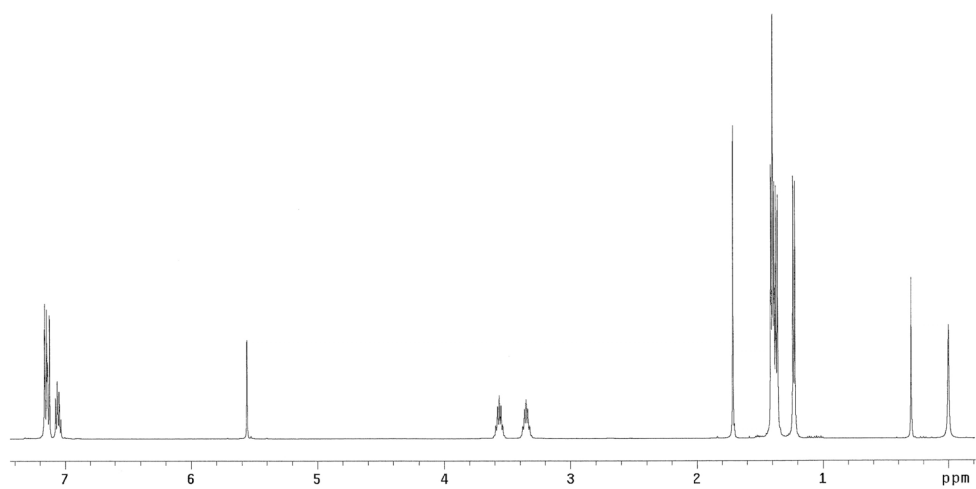


Supporting Information

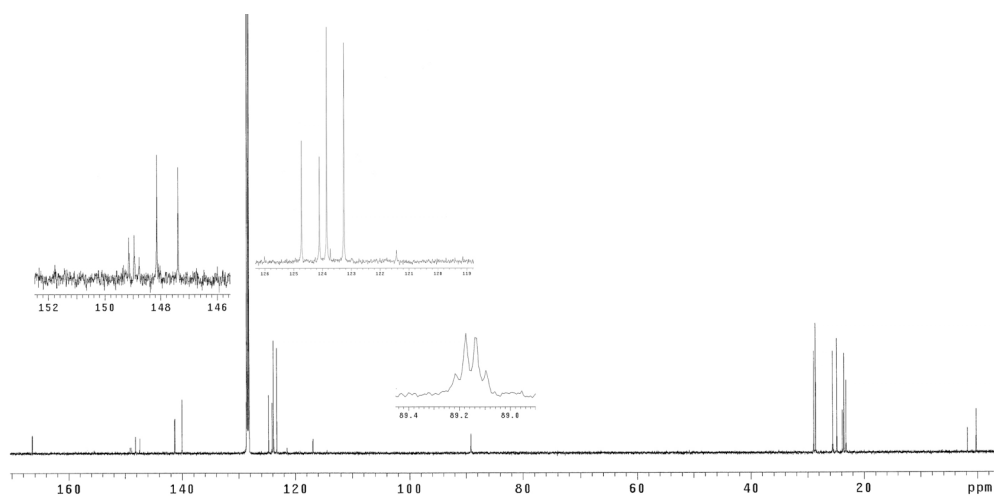
For

Electronic Tuning of β -Diketiminato Ligands with Fluorinated Substituents: Effects on the O₂-Reactivity of Mononuclear Cu(I) Complexes

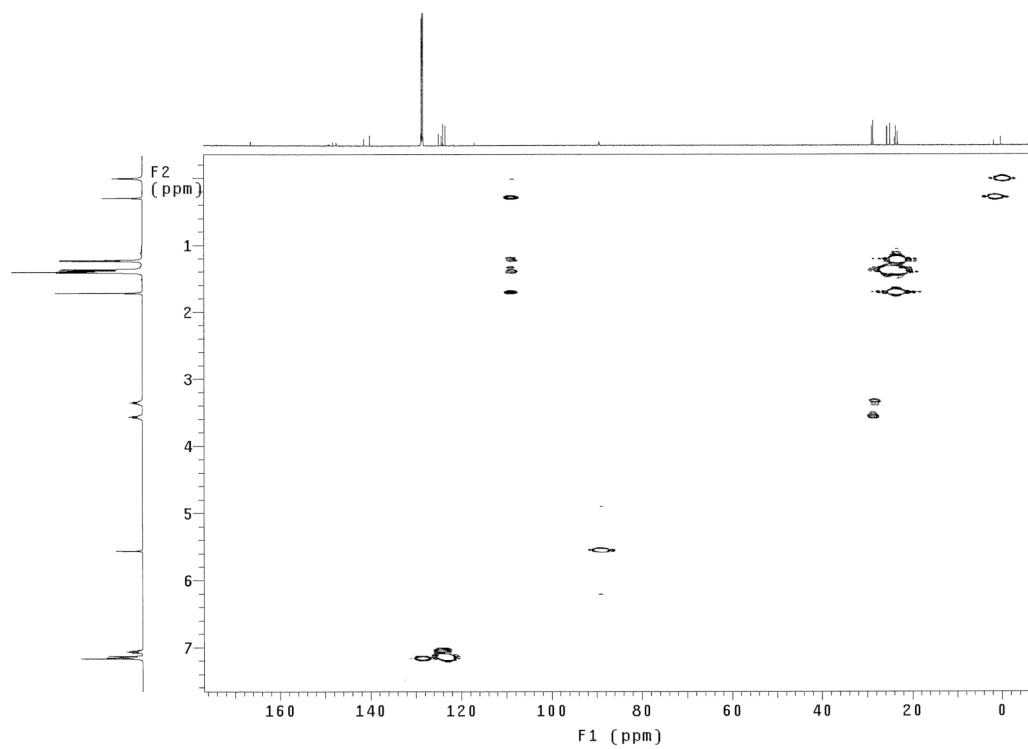
Lyndal M. R. Hill,^a Benjamin F. Gherman,^a Nermeen W. Aboeella,^a Christopher J. Cramer^a and William B. Tolman^{a,*}



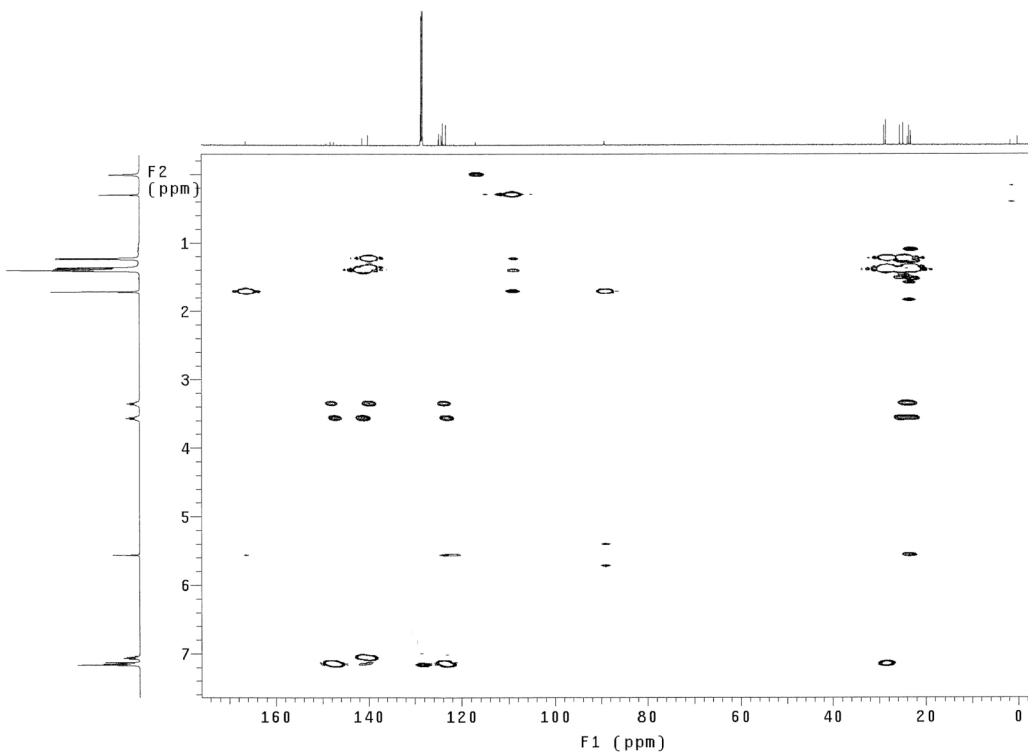
(a)



(b)



(c)



(d)

Figure S1. NMR spectra for $L^1Cu(CH_3CN)$ in benzene- d_6 . (a) 1H NMR spectrum (500 MHz). (b) ^{13}C NMR spectrum (125 MHz). The expanded regions are of the three quartets arising from C-F couplings (δ 89.16, 122.57 and 149.04 ppm). (c) HMQC (1H : 500 MHz). (d) HMBC (1H : 500 MHz).

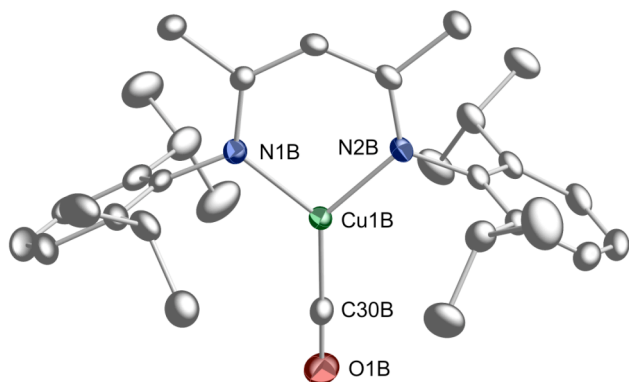


Figure S2. Representation of the X-ray structure of LCu(CO) (molecule B), showing all non-hydrogen atoms as 50 % ellipsoids. The asymmetric unit contains four molecules (A-D), resulting in $Z = 16$ and $Z' = 4$ for the monoclinic cell setting ($P2_1/n$).

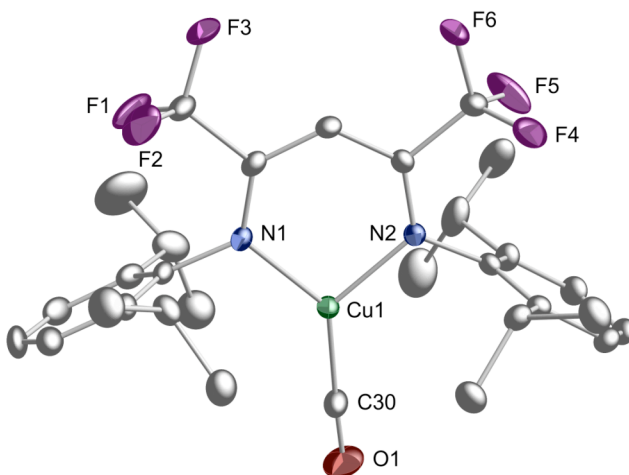


Figure S3. Representation of the X-ray structure of $L^2Cu(CO)$, showing all non-hydrogen atoms as 50 % ellipsoids.

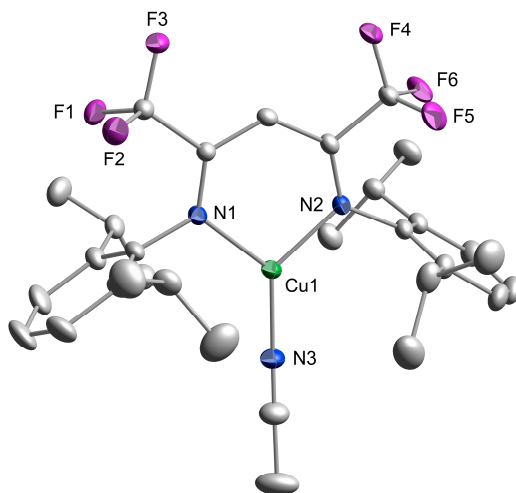


Figure S4. Representation of the X-ray structure of $L^2Cu(CH_3CN)$, showing all non-hydrogen atoms as 50% thermal ellipsoids.

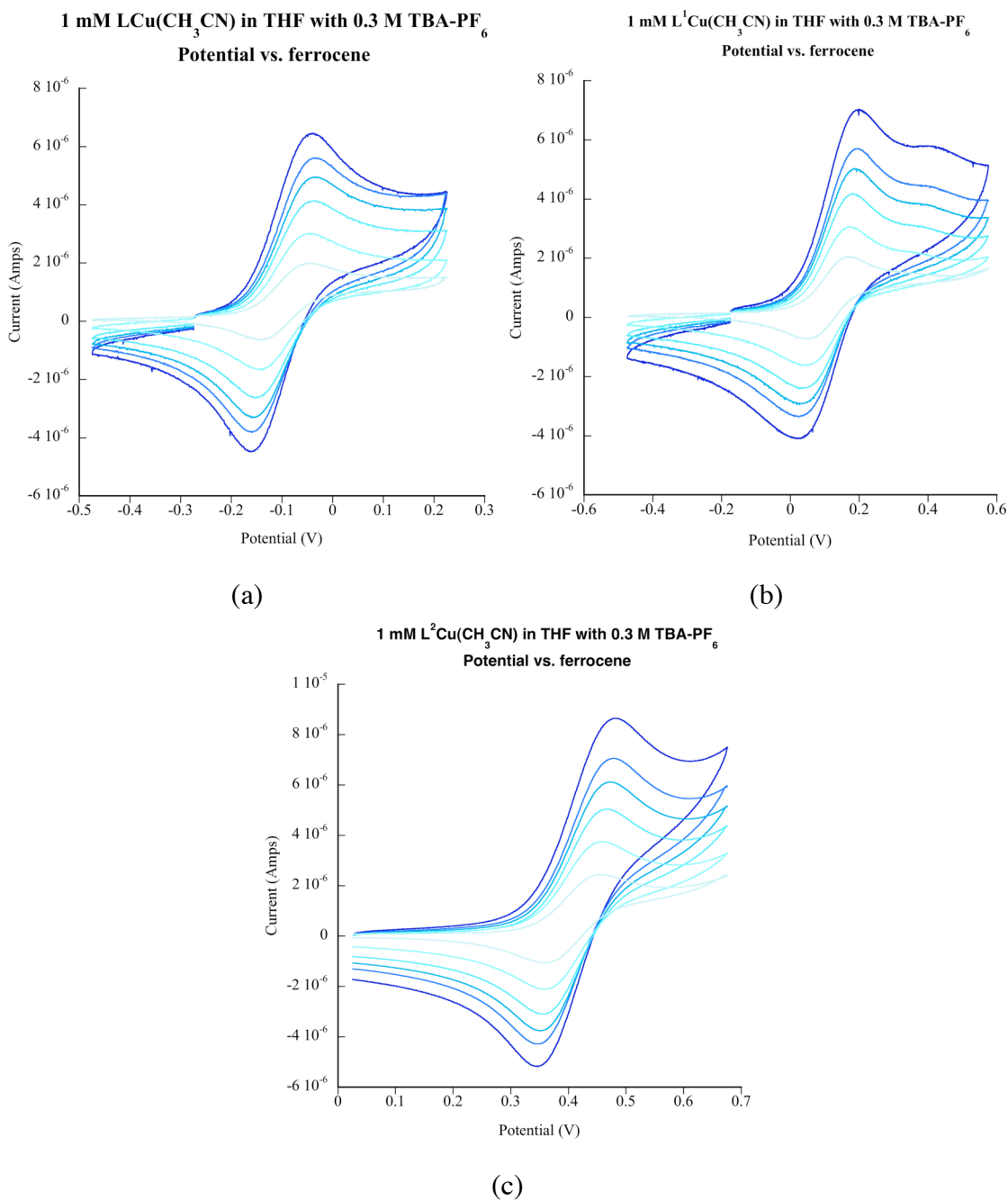


Figure S5. Cyclic voltammograms for (L, L¹ or L²)Cu(CH₃CN). Traces at six different scan rates are shown for each complex, with the darkest trace corresponding to the fastest scan rate, and the lightest the slowest scan rate. Scan rates: 300, 200, 150, 100, 50 and 20 mV/s.

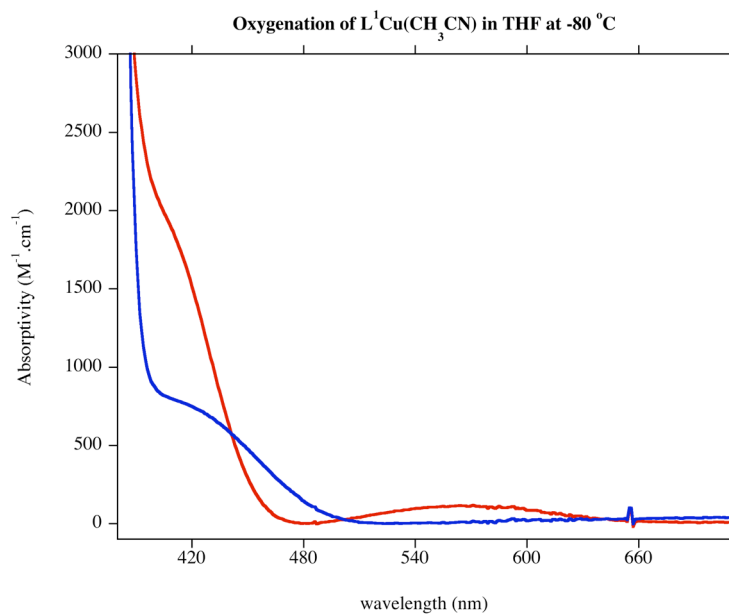


Figure S6. UV-Vis traces for $L^1Cu(CH_3CN)$ (blue) and $L^1Cu(O_2)$ (red); absorption coefficients were calculated based on the concentration of $L^1Cu(CH_3CN)$ (0.4 mM).

Table S1. Singlet-triplet free energy differences ($^1A - ^3A$, kcal/mol) at -80 °C in THF for 1:1 Cu-O₂ adducts supported by L, L¹, and L².

	end-on	side-on
LCuO ₂	+10.0 ^a	+6.9 ^a
L ¹ CuO ₂	+9.3	+4.1
L ² CuO ₂	+10.0	+2.9

^a -50 °C, THF (ref. 1).

Protonation of the 1:1 Cu-O₂ adducts leads to Cu(III)-hydroperoxide species. The singlet states for these CuO₂H⁺ structures are generally lower in energy than the triplets (Table S2), with the only exception being the η^2 LCuO₂H⁺ case, which retains a nontrivial degree of superoxide-like character.² The O–O bond lengths in CuO₂H⁺ shorten by ~0.004 Å and ~0.008 Å (Table S3) in the end-on and side-on cases with the addition of each CF₃ group to the ligand backbone in response to the decreasing ability of the β -diketiminato ligand to act as an electron donor. Mulliken population analysis supports this view as the magnitude of the Mulliken charge on the dioxygen unit in CuO₂H⁺ (Table S4) decreases in going from L to L². The large energetic preference for the end-on versus side-on isomer of LCuO₂H⁺ (10.3 kcal/mol) drops sharply to 2.0 kcal/mol and 0.4 kcal/mol with L¹ and L² (Table S5) as the electron donating character of the supporting ligand decreases and the presence of superoxide character in the side-on isomers² becomes less unfavorable. With the one-electron reduced forms CuO₂⁻ and the hydrogenated forms CuO₂H, free energy differences between the η^1 and η^2 isomers are small at ~1-2 kcal/mol (Table S5),² with a slight trend towards increasing preference for the end-on isomers as CF₃ groups are added to the ligand backbone.

Table S2. Singlet-triplet free energy differences ($^1A - ^3A$, kcal/mol) at -80 °C in THF for the protonated 1:1 Cu-O₂ adducts supported by L, L¹, and L².

	end-on	side-on
LCuO ₂ H ⁺	-7.9 ^a	+5.2 ^a
L ¹ CuO ₂ H ⁺	-8.7	-5.4
L ² CuO ₂ H ⁺	-4.3	-1.3

^a -50 °C, THF (ref. 2).

Table S3. O–O bond distances (Å) in the singlet end-on and side-on protonated 1:1 Cu-O₂ adducts supported by L, L¹, and L².

	end-on	side-on
LCuO ₂ H ⁺	1.404 ^a	1.438 ^a
L ¹ CuO ₂ H ⁺	1.401	1.431
L ² CuO ₂ H ⁺	1.397	1.420

^a Ref. 2.

Table S4. Mulliken charge populations on dioxygen in the singlet end-on and side-on protonated 1:1 Cu-O₂ adducts supported by L, L¹, and L².

	end-on	side-on
LCuO ₂ H ⁺	-0.63 ^a	-0.64 ^a
L ¹ CuO ₂ H ⁺	-0.62	-0.65
L ² CuO ₂ H ⁺	-0.60	-0.63

^a Ref. 2.

Table S5. Free energy differences (-80 °C, THF) between side-on and end-on ($\eta^2 - \eta^1$) isomers of LCuO₂H⁺ (singlets), LCuO₂⁻, and LCuO₂H supported by L, L¹, and L². All energies in kcal/mol.

	CuO ₂ H ⁺	CuO ₂ ⁻	CuO ₂ H
L	+10.3 ^{a,b}	-2.1 ^a	-1.3 ^a
L ¹	+2.0	-1.0	-0.9
L ²	+0.4	+0.1	+0.5

^a -50 °C, THF (ref. 2).

^b Lowest energy η^2 geometry is a triplet.

Table S6. Reduction potentials (-80 °C, THF) and pK_b (25 °C, H₂O) values for the singlet end-on 1:1 Cu-O₂ adducts supported by L, L¹, and L² and gas phase bond dissociation energies (BDEs) for a hydrogen atom bound to the oxygen moiety.

	E _o (V)	pK _b	BDE (kcal/mol)
LCuO ₂	-1.92 ^a	10.5 ^a	60.9 ^a
L ¹ CuO ₂	-1.71	16.1	60.1
L ² CuO ₂	-1.49	23.5	60.8

^a Ref. 2.

References

- (1) N. W. Aboelella, S. V. Kryatov, B. F. Gherman, W. W. Brennessel, V. G. Young, Jr., R. Sarangi, E. V. Rybak-Akimova, K. O. Hodgson, B. Hedman, E. I. Solomon, C. J. Cramer and W. B. Tolman, *J. Am. Chem. Soc.*, 2004, **126**, 16896.
- (2) B. F. Gherman, W. B. Tolman and C. J. Cramer, *J. Comput. Chem.*, 2006, in press.

Atomic Coordinates for Computed Structures.

1. L ¹ Cu(MeCN)			
Cu	-.0485744021	.1706789531	-.0861457426
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2. L²Cu(MeCN)

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3. L¹CuO₂ – side-on singlet

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H	2.2554560997	-1.0864761579	-3.7406499554
H	2.0959543579	1.9955251988	-4.2238394092
H	3.5955391865	1.1551368321	-3.8320934073
H	3.0636979548	2.5163461332	-2.8324483217
H	-5.4799454088	-1.9062882431	2.2121907519
H	-6.6887086939	-2.0575606601	.0657158636
H	-5.7313772500	-1.0290160619	-1.9647894961
H	-2.2527426358	-.0564441097	2.6709512311
H	-1.9060570059	-2.1585621535	3.9141801593
H	-1.9229204728	-2.4905977356	2.1670882391
H	-3.3339702708	-2.8814701231	3.1575912725
H	-3.3461395751	-.2512978627	4.8632747698
H	-4.7976315483	-.9411301678	4.1357360230
H	-4.3541572611	.7347447898	3.7908950634
H	-2.5253417996	.9154265220	-2.0107154678
H	-3.8725941588	1.6292489471	-3.9394800472
H	-4.7046116133	2.0777879329	-2.4412878604
H	-5.2577742398	.6887543599	-3.3834651956
H	-2.4095396807	-.4808524076	-4.0409280656
H	-3.7675727150	-1.4686226312	-3.4806967112
H	-2.2364450287	-1.5040121832	-2.5966259132

4. L¹CuO₂ – side-on triplet

Cu	-.5489122419	-.4989935801	.0436610528
O	.1994802371	-2.3498042132	-.3823727072
O	-1.0967339787	-2.4279396442	-.3129555177
N	.8678422466	.7962353616	.2391223196
N	-2.1139505501	.5854820325	.3494195333
C	1.6800430122	3.0744395458	.6843145696
C	.5431443214	2.0503531507	.5292101260
C	-.7517748454	2.5541375487	.7083235971
C	-1.9943380113	1.8775868753	.6238428896
C	-3.2439046522	2.7011266270	.8646064817
C	2.1995288277	.2933535906	.0318043543
C	2.8933051919	-.2979830057	1.1142368968
C	4.1291694095	-.9010399072	.8574995964
C	4.6670027032	-.9361511403	-.4253027333
C	3.9624441755	-.3695558900	-1.4821657195
C	2.7214365822	.2450858354	-1.2836928151
C	2.3088675262	-.3532364086	2.5240025755

C	3.2838778674	.1712269127	3.5932000123
C	1.8482572572	-1.7856696146	2.8642010614
C	1.9422266866	.7703741718	-2.4875267155
C	1.3809613188	-.4015331965	-3.3195446352
C	2.7727020604	1.7158654347	-3.3741825483
C	-3.3860577620	-.0766839008	.2759387992
C	-3.9161095371	-.6984890581	1.4327932118
C	-5.1142972854	-1.4116021077	1.3141791156
C	-5.7721278675	-1.5259537069	.0937223518
C	-5.2255266501	-.9321969019	-1.0392994918
C	-4.0299894189	-.2071816547	-.9779792554
C	-3.1880779850	-.6760572104	2.7752478427
C	-2.6032153775	-2.0671535678	3.0977318311
C	-4.0804273740	-.1806732418	3.9279648548
C	-3.4285718894	.3562549044	-2.2637482280
C	-4.4072791003	1.2685101664	-3.0255608342
C	-2.9233519655	-.7837005025	-3.1736794205
F	1.2390230783	4.3053080115	1.0100218324
F	2.3814295091	3.2035484404	-.4622848089
F	2.5460155737	2.7041425950	1.6506825318
H	-.8144978973	3.6052013275	.9431014395
H	-2.9987972998	3.7466814731	1.0543754573
H	-3.8036668212	2.3102847323	1.7202332679
H	-3.9135173364	2.6465728439	.0005704808
H	4.6748928100	-1.3611295540	1.6762378310
H	5.6266878928	-1.4138880724	-.6030009248
H	4.3780568220	-.4162211982	-2.4851974746
H	1.4245850926	.2899134545	2.5477193407
H	2.8017134825	.1694516411	4.5777973239
H	3.6021291848	1.1925254701	3.3707117877
H	4.1808417177	-.4540170201	3.6687800619
H	1.3747552259	-1.8156983734	3.8534999578
H	2.6975813198	-2.4786361611	2.8771151418
H	1.1304659819	-2.1646873227	2.1292588527
H	1.0905362857	1.3436340653	-2.1126742774
H	.7629953674	-.0307799102	-4.1460832308
H	.7687495226	-1.0735801554	-2.7091999922
H	2.1913405505	-1.0007129689	-3.7494085377
H	2.1491854600	2.1246522351	-4.1775238329
H	3.6129464372	1.1978156387	-3.8486925758
H	3.1745233642	2.5507710291	-2.7950677343
H	-5.5318057923	-1.8981388386	2.1915306849
H	-6.6992018071	-2.0883849543	.0231225701
H	-5.7298271272	-1.0447098220	-1.9952325292
H	-2.3470530812	.0187741409	2.6912893466
H	-2.0262706903	-2.0379204426	4.0294074796
H	-1.9442326669	-2.4193252009	2.2976967268
H	-3.3992428977	-2.8109736926	3.2185614972
H	-3.5008979265	-.1149921046	4.8554761879
H	-4.9195141274	-.8600477540	4.1141989034
H	-4.4969306168	.8099413968	3.7192049498
H	-2.5607439832	.9637372728	-1.9905001013

H	-3.9169484897	1.7020192366	-3.9040695729
H	-4.7648173586	2.0911197211	-2.3972185775
H	-5.2849275552	.7170606510	-3.3798573712
H	-2.4328251990	-.3791183990	-4.0659034218
H	-3.7513362856	-1.4196247985	-3.5060153901
H	-2.2070664538	-1.4248071805	-2.6508479562

5. L¹CuO₂ – end-on singlet

Cu	-.8951922830	-.6211673471	-.0347551010
O	-1.0474578251	-3.3296129855	.5678312250
O	-.9022428041	-2.1478610509	1.0234723969
N	.5963522687	.3309175757	-.8130092819
N	-2.3416649479	.5625455477	-.4973977327
C	1.5937063102	2.2307759333	-2.0164161522
C	.3815255535	1.4856743058	-1.4304441538
C	-.8564342637	2.1144529093	-1.6061278585
C	-2.1326054966	1.6869357352	-1.1667209379
C	-3.3114771056	2.5846097550	-1.4885798510
C	1.8682720704	-.2960224083	-.6014420901
C	2.5762844618	-.0358356395	.5990528782
C	3.7539009317	-.7490678626	.8393652529
C	4.2211625272	-1.7015331585	-.0615291749
C	3.5032431392	-1.9617898932	-1.2239184013
C	2.3183088503	-1.2793623478	-1.5168663624
C	2.0495215033	.9285424348	1.6583102092
C	3.1088227087	1.9405045882	2.1298307140
C	1.4722039909	.1412063135	2.8537976424
C	1.5239147923	-1.6508189435	-2.7646842870
C	.8532388146	-3.0297941869	-2.5894794856
C	2.3799508214	-1.6176351601	-4.0440421214
C	-3.6396848757	.1432843922	-.0617340773
C	-4.0825592031	.4877135633	1.2396820699
C	-5.3221713007	.0024216505	1.6675586863
C	-6.1042143982	-.8100251543	.8514190640
C	-5.6453588606	-1.1622632454	-.4138834234
C	-4.4126519923	-.7046609675	-.8934049121
C	-3.2187484027	1.3015119937	2.1997996568
C	-2.6667057007	.3993760747	3.3237593183
C	-3.9580004337	2.5174447284	2.7866172041
C	-3.9081823538	-1.1774214328	-2.2536236097
C	-4.9305496035	-.9423202212	-3.3800206252
C	-3.4907822489	-2.6621680027	-2.1914684347
F	1.2517201460	3.3687469720	-2.6533842841
F	2.2545096706	1.4667525414	-2.9115001581
F	2.4713481482	2.5739201564	-1.0489855052
H	-.8370938102	3.0510730275	-2.1409133673
H	-2.9954075242	3.4692960241	-2.0427455997
H	-3.8122562993	2.9050842084	-.5694279622
H	-4.0566843222	2.0445401847	-2.0810081820
H	4.3094148659	-.5642077433	1.7541651982
H	5.1364729029	-2.2480387192	.1484456454
H	3.8638124113	-2.7187361074	-1.9143478877

H	1.2296279534	1.5010097676	1.2161200846
H	2.6639378461	2.6494380057	2.8371098193
H	3.5161333045	2.5077566242	1.2888852763
H	3.9429899829	1.4502477089	2.6435235406
H	1.0223824239	.8223847178	3.5848919840
H	2.2578578554	-.4272978220	3.3640644787
H	.7063008982	-.5751265811	2.5385747241
H	.7275554750	-.9118398286	-2.8879312185
H	.2453739420	-3.2750566938	-3.4678882314
H	.2049265514	-3.0629879885	-1.7076513960
H	1.6046757002	-3.8186258200	-2.4725761756
H	1.7544604583	-1.8189667731	-4.9206789224
H	3.1690342501	-2.3773550034	-4.0266898531
H	2.8534316035	-.6415992411	-4.1791737296
H	-5.6759626872	.2543805456	2.6633979773
H	-7.0616709655	-1.1798456029	1.2072720581
H	-6.2486897700	-1.8160199899	-1.0370365897
H	-2.3612301562	1.6818948413	1.6381657310
H	-1.9894015198	.9637775141	3.9744214236
H	-2.1157045021	-.4557740718	2.9190869662
H	-3.4777472066	.0038890305	3.9450959530
H	-3.2796578316	3.1081111726	3.4119210516
H	-4.8027239945	2.2168417889	3.4154611866
H	-4.3467134589	3.1717779689	1.9996200449
H	-3.0133425488	-.5985232342	-2.5002894908
H	-4.4990996389	-1.2217518643	-4.3470232216
H	-5.2340135472	.1083562294	-3.4365976852
H	-5.8363956638	-1.5425430435	-3.2413648686
H	-3.0845283835	-2.9872131123	-3.1556368359
H	-4.3494675287	-3.3012316653	-1.9564889340
H	-2.7291425533	-2.8397353914	-1.4252119919

6. L¹CuO₂ – end-on triplet

Cu	-.7909283173	-.6681275363	-.1136165550
O	-2.5031454455	-2.7126279420	1.0849513866
O	-1.3574166040	-2.2699483270	.8333594982
N	.6899412686	.3323879657	-.8066424559
N	-2.3482224360	.4521619631	-.5003327478
C	1.5821081001	2.2783703301	-2.0172024327
C	.4138345247	1.4792935636	-1.4159286802
C	-.8567015256	2.0508785648	-1.5735111376
C	-2.1301858446	1.5964912428	-1.1368133636
C	-3.3059082482	2.5110695569	-1.4302381324
C	1.9934622314	-.2352952355	-.5995414604
C	2.6948591423	.0504457198	.5970177213
C	3.8869257348	-.6378791921	.8467855990
C	4.3779620713	-1.5857840156	-.0451118042
C	3.6717139207	-1.8635528004	-1.2110397963
C	2.4749968377	-1.2057105646	-1.5111813314
C	2.1521614449	1.0242023126	1.6395836362
C	3.2097365223	2.0331439707	2.1216607752
C	1.5424142049	.2561811035	2.8310457646

C	1.6879486913	-1.5918112996	-2.7598709025
C	.9484983680	-2.9278027837	-2.5390035806
C	2.5615606335	-1.6502519079	-4.0249729399
C	-3.6405099973	.0500825514	-.0486720673
C	-4.0498647826	.3825061480	1.2689705093
C	-5.2996255589	-.0644114408	1.7086513059
C	-6.1233505805	-.8341495605	.8923340312
C	-5.6928320345	-1.1872705037	-.3822045944
C	-4.4514019588	-.7685620230	-.8736316454
C	-3.1558836205	1.1702950802	2.2264469105
C	-2.7144464930	.2973522014	3.4200184929
C	-3.8237792450	2.4653988660	2.7255047383
C	-3.9951309911	-1.2288574244	-2.2561903360
C	-4.9596165653	-.7800959134	-3.3706948694
C	-3.7981072213	-2.7584418598	-2.2966739863
F	1.1890333621	3.4080650119	-2.6393935395
F	2.2538287610	1.5441696039	-2.9313177120
F	2.4680203052	2.6463500726	-1.0654783309
H	-.8710915891	2.9934970501	-2.0984195688
H	-2.9929596638	3.3934873322	-1.9895964513
H	-3.7786075013	2.8373414693	-.4983343106
H	-4.0738558433	1.9836454065	-2.0035279696
H	4.4362372406	-.4338518074	1.7614267455
H	5.3038454455	-2.1112767711	.1711989792
H	4.0533501384	-2.6125593542	-1.8987046068
H	1.3462896796	1.5985560905	1.1756915328
H	2.7553306955	2.7606962770	2.8032141790
H	3.6444468106	2.5792870886	1.2804087448
H	4.0253001945	1.5449916298	2.6661741632
H	1.1119502765	.9494252025	3.5625787750
H	2.3018504920	-.3449683574	3.3439078923
H	.7485989687	-.4261122372	2.5059774733
H	.9300190479	-.8226558091	-2.9275818746
H	.3433546277	-3.1889504570	-3.4147010315
H	.2809711153	-2.8808091581	-1.6704579415
H	1.6561717916	-3.7454704202	-2.3628075297
H	1.9388103138	-1.8458495902	-4.9050415832
H	3.3091708551	-2.4495665358	-3.9732190947
H	3.0879509406	-.7044347932	-4.1825938588
H	-5.6291336731	.1868997126	2.7133753633
H	-7.0903242470	-1.1706463613	1.2556841778
H	-6.3275596434	-1.8103648563	-1.0059422928
H	-2.2515455448	1.4562646082	1.6816078119
H	-2.0215898536	.8497452348	4.0648451640
H	-2.2134088374	-.6155253371	3.0851000171
H	-3.5719192195	-.0027430436	4.0326593043
H	-3.1324414284	3.0301840651	3.3606041093
H	-4.7189335484	2.2545601424	3.3204431978
H	-4.1232461752	3.1128631382	1.8953665805
H	-3.0229215665	-.7692593537	-2.4574240402
H	-4.5729914242	-1.0763297262	-4.3519803039
H	-5.0950600546	.3063966780	-3.3766192609

H	-5.9491923351	-1.2362049194	-3.2549418861
H	-3.4089757202	-3.0697590238	-3.2726864143
H	-4.7443744115	-3.2860499080	-2.1322125950
H	-3.0980298176	-3.0917175030	-1.5253948671

7. L¹CuO₂H⁺ – side-on singlet

Cu	-.1630697222	-1.0397960557	-.3451784875
O	.9154060262	-2.4714189681	-.7525888789
O	-.1328762037	-3.4129745996	-1.0020359332
N	1.3648019993	.1284882544	.1255273256
N	-1.5808094724	.1572241600	-.1417724681
H	-.0680078358	-4.0162567355	-.2390632430
C	-2.6807934899	2.2554107429	.4951763144
C	2.5932732056	-.4167184806	-.2465787926
C	3.2204894769	-1.3083438920	.6890661222
C	4.4840786496	-1.7942732511	.3705537368
C	5.0874450233	-1.4833713232	-.8473688322
C	4.4258425068	-.6940537288	-1.7927049146
C	3.1686552036	-.1587070240	-1.5380233916
C	2.5851796603	-1.6491358756	2.0274162402
C	3.2842094550	-.8944940390	3.1795519565
C	2.5750334787	-3.1676289791	2.2860237440
C	2.4106973193	.5526319854	-2.6515742614
C	1.7966034643	-.5028076162	-3.6036100729
C	3.2751010137	1.5524729520	-3.4399182868
C	-2.7692509106	-.6226379980	-.0935029926
C	-3.3006709116	-1.0404576976	1.1644241166
C	-4.4198102258	-1.8715949547	1.1458117146
C	-5.0007106385	-2.2824312556	-.0547818569
C	-4.4577559948	-1.8819773292	-1.2731837441
C	-3.3273643376	-1.0653358548	-1.3285248850
C	-2.6331866929	-.7025672884	2.4955553825
C	-1.8295404681	-1.9142456465	3.0157604292
C	-3.6328228737	-.2149428361	3.5600703688
C	-2.7540198456	-.6571213527	-2.6813962723
C	-3.7452211519	.2241947575	-3.4679025603
C	-2.3287216819	-1.8878907539	-3.5081676160
C	2.2540432378	2.4122639800	.4914540971
C	1.0734779710	1.4252967607	.2937847353
C	-.1804814203	2.0204462337	.3818601273
C	-1.4551395642	1.4173895218	.2244044121
F	1.8900547127	3.4288960866	1.2888186702
F	2.6366537730	2.9330218784	-.6888588414
F	3.3201864038	1.8243668536	1.0542750773
H	-.1848053006	3.0707391094	.6332354378
H	-2.4651170803	3.3146602808	.3478452684
H	-3.0135529721	2.1224261779	1.5302866361
H	-3.5055651028	1.9586062711	-.1571514825
H	5.0074439197	-2.4288280820	1.0774452856
H	6.0723090298	-1.8798891140	-1.0763463325
H	4.8976853530	-.5127762402	-2.7518916220
H	1.5450917565	-1.3103617034	1.9982648357

H	2.7827083018	-1.1070413597	4.1290022889
H	3.2716379677	.1864360245	3.0173665486
H	4.3291375443	-1.2069467337	3.2760379738
H	2.0183814644	-3.3847317741	3.2033652134
H	3.5840314525	-3.5698245291	2.4181077448
H	2.1060532245	-3.7014832268	1.4548496575
H	1.5836194839	1.1147564807	-2.2093764972
H	1.1732483133	-.0110359257	-4.3576907888
H	1.1904470834	-1.2353844785	-3.0631317760
H	2.5852147383	-1.0542211086	-4.1262553409
H	2.6454179601	2.1080104805	-4.1414611274
H	4.0439513745	1.0465769111	-4.0321969478
H	3.7682833499	2.2713490067	-2.7820213154
H	-4.8430207958	-2.2165087073	2.0834520029
H	-5.8753069144	-2.9258528639	-.0377894635
H	-4.9185832584	-2.2151637488	-2.1973751696
H	-1.9139380124	.1048484767	2.3319603715
H	-1.3153180648	-1.6613003815	3.9481854783
H	-1.0724215781	-2.2352489820	2.2895421308
H	-2.4836209899	-2.7699764799	3.2120214283
H	-3.0956689920	.1133141188	4.4548926138
H	-4.3216471054	-1.0074416561	3.8677064125
H	-4.2345674921	.6245165584	3.1983630395
H	-1.8567152030	-.0559928945	-2.5009970421
H	-3.2960946348	.5472185155	-4.4121998463
H	-4.0278472967	1.1190659503	-2.9043003787
H	-4.6623182395	-.3237029151	-3.7070179382
H	-1.8591598944	-1.5669327419	-4.4432028682
H	-3.1880974731	-2.5131207447	-3.7710996368
H	-1.6145572516	-2.5132083338	-2.9634220608

8. $L^1CuO_2H^+$ – side-on triplet

Cu	-.0241037405	-1.1706777896	.0342981136
O	.0049004082	-3.0508488935	-.1593318565
O	-.2938405075	-3.7391498123	.9959308980
N	1.4653510603	.1296889283	.0427639767
N	-1.5254985002	.0828652304	.0197977468
H	-.2413598162	-4.6720777648	.7112568136
C	-2.5644151510	2.2926995102	.3936852297
C	2.6256954818	-.4277312428	-.5238557959
C	3.2482308341	-1.5130220813	.1844405066
C	4.3260942492	-2.1555974189	-.4171172067
C	4.7797833118	-1.7758877039	-1.6805620393
C	4.1592414437	-.7322792112	-2.3667056842
C	3.0894412916	-.0269036261	-1.8211465777
C	2.8396162950	-1.8636153451	1.6095053695
C	3.5799838595	-.9540369720	2.6160199273
C	3.0472415610	-3.3454065965	1.9613258080
C	2.4037810747	1.0315951676	-2.6806677786
C	1.6676957246	.3699609347	-3.8655201936
C	3.3891923086	2.1099044147	-3.1738638615
C	-2.7831928511	-.5968156502	-.0633311400

C	-3.5455863500	-.8530109965	1.1073271370
C	-4.7165122966	-1.6028279064	.9628080102
C	-5.1264495280	-2.0841890210	-.2780642323
C	-4.3527612598	-1.8419399612	-1.4103549370
C	-3.1624924313	-1.1155230899	-1.3307021106
C	-3.0774607666	-.4537124249	2.5044289814
C	-2.5156567819	-1.6835440043	3.2503778572
C	-4.1800919962	.2323674501	3.3306433212
C	-2.3316664671	-.8886641964	-2.5914728088
C	-3.0950626149	-.0451377417	-3.6318396771
C	-1.8562971114	-2.2229880121	-3.2015160746
C	2.3248274400	2.4514723858	.4525002041
C	1.1937236632	1.4194003524	.2438645290
C	-.0822493092	1.9680118473	.4039163051
C	-1.3795204973	1.3656122558	.2623874269
F	2.1934258515	2.9900045376	1.6796217337
F	2.2426129625	3.4513970565	-.4455231508
F	3.5507866202	1.9165763776	.3730163172
H	-.1011611746	3.0283607397	.6270792051
H	-2.3632574856	3.2375032741	-.1182283201
H	-2.7486468088	2.5250704429	1.4487507870
H	-3.4685939248	1.8432765598	-.0176278406
H	4.8309957803	-2.9588206723	.1064459682
H	5.6180208066	-2.2965857608	-2.1336528960
H	4.5118865467	-.4708273348	-3.3589664811
H	1.7680381439	-1.6488006208	1.7172273485
H	3.2434945049	-1.1648080409	3.6358440955
H	3.4092610632	.1062361711	2.4111495269
H	4.6593703310	-1.1321803221	2.5713241800
H	2.5936031640	-3.5605059763	2.9332247849
H	4.1081324196	-3.6035400599	2.0395022770
H	2.5910158465	-4.0060682642	1.2184181120
H	1.6448796009	1.5448997951	-2.0861741806
H	1.1288106456	1.1257662849	-4.4457120202
H	.9437283759	-.3779597042	-3.5239976569
H	2.3691206278	-.1314587967	-4.5398556185
H	2.8453521189	2.8889372521	-3.7168346260
H	4.1356923611	1.6952356315	-3.8581821236
H	3.9177453246	2.5814009801	-2.3423182510
H	-5.3141732492	-1.8267078700	1.8404669798
H	-6.0442718354	-2.6586712540	-.3603890065
H	-4.6774649474	-2.2276446107	-2.3717948363
H	-2.2544562764	.2603299974	2.4068339781
H	-2.1214985445	-1.3901741831	4.2288646099
H	-1.7104719795	-2.1667006307	2.6867766738
H	-3.2969448229	-2.4332563214	3.4133404874
H	-3.7732891875	.5781221805	4.2859368778
H	-5.0029729554	-.4518911372	3.5588368777
H	-4.6019157267	1.0958208810	2.8069972433
H	-1.4390896595	-.3183101580	-2.3109637763
H	-2.4621428358	.1491153428	-4.5037152829
H	-3.4087777089	.9182395225	-3.2179729154

H	-3.9922468643	-.5642764388	-3.9842539391
H	-1.2197427326	-2.0376603699	-4.0732796137
H	-2.6998280331	-2.8346223636	-3.5374716342
H	-1.2842176346	-2.8151542863	-2.4794397018

9. $L^1CuO_2^-$ – side-on doublet

Cu	-.5504353881	-.5815882847	-.0085495632
O	.2382066698	-2.3520318202	-.4369413636
O	-1.1746485999	-2.4357864906	-.3631017821
N	.8851009112	.7987685108	.2213784030
N	-2.1312387185	.5942246824	.3345423425
C	1.6774772886	3.0818150316	.6935858041
C	.5544973686	2.0456451037	.5153558918
C	-.7454726674	2.5508194603	.6924458438
C	-1.9943226919	1.8797605868	.6105328018
C	-3.2306538201	2.7305833289	.8694781857
C	2.2208778388	.3309863533	.0391319781
C	2.9149541089	-.2439364525	1.1298681546
C	4.1959493455	-.7609924281	.9133826983
C	4.7798712407	-.7461754843	-.3497127515
C	4.0599710676	-.2396638195	-1.4276032007
C	2.7758720632	.2886034533	-1.2621615755
C	2.2461146873	-.4145782142	2.4894609645
C	3.1114892380	.0769541740	3.6620773202
C	1.8234551537	-1.8884283657	2.6724374900
C	1.9567587577	.6906066871	-2.4838584719
C	1.4813932823	-.5797608428	-3.2220538121
C	2.6988678846	1.6511809693	-3.4282851075
C	-3.4164617380	-.0182200116	.2896092920
C	-3.9480957317	-.6169522690	1.4589584463
C	-5.2018959598	-1.2324967377	1.3884887403
C	-5.9151209167	-1.2892218038	.1942719505
C	-5.3525454016	-.7578819951	-.9625068921
C	-4.1018822709	-.1310094124	-.9434561098
C	-3.1233560530	-.7094609116	2.7393183327
C	-2.5262014840	-2.1284166588	2.8616815561
C	-3.9064035613	-.3205429558	4.0047659795
C	-3.4453813118	.3054592440	-2.2489233809
C	-4.3609361706	1.1639293896	-3.1382712524
C	-2.9274864392	-.9381050294	-3.0038243508
F	1.2295984099	4.3239556112	1.0019873390
F	2.4194915102	3.2228415303	-.4311172768
F	2.5294345559	2.7359229372	1.6884615455
H	-.8072327399	3.6022779206	.9283594703
H	-2.9652502918	3.7720214367	1.0628813605
H	-3.7915392542	2.3463787849	1.7282652589
H	-3.9120900648	2.6940548981	.0130387261
H	4.7364158967	-1.2037274547	1.7464805355
H	5.7772580182	-1.1536324426	-.4983250768
H	4.4940899445	-.2750754702	-2.4238233881
H	1.3327943448	.1861421805	2.4844348180
H	2.5648269569	-.0267752773	4.6073737441

H	3.3830402130	1.1298475414	3.5382712159
H	4.0377989726	-.5018597934	3.7591592212
H	1.2324738554	-2.0105108282	3.5895899847
H	2.7057370250	-2.5364058936	2.7545575462
H	1.2296439244	-2.2321130979	1.8170843898
H	1.0642909313	1.2104226605	-2.1260145771
H	.7853493195	-.3204111197	-4.0305612560
H	.9832552435	-1.2690572720	-2.5297443336
H	2.3327511049	-1.1081311533	-3.6704108226
H	2.0482570555	1.9420953270	-4.2620561379
H	3.5939314139	1.1899474543	-3.8626885235
H	3.0084223589	2.5601447810	-2.9036241865
H	-5.6165740083	-1.6963797702	2.2801597636
H	-6.8888352943	-1.7724203790	.1592305720
H	-5.8851552626	-.8514021780	-1.9057251355
H	-2.2862107878	-.0127232412	2.6453675812
H	-1.8400187550	-2.1868111676	3.7163311605
H	-1.9830958789	-2.4044765126	1.9497388867
H	-3.3231288287	-2.8665845543	3.0195296979
H	-3.2488135980	-.3507964929	4.8816153343
H	-4.7381771701	-1.0074345472	4.2016092692
H	-4.3219152568	.6910635606	3.9296921925
H	-2.5741357055	.9141322152	-1.9912112130
H	-3.8184962556	1.4988280841	-4.0302620159
H	-4.7217489098	2.0535672351	-2.6091632939
H	-5.2384828035	.6052756018	-3.4846794107
H	-2.3541126019	-.6404603160	-3.8912368817
H	-3.7668691743	-1.5609629090	-3.3395017874
H	-2.2877978025	-1.5484844781	-2.3546438860

10. L¹CuO₂H – side-on doublet

Cu	.0273011685	-.9539797972	-.3408046830
O	.7108139030	-2.9471872511	-.9454628884
O	-.7068522577	-2.6576871635	-.7057883269
N	1.3962163869	.3761425550	-.0995833586
N	-1.5581631583	.1348134931	.0298779446
H	.9448097820	-3.5030748786	-.1818826805
C	-2.7124317782	2.2254408128	.5944015595
C	2.7320884127	-.1207872655	-.2861785368
C	3.4169378283	-.6902197710	.8145998222
C	4.6561579307	-1.2951342756	.5810614151
C	5.2055202205	-1.3487822925	-.6961136144
C	4.5132896832	-.7961016834	-1.7686673190
C	3.2697808416	-.1801098761	-1.5936763880
C	2.8175722933	-.7110021319	2.2191862305
C	3.8016442765	-.2213822594	3.2965039502
C	2.2866315781	-2.1176924020	2.5656428631
C	2.5102039828	.3489876281	-2.8077062510
C	1.9677302987	-.8173544206	-3.6600513440
C	3.3534642964	1.3085646247	-3.6668350334
C	-2.8261809552	-.5305727912	-.0365894135
C	-3.3497493567	-1.1496068533	1.1243572063

C	-4.5730045590	-1.8205742987	1.0251558558
C	-5.2586855835	-1.8999508573	-.1823728616
C	-4.7130968868	-1.3207713682	-1.3228721077
C	-3.4924022766	-.6382265555	-1.2813070991
C	-2.5885276823	-1.1669768714	2.4470465608
C	-2.0414253446	-2.5827559207	2.7264628277
C	-3.4302499672	-.6571658319	3.6302190762
C	-2.8926177769	-.0961069629	-2.5755729654
C	-3.8395059850	.8700638072	-3.3101691454
C	-2.4634023677	-1.2588692594	-3.4947546102
C	2.2038174632	2.6533510080	.3825833401
C	1.0713685282	1.6274018422	.2097514176
C	-.2218530891	2.1197210015	.4030267771
C	-1.4544392153	1.4218425831	.3228345417
F	1.7519493501	3.8916996731	.6620546365
F	2.9500958512	2.7560090232	-.7378232791
F	3.0334710590	2.3057895439	1.3914118082
H	-.2960696770	3.1676340585	.6476196565
H	-2.4761173236	3.2705839983	.7980132435
H	-3.2549636125	1.8137209412	1.4511189226
H	-3.3936503277	2.1768254624	-.2603791658
H	5.1977893782	-1.7367760941	1.4126558312
H	6.1683700216	-1.8261693842	-.8558950447
H	4.9419860946	-.8520414923	-2.7651136537
H	1.9627847829	-.0304373400	2.2302211397
H	3.3020111288	-.1739323495	4.2704937084
H	4.1795648564	.7759316901	3.0584378738
H	4.6604165819	-.8926616634	3.4043361356
H	1.8250775230	-2.1274778659	3.5594583310
H	3.0945588021	-2.8581440855	2.5617044069
H	1.5290203265	-2.4484787773	1.8456938651
H	1.6484333058	.9138531975	-2.4418334553
H	1.3619650394	-.4373467335	-4.4904778465
H	1.3503444625	-1.4991741407	-3.0674862341
H	2.7879593210	-1.4062710301	-4.0864743755
H	2.7458610316	1.7156545988	-4.4826867907
H	4.2110735516	.8017646503	-4.1226273397
H	3.7313999904	2.1447994673	-3.0735304688
H	-4.9888614538	-2.3013330451	1.9063048261
H	-6.2065654090	-2.4281886684	-.2379921858
H	-5.2376437153	-1.4123351128	-2.2699418741
H	-1.7271234554	-.5001682365	2.3472839361
H	-1.4080346499	-2.5842766443	3.6213337791
H	-1.4548786719	-2.9455501886	1.8766874086
H	-2.8584908072	-3.2939717184	2.8932026064
H	-2.8248390040	-.6267072411	4.5428051696
H	-4.2890249087	-1.3071328614	3.8296591417
H	-3.8144555507	.3518955944	3.4473641422
H	-1.9890503796	.4639358293	-2.3174954195
H	-3.3497818965	1.2777982511	-4.2011538270
H	-4.1350450290	1.7112767584	-2.6740560312
H	-4.7550829361	.3678679438	-3.6411801046

H	-1.9539124810	-.8764022157	-4.3868225962
H	-3.3325502954	-1.8368625270	-3.8294395999
H	-1.7891268592	-1.9400899188	-2.9675247380

11. L¹CuO₂H⁺ – end-on singlet

Cu	.2625120967	.0311497122	.4917794089
O	-1.3207426899	-2.1258894747	.9946379115
O	-.2834481954	-1.3672424631	1.5513384825
N	1.5562462594	.9134731114	-.5302472295
N	-1.2507105838	1.2053271028	.2023124606
H	-1.9279011214	-2.2280710460	1.7501198094
C	-2.3420478378	3.1127005174	-.8799211163
C	2.7480391853	.2555723234	-.1536750409
C	3.5408497368	.7363870167	.9415438684
C	4.6667265691	-.0051390449	1.2900230355
C	5.0090815003	-1.1770813064	.6128853029
C	4.2108211495	-1.6522119109	-.4259984566
C	3.0626063766	-.9719237525	-.8231357839
C	3.1357438351	1.9327729404	1.7958687187
C	4.3117181698	2.8830852845	2.0891001311
C	2.4851459875	1.4451290725	3.1107437209
C	2.2244093394	-1.5150893774	-1.9722335365
C	1.7258604057	-2.9457166771	-1.6820882225
C	3.0056834024	-1.4510682994	-3.3014118870
C	-2.4711685568	.5702643561	.4997919096
C	-2.8961083215	.5468721151	1.8643867077
C	-4.1068695989	-.0778090465	2.1561843723
C	-4.8610178285	-.7027845753	1.1587895662
C	-4.4060440543	-.7277988681	-.1568625368
C	-3.2045288467	-.1152050463	-.5212677363
C	-2.0985966629	1.2175080007	2.9771947152
C	-1.8087457989	.2510848605	4.1433381503
C	-2.8096660701	2.4914718563	3.4801697349
C	-2.7034910005	-.2582756618	-1.9556323771
C	-3.7506931197	.1888440558	-2.9947930650
C	-2.2561395823	-1.7103712908	-2.2398900516
C	2.5262069957	2.8245224523	-1.7497010799
C	1.3455710760	2.0967234082	-1.0791125447
C	.1060837979	2.7357542987	-1.1203961124
C	-1.1129738654	2.2808634569	-.5723076610
F	2.0932354900	3.6591751714	-2.7059109359
F	3.3725600758	1.9477242550	-2.3148429740
F	3.2169617009	3.5483976880	-.8487245062
H	.0642535324	3.6680279050	-1.6644186703
H	-2.0620405135	4.1596335685	-1.0116948476
H	-3.0826657616	3.0323243153	-.0829119336
H	-2.8067930586	2.7721300493	-1.8108227022
H	5.2861972257	.3250310321	2.1165654876
H	5.8960764752	-1.7295639053	.9089537895
H	4.4901612597	-2.5685747292	-.9349615605
H	2.3837717406	2.5120889282	1.2552882370
H	3.9476698143	3.7699608280	2.6164152409

H	4.7987754341	3.2106538635	1.1675294241
H	5.0674688818	2.4163184244	2.7282068037
H	2.1552362722	2.2986702212	3.7114576315
H	3.1936158876	.8642888103	3.7104775922
H	1.6132859077	.8043513922	2.9266812355
H	1.3437632825	-.8740935214	-2.0817579363
H	1.0785076287	-3.2877842921	-2.4955107726
H	1.1560843824	-2.9933747612	-.7482869584
H	2.5549135108	-3.6561837133	-1.6056935167
H	2.3767063752	-1.8032683088	-4.1250168027
H	3.8974400308	-2.0853873157	-3.2688487313
H	3.3255309819	-.4301200021	-3.5262657421
H	-4.4736060476	-.0768072851	3.1777733993
H	-5.7995032265	-1.1853859752	1.4156059039
H	-4.9870472540	-1.2481714834	-.9108749173
H	-1.1358460072	1.5269563129	2.5588309748
H	-1.1971572236	.7536422674	4.8993704635
H	-1.2628660714	-.6312566460	3.7977244745
H	-2.7275249421	-.0796980996	4.6384946739
H	-2.2021030360	2.9852440410	4.2449861144
H	-3.7803236861	2.2534226760	3.9270524921
H	-2.9811397711	3.2078413555	2.6703767803
H	-1.8220305243	.3766668775	-2.0842218688
H	-3.3115021867	.1680593021	-3.9968348558
H	-4.1170899909	1.2023040378	-2.8051514789
H	-4.6183190221	-.4778930150	-3.0069853285
H	-1.8473484530	-1.7835271267	-3.2530203289
H	-3.1024576630	-2.4021672057	-2.1719396766
H	-1.4975186245	-2.0480422230	-1.5297738526

12. L¹CuO₂H⁺ – end-on triplet

Cu	.0194525793	-.1509422860	.2781807549
O	.5514513034	-2.8854925377	.5512393980
O	.0517688467	-1.8045415959	1.2306194028
N	1.5409781997	.9363952881	-.2982621330
N	-1.4098463869	1.0688388739	-.2092726278
H	.5395194549	-3.5921445963	1.2267378736
C	-2.3581355025	3.1565359514	-1.0993024792
C	2.7538434642	.2203672480	-.1153185977
C	3.2769772828	.1601129520	1.2113629606
C	4.4349027722	-.5866143000	1.4214143794
C	5.0371642361	-1.2912168350	.3799548047
C	4.4821501163	-1.2631963707	-.8987902985
C	3.3383806700	-.5170996571	-1.1864863616
C	2.6449849959	.9219959444	2.3726013147
C	3.5665967798	2.0547890628	2.8699789541
C	2.2540092008	-.0210114387	3.5273918211
C	2.6880668882	-.6362477979	-2.5619331389
C	1.8957266508	-1.9588507640	-2.6595890921
C	3.6991960889	-.5232205235	-3.7166596622
C	-2.6414993567	.6985245977	.4045400813
C	-3.0510843172	1.3202487759	1.6217348134

C	-4.2207709310	.8548417853	2.2234138307
C	-4.9697853317	-.1778085211	1.6613713275
C	-4.5440520239	-.7879246704	.4842825642
C	-3.3720514881	-.3863861522	-.1586187774
C	-2.2067349805	2.3664815757	2.3472712884
C	-1.4838203875	1.7263642254	3.5529309213
C	-3.0238101827	3.5923177334	2.7959572049
C	-2.9386433169	-1.0891665737	-1.4418977077
C	-3.9350779043	-.8257223160	-2.5891570885
C	-2.7436072741	-2.6032936094	-1.2246696402
C	2.5830662954	2.8802118009	-1.4264657869
C	1.3546972191	2.0765407439	-.9409807943
C	.1016253961	2.6705492346	-1.1850614576
C	-1.1980370180	2.2327724270	-.8026620758
F	2.2584595265	4.1577810477	-1.6838296873
F	3.0962348205	2.3563290251	-2.5539684333
F	3.5470932879	2.8847194015	-.4912618331
H	.1351771179	3.6213619625	-1.6973072610
H	-2.0751751929	3.9172694668	-1.8278415097
H	-2.6909085855	3.6687824665	-.1915573045
H	-3.2100231577	2.5875100256	-1.4817754047
H	4.8761614648	-.6178373988	2.4125109186
H	5.9349634788	-1.8727351892	.5671527659
H	4.9440711882	-1.8476416530	-1.6871240504
H	1.7267915048	1.3954374060	2.0080364192
H	3.0764274649	2.6178103327	3.6706985835
H	3.8140072286	2.7491558683	2.0631025106
H	4.5038322233	1.6555992999	3.2709007979
H	1.7641257827	.5443764627	4.3266120958
H	3.1298354861	-.5107043891	3.9647561766
H	1.5658568538	-.8041315495	3.1920666727
H	1.9711094798	.1796976046	-2.6809625532
H	1.3875836648	-2.0272508473	-3.6270596301
H	1.1408287025	-2.0450673067	-1.8705718153
H	2.5624744641	-2.8227795522	-2.5676313796
H	3.1678047541	-.5037300113	-4.6730676783
H	4.3832591478	-1.3770993169	-3.7465174299
H	4.2960146378	.3886713258	-3.6393969711
H	-4.5477737006	1.2965379811	3.1590417076
H	-5.8798816325	-.5138945375	2.1489866290
H	-5.1337131105	-1.5941593826	.0596733615
H	-1.4295766455	2.7259052445	1.6667105536
H	-.8359040714	2.4603582086	4.0434484932
H	-.8645421108	.8747608374	3.2497583105
H	-2.2017569707	1.3626822930	4.2951769700
H	-2.3576405803	4.3524529323	3.2153931136
H	-3.7509270923	3.3353655725	3.5722966472
H	-3.5743900773	4.0451469435	1.9653355508
H	-1.9743724879	-.6700905759	-1.7501491590
H	-3.5847579620	-1.2973636988	-3.5126328825
H	-4.0570203444	.2451097792	-2.7808584045
H	-4.9230156554	-1.2375148159	-2.3585943721

H	-2.3841685581	-3.0728461338	-2.1459820867
H	-3.6818788881	-3.0959367967	-.9508277916
H	-2.0164456845	-2.8075167346	-.4334647541

13. $L^1CuO_2^-$ – end-on doublet

Cu	-.8460586014	-.4412916081	.3080684957
O	-1.1108252935	-3.0399327234	.7721074728
O	-.8990373994	-1.9556890156	1.5445069172
N	.6512200247	.4186097153	-.7001749414
N	-2.3635510720	.6252049835	-.4436460766
C	1.5936891449	2.2489826326	-2.0416036616
C	.4074996017	1.5210804349	-1.3904242918
C	-.8478854423	2.1245095919	-1.5970414088
C	-2.1413395482	1.6892783031	-1.1950949682
C	-3.3169066076	2.5266344286	-1.6807107073
C	1.9041067897	-.2572750678	-.6204396386
C	2.7360890214	-.0735560724	.5114187239
C	3.9106417377	-.8252981036	.6149609795
C	4.2647214814	-1.7581952805	-.3552003904
C	3.4146837836	-1.9685847396	-1.4366759039
C	2.2284808785	-1.2441597889	-1.5870330170
C	2.3195931733	.8431231131	1.6562514083
C	3.4205665486	1.8371290818	2.0631245244
C	1.8506879399	.0010773048	2.8622183049
C	1.2692289982	-1.6049233634	-2.7182368982
C	.5949754427	-2.9632695807	-2.4286284625
C	1.9405846930	-1.6041356585	-4.1033377458
C	-3.6740400064	.1715729150	-.1281872264
C	-4.2399130978	.4820469882	1.1357831207
C	-5.5040998874	-.0234683743	1.4544304698
C	-6.2076832137	-.8358734697	.5701561412
C	-5.6232185187	-1.1819454358	-.6442812417
C	-4.3597303901	-.7045188034	-1.0105884611
C	-3.4519607473	1.2609463956	2.1849519030
C	-2.9625070956	.3091098546	3.2977828013
C	-4.2393680322	2.4429999215	2.7760684583
C	-3.7043057194	-1.2259543623	-2.2866471641
C	-4.6033122332	-1.0850600025	-3.5280875536
C	-3.2565264188	-2.6899913614	-2.0877962885
F	1.2541618259	3.3991438172	-2.6735896906
F	2.2176689861	1.4855818109	-2.9710997401
F	2.5315723219	2.5915903935	-1.1243203856
H	-.8331933554	3.0361574507	-2.1752677960
H	-2.9809470885	3.4140188419	-2.2213839072
H	-3.9408382556	2.8413595654	-.8371795397
H	-3.9630332812	1.9410208976	-2.3435383350
H	4.5518626474	-.6893102881	1.4825081075
H	5.1812857269	-2.3350275730	-.2559048658
H	3.6666475910	-2.7277059941	-2.1733262854
H	1.4617328412	1.4269461610	1.3124344108
H	3.0550056621	2.5106742698	2.8478042943
H	3.7355937915	2.4449143101	1.2096079830

H	4.3065098213	1.3271923030	2.4600634860
H	1.4710407623	.6484216534	3.6632038523
H	2.6812083563	-.5866485619	3.2731338956
H	1.0577386000	-.6973728437	2.5759253174
H	.4795116781	-.8498350332	-2.7388994394
H	-.1348815395	-3.2031192706	-3.2124599188
H	.0746136193	-2.9601328489	-1.4642929613
H	1.3382309347	-3.7703817765	-2.4091892523
H	1.1981724828	-1.8123417167	-4.8835487007
H	2.7166316837	-2.3749272963	-4.1822947061
H	2.4020398449	-.6365148035	-4.3202753713
H	-5.9383676847	.2094512762	2.4238229480
H	-7.1891669262	-1.2199397082	.8379532756
H	-6.1488038380	-1.8570234706	-1.3152964702
H	-2.5650742318	1.6689334436	1.6921548343
H	-2.3320903643	.8484349079	4.0162557986
H	-2.3823477924	-.5223630681	2.8849707209
H	-3.8121486133	-.1130314817	3.8493938129
H	-3.6104479939	3.0086739195	3.4737853507
H	-5.1225318414	2.1084902244	3.3332647812
H	-4.5810458276	3.1306132305	1.9943262146
H	-2.8020703977	-.6348409613	-2.4646771861
H	-4.0644826822	-1.4074738411	-4.4268860900
H	-4.9254534765	-.0487353889	-3.6811142040
H	-5.5052524510	-1.7038032845	-3.4516161875
H	-2.7374619673	-3.0581421946	-2.9817671464
H	-4.1222059624	-3.3410444514	-1.9119278931
H	-2.5799377604	-2.7853745198	-1.2314387042

14. L¹CuO₂H – end-on doublet

Cu	.0893412731	-.0393043040	.4557394891
O	-.2174729059	-2.7351635929	.9286485047
O	.0191547379	-1.4953224119	1.5981065029
N	1.5577868426	.9165110423	-.3499846072
N	-1.3655170114	1.1214108152	-.0516734222
H	-.2931840512	-3.3391978472	1.6849520744
C	-2.3608162362	3.1281302119	-1.0487400335
C	2.8271697685	.2831336475	-.1244401693
C	3.5214143111	.5352119599	1.0856720169
C	4.6929174623	-.1839120507	1.3402764827
C	5.1650775959	-1.1399762218	.4470141266
C	4.4550262861	-1.4005299557	-.7199767157
C	3.2779984189	-.7106161686	-1.0276017973
C	2.9854408897	1.4887620525	2.1497700275
C	4.0315501958	2.5155401389	2.6181244654
C	2.4281871273	.6868957161	3.3461491463
C	2.4879452139	-1.0987054979	-2.2734371667
C	1.8333143138	-2.4846373766	-2.0869268715
C	3.3437089204	-1.0674695939	-3.5523663194
C	-2.6545817497	.6869891380	.4001192791
C	-3.0768124464	1.0143002951	1.7131278695
C	-4.3063960528	.5187156711	2.1584219829

C	-5.0977006518	-.2903974686	1.3491635155
C	-4.6538489484	-.6329921426	.0764545347
C	-3.4320731123	-.1660834600	-.4206848917
C	-2.1992687901	1.8111975140	2.6755259147
C	-1.6563027884	.8921110668	3.7914024020
C	-2.9236833300	3.0303642123	3.2734734709
C	-2.9498940994	-.6432666262	-1.7881203676
C	-3.9520190994	-.3238900131	-2.9123130638
C	-2.6285175433	-2.1527486777	-1.7549257470
C	2.5530141319	2.8043394981	-1.5708202692
C	1.3427403237	2.0622164187	-.9829006391
C	.1007273249	2.6812525310	-1.1684076387
C	-1.1722617249	2.2446455198	-.7264496789
F	2.2118330027	3.9401480252	-2.2122287244
F	3.2144098964	2.0361164245	-2.4622773285
F	3.4302667481	3.1504456930	-.6039652437
H	.1136745287	3.6138409141	-1.7106399413
H	-2.0550813960	4.0178905842	-1.6004800047
H	-2.8670112876	3.4394003111	-.1293508489
H	-3.0984557892	2.5801694143	-1.6432562917
H	5.2365397646	-.0028022576	2.2631811872
H	6.0749079187	-1.6915027927	.6678713590
H	4.8139960230	-2.1661551002	-1.4017633914
H	2.1538198840	2.0488333709	1.7134600830
H	3.5836670730	3.2089245247	3.3388444207
H	4.4175555944	3.0981834558	1.7777618610
H	4.8809817542	2.0344416848	3.1153554159
H	1.9641814266	1.3573672714	4.0786470834
H	3.2284925757	.1381945692	3.8561035376
H	1.6806801125	-.0476253339	3.0290327816
H	1.6829720770	-.3696666122	-2.4012096200
H	1.2144015040	-2.7366868757	-2.9560209336
H	1.2016575691	-2.5225014446	-1.1938428275
H	2.5951537140	-3.2663557668	-1.9835092009
H	2.7237387564	-1.2945063098	-4.4267865561
H	4.1470767151	-1.8117582237	-3.5215455100
H	3.7990605575	-.0852230865	-3.7015527930
H	-4.6428186290	.7584182235	3.1633700914
H	-6.0482226055	-.6674829727	1.7165533222
H	-5.2612637080	-1.2892774037	-.5406491670
H	-1.3384731501	2.1860626289	2.1141186921
H	-.9614081883	1.4399213018	4.4382566616
H	-1.1308201514	.0267008860	3.3751529153
H	-2.4710813547	.5149902477	4.4205760064
H	-2.2410037591	3.6026264887	3.9111075581
H	-3.7767761831	2.7329147483	3.8929857249
H	-3.2983307568	3.7006439363	2.4928641588
H	-2.0190279820	-.1168597292	-2.0185237336
H	-3.5430627195	-.6257920981	-3.8826532987
H	-4.1807660594	.7458994381	-2.9602821269
H	-4.8980824763	-.8590013841	-2.7749129852
H	-2.2155652185	-2.4778100392	-2.7168153443

H	-3.5329648617	-2.7426436833	-1.5654537296
H	-1.9043945954	-2.3926288338	-.9706272621
15. L ² CuO ₂ – side-on singlet			
Cu	-.5779334665	-.4356607727	.0393553078
O	.1780057188	-2.1054766224	-.3705221693
O	-1.1662809875	-2.1853449538	-.3015812321
N	.8458138894	.8054619000	.2229726912
N	-2.1187699634	.6235293436	.3659182678
C	1.7161584064	3.0664026632	.6540947764
C	.5561277500	2.0626191409	.5109136857
C	-.7313424296	2.5895938238	.7063166592
C	-1.9573255844	1.9072718554	.6359509984
C	-3.2113734092	2.7594589849	.9087335629
C	2.1679839261	.2603201980	.0230768868
C	2.8384568525	-.3321035579	1.1192216517
C	4.0754358112	-.9387254505	.8808812270
C	4.6251596361	-.9851313345	-.3950016783
C	3.9290596114	-.4360171977	-1.4665970958
C	2.6874832082	.1829839921	-1.2897336119
C	2.2254459247	-.4111211333	2.5144586797
C	3.1719563956	.0992350511	3.6142602804
C	1.7653654272	-1.8559288164	2.8125867127
C	1.9112424035	.6621526574	-2.5139935170
C	1.4039540274	-.5491760585	-3.3265335518
C	2.7262437348	1.6165251550	-3.4050728386
C	-3.3796644937	-.0759459660	.2897286273
C	-3.8762180604	-.7286548654	1.4423257965
C	-5.0543247014	-1.4711860865	1.3178034378
C	-5.7092139980	-1.5910846862	.0977429363
C	-5.1785351907	-.9800671070	-1.0331983621
C	-4.0036656409	-.2254236680	-.9702035865
C	-3.1318728339	-.7286790384	2.7744644837
C	-2.4755484714	-2.1072412079	3.0154571959
C	-4.0265670182	-.3341297901	3.9620011700
C	-3.4025466473	.3275743426	-2.2599182948
C	-4.3924104531	1.1954506037	-3.0577398018
C	-2.8583768717	-.8270178799	-3.1290609662
F	1.2871875157	4.3071952379	.9505920482
F	2.4250529578	3.1559693122	-.4882141403
F	2.5606209725	2.6953900190	1.6360936227
H	-.7848077956	3.6394457241	.9363504943
F	-2.9139604886	4.0520273558	1.1373969809
F	-3.8752770302	2.3088712626	1.9916642102
F	-4.0590453095	2.7288641425	-.1373930733
H	4.6080362491	-1.3991503767	1.7080387094
H	5.5844953726	-1.4679724338	-.5575062937
H	4.3478670137	-.5053252844	-2.4658027545
H	1.3365625580	.2262083076	2.5308790568
H	2.6675480936	.0732745928	4.5859366939
H	3.4904003530	1.1262760593	3.4206870812
H	4.0684655853	-.5231417342	3.6988462999

H	1.2446674482	-1.9037005191	3.7757409098
H	2.6234054085	-2.5360539296	2.8637192560
H	1.0957081436	-2.2307794539	2.0332518318
H	1.0330469461	1.2142220651	-2.1659539810
H	.7698766511	-.2177617633	-4.1568400205
H	.8300367116	-1.2380526992	-2.6999238662
H	2.2423411877	-1.1123622919	-3.7517019843
H	2.1108156887	1.9704574903	-4.2398813145
H	3.6021051889	1.1192523515	-3.8357564738
H	3.0742443459	2.4867876451	-2.8436380298
H	-5.4548635381	-1.9796292255	2.1899460797
H	-6.6199004149	-2.1782263648	.0241406983
H	-5.6757703285	-1.1054986635	-1.9900242077
H	-2.3287270970	.0114289343	2.7136728411
H	-1.8610311824	-2.0896168597	3.9222498030
H	-1.8464630373	-2.4029209834	2.1718904730
H	-3.2372733328	-2.8838905681	3.1451784079
H	-3.4308066260	-.2859700837	4.8798185266
H	-4.8226721240	-1.0672880853	4.1311536179
H	-4.4938769355	.6422436372	3.8038054820
H	-2.5537049922	.9647030524	-1.9942188007
H	-3.9021935908	1.6046454814	-3.9481781319
H	-4.7643391299	2.0297152026	-2.4583661683
H	-5.2551425932	.6140467245	-3.4000723530
H	-2.3464532617	-.4337443806	-4.0147678920
H	-3.6728714217	-1.4732510379	-3.4748788868
H	-2.1576849448	-1.4520086352	-2.5677436169

16. L²CuO₂ – side-on triplet

Cu	-.5799080838	-.4803413118	.0381960355
O	.1593467129	-2.3314530029	-.4087137812
O	-1.1325952067	-2.4115942589	-.3324041279
N	.8653688170	.7902909953	.2268798296
N	-2.1421544720	.6113972407	.3635316100
C	1.7119417841	3.0579737938	.6733247775
C	.5629555364	2.0441331684	.5183797285
C	-.7304479525	2.5656916424	.7021540335
C	-1.9648887148	1.8956960351	.6250002805
C	-3.2064997557	2.7719855296	.8756733502
C	2.1929217662	.2652257870	.0275943330
C	2.8655680407	-.3395822559	1.1155616085
C	4.0895245793	-.9684288933	.8660133953
C	4.6330330417	-1.0157760473	-.4131470545
C	3.9480659047	-.4331600762	-1.4735118373
C	2.7202688282	.2090481196	-1.2839174738
C	2.2735151663	-.3856491011	2.5222713484
C	3.2526589354	.1219234284	3.5966264061
C	1.7879178646	-1.8112661617	2.8581094815
C	1.9673492197	.7570015573	-2.4939551942
C	1.3970460933	-.3987647839	-3.3427840325
C	2.8301698671	1.6924970104	-3.3602215324
C	-3.4105529981	-.0702290085	.2953696823

C	-3.9102981095	-.7133929270	1.4521416788
C	-5.0719222852	-1.4828100654	1.3288351293
C	-5.7173009158	-1.6313290897	.1061017587
C	-5.1986215926	-1.0104527881	-1.0248133666
C	-4.0409380894	-.2283499711	-.9611555094
C	-3.1900705710	-.6570583942	2.7971457870
C	-2.4999767980	-2.0046777129	3.0956629892
C	-4.1193842835	-.2550612886	3.9563151765
C	-3.4673740431	.3639473300	-2.2458716711
C	-4.5013771599	1.1868857665	-3.0355629248
C	-2.8660311177	-.7472333964	-3.1315813225
F	1.2790326838	4.2911540533	.9971178841
F	2.4138064318	3.1763676767	-.4727453566
F	2.5703364537	2.6770314451	1.6412703998
H	-.7823575988	3.6161054682	.9312038323
F	-2.8967060011	4.0616610385	1.1080922672
F	-3.9016508421	2.3366029581	1.9463967328
F	-4.0373696376	2.7541280825	-.1865516225
H	4.6198177030	-1.4401763273	1.6879682965
H	5.5818569018	-1.5155127941	-.5850540515
H	4.3680319704	-.4887761525	-2.4734424888
H	1.3997593485	.2719454574	2.5439975716
H	2.7639230057	.1331109791	4.5771686822
H	3.5953584215	1.1356045357	3.3740658559
H	4.1345216638	-.5227074981	3.6800421828
H	1.3044738015	-1.8335600283	3.8411763777
H	2.6259010494	-2.5168720774	2.8800187591
H	1.0723548034	-2.1799912920	2.1165069815
H	1.1200713632	1.3443826193	-2.1292094305
H	.8036232829	-.0099690030	-4.1778155710
H	.7583902934	-1.0597543763	-2.7483701561
H	2.2019016068	-1.0136231870	-3.7605274181
H	2.2290071629	2.1142289055	-4.1732063282
H	3.6706000787	1.1612567696	-3.8201192791
H	3.2351126174	2.5188395461	-2.7706138154
H	-5.4700990136	-1.9854835086	2.2054053175
H	-6.6146045667	-2.2390671254	.0325208737
H	-5.6952668468	-1.1452318701	-1.9812468648
H	-2.4078458476	.1039948201	2.7315411083
H	-1.9295689145	-1.9492210760	4.0295526454
H	-1.8145442229	-2.2943531226	2.2929668743
H	-3.2370367803	-2.8085081411	3.1998537031
H	-3.5449595976	-.1599639754	4.8842492430
H	-4.8982773222	-1.0043946063	4.1325956412
H	-4.6092518651	.7012589898	3.7579190105
H	-2.6540167472	1.0420417836	-1.9728771212
H	-4.0297038035	1.6428315692	-3.9130984238
H	-4.9253840557	1.9853829010	-2.4217839095
H	-5.3263892346	.5636825476	-3.3969566670
H	-2.3952989664	-.3194161090	-4.0236835512
H	-3.6406340451	-1.4467224497	-3.4641983236
H	-2.1123263641	-1.3296319323	-2.5931047674

17. L²CuO₂ – end-on singlet

Cu	-.9467659807	-.5735933905	.0108757145
O	-.8071839325	-3.2519773418	.6750486966
O	-.8065582663	-2.0602682579	1.1098551998
N	.5739413252	.3290393638	-.7989998068
N	-2.3682246361	.6200635422	-.4961858005
C	1.6280376494	2.2076197869	-1.9885589431
C	.3941153085	1.4814740929	-1.4176557627
C	-.8357389783	2.1369447402	-1.6076741832
C	-2.1075725223	1.7179368338	-1.1800726138
C	-3.2794530534	2.6455990801	-1.5518611664
C	1.8360699798	-.3313454297	-.6038361604
C	2.5599045856	-.0936604120	.5914088598
C	3.7273172444	-.8316104595	.8125686268
C	4.1694648075	-1.7855971886	-.1011939100
C	3.4361708940	-2.0181515734	-1.2588490963
C	2.2611588390	-1.3068863066	-1.5377672481
C	2.0718182477	.8770516651	1.6647206670
C	3.1413735515	1.9012721912	2.0776517890
C	1.5605832154	.1021377487	2.8971790185
C	1.4644255328	-1.6426702917	-2.7956239389
C	.7644882949	-3.0135540122	-2.6437436182
C	2.3310770628	-1.6128236780	-4.0731267531
C	-3.6674780275	.1740207256	-.0735340588
C	-4.1260906712	.5029063909	1.2266226744
C	-5.3453243217	-.0369862908	1.6521447041
C	-6.0886882755	-.8819198816	.8344827828
C	-5.6101434255	-1.2131779493	-.4305473492
C	-4.3959135480	-.7060186673	-.9085767339
C	-3.3055232677	1.3592616110	2.1866734360
C	-2.6668478590	.4758451608	3.2786718609
C	-4.1237601572	2.4991391836	2.8162362169
C	-3.8571052228	-1.1738411077	-2.2577863913
C	-4.8791305927	-1.0224376821	-3.4006399786
C	-3.3592239883	-2.6337412251	-2.1586612763
F	1.3097949977	3.3574537512	-2.6129916348
F	2.2769022702	1.4393285516	-2.8855248302
F	2.5013768688	2.5205071772	-1.0091918767
H	-.7986424539	3.0692273351	-2.1432156905
F	-2.8795081926	3.7482633012	-2.2129972882
F	-3.9356949102	3.0626585584	-.4498560559
F	-4.1684890646	2.0115230320	-2.3431243967
H	4.2956225743	-.6639592014	1.7220873992
H	5.0767274888	-2.3535740094	.0953887295
H	3.7769082221	-2.7747663431	-1.9593174115
H	1.2292132722	1.4396311999	1.2562012069
H	2.7197477776	2.6145745950	2.7940923428
H	3.5124248694	2.4604000823	1.2161270119
H	3.9968018976	1.4223259957	2.5628729114
H	1.1412333669	.7907726836	3.6391900904
H	2.3766726757	-.4483984097	3.3756259971

H	.7890312772	-.6263271095	2.6339688764
H	.6808594682	-.8821026068	-2.9150571949
H	.1528624507	-3.2278886622	-3.5272634663
H	.1136513789	-3.0501000634	-1.7629194275
H	1.5030420618	-3.8218019615	-2.5409786132
H	1.6995616898	-1.7765414409	-4.9526374587
H	3.0947591199	-2.4045382969	-4.0651691252
H	2.8452869781	-.6527790962	-4.1963639112
H	-5.7156717285	.2018798998	2.6451075022
H	-7.0330547198	-1.2914320753	1.1875357575
H	-6.1851057362	-1.8885140309	-1.0556576302
H	-2.4943002173	1.8209555707	1.6174501155
H	-2.0215487760	1.0738329527	3.9312666893
H	-2.0619991746	-.3295909800	2.8565016912
H	-3.4364187707	.0095783211	3.9019454552
H	-3.4756882425	3.1313395032	3.4323162304
H	-4.9193207396	2.1196500472	3.4649040107
H	-4.5848851821	3.1277668609	2.0524393692
H	-2.9966904751	-.5496556174	-2.5119216487
H	-4.4176892562	-1.2953064736	-4.3558122259
H	-5.2395227427	.0081905444	-3.4764107420
H	-5.7476054111	-1.6762005787	-3.2652251862
H	-2.9111369717	-2.9536199960	-3.1056589737
H	-4.1885875468	-3.3144224079	-1.9353499665
H	-2.6106935887	-2.7637768388	-1.3689863421

18. L²CuO₂ – end-on triplet

Cu	-.9170777744	-.5761558175	.0137376603
O	-.8843700135	-3.4069621850	.7044042045
O	-.8747823378	-2.2145994301	1.0687137855
N	.6241600169	.3116787654	-.7788953304
N	-2.4091212546	.5674926251	-.4817924092
C	1.6015267429	2.2055722258	-2.0137594341
C	.3993941427	1.4507080253	-1.4132297928
C	-.8492269903	2.0749073579	-1.5979448328
C	-2.1258188826	1.6611691999	-1.1714635084
C	-3.2804191733	2.6066468922	-1.5558240044
C	1.9036671449	-.3192248125	-.6003690400
C	2.6188544776	-.0872190221	.5988437117
C	3.7844699231	-.8251817634	.8267304569
C	4.2341560986	-1.7704623062	-.0897970749
C	3.5127418019	-1.9932810238	-1.2576164705
C	2.3394440630	-1.2851606488	-1.5379479125
C	2.1211294263	.8870348426	1.6639947914
C	3.2037722466	1.8841485404	2.1127132195
C	1.5486980665	.1217319526	2.8745679724
C	1.5443235281	-1.6173421068	-2.7986216306
C	.8525757207	-2.9898578609	-2.6598455340
C	2.4048692565	-1.5727335009	-4.0742931592
C	-3.7231137593	.1548689826	-.0637098127
C	-4.1726954457	.4978074616	1.2333756424
C	-5.3912418660	-.0312519652	1.6718368085

C	-6.1451434954	-.8802206679	.8675417629
C	-5.6816994150	-1.2180537657	-.3995084963
C	-4.4706469114	-.7181930857	-.8907116168
C	-3.3423476350	1.3632402946	2.1780480710
C	-2.7007760394	.4937787899	3.2801479197
C	-4.1496817346	2.5196951383	2.7948970441
C	-3.9677340398	-1.1737649523	-2.2581933541
C	-5.0232635278	-1.0139668413	-3.3669275505
C	-3.4629169871	-2.6301383439	-2.1918951799
F	1.2499938070	3.3545632413	-2.6232257126
F	2.2421706638	1.4556381330	-2.9346768861
F	2.4974679434	2.5289566447	-1.0569872474
H	-.8241645640	3.0022856760	-2.1433578317
F	-2.8684118198	3.6834769511	-2.2517810222
F	-3.9138178701	3.0694396001	-.4573389495
F	-4.1975904776	1.9770013759	-2.3196624224
H	4.3447401799	-.6624056947	1.7430495196
H	5.1394383424	-2.3367066329	.1094544398
H	3.8612706196	-2.7405485756	-1.9644102116
H	1.3048924388	1.4709000746	1.2314676720
H	2.7821818731	2.6055222795	2.8213310135
H	3.6070351731	2.4376209408	1.2609944457
H	4.0371151050	1.3832587246	2.6163411657
H	1.1339276295	.8164131494	3.6132338478
H	2.3257757147	-.4701810659	3.3694803474
H	.7543345534	-.5692099710	2.5752926957
H	.7580746739	-.8656922171	-2.9106492178
H	.2318116937	-3.2016425059	-3.5378924192
H	.2117003120	-3.0320022755	-1.7734725385
H	1.5901840200	-3.7949864612	-2.5680871809
H	1.7783138054	-1.7465567836	-4.9565325447
H	3.1814367902	-2.3457830240	-4.0694142744
H	2.8949842879	-.6024081344	-4.1884720362
H	-5.7519651913	.2207857038	2.6648388361
H	-7.0869546878	-1.2829720724	1.2297236643
H	-6.2683034050	-1.8903565917	-1.0193396909
H	-2.5294648545	1.8100915775	1.5992357112
H	-2.0517093843	1.0976450338	3.9246221991
H	-2.0973147450	-.3158272187	2.8546704315
H	-3.4668459668	.0313895669	3.9127822839
H	-3.4962757275	3.1519836221	3.4063923865
H	-4.9524666658	2.1570014140	3.4458602141
H	-4.6003111186	3.1440828781	2.0188614772
H	-3.1161504392	-.5454844160	-2.5308606783
H	-4.5915234643	-1.2774322668	-4.3387821536
H	-5.3853900155	.0156607419	-3.4221447980
H	-5.8867520373	-1.6684289938	-3.2078976333
H	-3.0471602955	-2.9423806311	-3.1565817521
H	-4.2768279008	-3.3181301447	-1.9383374752
H	-2.6833245566	-2.7526125406	-1.4324733101

19. $L^2CuO_2H^+$ – side-on singlet

Cu	.1509919814	-.9336612111	-.2436900297
O	.1561643272	-3.4857705392	-.8233770113
O	-.8012268504	-2.4891233481	-.4985299228
N	1.3798877832	.4164319181	.0504681826
N	-1.5528978178	.0796810298	-.0627086433
H	.1182904821	-4.0829210188	-.0538390996
C	-2.7472957867	2.1572074598	.5213977000
C	2.6068489944	-.2157985850	-.2839508024
C	3.2219768017	-1.0499804401	.7013988988
C	4.3442868203	-1.7811525805	.3178938009
C	4.8336960363	-1.7238589476	-.9864759154
C	4.2071357765	-.9246061477	-1.9431499899
C	3.0861975398	-.1578154560	-1.6303812386
C	2.6970305698	-1.1604924902	2.1287893376
C	3.7580270280	-.7407526214	3.1643704930
C	2.1819255235	-2.5866936884	2.4176397280
C	2.3635856288	.6150641670	-2.7272955305
C	1.5527609648	-.3556830132	-3.6157291310
C	3.3179356386	1.4714141987	-3.5790606563
C	-2.6895426831	-.7283483980	-.0828002623
C	-3.2844031892	-1.1954871637	1.1406038324
C	-4.4499188638	-1.9415889241	1.0378507960
C	-5.0017529659	-2.2700756733	-.2060880515
C	-4.3743470219	-1.8827823260	-1.3860757653
C	-3.1961634478	-1.1404512985	-1.3646818291
C	-2.6414541454	-.9909800044	2.5064236277
C	-1.9101337779	-2.2881072532	2.9249198595
C	-3.6441351698	-.5661541894	3.5949383867
C	-2.5443793484	-.7240429097	-2.6714841804
C	-3.4015065842	.3337702234	-3.4024739968
C	-2.2665206909	-1.9388959200	-3.5789139900
C	2.1856818555	2.6808191700	.5210550319
C	1.0541128552	1.6588866079	.3180586983
C	-.2689393083	2.1087938663	.4466918761
C	-1.4399786056	1.3585387963	.2814393217
F	1.7219259176	3.8574183292	.9582131159
F	2.8495729540	2.8905220703	-.6300143752
F	3.0620662485	2.2106847148	1.4275764415
F	-2.5491001288	3.4688036229	.3380055034
F	-3.1769386491	1.9740791461	1.7829370318
F	-3.7264504261	1.7741309843	-.3117652427
H	-.3997390976	3.1526609821	.6819395433
H	4.8433738722	-2.4122481287	1.0460692012
H	5.7023158980	-2.3139203194	-1.2632735510
H	4.5922247077	-.9124397536	-2.9570645102
H	1.8504070442	-.4750818400	2.2351058127
H	3.3346624160	-.7827672162	4.1727130704
H	4.1074440051	.2784289057	2.9821251721
H	4.6265393740	-1.4066078901	3.1431760186
H	1.7449449003	-2.6395485780	3.4195812693
H	2.9901937157	-3.3234112125	2.3667682039
H	1.4141045998	-2.8922452663	1.6974674757

H	1.6533599587	1.2991799187	-2.2565931237
H	.9936566530	.1999985246	-4.3753496428
H	.8343202497	-.9447424037	-3.0324310742
H	2.2093940000	-1.0640108990	-4.1312631581
H	2.7412093149	2.0768378863	-4.2846866419
H	4.0057935356	.8564297448	-4.1674989969
H	3.9109002295	2.1460283975	-2.9565512886
H	-4.9382259112	-2.2948416146	1.9394478988
H	-5.9174176409	-2.8527277700	-.2477876358
H	-4.8043740569	-2.1724284383	-2.3384886634
H	-1.8896811480	-.2010278705	2.4250357132
H	-1.3753984055	-2.1344633922	3.8678698795
H	-1.1947483525	-2.6082955614	2.1622522727
H	-2.6254115010	-3.1042458043	3.0723065657
H	-3.1067799564	-.3367108455	4.5202027770
H	-4.3555418082	-1.3648240700	3.8274205116
H	-4.2104847133	.3198335242	3.3009501877
H	-1.5814103071	-.2603639232	-2.4364876446
H	-2.8966725436	.6569256372	-4.3181355331
H	-3.5779222577	1.2128863427	-2.7778931902
H	-4.3757044455	-.0771729212	-3.6865111538
H	-1.7249820280	-1.6153459459	-4.4735204708
H	-3.1922804533	-2.4152352894	-3.9166418339
H	-1.6647711169	-2.6888846808	-3.0591288204

20. L²CuO₂H⁺ – side-on triplet

Cu	-.0168430349	-1.0910620703	-.1747804742
O	.4517157479	-3.8360224480	.1379478333
O	-.1175638622	-2.9305880366	-.7084435365
N	1.3267061561	.3023856769	-.1772040982
N	-1.6000601126	.0081214475	.2405612177
H	.2576877940	-4.6932255599	-.2926746169
C	-2.7172791632	2.1911664620	.7111473026
C	2.6174800396	-.2837230302	-.3093713962
C	3.4097404276	-.5521873111	.8437074509
C	4.6329655839	-1.1922806206	.6411930549
C	5.0637316447	-1.5597948455	-.6328245733
C	4.2570552871	-1.3201049300	-1.7432976073
C	3.0141132697	-.7018654821	-1.6123747210
C	2.9085476331	-.3057998721	2.2641016757
C	3.9915775089	.2656259947	3.1960595550
C	2.3165809950	-1.6091360841	2.8444433602
C	2.1639128752	-.4297828980	-2.8496580484
C	1.8639769778	-1.7186976920	-3.6390931118
C	2.8168283074	.6376605988	-3.7519044777
C	-2.7818833737	-.7061307781	-.0631277659
C	-3.1944249411	-1.7233796553	.8530969397
C	-4.3365466001	-2.4548998841	.5371175608
C	-5.0328692629	-2.2319101344	-.6503875871
C	-4.5839649051	-1.2751930410	-1.5617459921
C	-3.4609902102	-.4915784317	-1.3049326775
C	-2.4873947525	-1.9380259866	2.1863798731

C	-2.2849491402	-3.4248105024	2.5310669422
C	-3.2413120723	-1.2096798831	3.3204007904
C	-2.9180347728	.4155840569	-2.4079903262
C	-4.0061142749	1.2790967021	-3.0710060181
C	-2.1755594012	-.4329895003	-3.4648549450
C	2.1528524869	2.6175319167	.1750485111
C	1.0350132581	1.5492675205	.1294265885
C	-.2637500027	2.0260139013	.4108976966
C	-1.4759329228	1.3121146980	.4251395991
F	1.6459069514	3.8414320779	-.0411211376
F	3.0857345081	2.3894078116	-.7616119876
F	2.7572241316	2.6286643452	1.3768275534
F	-2.4002993672	3.1515465827	1.5959289004
F	-3.7324041430	1.4807014359	1.2229425493
F	-3.1476522771	2.7952811174	-.4120604232
H	-.3385146608	3.0806612982	.6303335358
H	5.2588949763	-1.4220553220	1.4964974656
H	6.0261856676	-2.0467522606	-.7580207508
H	4.6044624917	-1.6155591448	-2.7280962064
H	2.1015728409	.4297828470	2.2296749222
H	3.5491570797	.5232087454	4.1631244308
H	4.4410993720	1.1690492252	2.7765883654
H	4.7911250878	-.4560440666	3.3896800187
H	1.9085307185	-1.4319598987	3.8448479172
H	3.0828254140	-2.3872835666	2.9241744713
H	1.5110156190	-2.0092070133	2.2163064028
H	1.2035629289	-.0197910365	-2.5164633325
H	1.2157194612	-1.4939490597	-4.4921401470
H	1.3589764486	-2.4641957236	-3.0154891571
H	2.7757401864	-2.1766326345	-4.0346687535
H	2.1707868752	.8581625982	-4.6075212290
H	3.7786663182	.2891143863	-4.1416202989
H	2.9925349854	1.5672912547	-3.2046629269
H	-4.6985009516	-3.2050287821	1.2314259287
H	-5.9200906453	-2.8160536438	-.8755885729
H	-5.1136074334	-1.1507618487	-2.4998471441
H	-1.4943150111	-1.4756767744	2.1188707352
H	-1.6938239499	-3.5150606598	3.4476246430
H	-1.7569679889	-3.9559047331	1.7348749862
H	-3.2341151988	-3.9386957874	2.7107159352
H	-2.6974440310	-1.3119095271	4.2647268940
H	-4.2396722889	-1.6386054729	3.4568851417
H	-3.3628705268	-.1451587910	3.1047026614
H	-2.1891379255	1.1058538034	-1.9788433038
H	-3.5442240704	1.9721293959	-3.7806763254
H	-4.5557121704	1.8668123326	-2.3318668981
H	-4.7254774419	.6759503000	-3.6331919057
H	-1.7369652583	.2135299745	-4.2320350259
H	-2.8592197371	-1.1290274865	-3.9619587843
H	-1.3686274105	-1.0271802171	-3.0198929699

21. $L^2CuO_2^-$ – side-on doublet

Cu	-.5758581151	-.5597194514	-.0046051954
O	.2166206800	-2.3309413528	-.4439716509
O	-1.1929081850	-2.4150529854	-.3703363704
N	.8782952344	.7985895480	.2119960860
N	-2.1540247229	.6170472223	.3586478013
C	1.7022514010	3.0767745185	.6627319620
C	.5686403270	2.0467079584	.5023342271
C	-.7292682558	2.5658071664	.6927918003
C	-1.9683679681	1.8946808188	.6248539865
C	-3.1958207098	2.7824965413	.9019063982
C	2.2105467192	.3103279430	.0339005326
C	2.8921373693	-.2668914285	1.1309979649
C	4.1680989071	-.7985931950	.9200704919
C	4.7546646265	-.7973121331	-.3415785212
C	4.0432354214	-.2901325996	-1.4242965062
C	2.7644512395	.2533029846	-1.2662060110
C	2.2192821690	-.4282751845	2.4901572581
C	3.0856906793	.0635683529	3.6618371213
C	1.7915004458	-1.9004135308	2.6776406925
C	1.9544569859	.6547003680	-2.4943609715
C	1.4816068811	-.6169416549	-3.2324903294
C	2.7070683104	1.6102707679	-3.4356831866
C	-3.4298983931	-.0264620327	.3062599179
C	-3.9372627476	-.6631588849	1.4628062633
C	-5.1553797990	-1.3438183043	1.3706030085
C	-5.8487655622	-1.4297104754	.1673696192
C	-5.3023330979	-.8582646345	-.9774904248
C	-4.0878447165	-.1663367775	-.9378549780
C	-3.1280712863	-.7263959291	2.7537935442
C	-2.4996422400	-2.1301883645	2.8927386077
C	-3.9393190316	-.3435875909	4.0028871154
C	-3.4462462607	.3136120401	-2.2352562838
C	-4.3848083213	1.1763725948	-3.0960660382
C	-2.9085971453	-.9021030710	-3.0209372090
F	1.2621057351	4.3227126354	.9602496592
F	2.4350618959	3.1980706073	-.4687611042
F	2.5562090528	2.7330374414	1.6550453004
H	-.7811681460	3.6157165575	.9225896590
F	-2.8829650267	4.0784759717	1.1408509652
F	-3.8876814112	2.3575413080	1.9852662548
F	-4.0565257902	2.7906644026	-.1421751447
H	4.7015077491	-1.2428067910	1.7566840780
H	5.7478274136	-1.2164171841	-.4853548718
H	4.4793424944	-.3371334851	-2.4189546742
H	1.3081334438	.1756418184	2.4840928444
H	2.5375412874	-.0358310931	4.6064786013
H	3.3615623489	1.1150161287	3.5357598894
H	4.0094013953	-.5188693253	3.7610990973
H	1.2012260968	-2.0172849593	3.5956045333
H	2.6718497567	-2.5509150915	2.7609555950
H	1.1961840743	-2.2446854762	1.8235665142
H	1.0604763103	1.1787299400	-2.1460476325

H	.7949050482	-.3579048439	-4.0486688450
H	.9746163675	-1.3015527330	-2.5422389189
H	2.3356093568	-1.1497824029	-3.6702940215
H	2.0639216665	1.9008079407	-4.2750829261
H	3.6034516764	1.1440756587	-3.8616274772
H	3.0163716002	2.5196456522	-2.9116054584
H	-5.5555079683	-1.8353148909	2.2537741191
H	-6.7943956488	-1.9643657052	.1160440498
H	-5.8173799692	-.9699720079	-1.9283719334
H	-2.3069006939	-.0100962088	2.6677906949
H	-1.8122926027	-2.1638418202	3.7478306382
H	-1.9532201818	-2.4057290905	1.9829801779
H	-3.2787282995	-2.8848716838	3.0595371179
H	-3.2976505603	-.3627871156	4.8919964778
H	-4.7650555021	-1.0415384353	4.1853514013
H	-4.3616007945	.6614354080	3.9077551519
H	-2.5858883322	.9337747231	-1.9701143269
H	-3.8605956274	1.5288495984	-3.9925259786
H	-4.7384494583	2.0506511566	-2.5411928078
H	-5.2626569659	.6133721937	-3.4348872904
H	-2.3301602816	-.5731823556	-3.8938976808
H	-3.7362527818	-1.5250978421	-3.3837081154
H	-2.2706720863	-1.5248209317	-2.3826290680

22. L²CuO₂H – side-on doublet

Cu	-.0284691159	-1.0371815561	-.2365853509
O	-.1106964693	-3.3981088314	-1.6770223889
O	-.0368772536	-2.8853688600	-.3561274869
N	1.3702281646	.2834250676	-.0685943858
N	-1.5926358915	.0836504049	.0217129330
H	-.2489890343	-4.3445237852	-1.5068213584
C	-2.7058567521	2.2199721186	.5256994671
C	2.6892990178	-.2615886082	-.2394221353
C	3.3458312545	-.8421522710	.8714454267
C	4.5774428567	-1.4676705575	.6559660063
C	5.1409174014	-1.5421152361	-.6134931173
C	4.4655511218	-.9968537519	-1.7004362664
C	3.2320185967	-.3570477328	-1.5448502096
C	2.7150316603	-.8860649005	2.2593780360
C	3.6615540559	-.3863944274	3.3649444943
C	2.2167311551	-2.3146943023	2.5664735210
C	2.4844804675	.1429275643	-2.7784574570
C	1.9484395354	-1.0497426193	-3.5992671495
C	3.3392717031	1.0707316732	-3.6601230933
C	-2.8371730171	-.6387256330	-.0366475509
C	-3.2940620974	-1.3106865382	1.1247709793
C	-4.4423363313	-2.1008466833	1.0208573419
C	-5.1142682998	-2.2490354445	-.1882437261
C	-4.6330477773	-1.6100318124	-1.3247893074
C	-3.4892394761	-.8046776151	-1.2823982803
C	-2.5371087337	-1.2686561714	2.4498675974
C	-1.8673956424	-2.6325927212	2.7271311392

C	-3.4260594886	-.8449616940	3.6330814660
C	-2.9572777428	-.2014265219	-2.5795162720
C	-4.0249084826	.6129360139	-3.3344514807
C	-2.3717608689	-1.3034058045	-3.4888400994
C	2.2221053021	2.5512143964	.3587012284
C	1.0715462709	1.5411078583	.2015989152
C	-.2234813156	2.0623491154	.3645066012
C	-1.4449108563	1.3699577323	.2848668691
F	1.7884778830	3.8015666083	.6053726082
F	2.9754228456	2.6111124549	-.7583929017
F	3.0339831028	2.2084238015	1.3807506924
F	-2.4217696894	3.5114700514	.7802133011
F	-3.4140562781	1.7599636401	1.5771678784
F	-3.5167655725	2.2009752439	-.5527586807
H	-.2879333734	3.1137691906	.5845730825
H	5.0975522092	-1.9171497790	1.4968579298
H	6.0970131539	-2.0376196728	-.7575214385
H	4.8983967049	-1.0798435933	-2.6930814640
H	1.8424020829	-.2266553441	2.2559618733
H	3.1417570079	-.3769107422	4.3292314289
H	4.0143992035	.6270212139	3.1571721509
H	4.5380818840	-1.0340527419	3.4754323846
H	1.6959125032	-2.3439912117	3.5301261521
H	3.0556648304	-3.0182011726	2.6174734624
H	1.5309146004	-2.6792044878	1.7947019333
H	1.6218203254	.7229626567	-2.4391219301
H	1.3532155754	-.6962397853	-4.4488271555
H	1.3210070092	-1.7149707977	-2.9976121441
H	2.7732950090	-1.6518500534	-3.9972000308
H	2.7417028996	1.4503880309	-4.4961615742
H	4.2006669926	.5470401056	-4.0887001112
H	3.7128265573	1.9258261788	-3.0911702972
H	-4.8084471135	-2.6216932661	1.9008446349
H	-6.0022864195	-2.8724974815	-.2461018283
H	-5.1469231190	-1.7491459185	-2.2714042599
H	-1.7400104380	-.5249461436	2.3613672725
H	-1.2478016926	-2.5802478199	3.6296839610
H	-1.2353034992	-2.9492342275	1.8913821871
H	-2.6195704019	-3.4142999471	2.8853773430
H	-2.8283275017	-.7787344062	4.5490144146
H	-4.2259771772	-1.5697937204	3.8181280212
H	-3.8878118755	.1292521148	3.4551720963
H	-2.1425332598	.4826943511	-2.3245877482
H	-3.5862218806	1.0760315479	-4.2251262414
H	-4.4414220781	1.4041613757	-2.7073255275
H	-4.8520797975	-.0211067856	-3.6715863371
H	-1.9230119283	-.8606950285	-4.3853375696
H	-3.1545267138	-1.9968867603	-3.8186658774
H	-1.6067504772	-1.8920841206	-2.9743034794

23. $L^2CuO_2H^+$ – end-on singlet

Cu	-.0571636433	-.0465477258	.9052104638
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O	1.4106276707	-2.2045049606	1.6600360636
O	.5969793498	-1.1942831208	2.1783395301
N	1.4692919283	.5098940825	-.2591025678
N	-1.4210673508	1.0349191460	.1664834064
H	2.1675520849	-2.2012924823	2.2747280939
C	-2.2429610214	3.0513497227	-1.0472381402
C	2.6599364728	-.1860406564	-.0134044180
C	3.6264628764	.2958730924	.9304309116
C	4.7918632879	-.4472333747	1.0810083283
C	5.0142064932	-1.6243899923	.3542178591
C	4.0449360862	-2.1131371556	-.5139295286
C	2.8369088678	-1.4371599638	-.6961595868
C	3.3904857888	1.5105126095	1.8230838936
C	4.6021364978	2.4605769833	1.8752482211
C	2.9995825460	1.0520011849	3.2476639619
C	1.8086784729	-1.9630449103	-1.6828664038
C	1.5521951771	-3.4735991579	-1.5307207880
C	2.2270531872	-1.6169375646	-3.1308356162
C	-2.6677904354	.3915411004	.3486049541
C	-3.1694068304	.3006401266	1.6853956300
C	-4.3658030585	-.3858029636	1.8832162830
C	-5.0356261062	-.9895183781	.8216737678
C	-4.5165859223	-.9198973627	-.4722753090
C	-3.3344171699	-.2391848410	-.7504915157
C	-2.5037858149	1.0055749674	2.8626938265
C	-2.2409089643	.0483714671	4.0414855637
C	-3.3339082803	2.2317130214	3.2973718906
C	-2.7580530278	-.3069026701	-2.1619484558
C	-3.7831258484	.0836501193	-3.2438280004
C	-2.1867960644	-1.7163133904	-2.4300496232
C	2.5501535382	2.3188780854	-1.6019799200
C	1.3332822030	1.6731607628	-.8862404624
C	.1532464695	2.4164955097	-1.0271340048
C	-1.1354260145	2.0752682443	-.5922079205
F	2.1446024253	2.9696878326	-2.7033322976
F	3.4644381589	1.4157754831	-1.9828393027
F	3.1477002452	3.2105798806	-.7913688237
F	-1.8051241790	4.3126872138	-.9031888792
F	-3.3642740455	2.9182069897	-.3272160661
F	-2.5464805758	2.8657506767	-2.3443766802
H	.2351427589	3.3313506085	-1.5949481546
H	5.5502862521	-.1093897721	1.7790272006
H	5.9459692064	-2.1669032670	.4855159959
H	4.2259347202	-3.0361962515	-1.0531713586
H	2.5475999298	2.0801881890	1.4223569830
H	4.3379040946	3.3621083315	2.4361159125
H	4.9240727852	2.7639421834	.8769057787
H	5.4554647609	2.0033586854	2.3857304079
H	2.7759944735	1.9219431573	3.8735601785
H	3.8252970145	.5077191606	3.7191585279
H	2.1217106986	.3986634725	3.2407735124
H	.8642460932	-1.4456035895	-1.4840087925

H	.7307057125	-3.7732564341	-2.1888597796
H	1.2811456440	-3.7308992615	-.5034861942
H	2.4237144240	-4.0706206495	-1.8170373182
H	1.4500177801	-1.9355618331	-3.8326994726
H	3.1547150607	-2.1323196590	-3.4008254148
H	2.3931683613	-.5446590284	-3.2630128038
H	-4.7872962853	-.4443063338	2.8810113994
H	-5.9633621578	-1.5242898810	1.0014149728
H	-5.0413180856	-1.4201756753	-1.2791308316
H	-1.5313717449	1.3868737195	2.5282083829
H	-1.7201519378	.5814267768	4.8431518016
H	-1.6205231022	-.8018114328	3.7404982987
H	-3.1718014046	-.3442844651	4.4619995216
H	-2.8195556605	2.7725101527	4.0978495460
H	-4.3162626439	1.9295369925	3.6746096246
H	-3.4920413826	2.9209382541	2.4627097515
H	-1.9256227356	.3958855229	-2.2437467734
H	-3.2949574568	.1072355755	-4.2229571428
H	-4.2110014956	1.0707546346	-3.0551219481
H	-4.6035566735	-.6375100378	-3.3079537523
H	-1.7093484109	-1.7499752107	-3.4147222938
H	-2.9777976488	-2.4728264534	-2.4144225376
H	-1.4430753142	-2.0011253463	-1.6778386124

24. $L^2CuO_2H^+$ – end-on triplet

Cu	.0314585568	-.3905737244	.3747626449
O	.5750693171	-3.1226309829	.6260211726
O	.0688542329	-2.0791351558	1.3409602877
N	1.5485278799	.6869532518	-.1851001808
N	-1.4115644126	.8014220454	-.1588052689
H	.5793831707	-3.8639859716	1.2657077007
C	-2.3262958342	2.8168274878	-1.2764858563
C	2.7479788175	-.0522427676	-.0143978229
C	3.2732725710	-.1535679717	1.3084798275
C	4.4284799155	-.9112612234	1.4873013584
C	5.0207167273	-1.5878058342	.4209289843
C	4.4590846566	-1.5204929961	-.8537937882
C	3.3165488587	-.7619435293	-1.1113689023
C	2.6626258266	.5837240123	2.4967384506
C	3.5796697206	1.7336124101	2.9687152327
C	2.3299403431	-.3720813722	3.6604329356
C	2.6583472546	-.8216134542	-2.4890988334
C	1.8628906403	-2.1369576643	-2.6470893210
C	3.6607435270	-.6516728848	-3.6450910905
C	-2.6373190881	.4424445068	.4657734689
C	-3.0502297838	1.1007595933	1.6638638224
C	-4.2108020679	.6326890099	2.2785908424
C	-4.9403282878	-.4331846106	1.7502437250
C	-4.5080953888	-1.0761100510	.5914123653
C	-3.3477470486	-.6751299743	-.0665336359
C	-2.2127301106	2.1752639261	2.3529841270
C	-1.3647315138	1.5426403642	3.4789583636

C	-3.0551393800	3.3403997891	2.8999430949
C	-2.9173249113	-1.3893091428	-1.3440595456
C	-3.9437978150	-1.1840910093	-2.4769451450
C	-2.6705105974	-2.8907584383	-1.0965072144
C	2.6156424068	2.6435155882	-1.2677838689
C	1.3800288240	1.8296686880	-.8189353704
C	.1313761844	2.4057880194	-1.1245091260
C	-1.1513883255	1.9284474454	-.8015102350
F	2.3081077539	3.9420967142	-1.4005266180
F	3.0834409405	2.2058956730	-2.4501410313
F	3.6054490543	2.5455495525	-.3656612521
F	-1.9472612920	3.6254815974	-2.2772510269
F	-2.7989995882	3.5890104342	-.2827937985
F	-3.3350274229	2.0529522759	-1.7274505365
H	.1636308536	3.3429245053	-1.6586456874
H	4.8764279991	-.9732570919	2.4739929692
H	5.9192176026	-2.1753355746	.5842389709
H	4.9137326687	-2.0829023082	-1.6617919424
H	1.7233281896	1.0413847808	2.1666785735
H	3.1120474930	2.2749229013	3.7974478940
H	3.7746028181	2.4444103672	2.1620574020
H	4.5426243610	1.3499429831	3.3202893628
H	1.8550131277	.1822395899	4.4761311635
H	3.2278661242	-.8458453324	4.0699463512
H	1.6451209706	-1.1681607630	3.3469099314
H	1.9416659231	-.0011721892	-2.5679129536
H	1.3590630834	-2.1607308340	-3.6190051210
H	1.1008332950	-2.2527723423	-1.8674354802
H	2.5252899835	-3.0072661317	-2.5896140979
H	3.1219137418	-.5824010458	-4.5949017695
H	4.3432035683	-1.5033343736	-3.7252880921
H	4.2592523371	.2548613420	-3.5269052430
H	-4.5492133119	1.1011315284	3.1962058946
H	-5.8460562687	-.7658377958	2.2481404712
H	-5.0898549032	-1.8992931557	.1888153621
H	-1.5164693069	2.5979235550	1.6256312504
H	-.7365561428	2.3035335408	3.9543241395
H	-.7063229491	.7513142839	3.1005252747
H	-2.0012757382	1.0994898495	4.2519843026
H	-2.3951058614	4.1331243166	3.2650872125
H	-3.6833998491	3.0339257528	3.7422247276
H	-3.7021537547	3.7647354223	2.1286101966
H	-1.9745075884	-.9448805247	-1.6809112699
H	-3.5973129093	-1.6743279327	-3.3923049222
H	-4.0901891428	-.1227625210	-2.6919511207
H	-4.9166823030	-1.6140560856	-2.2177967593
H	-2.3316126017	-3.3732369537	-2.0186262200
H	-3.5848331959	-3.3996133729	-.7752018493
H	-1.9108153631	-3.0582803609	-.3273931580
25.	L ² CuO ₂ ⁻ – end-on doublet		
Cu	-.8866810430	-.4030913597	.3237523562

O	-1.0251859118	-3.0062991272	.8091496767
O	-.8259891983	-1.9096930176	1.5664343081
N	.6376047355	.4063773084	-.7150133957
N	-2.3857449827	.6633044386	-.4412792041
C	1.6107128705	2.2073879310	-2.0790865547
C	.4184226371	1.5062228108	-1.4064999907
C	-.8302444829	2.1386264938	-1.6033110408
C	-2.1116283574	1.7182241106	-1.1843155936
C	-3.2718314076	2.6139723156	-1.6489351126
C	1.8822122849	-.2873657212	-.6249615328
C	2.6859059393	-.1324263201	.5309811424
C	3.8551476738	-.8902502008	.6457886471
C	4.2280631954	-1.8047373105	-.3340900355
C	3.4009961739	-1.9912361514	-1.4365223871
C	2.2192844706	-1.2609369726	-1.5997936235
C	2.2565892362	.7662951945	1.6857180988
C	3.3353139130	1.7905062916	2.0775963233
C	1.8300954726	-.0921359126	2.8962816568
C	1.2794437990	-1.6185064488	-2.7481816554
C	.6094825316	-2.9809600558	-2.4678157845
C	1.9718634042	-1.6186803020	-4.1226284077
C	-3.6928243971	.1866737821	-.1158438217
C	-4.2472498765	.4830949650	1.1539338238
C	-5.4808079277	-.0768061739	1.4980308574
C	-6.1583896768	-.9297576489	.6326685122
C	-5.5792940515	-1.2567354289	-.5885833387
C	-4.3456266531	-.7275287354	-.9812659825
C	-3.4843064755	1.3111361404	2.1819220164
C	-2.9427284369	.3966836388	3.3017540652
C	-4.3205334188	2.4658369418	2.7588844020
C	-3.6930376493	-1.2399652987	-2.2622168459
C	-4.6083097973	-1.1290745445	-3.4946674884
C	-3.2133585600	-2.6931771940	-2.0576120730
F	1.2953249883	3.4032560613	-2.6316493000
F	2.1441956159	1.4605096892	-3.0754157518
F	2.6057669092	2.4515461610	-1.1939990962
H	-.8043563285	3.0502406215	-2.1752258112
F	-2.8691128152	3.7217155627	-2.3157027837
F	-4.0095380659	3.0527724227	-.6010420133
F	-4.1176372806	1.9605482304	-2.4805105640
H	4.4754339973	-.7743159784	1.5312219230
H	5.1396020678	-2.3877237255	-.2255752914
H	3.6650129750	-2.7398979256	-2.1792458328
H	1.3770380398	1.3269311793	1.3577418765
H	2.9671291435	2.4449176750	2.8769491870
H	3.6131792447	2.4154356154	1.2236447526
H	4.2442672413	1.3023189889	2.4488784676
H	1.4452870544	.5440896573	3.7035442158
H	2.6831010091	-.6558053941	3.2947259701
H	1.0523631855	-.8117235711	2.6208840015
H	.4866985212	-.8671532886	-2.7828903318
H	-.1158555527	-3.2217216964	-3.2549257724

H	.0881968127	-2.9838672978	-1.5044992567
H	1.3572955872	-3.7836650848	-2.4482306372
H	1.2406565206	-1.8248205985	-4.9135586982
H	2.7454663982	-2.3927186514	-4.1894692970
H	2.4406012140	-.6535567917	-4.3333504682
H	-5.9096180360	.1460073416	2.4719370121
H	-7.1157852850	-1.3582294028	.9192886573
H	-6.0843940098	-1.9597614744	-1.2463216331
H	-2.6214700519	1.7524551413	1.6760863830
H	-2.3334699228	.9725543148	4.0099280409
H	-2.3263766213	-.4108129793	2.8934048499
H	-3.7660407006	-.0607744312	3.8645377963
H	-3.7178767163	3.0615014302	3.4550762078
H	-5.1926192520	2.1001394733	3.3140136341
H	-4.6794565777	3.1266901104	1.9642695106
H	-2.8073383732	-.6297193915	-2.4568936685
H	-4.0738144800	-1.4612737461	-4.3928615713
H	-4.9387106894	-.0990694723	-3.6546988282
H	-5.5001020193	-1.7597410950	-3.3978749529
H	-2.6897424906	-3.0536899142	-2.9518196008
H	-4.0650874449	-3.3615650052	-1.8792479636
H	-2.5338863826	-2.7758149001	-1.2020580044

26. L²CuO₂H – end-on doublet

Cu	.0596077394	-.2821286563	.5144440246
O	-.0121389969	-2.9955040198	1.0209075236
O	.1207717339	-1.7354156995	1.6623395461
N	1.5624595482	.6375665408	-.2962753870
N	-1.3793465345	.8920178950	-.0165685944
H	.1271515001	-3.6001395389	1.7683464552
C	-2.3028203951	2.9224299911	-1.0524891430
C	2.8218769514	-.0249021758	-.0830871582
C	3.5222220727	.1985411531	1.1274131175
C	4.6826024165	-.5442620274	1.3654058612
C	5.1354735450	-1.4939617412	.4557371467
C	4.4167889555	-1.7249252047	-.7120592189
C	3.2494943891	-1.0118012759	-1.0043468747
C	3.0113782463	1.1484379789	2.2073398707
C	4.0718233373	2.1693101333	2.6566576178
C	2.4775987226	.3447371892	3.4132528927
C	2.4505811714	-1.3707609430	-2.2541049005
C	1.7931447601	-2.7583584073	-2.0927058313
C	3.2986677936	-1.3178424703	-3.5377386693
C	-2.6712472540	.4404682087	.4273377938
C	-3.1018960420	.7625956850	1.7373250534
C	-4.3094498298	.2200761732	2.1868216866
C	-5.0650897756	-.6300386626	1.3861624845
C	-4.6089502376	-.9651428514	.1158657794
C	-3.4086527025	-.4527542477	-.3870250080
C	-2.2568988797	1.6005616357	2.6926791818
C	-1.6387432276	.6985121414	3.7828661525
C	-3.0399636971	2.7657890500	3.3229178538

C	-2.9026938116	-.9295355227	-1.7452962651
C	-3.9389166485	-.7413299726	-2.8676655942
C	-2.4489528064	-2.4027494959	-1.6595476106
C	2.6032672758	2.5111658032	-1.5062892764
C	1.3761860337	1.7820372346	-.9291339333
C	.1407025072	2.4241168264	-1.1274340439
C	-1.1269714817	1.9957316777	-.6963150688
F	2.2774288567	3.6505502696	-2.1468105849
F	3.2621010044	1.7370640359	-2.3922965402
F	3.4725451139	2.8430400753	-.5289489067
F	-1.9179722831	4.0030454538	-1.7572917574
F	-2.9157886691	3.3757957745	.0610667557
F	-3.2272947689	2.2783831495	-1.7939514002
H	.1696896611	3.3539686695	-1.6686284047
H	5.2332577825	-.3853178307	2.2879892659
H	6.0374004729	-2.0630213550	.6637463067
H	4.7608328250	-2.4847533318	-1.4077156360
H	2.1723651982	1.7140306045	1.7919866849
H	3.6423195850	2.8610892660	3.3897264000
H	4.4435733936	2.7540082474	1.8114748717
H	4.9287389122	1.6812914822	3.1336086100
H	2.0301155444	1.0150895977	4.1559750941
H	3.2881706422	-.2046446676	3.9060908902
H	1.7230094478	-.3876182975	3.1091844873
H	1.6464391291	-.6376418175	-2.3639966249
H	1.1576258205	-2.9844864136	-2.9566900926
H	1.1796604303	-2.8165956746	-1.1887410613
H	2.5534546265	-3.5453544299	-2.0250372538
H	2.6721921155	-1.5276206953	-4.4116911555
H	4.0993753758	-2.0653566885	-3.5250990438
H	3.7565986888	-.3350108971	-3.6730347671
H	-4.6565577592	.4572234978	3.1882263486
H	-5.9987983777	-1.0430793358	1.7576911546
H	-5.1893432660	-1.6503031090	-.4950829362
H	-1.4328697678	2.0367687778	2.1213708272
H	-.9642474408	1.2759455004	4.4252166654
H	-1.0733870951	-.1325283619	3.3487077113
H	-2.4184405817	.2661505905	4.4204932403
H	-2.3763139541	3.3687996041	3.9524739589
H	-3.8570818291	2.4100537807	3.9597936642
H	-3.4679505783	3.4164888416	2.5560560598
H	-2.0260434970	-.3312719723	-2.0092378630
H	-3.5106194528	-1.0426484931	-3.8299662980
H	-4.2549730938	.3019239638	-2.9458299653
H	-4.8318265730	-1.3542267573	-2.7033432943
H	-2.0189590333	-2.7284274872	-2.6135943599
H	-3.2965595247	-3.0602931621	-1.4340741023
H	-1.7000919962	-2.5553735785	-.8760789324