Supporting Information

For

Characterization of a 1:1 Cu/O_2 Adduct Supported by an Anilido-Imine Ligand

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Figure S1. Interaction between H18A and H34B in the crystal structure of $L^2Cu(MeCN)$.

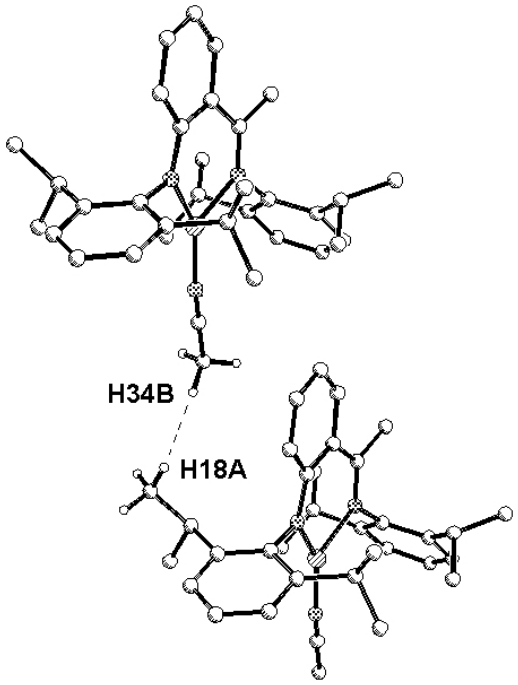

Figure S2. Optimized geometries for the end-on and side-on triplet states of L^2CuO_2. Hydrogen atoms are omitted for clarity. Single numbers denote distances (Å). Gray represents C, blue N, red O, and pink Cu.

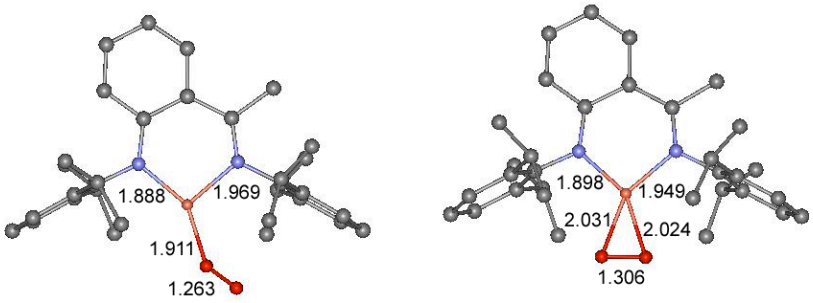

Figure S3. Key frontier orbitals showing partial occupation in the side-on singlet L^4CuO_2 CASSCF wave function. Occupation numbers are shown in parentheses. Orange represents C, blue N, red O, white H, and yellow Cu.

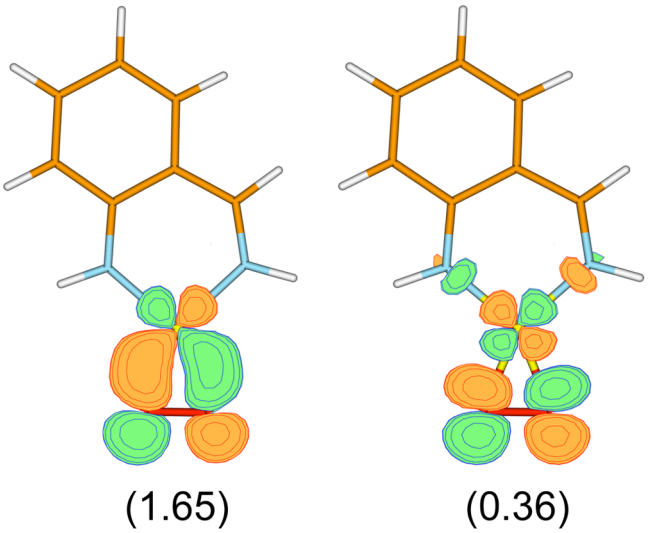

Table S1. Summary of X-ray Crystallographic Data.

	$L^2Cu(MeCN)$	L^2CuO_2
Empirical Formula	$C_{34}H_{44}CuN_3$	$C_{32}H_{41}CuN_2O_2$
Formula weight	558.26	549.21
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	C2/c
Temperature	-100 °C	-100 °C
a (Å)	10.1334(5)	36.846(6)
b (Å)	20.1075(11)	9.2961(14)
c (Å)	15.9863(9)	24.176(4)
α (deg)	90	90
β (deg)	105.5080(10)	125.372(2)
γ (deg)	90	90
V (Å^3)	3138.7(3)	6752.2(18)
Z	4	8
D_{calc} (g/cm^3)	1.181	1.081
Crystal dimensions	0.4 x 0.3 x 0.2	0.2 x 0.2 x 0.05
θ range (deg)	1.67 to 25.08	1.69 to 25.10
Absorption coeff (mm^{-1})	0.721	0.673
Reflections collected	30253	16127
Unique Reflections	4328	5988
Parameters	345	343
$R1$, $wR2$ (for $I > 2\sigma(I)$)[a]	0.0369, 0.1037	0.0446, 0.1102
Goodness-of-fit	1.015	0.973
Largest peak, hole (e$^-$ Å^{-3})	0.360, -0.235	0.470, -0.284

[a] $R1 = \Sigma||F_o| - |F_c||/ \Sigma |F_o|$; $wR2 = [\Sigma [w(F_o^2 - F_c^2)^2]/ [\Sigma [w(F_o^2)^2]]^{1/2}$, where $w = 1/\sigma^2(F_o^2) + (aP)^2 + bP$.

Table S2. Mulliken charge populations from DFT calculations on the singlet 1:1 Cu/O_2 adducts for the (a) anilido-imine system using L^2 and (b) β-diketiminate system reported previously.[1] Both sets of calculations utilized the same basis sets.

(a)

dioxygen coordination mode	**Cu**	**amide N**	**Δ**
η^1	0.51	-0.81	1.32
η^2	0.70	-0.84	1.54

(b)

dioxygen coordination mode	**Cu**	**N**	**Δ**
η^1	0.52	-0.74	1.26
η^2	0.68	-0.75	1.43

[1] Aboelella, N. W.; Kryatov, S. V.; Gherman, B. F.; Brennessel, W. W.; Young, V. G., Jr.; Sarangi, R.; Rybak-Akimova, E. V.; Hodgson, K. O.; Hedman, B.; Solomon, E. I.; Cramer, C. J.; Tolman, W. B. *J. Am. Chem. Soc.*

2004, *126*, 16896-16911.

Atomic Coordinates for Computed Structures.

1) $L^2Cu(MeCN)$ (B3LYP/DZP level)

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

2) L^2CuO_2 side-on singlet (B3LYP/DZP level)

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

3) L^2CuO_2 side-on triplet (B3LYP/DZP level)

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

4) L^2CuO_2 end-on singlet (B3LYP/DZP level)

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	3.3891110617
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

5) L^2CuO_2 end-on triplet (B3LYP/DZP level)

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

6) L^2CuO_2 side-on singlet (B3LYP/TZP level)

Cu	-.0057300849	-2.3711768989	.8835524336
O	.8233590779	-3.9447133802	1.4668483203
O	-.5159292114	-4.1195638763	1.2936592187
N	1.3138277546	-1.0216250373	.6521876652
N	-1.4970868134	-1.3711184670	.3555055269
C	2.2626190204	1.1373851704	.0605849387
C	1.0792515248	.2089752896	.2588767956
C	-.2480365757	.7296753015	.0092121774
C	-1.4625536770	-.0530474248	.0597949161
C	-2.6833353779	.6296747943	-.2404320346
C	2.6534693034	-1.4738177094	.9324117775
C	3.1747104216	-1.2790191515	2.2244419129
C	4.4719608443	-1.7254724806	2.4758533512
C	5.2182955082	-2.3582430094	1.4904768272
C	4.6714464728	-2.5628283478	.2310244007
C	3.3806797998	-2.1306293661	-.0753353390
C	2.3456246024	-.6566088614	3.3410052388
C	3.0820638960	.4798006853	4.0685964216
C	1.8816130480	-1.7456893506	4.3274651185
C	2.8011817756	-2.3814795364	-1.4615722522
C	2.6325146768	-3.8891061178	-1.7231445694
C	3.6357392975	-1.7090350680	-2.5661618724
C	-2.7413340027	-2.0780273741	.2893278539
C	-3.5124865663	-2.2381435202	1.4574667626
C	-4.7029153837	-2.9613546490	1.3727323638
C	-5.1294400121	-3.5058613808	.1692934203
C	-4.3659253202	-3.3277542258	-.9771218393
C	-3.1683668262	-2.6136206664	-.9436744463
C	-3.0764849162	-1.6529662152	2.7931504372
C	-2.7351433168	-2.7657172219	3.8005586846
C	-4.1249821815	-.6827414923	3.3648762168
C	-2.3459662010	-2.4557205744	-2.2154572903
C	-3.1674514596	-1.8789813877	-3.3809182403
C	-1.6881172352	-3.7923203611	-2.6037279405
C	-2.7266197451	1.9635395860	-.5516979733
C	-.3588526792	2.1095489568	-.3168005233
C	-1.5507313950	2.7294409817	-.5912277433
H	2.2384879663	1.5762306644	-.9372919705
H	3.2034181159	.6138864669	.1874015021
H	2.2283336716	1.9565667916	.7835946253
H	-3.6018381248	.0624206614	-.2087209507
H	4.9024316450	-1.5815770566	3.4598879399
H	6.2251617299	-2.6974681796	1.7069821695
H	5.2567421716	-3.0672754040	-.5292125067
H	1.4479552679	-.2242748731	2.8961791957

H	2.4173254398	.9541894384	4.7958169929
H	3.4224763528	1.2488710398	3.3699694252
H	3.9560024982	.1160785916	4.6153676679
H	1.2196767490	-1.3187138119	5.0866904399
H	2.7359845678	-2.1967541271	4.8404146674
H	1.3471981281	-2.5441076014	3.8079157222
H	1.8056645291	-1.9349876264	-1.4958007900
H	2.1426479556	-4.0555626739	-2.6867307537
H	2.0282398667	-4.3525009009	-.9408633910
H	3.5999648825	-4.3983768630	-1.7487051869
H	3.1591988805	-1.8482405991	-3.5405347343
H	4.6407540042	-2.1352736253	-2.6264805524
H	3.7403140571	-.6346569663	-2.3920416764
H	-5.3062297662	-3.0995473451	2.2630174187
H	-6.0572116515	-4.0658524168	.1236088135
H	-4.7070932636	-3.7519843288	-1.9145299505
H	-2.1655604963	-1.0781699230	2.6177405248
H	-2.3528451996	-2.3352831310	4.7312062858
H	-1.9807148611	-3.4414339660	3.3928142988
H	-3.6204643801	-3.3589470735	4.0482683704
H	-3.7596170632	-.2314674550	4.2920058798
H	-5.0645911869	-1.1928299016	3.5952978336
H	-4.3448734688	.1237159981	2.6607277100
H	-1.5454388104	-1.7456084035	-2.0044944953
H	-2.5227360895	-1.7007997523	-4.2465557533
H	-3.6319288184	-.9289182073	-3.1057026171
H	-3.9601530013	-2.5613211437	-3.6998166496
H	-1.0444306952	-3.6652803438	-3.4798972423
H	-2.4423495736	-4.5457244695	-2.8491840557
H	-1.0834027754	-4.1846447992	-1.7829144027
H	-3.6856019090	2.4256037523	-.7627533410
H	.5348483166	2.7148579954	-.3418488408
H	-1.5806572271	3.7853113500	-.8299437614

7) L^2CuO_2 end-on singlet (B3LYP/TZP level)

Cu	-.1332935411	-2.1738620988	.2554294241
O	.4710805181	-4.8259501725	-.2561673230
O	.1266879576	-3.9567082327	.6128174504
N	1.3155538771	-.8923591868	.1713135714
N	-1.5314615367	-.9364852934	-.0319940920
C	2.4379768465	1.2597656737	.0479839023
C	1.1892627227	.3983895307	-.0147670657
C	-.0828363819	1.0446392210	-.2832001751
C	-1.3686369528	.3763336683	-.2978616666
C	-2.5129975194	1.1824172588	-.5960345620
C	2.5747261667	-1.5278474194	.4266095346
C	3.0215541916	-1.6585125459	1.7577197275
C	4.2141394798	-2.3449405075	1.9813524819
C	4.9379807199	-2.8938778182	.9291643823
C	4.4732536699	-2.7645341119	-.3723008993
C	3.2864095898	-2.0855705634	-.6536849891
C	2.2258288148	-1.1079382116	2.9356336123
C	3.0618110070	-.1654429352	3.8183656481
C	1.6189007041	-2.2543191859	3.7661358576
C	2.8092512876	-1.9524836441	-2.0950261158
C	2.5831014859	-3.3234483308	-2.7557274036
C	3.7757439876	-1.0897503238	-2.9278963852
C	-2.8220225231	-1.5399013903	-.0970604630
C	-3.5997607089	-1.6450575345	1.0787599880
C	-4.8303733481	-2.2975328927	1.0072874841
C	-5.2955000799	-2.8289325473	-.1892747352
C	-4.5285030336	-2.7073383807	-1.3413065654
C	-3.2898702274	-2.0650801856	-1.3227709316
C	-3.1309162878	-1.0632324180	2.4057493769
C	-2.8969884661	-2.1687993334	3.4506495460
C	-4.1044050297	.0038050718	2.9379854830
C	-2.4705663583	-1.9662529018	-2.6028182711
C	-3.2641216950	-1.3159277653	-3.7496403266
C	-1.9243580593	-3.3452255612	-3.0177708917
C	-2.4241685198	2.5224586822	-.8714014662
C	-.0584371294	2.4368980389	-.5691769912
C	-1.1796106806	3.1728447346	-.8635077965
H	2.3240632115	2.0458464382	.7964006640
H	2.6215524856	1.7431930322	-.9136083223
H	3.3103018418	.6657504140	.3006783429
H	-3.4807256436	.7013660847	-.6006172224
H	4.5816832912	-2.4556623451	2.9950881279
H	5.8619249263	-3.4263785934	1.1250090146
H	5.0415567865	-3.1994064681	-1.1865783489
H	1.3944749044	-.5234978341	2.5381234313

H	2.4387090748	.2677826293	4.6057745011
H	3.4880448748	.6551310518	3.2354858987
H	3.8871453836	-.6915012954	4.3052252922
H	.9897075573	-1.8563627056	4.5675582254
H	2.4006484398	-2.8657080596	4.2252998879
H	1.0076346537	-2.9145299963	3.1462056264
H	1.8456604058	-1.4402826304	-2.0818508981
H	2.1841521394	-3.1923714258	-3.7658195744
H	1.8751223128	-3.9250269152	-2.1818812235
H	3.5162098999	-3.8873610994	-2.8403932387
H	3.3858767710	-.9490665713	-3.9400844236
H	4.7585196535	-1.5618530853	-3.0130097534
H	3.9200649438	-.1025332574	-2.4811969126
H	-5.4386030568	-2.3876261008	1.9006600497
H	-6.2558143616	-3.3318686576	-.2251858055
H	-4.9006577224	-3.1192208283	-2.2725804664
H	-2.1732635674	-.5726705600	2.2270389228
H	-2.5036428334	-1.7433169315	4.3787482996
H	-2.1829400588	-2.9118210585	3.0867061871
H	-3.8260190692	-2.6926165996	3.6929982889
H	-3.7163463732	.4489705414	3.8589234039
H	-5.0858521321	-.4220593758	3.1653272177
H	-4.2470298405	.8060564217	2.2100685811
H	-1.6137583428	-1.3231687896	-2.3974731403
H	-2.6235574962	-1.1845430063	-4.6264263030
H	-3.6445871593	-.3335401936	-3.4596465034
H	-4.1157242715	-1.9298512565	-4.0557077712
H	-1.3143425544	-3.2602064662	-3.9222314082
H	-2.7381933791	-4.0449626248	-3.2289310632
H	-1.3041574345	-3.7848047588	-2.2323138178
H	-3.3291945115	3.0787648119	-1.0937351248
H	.8893045871	2.9544448366	-.5678767742
H	-1.1029996221	4.2307271089	-1.0825800402

Vibrational Frequencies. Vibrational frequencies were computed for truncated models only, owing to the prohibitive cost of computing frequencies for the entire ~80 atom model. Isopropyl groups on the phenyl rings were replaced with hydrogen atoms. Before frequencies were computed, the positions of these hydrogen atoms were optimized, while freezing the rest of the structure. Imaginary frequencies attributable to numerical noise from the computation are indicated by "()". Imaginary frequencies which are artifacts of the truncated model are indicated by "<>".

1) $L^2Cu(MeCN)$ (B3LYP/DZP level)

24.56	26.84	37.92	40.35	48.98	56.73
57.52	67.14	85.19	87.31	111.54	121.19
127.26	147.36	169.23	193.30	207.70	228.10
233.32	241.59	267.02	292.45	304.53	377.49
386.77	393.95	416.47	425.69	428.27	446.43
482.66	498.56	514.61	532.72	535.27	554.92
599.09	601.04	628.69	629.56	656.31	667.88
716.70	718.99	739.54	748.50	755.93	768.87
803.53	842.06	843.60	845.59	851.60	861.86
888.99	914.93	924.16	941.99	953.46	963.73
967.76	981.84	983.76	987.49	992.94	1003.13
1004.14	1046.92	1049.61	1050.60	1055.21	1057.35
1058.66	1090.33	1093.85	1095.53	1161.63	1181.85
1186.47	1187.06	1188.68	1199.24	1221.17	1229.07
1268.28	1286.25	1294.94	1310.70	1340.16	1343.70
1381.78	1411.73	1414.95	1417.12	1473.53	1476.14
1478.57	1479.56	1481.50	1502.05	1504.70	1506.88
1512.46	1515.31	1567.61	1613.47	1621.27	1624.97
1631.94	1634.84	1667.34	2362.50	3058.87	3058.95
3122.85	3138.31	3139.87	3164.25	3170.98	3171.35
3171.93	3178.09	3179.51	3188.30	3192.97	3193.32
3197.94	3198.87	3199.28	3204.46	3220.30	3237.65

2) L^2CuO_2 side-on singlet (B3LYP/DZP level)

<-128.43>	(-20.09)	48.08	56.48	60.89	66.15
79.41	80.01	89.69	113.98	127.80	157.43
158.99	188.19	219.64	231.93	234.73	263.21
298.83	328.97	400.43	413.71	421.17	424.62
431.36	456.40	496.17	499.12	507.56	519.83
520.21	534.37	572.05	605.49	616.41	626.45
633.06	661.13	679.88	714.14	716.72	745.35
747.37	761.73	777.10	806.12	840.78	841.68
853.04	871.60	884.05	895.61	921.11	929.78
938.27	966.85	969.57	992.25	996.20	998.84
1000.60	1006.32	1008.21	1048.38	1049.48	1050.24
1059.26	1092.62	1094.86	1103.14	1107.03	1161.98
1182.97	1189.28	1190.54	1192.38	1204.18	1225.52
1233.10	1273.59	1292.06	1299.90	1305.45	1339.57
1341.40	1388.76	1408.73	1423.99	1461.76	1481.82
1482.37	1483.05	1495.25	1509.91	1513.09	1531.52
1558.96	1606.19	1626.88	1630.57	1633.02	1634.99
1666.90	3081.36	3134.01	3176.12	3180.93	3181.67
3185.90	3191.36	3199.19	3203.00	3206.53	3212.94
3213.56	3215.30	3216.19	3222.20	3238.03	3261.36

3) L^2CuO_2 side-on triplet (B3LYP/DZP level)

<-146.30>	10.18	50.29	54.09	59.59	65.22
75.38	75.99	81.86	108.59	112.97	123.30
147.83	156.75	209.50	217.41	232.51	245.37
282.35	301.59	330.27	375.90	398.48	411.13
425.25	426.69	435.42	491.22	497.39	515.44
524.54	532.49	560.27	601.97	614.88	628.33
632.23	659.31	674.86	715.69	718.36	743.56
746.12	761.17	773.27	802.16	841.17	843.08
854.85	860.42	876.88	891.44	918.37	923.73
932.84	964.13	967.85	989.47	992.44	993.63
998.48	1005.14	1006.35	1046.89	1049.52	1050.38
1055.59	1091.39	1093.70	1101.51	1160.65	1181.70
1188.36	1189.31	1191.70	1202.20	1221.30	1225.31
1236.89	1268.76	1292.13	1296.79	1303.69	1339.31
1341.07	1383.58	1411.58	1423.80	1461.70	1481.35
1481.58	1484.34	1496.13	1508.63	1512.27	1532.32
1557.21	1603.02	1625.80	1628.81	1632.93	1634.88
1672.35	3079.01	3130.83	3174.59	3177.63	3179.60
3183.03	3188.43	3198.46	3201.42	3204.42	3210.48
3211.07	3213.08	3213.95	3218.86	3228.82	3261.63

4) L^2CuO_2 end-on singlet (B3LYP/DZP level)

26.26	35.23	47.87	50.72	56.36	65.42
69.43	82.29	90.10	111.08	136.18	149.54
195.39	207.27	215.67	222.83	231.93	245.20
253.17	290.47	314.20	375.84	415.17	421.17
424.72	433.27	457.13	493.45	495.60	516.59
524.18	535.06	557.62	601.29	603.78	625.87
629.44	660.66	673.94	716.45	718.31	747.41
751.78	760.36	772.13	807.02	845.14	845.55
852.21	856.32	873.49	893.70	922.89	932.23
949.99	970.58	973.42	988.99	989.92	997.86
1002.21	1004.62	1006.03	1048.42	1049.31	1050.48
1062.35	1093.45	1096.53	1097.25	1161.65	1182.23
1188.95	1190.18	1192.34	1201.56	1221.93	1230.06
1272.40	1284.46	1292.10	1297.24	1312.64	1341.58
1344.41	1390.94	1409.29	1415.54	1468.16	1481.12
1482.98	1498.67	1503.22	1505.24	1511.30	1515.42
1566.89	1614.98	1621.70	1627.24	1630.28	1634.76
1666.80	3064.31	3126.71	3175.33	3176.85	3180.48
3183.78	3184.56	3187.77	3194.51	3198.42	3201.22
3203.88	3204.07	3207.34	3210.41	3225.04	3236.84

5) L^2CuO_2 end-on triplet (B3LYP/DZP level)

18.52	45.55	47.87	54.39	57.45	62.75
65.49	84.51	89.63	101.94	115.20	138.17
150.37	194.22	216.36	220.74	231.99	239.04
262.02	290.99	312.58	372.50	384.01	414.89
421.88	425.66	436.41	485.91	494.28	515.69
529.53	534.03	557.05	600.34	602.24	626.96
629.79	659.73	676.92	714.58	715.99	745.02
752.77	759.92	770.39	804.44	839.79	840.83
851.92	856.07	876.71	890.86	916.98	932.00
945.25	964.24	965.49	987.06	989.01	993.33
995.75	1004.14	1005.39	1048.98	1049.30	1050.66
1060.44	1090.89	1094.24	1096.89	1160.24	1181.25
1187.70	1189.34	1191.45	1201.18	1220.69	1228.67
1267.28	1289.61	1295.99	1305.66	1318.62	1339.16
1341.80	1382.50	1411.00	1415.71	1470.12	1480.60
1482.33	1500.28	1504.16	1506.25	1511.07	1515.08
1569.77	1614.45	1623.11	1626.95	1631.70	1634.93
1670.63	3066.32	3129.69	3175.08	3176.64	3177.35
3178.21	3184.74	3186.59	3198.27	3201.54	3203.78
3209.98	3212.80	3213.15	3215.99	3221.65	3242.74

6) L^2CuO_2 side-on singlet (B3LYP/TZP level, scaled by 0.97)

(-20.86)	33.87	45.72	53.36	61.57	69.05
74.66	105.19	115.24	125.78	156.17	166.77
189.64	195.08	212.95	222.13	231.31	256.15
291.91	322.09	371.86	405.31	408.01	411.33
422.97	452.27	489.80	494.56	499.63	510.95
518.70	524.14	559.23	590.21	602.76	610.65
617.30	644.54	666.04	695.61	696.55	730.97
736.10	756.86	757.85	788.95	815.99	816.14
842.11	848.32	861.73	872.45	900.59	914.66
928.16	946.35	948.57	965.46	968.68	971.82
976.69	979.27	981.51	1014.96	1015.74	1022.88
1030.13	1041.12	1057.70	1061.00	1063.53	1126.60
1146.10	1151.78	1152.90	1154.91	1167.01	1187.59
1193.28	1233.80	1243.70	1251.36	1271.36	1297.01
1299.90	1346.01	1360.61	1369.51	1416.74	1432.68
1435.83	1446.31	1451.23	1454.91	1461.65	1464.75
1511.63	1557.04	1569.43	1574.07	1575.47	1578.40
1609.27	2958.12	3014.45	3062.16	3064.81	3067.65
3073.66	3079.19	3081.37	3084.67	3089.25	3089.32
3102.13	3105.50	3106.11	3108.36	3120.07	3124.93

7) L^2CuO_2 end-on singlet (B3LYP/TZP level, scaled by 0.97)

17.83	29.97	42.09	48.18	48.88	59.95
67.27	77.15	89.79	109.56	139.56	149.39
189.97	198.76	203.54	220.89	224.18	241.74
258.22	288.38	311.73	362.85	403.31	408.38
411.08	421.50	457.27	485.09	488.08	505.59
513.96	520.18	543.83	585.74	594.26	609.91
614.09	642.92	660.30	699.47	699.92	727.62
734.29	747.18	753.01	785.12	820.52	820.80
833.75	837.06	853.62	867.39	898.32	909.82
924.81	951.93	952.21	960.00	965.12	976.45
977.33	978.66	980.52	1013.38	1014.91	1018.84
1027.45	1057.95	1060.21	1061.73	1124.63	1145.17
1151.22	1152.56	1154.82	1163.84	1183.57	1190.12
1225.85	1231.79	1237.96	1246.46	1270.09	1298.10
1301.70	1340.23	1358.27	1367.02	1416.16	1431.26
1434.42	1445.73	1450.41	1451.40	1458.45	1461.85
1510.39	1556.06	1562.45	1568.30	1571.61	1576.01
1605.55	2960.96	3013.15	3060.83	3062.81	3066.48
3070.59	3070.69	3075.65	3080.95	3084.74	3087.73
3089.13	3092.13	3093.06	3096.60	3112.48	3123.04