-5.4170389154
H	.9938089230	-4.8123288912	-.9235776459
H	.8228325038	-6.4662615395	-2.7425313961
H	1.1105284661	-5.7743368743	-5.0924070099
H	1.8538331610	-1.2041609883	-1.4161838799
H	2.2558616764	-1.8051406542	.9125421750
H	3.2785249623	-2.8342503575	-.1057122322
H	1.8119110793	-3.4864984435	.6310707350
H	-.0749434692	-1.0821956592	.1042032906
H	-.5307588787	-2.7488651108	-.2847266186
H	-.6256192305	-1.5011511925	-1.5301099588
H	1.7810513205	-2.2319226713	-6.1455760617
H	.4934521811	-3.2936403510	-7.9443833152
H	-.5048907532	-3.2303568802	-6.4756369784

H	.2358148298	-4.7512062826	-6.9858106750
H	3.0325000293	-3.6247483584	-7.7579886443
H	2.8484685170	-5.0443829006	-6.7208257765
H	3.8161876472	-3.6704859198	-6.1694658877
H	-3.0527671223	3.6043116257	-4.6449618681
H	-2.6921695036	4.2903128834	-6.9847935459
H	-.7117253530	3.5051208560	-8.2239317890
H	-.7621308811	1.3102075166	-2.7672029157
H	-3.0674447091	1.0932660224	-1.8672888950
H	-2.9622938325	.4830894882	-3.5335928761
H	-3.7127688929	2.0598554254	-3.1927082239
H	-1.5181169882	2.9423869653	-1.0729557230
H	-2.1111505790	4.0282162833	-2.3354726715
H	-.3774709281	3.7112030261	-2.1903716524
H	2.0305364507	1.4348568817	-6.7610714144
H	2.8390108321	2.5031524759	-8.7894723622
H	2.3223671091	3.7815262054	-7.6756342012
H	1.3105842265	3.3368480908	-9.0530855668
H	1.5610138654	.2777846555	-8.8907260776
H	-.0129804308	1.0815537884	-9.0103387339
H	.2866061829	-.0754107905	-7.7090758895
N	1.9011232720	-1.4231908757	-3.9170446674
N	.8613685165	1.2360997616	-4.5258101449
O	-1.4626105489	-1.1317325146	-4.8180133266
Cu	.2375823941	-.6230912966	-4.5057896457

144.L¹CuOH⁺ / cyclohexadiene complex

C	-6.9701623847	.5064294228	-1.9846168605
C	-.0320399179	-2.5643014104	-3.1028982583
C	.0013391336	-2.9215834126	-1.7220936877
C	-.6244425096	-4.1109135911	-1.3470389669
C	-1.2653190558	-4.9216475147	-2.2835470418
C	-1.3253100956	-4.5376245833	-3.6215128970
C	-.7395630129	-3.3483410671	-4.0581080257
C	.5512646556	-1.9889383283	-.6462863625
C	1.4326736752	-2.7097054643	.3894301967
C	-.6140052592	-1.2471306066	.0470024153
C	-.8439312328	-2.9444943390	-5.5245872946
C	-6.0846939897	-.6529895795	-1.6229825768
C	-2.3140515218	-2.8422006318	-5.9777955395
C	-.0486091058	-3.9021522093	-6.4344022234
C	-.3011705326	2.6837955032	-4.2972661130
C	-.9759610740	3.4116764048	-3.2717431106
C	-1.7155264604	4.5335685827	-3.6477493753
C	-1.8315711104	4.9081261524	-4.9846665663
C	-1.2119321976	4.1551264014	-5.9822391937
C	-.4397937894	3.0347759451	-5.6742345740
C	-.8878739070	3.0283860296	-1.7985207173
C	-2.2855164451	2.7527691498	-1.2073234931
C	-6.6306809874	-1.9757091880	-2.0843101296
C	-.1323101141	4.0983341265	-.9831931210
C	.0949779527	2.1611343028	-6.8064298560
C	.8386601276	2.9663538413	-7.8872799772
C	-1.0563998396	1.3414511195	-7.4313540762
C	-7.8058016271	-2.1117225915	-2.7100382374
C	2.8407969737	-2.2389435474	-3.2725032681
C	-8.7123172313	-.9564074440	-3.0291786412
C	-8.1448837635	.3707256442	-2.6114269178
C	1.8627746506	-1.1194577994	-3.5544799528
C	2.4052213682	.1608919621	-3.8322193862
C	1.7404581090	1.3929310017	-4.0529211835
C	2.6009583751	2.5802734709	-4.4289628401
H	-8.7411852859	1.2526788030	-2.8364537829
H	-6.6220887428	1.4984121027	-1.7038528569

H	-5.9361434687	-.6771641692	-.5288716547
H	-5.0661162235	-.4964315738	-2.0169388809
H	-8.9450965930	-.9450286707	-4.1072888189
H	-3.1784075314	-.0424198726	-4.0791851729
H	3.7871196570	-2.0577924143	-3.7860115718
H	2.4350531095	-3.2016608963	-3.5899502768
H	3.0519557281	-2.3057636699	-2.1999030557
H	3.4862646212	.2021099387	-3.8924536738
H	3.5813127176	2.5006189086	-3.9538707151
H	2.1297971631	3.5175064174	-4.1272048515
H	2.7601360250	2.6176767461	-5.5117117617
H	-.6285712365	-4.4030701489	-.3022605792
H	-1.7359096729	-5.8470275979	-1.9649123777
H	-1.8414427163	-5.1712200185	-4.3357666195
H	1.1711368608	-1.2262895257	-1.1265544980
H	1.8745909572	-1.9810987763	1.0760253669
H	2.2470965454	-3.2681419997	-.0831954965
H	.8562814774	-3.4150370567	.9957887124
H	-.2262801797	-.5232348169	.7715259460
H	-1.2582629844	-1.9499220330	.5854394473
H	-1.2434410987	-.7120888249	-.6723941703
H	-.3963710614	-1.9505030738	-5.6312030468
H	-2.3673899241	-2.4658860582	-7.0047347586
H	-2.8830936558	-2.1653090575	-5.3323528409
H	-2.8150635952	-3.8154035741	-5.9601762053
H	-.1077617335	-3.5738912830	-7.4771351919
H	-.4477302908	-4.9205309304	-6.3825579874
H	1.0082816092	-3.9438264400	-6.1516925507
H	-2.2143580560	5.1210510885	-2.8836781303
H	-2.4200728251	5.7803525963	-5.2533652918
H	-1.3484132658	4.4381501907	-7.0206996006
H	-.3104361053	2.1006923079	-1.7239425412
H	-2.1909467770	2.4384947920	-.1622598836
H	-2.7944806040	1.9586690083	-1.7610098908
H	-2.9144477293	3.6492460791	-1.2238087718
H	-.0398947983	3.7831556187	.0611555004
H	-.6639616494	5.0557428373	-.9940206503
H	.8750011721	4.2719124729	-1.3758892701
H	.8040048131	1.4400481344	-6.3900949915
H	-6.0289895666	-2.8576596652	-1.8734478441
H	1.285542863	2.2874336004	-8.6200744223
H	1.6374742281	3.5805810345	-7.4604774846
H	.1652017144	3.6337041056	-8.4336669795
H	-.6724159412	.6767886835	-8.2123644648
H	-1.8064942510	1.9973083430	-7.8850939719
H	-1.5658904252	.7260758416	-6.6810015865
H	-8.1473517116	-3.1011489584	-3.0075295946
H	-9.6950401306	-1.1100307111	-2.5512757216
N	.5577991413	-1.3530845655	-3.5565025550
N	.4302440578	1.5336467721	-3.9058087298
O	-2.5805365220	.0306699614	-3.3232008953
Cu	-.7930666921	.0428944905	-3.6161712583

145.L¹CuOH⁺ / dopamine complex

C	-2.2689090500	-5.5236637382	4.7481893720
C	3.1226964641	-8.1198041212	3.2798470767
C	2.9526376849	-8.5754387148	4.6186208940
C	2.1827243100	-9.7227182997	4.8206770692
C	1.5912935383	-10.4006536869	3.7564135756
C	1.7349787562	-9.9203107250	2.4565989765
C	2.4760844723	-8.7670109410	2.1898501484
C	3.4653291645	-7.7985358356	5.8285633663
C	4.2481991452	-8.6806468701	6.8200513854
C	2.2923783899	-7.0898378326	6.5439228739

C	2.5896939302	-8.2586216017	.7556503734
C	-3.4733585124	-5.9610219696	3.9478792079
C	1.2012008547	-7.9629895387	.1526965065
C	3.3807246471	-9.2367587091	-.1354357907
C	3.6049607589	-2.7989981327	2.3581889051
C	2.9293588398	-2.0272541114	3.3450533318
C	2.3486664132	-.8208662775	2.9485629534
C	2.3895304167	-.4038080268	1.6205488168
C	3.0092641710	-1.1973616866	.6556720014
C	3.6239030092	-2.4047224613	.9891611723
C	2.8345003423	-2.4709669721	4.8012257167
C	1.3670266056	-2.7161396991	5.2071107136
C	-3.3756478271	-6.9770784330	2.9915583753
C	3.5237298187	-1.4704594723	5.7500044754
C	4.1646125371	-3.3022140057	-.1218494641
C	5.0898016252	-2.5571425316	-1.1015256877
C	2.9976493536	-3.9743023254	-.8791015923
C	-4.5037918118	-7.4166460309	2.3009055832
C	6.0057720571	-8.1253157395	3.3868500914
C	-5.7670794165	-6.8321477213	2.5684349924
C	-5.8778100753	-5.8189186412	3.5152599289
C	5.1968012311	-6.8746929686	3.1134698451
C	-4.7403337664	-5.3913103003	4.1966479933
C	5.9189463826	-5.6631652113	2.9676762581
C	-2.0276255063	-6.4315549428	5.9753246309
C	5.4384954110	-4.3479602826	2.7559815249
C	6.4676079197	-3.2607122666	2.5319815540
H	-1.3566360592	-5.5231436836	4.1403957998
H	-2.4206175991	-4.4953452712	5.0999684040
H	-2.4219522242	-7.4447298882	2.7667457715
H	-6.8461923555	-5.3670288039	3.7154555259
H	-4.8311858933	-4.5999630461	4.9346275263
H	-1.7689758026	-7.4363695127	5.6220531061
H	-2.9710009611	-6.5310698886	6.5389213935
H	-5.2752730544	-8.5723428264	1.0103726541
H	-7.6315778733	-6.9135563285	2.0687457035
H	-.5776330974	-6.6413928752	7.4131687727
H	-1.2094115161	-5.1381499624	7.3457563189
H	.4462947850	-5.3490319683	2.0494531973
H	7.0193842977	-8.0198298474	2.9959267205
H	5.5347944994	-9.0020409975	2.9371882811
H	6.0803178684	-8.3072575104	4.4638974595
H	6.9966275108	-5.7597763265	3.0170019109
H	7.4041010741	-3.5124785058	3.0335737927
H	6.1070800907	-2.2989063781	2.9027518052
H	6.6828066347	-3.1453913485	1.4645573330
H	2.0294403949	-10.0869172743	5.8318012319
H	1.0061333389	-11.2966486376	3.9424333955
H	1.2608513730	-10.4504510414	1.6363750236
H	4.1441901239	-7.0160355069	5.4760700997
H	4.6730886726	-8.0623943553	7.6172674333
H	5.0680467529	-9.2206670507	6.3361662961
H	3.6020919427	-9.4244801116	7.2970851402
H	2.6717514744	-6.4599768365	7.3557128899
H	1.6113185376	-7.8263612262	6.9875371514
H	1.7060132288	-6.4618226911	5.8669866449
H	3.1474083311	-7.3168145513	.7772278177
H	1.3047227090	-7.5159740930	-.8416931905
H	.6355458862	-7.2708951506	.7846417399
H	.6040127121	-8.8739422509	.0426449668
H	3.4813159655	-8.8342950018	-1.1488821657
H	2.8737518570	-10.2045971661	-.2114478131
H	4.3859600491	-9.4181218429	.2581888147
H	1.8499184488	-.2027908189	3.6886805504

H	1.9243063209	.5338584053	1.3314488193
H	2.9974580395	-.8755574400	-.3806451092
H	3.3656267939	-3.4238306720	4.8973391150
H	1.3178261238	-3.0844766903	6.2371880992
H	.8961218276	-3.4606849849	4.5582255979
H	.7801612154	-1.7925014474	5.1565376252
H	3.4883427305	-1.8405660736	6.7798731953
H	3.0276646622	-.4940846229	5.7332948756
H	4.5737036970	-1.3151255741	5.4810169569
H	4.7493995474	-4.1074532490	.3313250735
H	5.5269117462	-3.2627148940	-1.8151199669
H	5.9076794462	-2.0475096665	-.5827709170
H	4.5471280433	-1.8044927722	-1.6817148052
H	3.3805987907	-4.6581746719	-1.6441344918
H	2.3688726578	-3.2286948930	-1.3768302556
H	2.3558106961	-4.5480227373	-.2009350756
N	-.9097534811	-5.9248761155	6.7746869212
N	3.8780629316	-6.9447370980	2.9993821858
N	4.1462096528	-4.0529291934	2.7617567839
O	-6.7971169250	-7.3408117300	1.8328244315
O	.9152825852	-5.3351910858	2.8939542414
O	-4.3935582041	-8.3976007590	1.3772802663
Cu	2.7282553757	-5.3680675342	2.8608835358

146.L¹CuOH⁺ / formylglycine complex

C	1.7400958223	-2.4576015373	.2896775896
C	1.4059123661	-2.8222590936	1.6199971727
C	.6542556652	-3.9835519759	1.8208584704
C	.2318649456	-4.7672655733	.7504506309
C	.5514974148	-4.3893048090	-.5491820273
C	1.2980449339	-3.2346476211	-.8083927983
C	1.7719483338	-1.9423561472	2.8122814339
C	2.3818252932	-2.7331877356	3.9826334067
C	.5397996046	-1.1388605985	3.2775557517
C	1.5640660385	-2.8245250210	-2.2528173953
C	-3.2973989544	-.6392704501	1.1765861498
C	.2482973741	-2.4254343763	-2.9514092788
C	2.2947727520	-3.9196264977	-3.0512403586
C	2.0376737756	2.9053268151	-.6776503066
C	1.4807490240	3.7270166518	.3319501105
C	.8769663412	4.9310369090	-.0497675459
C	.8072160475	5.3130129622	-1.3856529981
C	1.3315705070	4.4808182996	-2.3721546083
C	1.9453445210	3.2684421270	-2.0473532236
C	1.4625335605	3.3039835819	1.7974129693
C	.0323658419	2.9210238124	2.2312641125
C	-3.4009883479	.1433766111	2.4624861904
C	2.0609845717	4.3742408070	2.7270202245
C	2.4186011498	2.3372761742	-3.1622615187
C	3.3189128509	3.0371636866	-4.1952525836
C	1.2101243072	1.6741005812	-3.8574154634
C	4.5886718536	-2.3560351362	.3596902204
C	-5.5646201135	-1.0732610064	.3077764069
C	3.7582762883	-1.1098345597	.1242803980
C	4.4388123481	.1165320709	-.0014129582
C	3.8945887821	1.3967781627	-.2169023481
C	4.8576191769	2.5609452723	-.3353803116
H	-3.3198022834	-1.7097904810	1.3970393865
H	-6.3486268005	-.6276795581	-.3341159693
H	-.9747059236	.2758070992	-1.1177543757
H	5.6557015741	-2.1347870627	.3094318099
H	4.3501001389	-3.1241786239	-.3825227595
H	4.3665495289	-2.7868767331	1.3416864214
H	5.5172203735	.0683288000	.0771468798

H	5.8805123412	2.2495951928	-.1187811485
H	4.5761847466	3.3635941755	.3530950258
H	4.8290240078	2.9863233628	-1.3441194808
H	.3818426012	-4.2736396702	2.8313704501
H	-.3558354270	-5.6634225488	.9295238971
H	.2039818196	-4.9966832313	-1.3804776645
H	2.5239959385	-1.2204803018	2.4816921249
H	2.7071259136	-2.0458853101	4.7710303668
H	3.2504287860	-3.3206070782	3.6659050851
H	1.6595874055	-3.4222270916	4.4333741463
H	.8056686968	-.4567184151	4.0924200726
H	-.2482284460	-1.8054940806	3.6435335335
H	.1113932987	-.5460987818	2.4636577502
H	2.2092034519	-1.9410342884	-2.2353510788
H	.4404399370	-2.0663429303	-3.9688520928
H	-.2637446552	-1.6320389598	-2.3975433711
H	-.4386924473	-3.2763421058	-3.0189268632
H	2.5223772076	-3.5676536866	-4.0634385582
H	1.6856690984	-4.8248637315	-3.1486778627
H	3.2369374742	-4.2047228990	-2.5719074592
H	.4419465789	5.5718652324	.7118851390
H	.3302579813	6.2495682361	-1.6610956064
H	1.2487991199	4.7735058198	-3.4152562830
H	2.0819973313	2.4063733355	1.8868427914
H	.0302973352	2.5424931858	3.2594858088
H	-.3837298261	2.1476503145	1.5783582700
H	-.6369797621	3.7876456778	2.1958008560
H	2.0938415311	4.0053329255	3.7577572348
H	1.4643033450	5.2930964424	2.7270759383
H	3.0807787736	4.6408478234	2.4297231330
H	3.0068744951	1.5360938765	-2.7068319591
H	3.6921895869	2.3106714147	-4.9254245359
H	4.1833379674	3.5128421687	-3.7206007209
H	2.7792642900	3.8100810262	-4.7531449127
H	1.5432343637	.9558440925	-4.6154872483
H	.5822056161	2.4225688002	-4.3537210460
H	.5810333700	1.1399558012	-3.1376545442
H	-4.4507386805	.5888440250	-.1157989532
H	-2.3421283262	-.3912130645	.6902439914
N	-4.4198217707	-.3246522572	.3143116868
N	2.4357006149	-1.2279360127	.0577242764
N	2.5902695350	1.6321173995	-.3292678564
O	-.5933726303	.3371107603	-.2327391863
O	-2.5943537329	.0650684936	3.4217747408
O	-4.3216808994	.9884798292	2.6629984709
O	-5.7111546607	-2.1241015825	.9044046264
Cu	1.2485311290	.2683580358	-.1915770282

147.L¹CuOH⁺ / methane t.s.

C	-3.9153394348	-.4236636400	1.5870294525
C	.5365459120	-3.2526192773	-.1783045624
C	.3702955199	-3.7940864227	1.1256156279
C	-.2861133850	-5.0211765163	1.2387613812
C	-.7655565976	-5.6947417782	.1156958964
C	-.6182943188	-5.1357516254	-1.1528814232
C	.0124297207	-3.9031313211	-1.3278618834
C	.7973208922	-3.0428701570	2.3829456370
C	1.5570645442	-3.9287956353	3.3858128002
C	-.4260477279	-2.3865313261	3.0553654534
C	.1961081225	-3.3158245371	-2.7218896513
C	-1.0949997634	-3.3528806057	-3.5567446606
C	1.3515340941	-4.0130731280	-3.4686473713
C	.6623342817	2.0564707172	-1.0389066203
C	-.0914303978	2.8820894895	-.1554080432

C	-.7133649549	4.0138147705	-.6845596418
C	-.6306224446	4.3122292345	-2.0429481057
C	.0783010705	3.4737458471	-2.9045391378
C	.7378025732	2.3378463764	-2.4364064057
C	-.1623925592	2.6013254563	1.3396954808
C	-1.6179558695	2.4640977576	1.8236753202
C	.6031971222	3.6682614619	2.1459284648
C	1.4135749814	1.3973137570	-3.4302611929
C	2.3494836492	2.1305269624	-4.4081079656
C	.3553336974	.5819513536	-4.2020191017
C	3.3793042323	-3.0369287832	.0824303441
C	2.4920847317	-1.8396714638	-.1956414313
C	3.1402829350	-.5867283566	-.2675762754
C	2.5810830762	.6841509330	-.4817182615
C	3.5374675302	1.8393991039	-.6908764627
H	-3.8613247987	.6109926198	1.9248863282
H	-4.8077045162	-.6559591507	1.0068188721
H	-2.5728349978	-.8960699095	-.9305133164
H	4.3912672342	-2.8478034921	-.2803119146
H	2.9904791862	-3.9400081431	-.3907354231
H	3.4423378566	-3.2268662764	1.1587414798
H	4.2188940989	-.6142669216	-.1753556377
H	4.4660372173	1.6611406309	-.1449003022
H	-3.6886010360	-1.1591925406	2.3587524619
H	3.0989246577	2.7814012328	-.3565497328
H	3.7927714283	1.9462430569	-1.7501220580
H	-.4291284882	-5.4604213984	2.2203420571
H	-1.2594968513	-6.6545194087	.2307169411
H	-.9960793825	-5.6708985297	-2.0177384815
H	1.4704231146	-2.2322451480	2.0895568488
H	1.9277493152	-3.3207468217	4.2165248547
H	2.4127030412	-4.4283604480	2.9212137881
H	.9140301605	-4.7037804848	3.8134221918
H	-.1146321782	-1.7963230823	3.9233656072
H	-2.9062071424	-.5819651554	.7470529650
H	-1.1367010542	-3.1457594644	3.3977829565
H	-.9542831821	-1.7255108241	2.3608156047
H	.4822503603	-2.2660474672	-2.6008926290
H	-.9426868498	-2.8305059373	-4.5063068035
H	-1.9281287920	-2.8716659862	-3.0328903651
H	-1.4013621524	-4.3756104942	-3.7955951840
H	1.4974590975	-3.5620400373	-4.4555387843
H	1.1402514590	-5.0776098473	-3.6121881143
H	2.2937982318	-3.9314991880	-2.9180664129
H	-1.2632801211	4.6773422070	-.0250758917
H	-1.1224538482	5.1970377453	-2.4347113630
H	.1109482088	3.7093706719	-3.9630583513
H	.3346264306	1.6435652702	1.5216968372
H	-1.6376193371	2.2150266887	2.8896914051
H	-2.1296284082	1.6686575950	1.2726547976
H	-2.1830954934	3.3916468144	1.6898963893
H	.5871782393	3.4215039914	3.2120889367
H	.1550217720	4.6593790440	2.0236554044
H	1.6489492066	3.7337991575	1.8299633323
H	2.0226132706	.6800340219	-2.8742337962
H	2.8847449026	1.4048523860	-5.0278312072
H	3.0900570623	2.7403120368	-3.8818687491
H	1.7975081523	2.7900465491	-5.0842813872
H	.8401893104	-.1227992491	-4.8852472056
H	-.2927129682	1.2359112208	-4.7939628803
H	-.2835977823	.0078967434	-3.5215155976
N	1.1857231915	-2.0082598948	-.3834221048
N	1.2673685261	.8984015877	-.4966625759
O	-2.0310000329	-.7433856359	-.1408079386

Cu - .0906243633 - .4956748247 - .3895723609

148.L¹CuOH⁺ / cyclohexane t.s.

C	-4.4698396714	-1.1644582322	2.3313883034
C	1.3693464471	-1.5497992822	3.5540471855
C	1.3845653028	-2.9931998962	-2.1481894132
C	-3.0900981687	-1.2974713616	1.6252927440
C	-.0083290489	-3.0075420522	-2.8056199364
C	2.3825599542	-3.8308181553	-2.9732487009
C	2.2839633067	2.6294102267	-.4455029834
C	1.7072948856	3.4119869385	.5966848752
C	1.0719327754	4.6046424772	.2474886578
C	.9695308929	5.0055368631	-1.0825338092
C	1.5058434348	4.2126541382	-2.0961733761
C	2.0129470148	-2.7322239438	.3354233645
C	2.1720784076	3.0195913011	-1.8125916503
C	1.8195562925	3.0102061085	2.0640133921
C	.4438892468	2.9564208888	2.7550460053
C	-2.5772405742	.0839784474	1.2628221647
C	2.7816391868	3.9445321410	2.8249335787
C	2.6559575005	2.1368478765	-2.9605308875
C	3.4852074769	2.9104120747	-4.0018594632
C	1.4618284720	1.4266283579	-3.6339778708
C	-3.5191781452	.8783744352	.3793990545
C	4.8710047523	-2.6422010151	.2611045717
C	1.9368662318	-3.1497189414	1.6939572967
C	-4.8994643135	1.0082095207	1.0861535434
C	4.0129056827	-1.4073115479	.0534301750
C	-5.4586102728	-.3684078136	1.4696144341
C	4.7001179248	-.1813098759	-.0791005139
C	4.1832848547	1.1242950431	-.2010527195
C	5.1691239638	2.2451739250	-.4576622285
C	1.2341754227	-4.3225873738	1.9784452182
C	.6221536059	-5.0652625523	.9712611903
C	.6772923809	-4.6269482855	-.3501042186
C	1.3445573586	-3.4507563547	-.6942740596
C	2.5040647654	-2.3169874787	2.8412223959
C	3.3133483335	-3.1506595425	3.8513102079
H	-2.3832074666	-1.8269320650	2.2724727162
H	-3.2187834918	-1.9000982095	.7162532238
H	-2.2501540699	.6545510306	2.1436015156
H	-1.4994304971	-.0875464386	.6803589506
H	-3.1170617098	1.8729770320	.1576288324
H	-3.6670470102	.3599075959	-.5780571082
H	-5.5895511371	1.5415083574	.4223899669
H	-4.7829733151	1.6254639253	1.9865551594
H	-6.4063553226	-.2467100452	2.0081167768
H	-.7256545601	-.6342180983	-.8674428964
H	5.8592907514	-2.4943054484	-.1786122266
H	4.4083399716	-3.5249766791	-.1838671476
H	5.0078969072	-2.8434456315	1.3287598381
H	5.7805792692	-.2559793963	-.0944074992
H	6.1371808757	2.0099564902	-.0103051215
H	4.8058428081	3.1908608116	-.0500534207
H	5.3262464818	2.3842206125	-1.5329006807
H	1.1579602624	-4.6611924975	3.0068295045
H	.0930904612	-5.9810939113	1.2180313875
H	.1909257188	-5.2115366437	-1.1247822376
H	3.1798801035	-1.5648443489	2.4244983512
H	3.7859804751	-2.4930274827	4.5877329392
H	4.1005852455	-3.7328245727	3.3622094678
H	2.6797752732	-3.8515438254	4.4039313730
H	1.7760843120	-.9095336912	4.3441329532
H	.6568819087	-2.2422168781	4.0148178396

H	.8117681081	-.9178003569	2.8539129598
H	1.7454313908	-1.9595937132	-2.1577402626
H	.0372372409	-2.5531845903	-3.8004885036
H	-.7444087646	-2.4548334600	-2.2101422536
H	-.3951526367	-4.0236991406	-2.9312112252
H	2.4237860633	-3.4722064222	-4.0071305286
H	2.0866235764	-4.8849831732	-2.9939424728
H	3.3937288684	-3.7765227443	-2.5578228236
H	.6508342894	5.2318916141	1.0270528410
H	.4651623663	5.9342963275	-1.3322518768
H	1.3961107922	4.5282997726	-3.1288437184
H	2.2457542881	2.0028810962	2.1022932842
H	.5521654141	2.5957392698	3.7831754059
H	-.2410443915	2.2834699210	2.2282011798
H	-.0296138663	3.9422748736	2.8033433129
H	2.8879051929	3.6179837445	3.8644714638
H	2.4106367959	4.9747487073	2.8336135527
H	3.7776406640	3.9530966638	2.3707069284
H	3.2992824715	1.3536196098	-2.5499761206
H	-5.6893756431	-.9368001093	.5579783400
H	3.8935764080	2.2189171854	-4.7455010158
H	4.3213104686	3.4433409144	-3.5385703151
H	2.8811541587	3.6467153908	-4.5410188066
H	1.8096529676	.7599960087	-4.4301191485
H	.7692023378	2.1496460470	-4.0773966837
H	.8945088119	.8259644135	-2.9125752402
H	-4.8556635436	-2.1676046598	2.5470209452
H	-4.3312023455	-.6625691903	3.2980043773
N	2.6889511211	-1.5354527546	-.0193481874
N	2.8874734208	1.3954553734	-.0870237536
O	-.3412323437	-.4142987885	-.0043399351
Cu	1.5157984347	.0580933905	-.0285430380

149.L¹CuOH⁺ / acetonitrile t.s.

C	1.6264080404	-2.8833642114	.6591625010
C	1.4305932788	-3.4414830513	1.9534276657
C	.7526293007	-4.6583517672	2.0337543983
C	.2833787126	-5.3071222690	.8908851320
C	.4579352504	-4.7316897873	-.3674324122
C	1.1056015492	-3.5056588300	-.5121525136
C	1.8423431498	-2.7123664493	3.2280444131
C	2.5588856117	-3.6249980734	4.2385161005
C	.6187713343	-2.0367733230	3.8791607693
C	1.3210382862	-2.8990180015	-1.8925714704
C	-3.9116248404	-.8736212618	1.9240905297
C	.0426659083	-2.8966166161	-2.7470602497
C	2.4762118265	-3.6083192838	-2.6301143812
C	1.7649673982	2.4116495925	-.2167021934
C	1.0105321964	3.2531533502	.6524892079
C	.4106573389	4.3876996572	.1054111038
C	.5088259701	4.6695089967	-1.2554365472
C	1.2125072250	3.8127164091	-2.1041376351
C	1.8560936834	2.6758231521	-1.6196418211
C	.9138728529	2.9785658177	2.1462872917
C	-.5441686415	2.9755913361	2.6379660280
C	-2.7409845937	-.5124910332	2.6342229608
C	1.7701155191	3.9796973690	2.9475329520
C	2.5323513783	1.7217060620	-2.6008325046
C	3.4787838355	2.4425585836	-3.5792710837
C	1.4761727490	.9085482040	-3.3774748532
C	4.4684312730	-2.6661357545	1.0060798010
C	3.5857824773	-1.4754148734	.6893391621
C	4.2325862829	-.2231059464	.5981788312
C	3.6709520176	1.0433565511	.3529805145

C	4.6302844747	2.1907508875	.1169776066
H	-1.4620196361	-.6123277440	-.0110929986
H	5.4847018290	-2.4875511936	.6502125693
H	4.0830671235	-3.5793080982	.5494811520
H	4.5191822655	-2.8304476797	2.0870965804
H	5.3107782884	-.2469592120	.6963988745
H	5.5536192400	2.0286957873	.6766156795
H	-1.7307261746	-.4332028203	1.6579697414
H	4.1897076042	3.1433312387	.4164540903
H	4.8959168162	2.2630314109	-.9424486833
H	.5797386642	-5.1093652097	3.0049349220
H	-.2293065224	-6.2593487671	.9830399628
H	.0836814464	-5.2472557938	-1.2455691369
H	2.5378597979	-1.9120721779	2.9590241441
H	2.9155406087	-3.0347266488	5.0878058521
H	3.4182332951	-4.1334353460	3.7909563129
H	1.8901439398	-4.3936164338	4.6369161523
H	.9242257733	-1.4582082585	4.7568337514
H	-2.4057566535	-1.2667594197	3.3471846127
H	-.1119289347	-2.7853256429	4.2030607660
H	.1200513960	-1.3617226937	3.1778383776
H	1.6295165848	-1.8588576095	-1.7501517072
H	.2215299883	-2.3628196389	-3.6853849854
H	-.7890810438	-2.4061675203	-2.2302803756
H	-.2804733529	-3.9089899876	-3.0069930416
H	2.6503177294	-3.1421028725	-3.6051256442
H	2.2452991071	-4.6650274858	-2.7987913624
H	3.4090375806	-3.5579400004	-2.0597790300
H	-.1400141775	5.0639159938	.7504944448
H	-2.7766015763	.4899998959	3.0639174676
H	.0289583630	5.5546391809	-1.6607423515
H	1.2529776110	4.0354784319	-3.1649639618
H	1.3308003527	1.9831097501	2.3297889171
H	-.5787853803	2.7162524686	3.7008873984
H	-1.1453021891	2.2505034853	2.0813916704
H	-1.0140138201	3.9574123106	2.5276444159
H	1.7318290324	3.7421085471	4.0150882342
H	1.4064906146	5.0039003914	2.8173059933
H	2.8179951567	3.9547128368	2.6326757667
H	3.1359451037	1.0063615296	-2.0365216889
H	4.0130837188	1.7085579560	-4.1898652028
H	4.2200627265	3.0533019843	-3.0550593562
H	2.9345752694	3.0987985463	-4.2645894053
H	1.9646912307	.1935309355	-4.0472309909
H	.8434303960	1.5628956052	-3.9850121360
H	.8216352190	.3475064600	-2.7016905541
N	-4.8356595512	-1.1763485028	1.2721638197
N	2.2840126635	-1.6459491465	.4747573008
N	2.3569314541	1.2551037582	.3421892905
O	-.9058490245	-.4253817744	.7600158865
Cu	.9907082623	-.1324061226	.4710556456

150.L¹CuOH⁺ / toluene t.s.

C	-5.8519494212	-1.9615993422	.0160129325
C	.9417876000	-1.8851590261	3.6093706854
C	1.4030346937	-2.9871730736	-2.1512404629
C	-5.3501298343	-1.1018434517	-.9720658112
C	.0797395107	-2.9371753614	-2.9374397149
C	2.4647490185	-3.7983767252	-2.9216121971
C	2.3174589832	2.4066293599	-.4529617906
C	1.7051533995	3.2409043015	.5301279723
C	1.0728857977	4.4080920411	.0988867446
C	1.01244461340	4.7399406597	-1.2524669633
C	1.5929274870	3.9049820346	-2.2069127821

C	1.8346184254	-2.8897432179	.3840904130
C	2.2540691473	2.7315648274	-1.8413717504
C	1.7890173972	2.9326815045	2.0220995289
C	.3929413880	2.8329615209	2.6665590843
C	-4.3232911775	-.2219493200	-.6687249081
C	2.6623877745	3.9693820111	2.7579708612
C	2.7988224547	1.8073347044	-2.9263615391
C	3.7001128625	2.5438067785	-3.9354104871
C	1.6429710256	1.0849551968	-3.6506751625
C	-3.7740883313	-.1683105277	.6373736335
C	4.7005524356	-2.9013187988	.4935651274
C	1.6395126927	-3.3729815657	1.7069170831
C	-4.2876635483	-1.0548517942	1.6169730708
C	3.9044604646	-1.6336556433	.2443679368
C	-5.3162489517	-1.9328424724	1.3112997568
C	4.6487357199	-.4391259521	.1211400452
C	-2.6626004472	.7308683827	.9463717831
C	4.1834275060	.8743468713	-.0620169155
C	5.2054568418	1.9631048335	-.3136755852
C	.8820215589	-4.5359907769	1.8729526657
C	.3235098000	-5.1977032704	.7817520274
C	.4903581999	-4.6891171137	-.5055224927
C	1.2238955566	-3.5227035331	-.7334844808
C	2.1285811427	-2.6089703229	2.9346400642
C	2.8731244317	-3.4988143460	3.9461322387
H	-3.8718419721	-1.0297890124	2.6205060602
H	-5.7096277245	-2.5967080807	2.0748779229
H	-6.6573206841	-2.6496471320	-.2226196369
H	-2.5483579022	.9520326825	2.0108033026
H	-2.6317954390	1.6370903278	.3355345256
H	-1.6138266738	.1882720178	.6746352438
H	-.6855524464	-1.2517623947	-.1048648001
H	5.7164132928	-2.7941395630	.1087777930
H	4.2282862142	-3.7667699868	.0253154566
H	4.7692062499	-3.1039193068	1.5677614511
H	5.7248051683	-.5553250432	.1527727941
H	6.1624055704	1.7008742198	.1416796865
H	4.8667089801	2.9199812407	.0900714524
H	5.3734499992	2.0966624672	-1.3876962707
H	.7182000013	-4.9266317519	2.8723871129
H	-.2518913663	-6.1060070503	.9349769648
H	.0442482361	-5.2119900092	-1.3457364020
H	2.8264222184	-1.8344054682	2.6026031110
H	3.2836219921	-2.8858473504	4.7548811897
H	3.7009277496	-4.0429194050	3.4805040815
H	2.2092749451	-4.2382533808	4.4051850646
H	1.2929739588	-1.2700680660	4.4451015414
H	.2196813171	-2.6076597043	4.0054797902
H	.4130388885	-1.2416178913	2.8985711468
H	1.7722144244	-1.9595567167	-2.0700622037
H	.2364267349	-2.4464489270	-3.9035206796
H	-.6913915044	-2.3740037552	-2.3990920291
H	-.3203437712	-3.9354035132	-3.1417539308
H	2.6081050553	-3.3883644464	-3.9268287701
H	2.1590407879	-4.8448499675	-3.0254666594
H	3.4327759837	-3.7832474458	-2.4111557477
H	.6233751855	5.0718753259	.8310914075
H	.5100379487	5.6506773324	-1.5649460725
H	1.5216603123	4.1704696712	-3.2568401252
H	2.2711252301	1.9570742507	2.1366811852
H	.4834761302	2.5572529050	3.7224427719
H	-.2185338923	2.0729573570	2.1695091835
H	-.1485338335	3.7834047392	2.6193178914
H	2.7515247825	3.7078029679	3.8174424348

H	2.2264185134	4.9722649613	2.6984422175
H	3.6712958080	4.0192675323	2.3362663584
H	3.4063943597	1.0331382271	-2.4498916553
H	4.1495086414	1.8276335818	-4.6305270910
H	4.5096714954	3.0857919833	-3.4366714113
H	3.1375390118	3.2676516541	-4.5333760814
H	2.0362639967	.3855778674	-4.3960346357
H	.9934539802	1.7983171387	-4.1687166575
H	1.0209798235	.5194374777	-2.9478053208
H	-3.9369844044	.4492102190	-1.4311537477
H	-5.7704065040	-1.1239559940	-1.9728120757
N	2.5795669057	-1.7044934398	.1376113712
N	2.8919696943	1.1872971103	-.0149160192
O	-.3500464957	-.4526160383	.3246459401
Cu	1.4801685760	-.0711285252	.1721496295

151.L¹CuOH⁺ / phenol t.s.

C	-3.5918859007	-.8658238321	2.3213463910
C	1.7413837484	-1.3835747029	3.5813899553
C	2.0724854132	-2.9034055935	-2.1555402371
C	-2.6900325903	-.3821493521	1.3154622003
C	.7189398277	-2.7893809519	-2.8828858144
C	3.0098068742	-3.8772086370	-2.8992152321
C	2.7527194808	2.7099303229	-.5762221862
C	2.0373411466	3.4840673396	.3799201301
C	1.3848714763	4.6379395891	-.0609212372
C	1.4021999167	5.0079033031	-1.4033224149
C	2.0760099645	4.2215975067	-2.3367436111
C	2.5150857494	-2.5748214827	.3651829526
C	2.7596284410	3.0652835012	-1.9571788917
C	2.0082044372	3.1104828237	1.8582069738
C	.5678970623	2.9801881488	2.3907948066
C	-3.2248929156	.2666869988	.1495686987
C	2.8225236320	4.1129345442	2.7001187662
C	3.4011458283	2.1874873585	-3.0306077782
C	4.3330435160	2.9747167662	-3.9702742915
C	2.3178639071	1.4419625164	-3.8399778000
C	-4.5872592218	.3960849997	.0059037469
C	5.3910585361	-2.4843798473	.4106315950
C	2.3503080535	-2.9738870858	1.7214614984
C	-5.4606666236	-.1016619017	.9976251234
C	4.5417808794	-1.2529608821	.1626228906
C	-4.9499617106	-.7276865871	2.1519324532
C	5.2160407514	-.0193984903	.0583157051
C	4.6702626284	1.2653375371	-.1213928303
C	5.6377386759	2.4185384588	-.2908068410
C	1.6016489948	-4.1242547630	1.9800186756
C	1.0279838826	-4.8658385731	.9495867368
C	1.1821391222	-4.4551009614	-.3721176190
C	1.9067986612	-3.3058291915	-.6935846736
C	2.8875140592	-2.1517457089	2.8900057720
C	3.6628282337	-3.0033489256	3.9125603178
H	-2.5376766392	.6604858712	-.5911316506
H	-4.9980387359	.8853753574	-.8715491912
H	-6.5332481378	.0033022789	.8692093629
H	-.2466366281	-.0543544995	-1.1797573208
H	6.3993185120	-2.3362947530	.0190865806
H	4.9511894026	-3.3684104863	-.0554361935
H	5.4762725587	-2.6855127043	1.4839559301
H	6.2961581001	-.0676781368	.1174887652
H	6.5798698801	2.2029635878	.2170021144
H	5.2200354616	3.3467396431	.1047510706
H	5.8614581985	2.5804951942	-1.3507407415
H	1.4576400036	-4.4449946431	3.0070415808

H	.4569026468	-5.7612089759	1.1776457899
H	.7324574728	-5.0418089092	-1.1675411742
H	3.5813804293	-1.4037809598	2.4965722265
H	4.1240455664	-2.3581862033	4.6670866051
H	4.4557244091	-3.5892614500	3.4372994586
H	3.0075277249	-3.7029778799	4.4413033541
H	2.1358425887	-.7458472438	4.3796949131
H	1.0200387670	-2.0756303180	4.0288589413
H	1.1922712227	-.7504627582	2.8767447413
H	2.5435108904	-1.9159153737	-2.1760929689
H	.8627245391	-2.3869620544	-3.8912624377
H	.0332695976	-2.1276821051	-2.3427130852
H	.2246216648	-3.7608283988	-2.9875661735
H	3.1420028587	-3.5646723092	-3.9404314695
H	2.5995560320	-4.8928109961	-2.9042767067
H	3.9987268970	-3.9208200676	-2.4319993622
H	.8547650781	5.2571092526	.6562271349
H	.8838477617	5.9060944271	-1.7260013485
H	2.0620877700	4.5117900362	-3.3829090912
H	2.4844137275	2.1307379616	1.9643317679
H	.5820878976	2.6665779299	3.4400796189
H	-.0028982547	2.2391962628	1.8214620105
H	.0267831375	3.9308786301	2.3424153377
H	2.8305410830	3.8115288598	3.7527466218
H	2.3936509847	5.1191535697	2.6433276581
H	3.8607246567	4.1742934879	2.3583445188
H	4.0053250531	1.4214612357	-2.5376404210
H	-.7385225634	-.2566018302	.6382749782
H	4.8458954553	2.2888251313	-4.6521887991
H	5.0938652536	3.5312971092	-3.4145146190
H	3.7817634682	3.6930860509	-4.5852709440
H	2.7790522089	.7816340634	-4.5821210472
H	1.6664645840	2.1433302798	-4.3720665427
H	1.6837452461	.8279680615	-3.1895140055
H	-5.6334139556	-1.1028571351	2.9066513638
H	-3.1620792212	-1.3443563964	3.1945193336
N	3.2228725044	-1.3838701274	.0450017630
N	3.3615716920	1.5023920303	-.1396293637
O	-1.4220509444	-.5520139767	1.4944665710
O	.1094756825	.0266474490	-.2883288337
Cu	2.0193683576	.1440912294	-.1230716338

152.L¹CuOH⁺ / isopropylbenzene t.s.

C	-7.2129550689	.4177196397	-5.0519187854
C	-.6030132480	-2.4836667272	-3.1916441419
C	-.5226704196	-2.7397338002	-1.7931091576
C	-1.2462628744	-3.8219191866	-1.2889989944
C	-2.0205088569	-4.6303282842	-2.1200589439
C	-2.1147728817	-4.3474533194	-3.4822922732
C	-1.4332192391	-3.2658342972	-4.0409452725
C	.2232841604	-1.8205683332	-.8287978009
C	1.0838501211	-2.5860719734	.1920694645
C	-.7646226277	-.8818950125	-.1051637245
C	-1.5408691676	-2.9598162732	-5.5282109693
C	-6.0858348419	.3459135105	-4.2340033353
C	-2.9710134560	-3.1121083796	-6.0726781849
C	-.5539125061	-3.8181349616	-6.3462331425
C	-.1100159491	2.8222924296	-4.4032740699
C	-.6490984927	3.6009691316	-3.3439439539
C	-1.1222892294	4.8799133209	-3.6436128147
C	-1.1108325625	5.3635011357	-4.9498814479
C	-.6365099729	4.5625177687	-5.9890707171
C	-.1284538222	3.2849712721	-5.7486516363
C	-.7409141338	3.0690957319	-1.9186248653

C	-2.2227575199	2.9641762543	-1.5118665074
C	-6.1695803396	-.1608721870	-2.9282156553
C	.0733760977	3.9033993051	-.9157754797
C	.2756552160	2.3914864936	-6.9166170968
C	1.1554125862	3.1084408963	-7.9547895579
C	-.9830707000	1.7947833155	-7.5814331334
C	-7.4238428327	-.5893133465	-2.4594760424
C	2.2425574645	-2.5570019418	-3.5320391474
C	-8.5524600187	-.5093019837	-3.2733448642
C	1.4133698801	-1.3081296629	-3.7768727989
C	-8.4513590370	-.0116036576	-4.5743159770
C	2.1345799696	-.1225270237	-4.0078178051
C	-4.9575210825	-.2287115162	-2.0319303438
C	-4.8508913640	.9305766454	-1.0401760023
C	1.6704272728	1.2049336213	-4.1669093431
C	-4.6859484829	-1.5960184139	-1.4212008159
C	2.7188537763	2.2638066841	-4.4321234066
H	-9.5134601668	-.8374723044	-2.8889151815
H	-9.3308099594	.0428672598	-5.2079048734
H	-5.1313832914	.7107293678	-4.6036712451
H	-7.1225582355	.8112934741	-6.0598385601
H	-7.5193825053	-.9775063729	-1.4496896954
H	-3.9733230321	-.0808859138	-2.7742831064
H	-3.7750593388	-1.5841153993	-.8170789412
H	-4.5887685669	-2.3681456025	-2.1880675708
H	-5.5133394369	-1.8877004808	-.7596239383
H	-3.8284719889	1.0553694508	-.6675288303
H	-5.5173069341	.7449179846	-.1866089505
H	-5.1577871933	1.8738005758	-1.4993182057
H	-3.3544797838	-.5911913555	-4.4046717605
H	3.1834129939	-2.4904771364	-4.0820655785
H	1.7081009712	-3.4556742777	-3.8429472379
H	2.4859324594	-2.6638829515	-2.4704512607
H	3.2111045240	-.2388529672	-4.0418384430
H	3.6568644729	1.9969533320	-3.9411762866
H	2.3935451500	3.2426780352	-4.0760583644
H	2.9188577610	2.3485586531	-5.5054700021
H	-1.2117214892	-4.0364629637	-.2260924142
H	-2.5604249457	-5.4748858298	-1.7031779129
H	-2.7277804490	-4.9798238088	-4.1155557315
H	.8954805487	-1.1801765173	-1.4050378033
H	1.6806396056	-1.8819265002	.7796982413
H	1.7672898681	-3.2887487290	-.2941945531
H	.4697366620	-3.1556511113	.8960700893
H	-.2231721463	-.1890220349	.5474735307
H	-1.4629787965	-1.4518034653	.5165542904
H	-1.3514728808	-.2942338740	-.8181215738
H	-1.2362646153	-1.9158088910	-5.6675736479
H	-3.0231394754	-2.7360467370	-7.0989092022
H	-3.7035790101	-2.5653156019	-5.4685451238
H	-3.2904553732	-4.1584161031	-6.0982113484
H	-.6170682036	-3.5658595655	-7.4095979428
H	-.7801209767	-4.8836724718	-6.2361283097
H	.4789853614	-3.6588464000	-6.0225634830
H	-1.5105460597	5.5047316839	-2.8454784439
H	-1.4865433418	6.3594318597	-5.1628292294
H	-.6680647651	4.9406059732	-7.0054031387
H	-.3236058534	2.0578939609	-1.9131968513
H	-2.3624192869	2.3642778722	-.6045416971
H	-2.8053241900	2.4869674111	-2.3045415445
H	-2.6600148031	3.9512748842	-1.3287415140
H	-.0047607480	3.4717452633	.0871625753
H	-.2900496745	4.9345347495	-.8619732943
H	1.1324731970	3.9355922662	-1.1896097560

H	.8530174038	1.5493980564	-6.5254240498
H	1.4984112349	2.3956930248	-8.7107173533
H	2.0358814606	3.5651703041	-7.4925068782
H	.6081379933	3.8978699105	-8.4785911123
H	-.7038654686	1.1109158610	-8.3894515977
H	-1.6150495691	2.5820318522	-8.0045576414
H	-1.5894353219	1.2384424706	-6.8568311159
N	.0799155353	-1.3906695572	-3.7731359619
N	.3882524650	1.5286689102	-4.0836504951
O	-2.8974385094	-.2036489086	-3.6427292154
Cu	-1.0645332294	.2552846584	-3.9399576761

153.L¹CuOH⁺ / cyclohexadiene t.s.

C	-3.7200764875	-.1328459800	1.6825787399
C	1.1677480924	-1.4571512531	3.8517107382
C	1.3130301822	-3.0626116027	-1.8584181861
C	-2.5404822655	-.9972583618	1.8239686412
C	-.0773274556	-2.9103107164	-2.5060410158
C	2.1789808480	-4.0614413974	-2.6519848350
C	1.9487143290	2.5517500832	-.5529870311
C	1.3839186476	3.4068832102	.4321993018
C	.7071837354	4.5497552805	.0014153680
C	.5576174506	4.8324638228	-1.3536933737
C	1.0831431749	3.9655330518	-2.3101615358
C	1.8373571900	-2.7047521425	.6437607703
C	1.7803833426	2.8134782082	-1.9425174724
C	1.4988939287	3.1117912611	1.9239101536
C	.1062323242	2.9128531082	2.5568515360
C	-2.7256088710	-2.4110827965	1.4712376204
C	2.2954819381	4.2007696463	2.6664379858
C	2.2549837109	1.8454744291	-3.0243061911
C	3.0710309937	2.5362904372	-4.1320449949
C	1.0567049278	1.0830466216	-3.6301357060
C	-3.8748687241	-2.8690987034	.9213625763
C	4.7158942415	-2.5775582922	.5067801928
C	1.7207437606	-3.0902341152	2.0078929826
C	-5.0569662323	-1.9882242815	.6830475237
C	-4.8772012947	-.5774753437	1.1377240829
C	3.8391121970	-1.3661230580	.2652558496
C	4.4817387176	-.1364174525	.0178315724
C	3.9005754720	1.1248541692	-.2056877668
C	4.8280929141	2.2700964481	-.5574212024
C	1.0031828174	-4.2528931164	2.3034208345
C	.4141416896	-5.0187205534	1.2981261482
C	.5185010390	-4.6188693661	-.0322480376
C	1.2122603843	-3.4581511758	-.3879064342
C	2.2908845342	-2.2464323501	3.1454597518
C	3.0942560569	-3.0778075986	4.1621743354
H	-5.7272468432	.0926234029	1.0386519448
H	-3.6384687604	.8978506352	2.0165451700
H	-1.9934578123	-.8468147025	2.7674045057
H	-1.6834840968	-.5400868702	1.1146728080
H	-5.3300916988	-2.0060603388	-.3890705985
H	-1.0489355854	-.0434671004	-.6919184776
H	5.7015728414	-2.4351069750	.0608434643
H	4.2631936223	-3.4816386616	.0935641178
H	4.8532291289	-2.7420157903	1.5813915497
H	5.5629475306	-.1696693164	-.0231516309
H	5.8331452087	2.0772104741	-.1782966930
H	4.4634063989	3.2129179880	-.1441926384
H	4.8955298870	2.3900096796	-1.6440167047
H	.9043804459	-4.5691596938	3.3373413026
H	-.1235032997	-5.9277225423	1.5534059456
H	.0595728418	-5.2236739617	-.8086609588

H	2.9742275914	-1.5095014506	2.7141809593
H	3.5733073248	-2.4179786391	4.8923496920
H	3.8762086608	-3.6677977295	3.6740906144
H	2.4570208913	-3.7704668550	4.7212853236
H	1.5798523779	-.8323881380	4.6511552862
H	.4324622979	-2.1345647787	4.3006957157
H	.6380886842	-.8014158369	3.1508642916
H	1.8048291503	-2.0865903864	-1.9076875852
H	.0192092136	-2.5416808171	-3.5325280251
H	-.6996819501	-2.2032178464	-1.9467590831
H	-.6152342158	-3.8632654157	-2.5497447798
H	2.2702183772	-3.7444864722	-3.6962246383
H	1.7367912101	-5.0636132069	-2.6462622733
H	3.1875785737	-4.1411468781	-2.2344360123
H	.2854071311	5.2278466166	.7372136114
H	.0223756574	5.7241048314	-1.6668266867
H	.9388523829	4.1875523239	-3.3630655167
H	2.0471667260	2.1712970693	2.0357076050
H	.2045373894	2.6256605989	3.6096049345
H	-.4545511539	2.1315488634	2.0332497929
H	-.4866097830	3.8330395562	2.5200705422
H	2.4020611620	3.9393512648	3.7244617417
H	1.7925145380	5.1721725865	2.6147004872
H	3.2985666976	4.3223278452	2.2455445612
H	2.9035901124	1.0982194213	-2.5584821364
H	-1.8970296209	-3.0922186817	1.6456048460
H	3.4708594314	1.7899681104	-4.8260439460
H	3.9128324609	3.1030858753	-3.7225784926
H	2.4593147644	3.2299231113	-4.7176323736
H	1.4000249076	.3528829544	-4.3710729177
H	.3626186698	1.7677083543	-4.1290854189
H	.4933493531	.5437258225	-2.8597876150
H	-3.9736317290	-3.9193269431	.6586838241
H	-5.9519297576	-2.4241723488	1.1633938702
N	2.5165809089	-1.5020861967	.2915735110
N	2.5929337098	1.3611663917	-.1182832858
O	-.6034834170	.0469296340	.1617837683
Cu	1.2950568899	-.0126546599	.1588348074

154.L¹CuOH⁺ / dopamine t.s.

C	-2.4399509630	-.1433572884	1.3969124320
C	1.6732160632	-1.6820306992	3.7584109546
C	1.3345646094	-2.9888654045	-2.0516299495
C	-3.2973776025	-.9213207664	.5210308040
C	-.0686562895	-2.7129943416	-2.6261167810
C	2.0889090793	-4.0082059225	-2.9290510802
C	2.6914120900	2.5769324067	-.1693240262
C	2.3353077596	3.3660468859	.9582277157
C	1.7911709415	4.6324929069	.7292573819
C	1.5837528087	5.1081262681	-.5626195327
C	1.9234852047	4.3193783571	-1.6605417270
C	2.0147587445	-2.7867359018	.4278140719
C	2.4814403353	3.0491162276	-1.4959099154
C	2.5762052671	2.8912178704	2.3883879674
C	1.2762640712	2.8588120806	3.2141532004
C	-3.0837404242	-2.3065318220	.3064462991
C	3.6483722718	3.7505632150	3.0895123729
C	2.7865009911	2.1898961504	-2.7208225925
C	3.5802064920	2.9503641671	-3.7990401195
C	1.4883831010	1.6055515464	-3.3152145968
C	-3.9079715495	-3.0243231344	-.5375229288
C	4.8494318840	-2.9326291934	.1096669737
C	1.9465526348	-3.2299155001	1.7770643107
C	-4.9811787713	-2.3652287614	-1.2007916903

C	-5.1940123785	-.9960567216	-1.0210728484
C	4.0997142832	-1.6152845194	.0403600014
C	-4.3511911860	-.2797742847	-.1857897528
C	4.8768719815	-.4478637576	-.0808330468
C	-2.0267153341	-.7250615201	2.7524469121
C	4.4501231934	.8910634442	-.1020728038
C	5.5011667699	1.9593659805	-.3200622276
C	1.1463478842	-4.3393937123	2.0656712988
C	.4347279097	-5.0016566609	1.0679834785
C	.5059036259	-4.5533575525	-.2485376925
C	1.2783704445	-3.4417050473	-.5953625353
C	2.6658500210	-2.5095457940	2.9163350134
C	3.4675231960	-3.4690460756	3.8155430445
H	-1.2648712904	-.1074633713	.7915801954
H	-2.7309386018	.9096259184	1.4634138154
H	-2.2654364557	-2.8295850904	.7888588977
H	-6.0143326918	-.5034694752	-1.5367500068
H	-4.5100884583	.7850527069	-.0473155632
H	-1.4042627395	-1.6157653672	2.6122904677
H	-2.9513747532	-1.0686122315	3.2528549155
H	-4.3718178463	-4.6793702874	-1.3510272350
H	-6.4457379916	-2.6750779861	-2.4214043258
H	-.8019440782	-.1990078972	4.3098273818
H	-1.8652501916	.9750105231	3.8963920154
H	-.5688390645	-.1429061992	-.7946423815
H	5.8478430113	-2.8274016973	-.3179496540
H	4.3131561761	-3.7208209970	-.4231608276
H	4.9609328982	-3.2594675414	1.1487705489
H	5.9452540533	-.6014452565	-.1625780463
H	6.4929867106	1.5826328647	-.0652198178
H	5.2905739513	2.8476648089	.2799700080
H	5.5184120031	2.2719502533	-1.3699745996
H	1.0794386698	-4.6954080398	3.0893407805
H	-.1733958177	-5.8669729774	1.3158664673
H	-.0500420220	-5.0787627150	-1.0195117254
H	3.3766014754	-1.8018723166	2.4810514525
H	4.0514460458	-2.9005047728	4.5465421380
H	4.1607057351	-4.0863717397	3.2356534941
H	2.8151472147	-4.1453599840	4.3774988351
H	2.2032634542	-1.1303371258	4.5428764798
H	.9407399056	-2.3366017856	4.2466464514
H	1.1267067012	-.9565370507	3.1471358257
H	1.8980264811	-2.0513344295	-2.0851571727
H	.0071429765	-2.3142252740	-3.6435912018
H	-.6132175678	-1.9921972398	-2.0086757523
H	-.6769846214	-3.6224648329	-2.6746682707
H	2.1550047739	-3.6508824435	-3.9622990676
H	1.5776683900	-4.9769408975	-2.9421518641
H	3.1078992768	-4.1760564479	-2.5663029178
H	1.5297778581	5.2594914721	1.5765857869
H	1.1576577845	6.0954479894	-.7158987335
H	1.7494712167	4.7003354754	-2.6621203934
H	2.9588031037	1.8672921665	2.3385617064
H	1.4908672446	2.5175039297	4.2329753936
H	.5363368219	2.1755011138	2.7859536229
H	.8217253470	3.8526504944	3.2918864178
H	3.8531677864	3.3596738218	4.0918844387
H	3.3196244020	4.7896424949	3.1993405743
H	4.5909664253	3.7578822382	2.5325896893
H	3.4019801972	1.3437490728	-2.4029504674
H	3.8685678757	2.2686298061	-4.6056379036
H	4.4929950880	3.3934691975	-3.3886957679
H	2.9935696938	3.7573745301	-4.2492487143
H	1.7107963133	.9649826596	-4.1751726862

H	.8134811770	2.4007632115	-3.6495558430
H	.9475470877	1.0012370077	-2.5764807819
N	-1.2625799788	.2464745177	3.5227473848
N	2.7683770141	-1.6258549353	.0875037982
N	3.1793762424	1.2566819211	.0535765496
O	-5.7271850289	-3.1659891153	-1.9984568284
O	-.2056742875	-.2561436067	.0959162701
O	-3.6930254165	-4.3418859049	-.7456498826
Cu	1.7177727215	.0407979837	.1390401896

155.L¹CuOH⁺ / formylglycine t.s.

C	1.4911803316	-2.4472698938	.3278756140
C	1.3316555204	-2.8503939880	1.6809601307
C	.5800950905	-4.0020417011	1.9309078249
C	.0008218482	-4.7319395966	.8958312437
C	.1428186624	-4.3064016572	-.4226973364
C	.8683942614	-3.1547477556	-.7311483262
C	1.8614841988	-2.0302296331	2.8553070944
C	2.6280873815	-2.8895788781	3.8784053358
C	.7190725906	-1.2654548125	3.5528205804
C	.9921116565	-2.6787572290	-2.1728689522
C	-2.9148675732	-.5196428113	1.5212058060
C	-.3523551224	-2.7112388920	-2.9200363099
C	2.0663366536	-3.4774422047	-2.9363484054
C	1.8897387388	2.8712016230	-.6693928905
C	1.2088549628	3.6620677430	.2908934399
C	.7098180202	4.9043822604	-.1122006840
C	.8495128161	5.3438627606	-1.4251408707
C	1.4818057545	4.5348676478	-2.3692835753
C	2.0081302406	3.2887759186	-2.0218345587
C	1.0144842519	3.1845828845	1.7229985556
C	-.4811909544	3.0607716790	2.0699363002
C	-2.9335591818	.6781786428	2.5514277053
C	1.7639693345	4.0724134167	2.7326543654
C	2.6058156575	2.3875918662	-3.0986625620
C	3.6027391965	3.1177994275	-4.0152681790
C	1.4853218423	1.7300384251	-3.9296409083
C	4.3591236635	-2.3892187292	.4585778500
C	-4.3370725214	-1.4828320613	-.2349707033
C	3.5297427576	-1.1531655945	.1663849838
C	4.2236107224	.0642791617	.0694257118
C	3.6971861420	1.3481599079	-.1539203908
C	4.6981655867	2.4803543527	-.2813998964
H	-2.6085849742	-1.5104665977	1.8747829824
H	-5.3222587574	-1.3270867944	-.7103638721
H	-1.3522951393	-.2700076240	-.8649128896
H	5.3835824905	-2.2460758842	.1092962112
H	3.9358405807	-3.2746338939	-.0190878668
H	4.3960843528	-2.5821354499	1.5352085032
H	5.2997004578	.0060827778	.1740725678
H	5.6046567725	2.2430364406	.2788536939
H	4.2858715471	3.4206439333	.0891473810
H	4.9817468945	2.6324974762	-1.3280587880
H	.4329605759	-4.3267243982	2.9559438423
H	-.5767297782	-5.6239841158	1.1183901002
H	-.3300019859	-4.8713566383	-1.2190921955
H	2.5631057497	-1.2854024488	2.4696709177
H	3.0723549067	-2.2486578780	4.6466169654
H	3.4313443284	-3.4691212989	3.4113572099
H	1.9660940463	-3.5954641694	4.3895837026
H	1.1170108818	-.6488092961	4.3659285544
H	-.0092809726	-1.9578970389	3.9869821828
H	.1651920742	-.6056063153	2.8813868561
H	1.3339565395	-1.6389360806	-2.1433339761

H	- .2514419537	-2.2281809121	-3.8978462811
H	-1.1409275536	-2.2042899722	-2.3553526636
H	-.6947744516	-3.7352623786	-3.0994419554
H	2.1677204791	-3.1055202227	-3.9618569165
H	1.8031963969	-4.5396136067	-2.9858654036
H	3.0439730041	-3.3971514810	-2.4506834293
H	.1989968161	5.5296709545	.6133527643
H	.4545432898	6.3116491155	-1.7197227102
H	1.5587905723	4.8787009671	-3.3960825931
H	1.4494791926	2.1838297660	1.7970110100
H	-.6263613718	2.4477420722	2.9657372584
H	-1.0272609295	2.5578302071	1.2678790019
H	-.9411802239	4.0422607637	2.2281260399
H	1.6303118060	3.6831254217	3.7469214980
H	1.3863552815	5.1005712507	2.7182568979
H	2.8382638411	4.1076239779	2.5200823712
H	3.1492180360	1.5771443652	-2.6060118747
H	4.0752745688	2.4063304127	-4.7002734071
H	4.3925177976	3.6130013811	-3.4415446178
H	3.1111253988	3.8807150742	-4.6272246670
H	1.9076252788	1.0460174022	-4.6738050066
H	.8928959478	2.4844696186	-4.4577620401
H	.8025644706	1.1587674489	-3.2917471253
H	-4.6532859069	.2709200545	.8855303389
H	-1.8212103854	-.2399529946	.8018244957
N	-4.0685246843	-.5566554088	.7350850001
N	2.2139638763	-1.2686607049	-.0024314251
N	2.3947885762	1.6041731993	-.2546429764
O	-.8977170898	-.0680167096	-.0359126540
O	-1.9733242552	.6977768394	3.3409665039
O	-3.9233947212	1.4215480813	2.3849185310
O	-3.5737191207	-2.3807779415	-.5601657889
Cu	1.0007993148	.2682649161	-.1448708210