Supporting Information

for

Dioxygen Activation at a Single Copper Site: Structure, Bonding, and Mechanism of Formation of 1:1 Cu/O_2 Adducts

Nermeen W. Aboelella,[a] Sergey V. Kryatov,[b] Benjamin F. Gherman,[a] William W. Brennessel,[a] Victor G. Young, Jr.,[a] Ritimukta Sarangi,[c] Elena V. Rybak-Akimova,[b] Keith O. Hodgson,[c] Britt Hedman,[c] Edward I. Solomon,[c] Christopher J. Cramer,[a] and William B. Tolman[a,]*

[a] *Department of Chemistry, Center for Metals in Biocatalysis, and Supercomputer Institute, University of Minnesota, 207 Pleasant St. SE, Minneapolis, MN 55455;* [b] *Department of Chemistry, Tufts University, 62 Talbot Ave, Medford, MA, 02155;* [c] *Department of Chemistry, Stanford University, Stanford, CA 94305.* [d] *Stanford Synchrotron Radiation Laboratory, Stanford University, Stanford, CA 94305.*

E-mail: tolman@chem.umn.edu

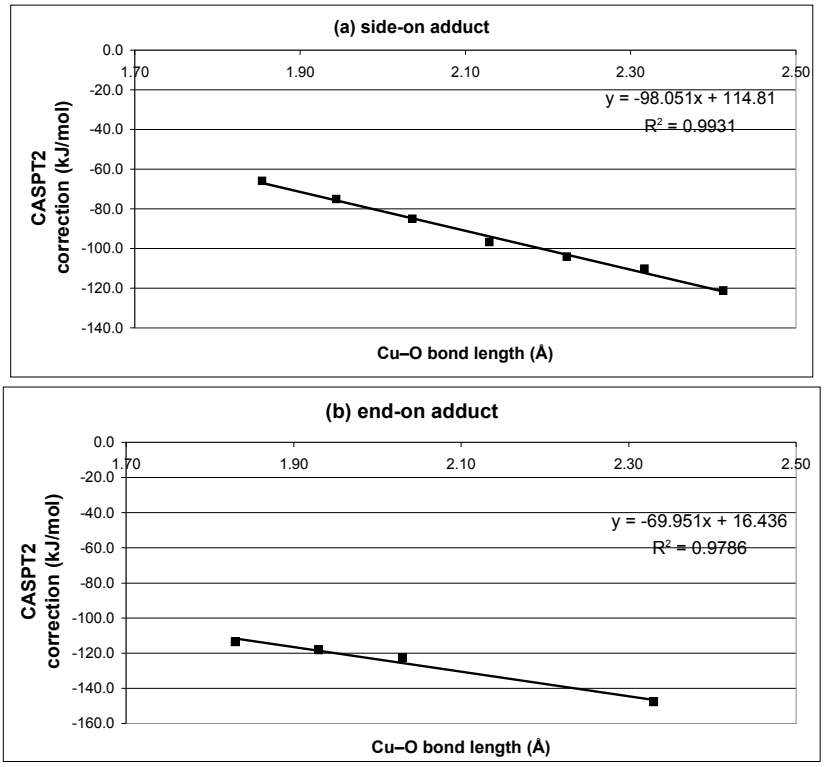

Figure S1. Linear correlation between CASPT2 energy correction and Cu–O bond distance for the singlet side-on (a) and end-on (b) Cu/O_2 adducts.

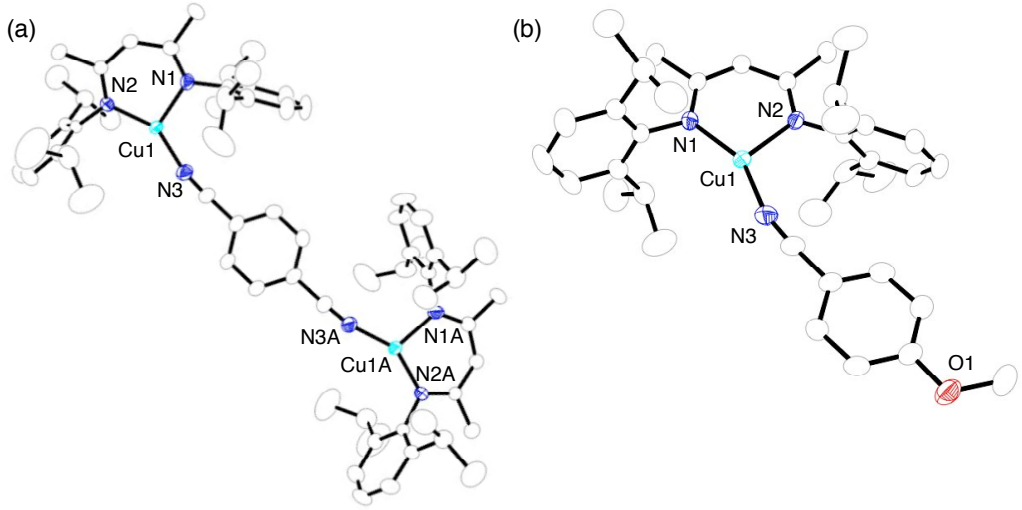

Figure S2. Representations of the X-ray crystal structure of (a) $[(L^1Cu)_2(p\text{-NC-}C_6H_4\text{-CN})]$ and (b) $L^1Cu(p\text{-NC-}C_6H_4\text{-OMe})$ with all nonhydrogen atoms shown as 50% thermal ellipsoids. Selected bond distances (Å) and angles (deg) are as follows. $[(L^1Cu)_2(p\text{-NC-}C_6H_4\text{-CN})]$: Cu1-N3, 1.846(3), Cu1-N2, 1.891(2), Cu1-N1, 1.964(2), N3-Cu1-N2, 147.51(12), N3-Cu1-N1, 113.01(11), N2-Cu1-N1, 99.05(10). $L^1Cu(p\text{-NC-}C_6H_4\text{-OMe})$: (molecule A) Cu1A-N3A, 1.855(2), Cu1A-N1A, 1.9009(17), Cu1A-N2A, 1.9779(18), N3A-Cu1A-N1A, 147.18(9), N3A-Cu1A-N2A, 112.85(8), N1A-Cu1A-N2A, 99.97(8); (molecule B) Cu1B-N3B, 1.864(2), Cu1B-N1B, 1.9003(18), Cu1B-N2B, 1.9913(18), N3B-Cu1B-N1B, 150.49(9), N3B-Cu1B-N2B, 110.97(8), N1B-Cu1B-N2B, 98.49(8).

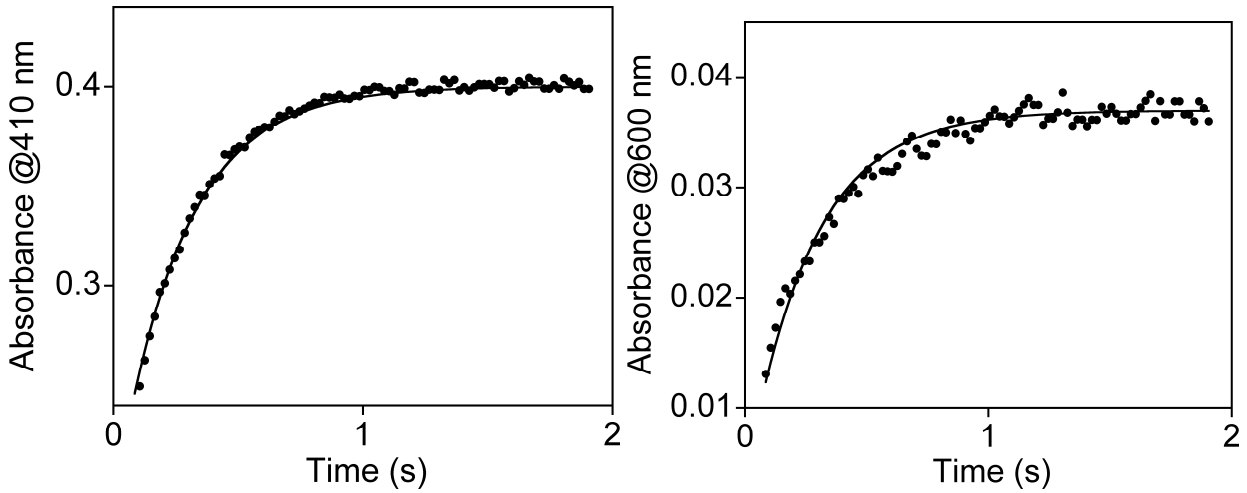

Figure S3. Kinetic traces with single-exponential fits to $A_t = A_\infty - (A_\infty - A_0)\exp(-kt)$, $k = 3.73\ s^{-1}$.

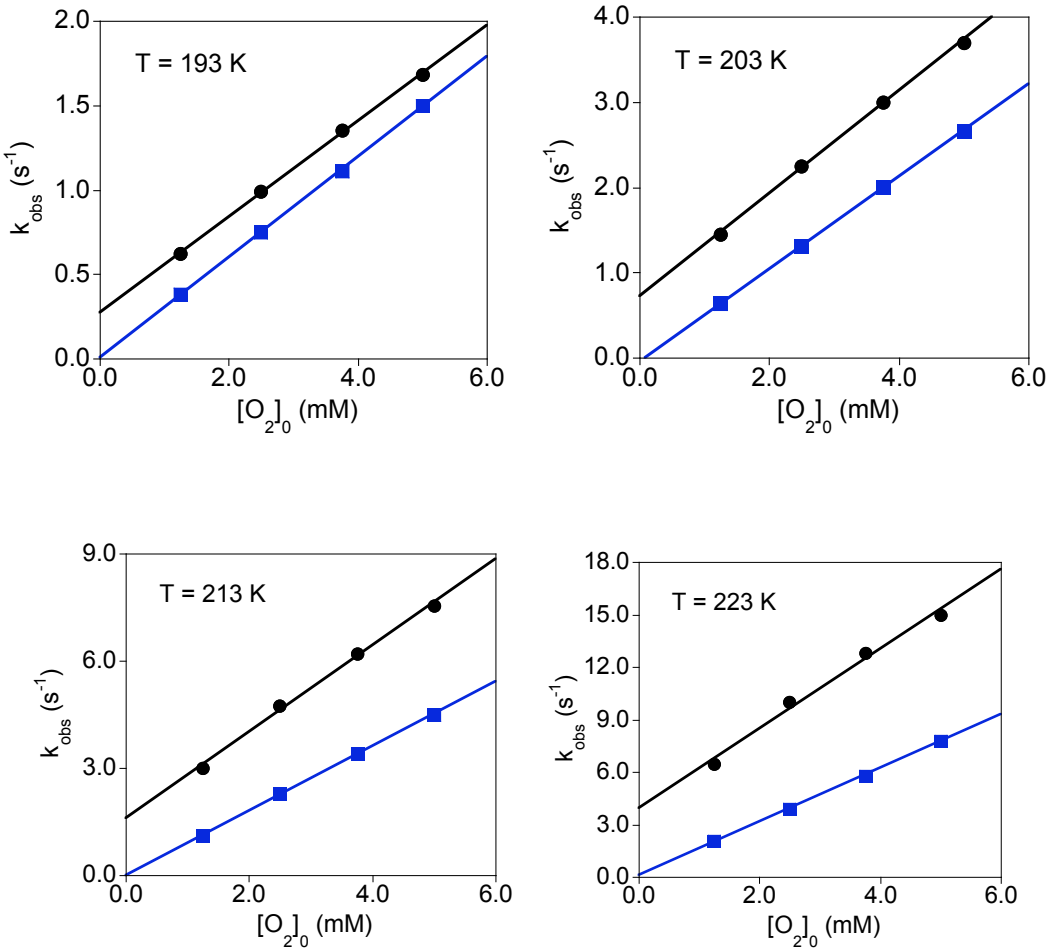

Figure S4. Plots of pseudo-first order rate constants (k_{obs}) for the oxygenation of $L^1Cu(MeCN)$ in neat THF (●) and THF/MeCN (■, [MeCN] = 120 mM) at different temperatures and varying $[O_2]_0$. The data are listed in Table S4.

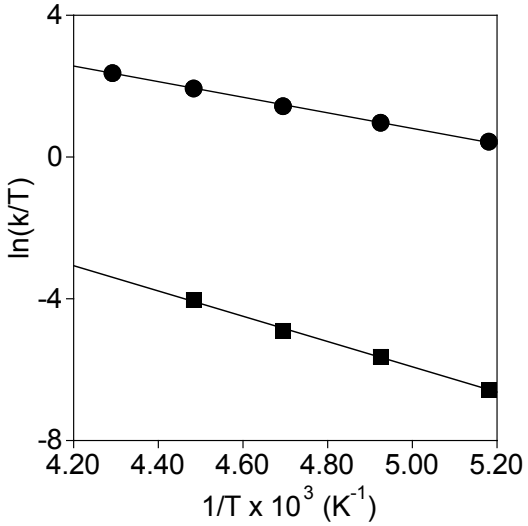

Figure S5. Eyring plots of the temperature dependencies of the rate constants for the oxygenation of $L^1Cu(MeCN)$. Data are for the second-order rate constant k_A (●, conditions: THF/MeCN v/v 160:1, values obtained from slopes of linear fits in Figure 6a) and the first order rate constant k_B (■, conditions: neat THF, values obtained from y intercepts of linear fits in Figure 6b).

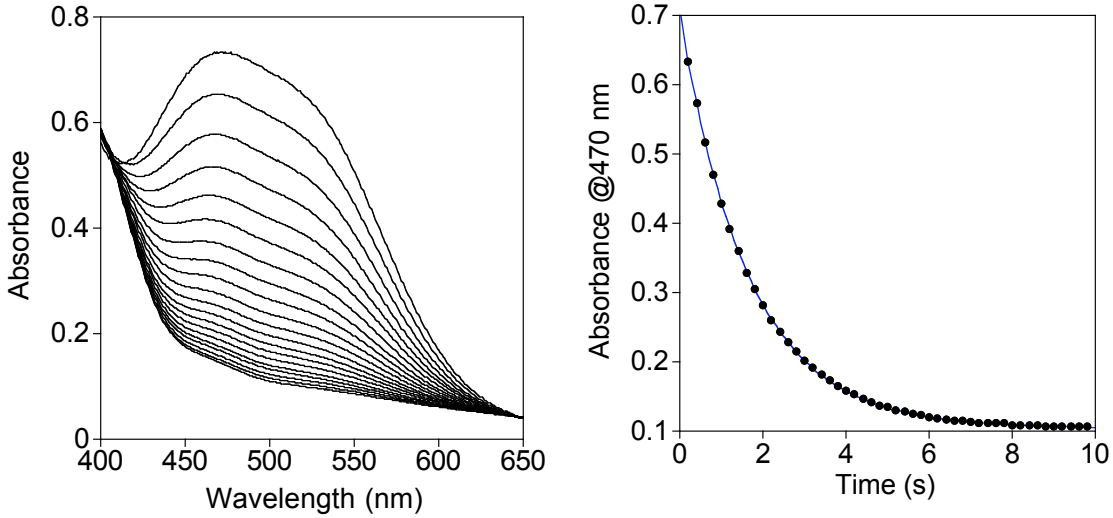

Figure S6. (left) Stopped-flow time-resolved UV-vis spectra of the reaction of $L^1Cu(MeCN)$ (0.25 mM) with O_2 (~ 5 mM) in THF and $[p\text{-NC-}C_6H_4CN]_0$ = 50 mM at 203 K recorded every 0.02 s (approximately every 4th spectrum shown). (right) Absorbance data at 470 nm as a function of time, fit to $A_t = A_\infty - (A_\infty - A_0)\exp(-kt)$, $k = 0.6$ s^{-1}.

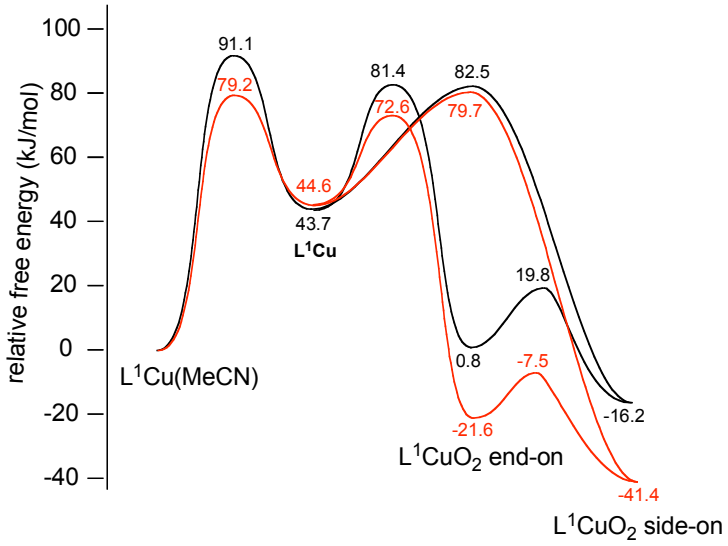

Figure S7. Calculated reaction energy profile (black line: 298 K, gas phase; red line: 223 K, THF) for the oxygenation mechanism involving dissociation of MeCN from $L^1Cu(MeCN)$ to yield the intermediate "L^1Cu". Full details on the protocol used to compute relative energies for all stationary points are provided in Table S7.

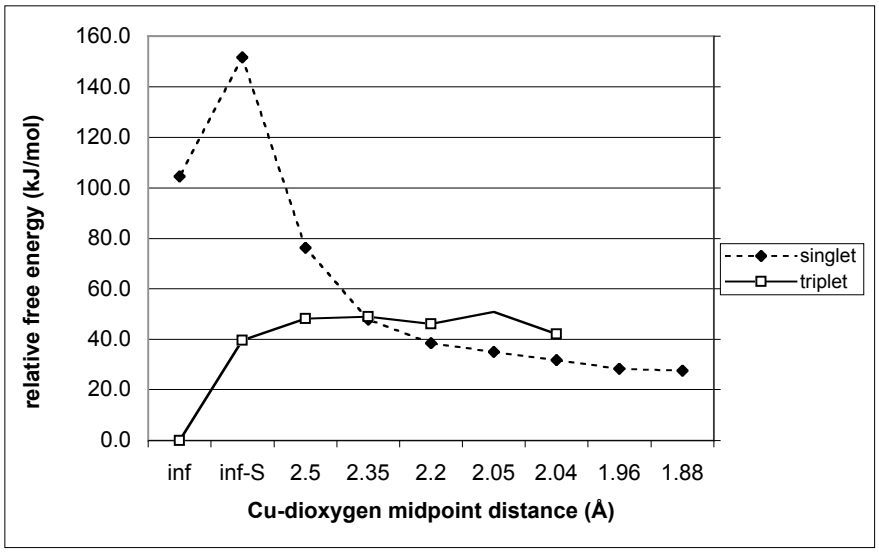

Figure S8. Calculated reaction coordinate for the side-on reaction (pathway A) of $L^1Cu(MeCN)$ with O_2 (298 K, gas phase). The "inf-S" label refers to a state whose enthalpy is equal to $L^1Cu(MeCN)$ and O_2 at inifinte separation, but whose entropy is that of $L^1Cu(MeCN)(O_2)$. The triplet/singlet crossing occurs at 2.36 Å. Cu-O1/O2 distances are reported in Table S4.

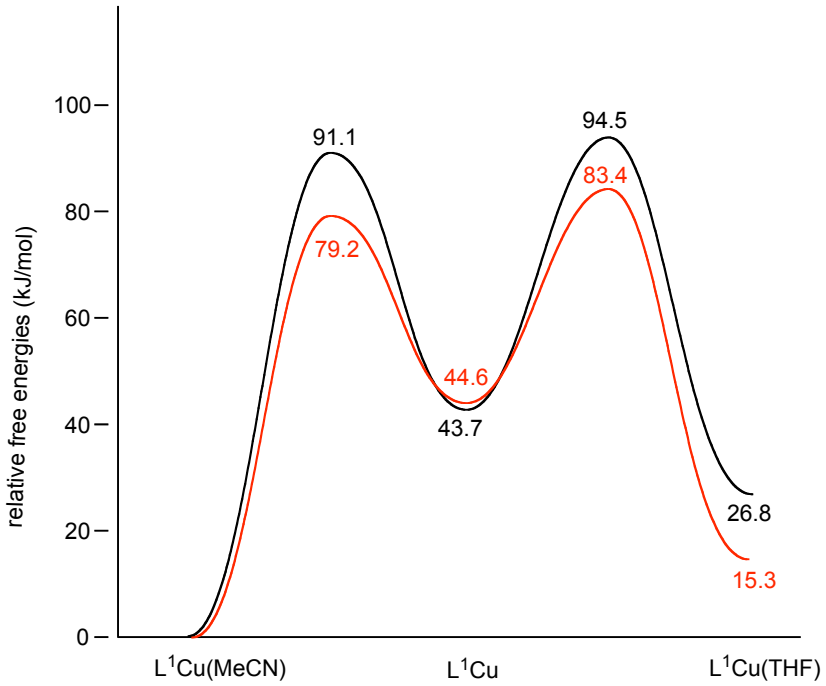

Figure S9. Calculated reaction energy profile for the dissociative mechanism for the ligand substitution step of pathway B, $L^1Cu(MeCN) \rightarrow L^1Cu(THF)$ (black line: 298 K, gas phase; red line: 223 K, THF).

Table S1. Selected properties of synthetic 1:1 Cu/O_2 adducts derived from experiment or theory (t).[a] All references are listed at the end of the Supporting Information (p. S51).

Complex	Cu-O (Å)	O-O (Å)	$\nu(^{16}O_2)$[b]	$\Delta\nu$ ($^{18}O_2$, $^{16}O^{18}O$)[b]	ref
$TpCuO_2$	1.84(1) 1.857 (t)[c]	1.22(3) 1.362 (t)[c]	1112	52, -	1,2
$Tp'CuO_2$	-	-	1043	59, -	1
$Tp''CuO_2$	1.983 (t)[d]	1.329 (t)[d]	-	-	3
$(dpha)(Et_3N)CuO_2$[e]	-	-	964	55, 22/25	4
$(N_3O)CuO_2$	-	-	1120	62, 27	5
$(L^{Me,Bn})CuO_2$	-	-	1120	61, -	6
L^1CuO_2	1.83*[f]	1.358 (t)	968 1042 (t)	51, 25	3,7, *this work
L^2CuO_2	1.852(8) 1.821(5)*	1.44(2) 1.392(12)* 1.376 (t)	961 1013 (t)	49, 24 57, 28 (t)	3,7,8, *this work

[a] Abbreviations: Tp = tris(3-*tert*-butyl-isopropyl-1-pyrazolyl)hydroborate, Tp' = tris(3-adamantyl-5-isopropyl-1-pyrazolyl)hydroborate, Tp'' = tris(1-pyrazolyl)hydroborate, dphaH = 2,4-bis(*tert*-butyl)-6-(2-hydroxy-4,6-bis{*tert*-butyl}phenylimino)cyclohexa-2,4-dienone, N_3O = 1-(2-hydroxy-3,5-di-*tert*-butylbenzyl)-4,7-diisopropyl-1,4,7-triazacyclononane, $L^{Me,Bn}$ = tris(*N*-benzyl-*N*-methylaminoethyl)amine, L^1 and L^2 = bis(2,6-diisopropylphenyl)-substituted β-diketiminates. [b] Units = cm^{-1}. Unless indicated otherwise, determined by resonance Raman spectroscopy. [c] Singlet geometry by DFT using BP86 functional, ref. 1. [d] Singlet geometry by DFT using mPWPW91 functional, ref. 3. [e] Values determined by FTIR spectroscopy. [f] Average Cu-N/O distance determined by EXAFS.

Table S2. X-ray crystallographic data.

Compound	$[(L^1Cu)_2(p\text{-}NC\text{-}C_6H_4\text{-}CN)]^a$	$L^1Cu(p\text{-}NC\text{-}C_6H_4\text{-}OMe)$	L^2CuO_2
Empirical formula	$C_{66}H_{86}Cu_2N_6$	$C_{37}H_{48}CuN_3O$	$C_{35}H_{53}CuN_2O_2$
Formula weight	1090.49	614.32	597.33
Temperature (K)	173(2)	173(2)	100(2)
Crystal system	tetragonal	Triclinic	orthorhombic
Space group	$P\bar{4}2(1)c$	$P\bar{1}$	*Imm*2
a(Å)	16.6331(8)	8.8419(8)	15.464(4)
b(Å)	16.6331(8)	20.1670(18)	17.324(4)
c(Å)	23.423(2)	20.2321(18)	8.763(2)
α(deg)	90	102.313(2)	90
β(deg)	90	96.573(2)	90
γ(deg)	90	97.252(2)	90
V(Å^3)	6480.2(8)	3459.1(5)	2347.7(10)
Z	4	4	2
D_{calc} (mg/m^3)	1.118	1.180	0.845
Abs coeff (mm^{-1})	0.697	0.662	0.261
Crystal shape and color	purple prism	yellow block	green needle
Crystal size (mm^3)	0.37 x 0.25 x 0.19	0.35 x 0.3 x 0.25	0.10 x 0.02 x 0.01
θ range (deg)	1.50 to 25.09°	1.05 to 25.07°	2.10 to 21.63°
Reflcns collected	39518	29164	13214
Independent reflcns	5759 [*R*(int) = 0.0701]	12187 [*R*(int) = 0.0378]	2804 [*R*(int) = 0.041]
Observed reflecns	4822	9682	2526
Completeness to theta = 21.63°	99.9 %	99.3 %	95.1 %
Data / restraints / parameters	5759 / 1 / 344	12187 / 0 / 784	2804 / 286 / 195
Goodness-of-fit on F^2	1.059	1.036	1.291
*R*1, w*R*2 (for $I > 2\sigma(I)$)^b	0.0387, 0.0886	0.0382, 0.0975	0.0936, 0.2338
largest peak, hole (e/Å^{-3})	0.357, -0.369	0.482, -0.343	1.296, -1.796

[a] Due to an inability to identify disordered solvent, various fields (e.g., formula, formula weight, and density) are incorrect; see Experimental section for details. [b] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR2 = [\Sigma w(F_o^2 - F_c^2)^2/ \Sigma w(F_o^2)^2]^{1/2}$, where $w = 1/[\sigma^2(F_o^2 + (aP)^2 + bP]$, $P = (F_o^2 + 2F_c^2)/3$, and *a* and *b* are constants given in the supporting information (CIF).

Table S3. Values of pseudo-first order rate constants for the oxygenation of $L^1Cu(MeCN)$ in THF-MeCN (v/v 160:1; [MeCN] = 120 mM) at different concentrations of $L^1Cu(MeCN)$.[a]

$[L^1Cu(MeCN)]_0$, M	k_{obs} (s^{-1})
0.10	2.56
0.15	2.68
0.25	2.66
0.40	2.47

[a] Conditions: T = 203 K; $[O_2]_0$ = 5 mM. All concentrations are after mixing. The standard deviation in the values of the rate constants is ≤ 5%.

Table S4. . Values of pseudo-first order rate constants for the oxygenation of **1** in neat THF and THF/MeCN.[a]

O_2 sat. (%)	$[O_2]_0$ (mM)	T (K)	k_{obs} (s^{-1}) THF	k_{obs} (s^{-1}) THF/MeCN
25	1.25	193	0.62	0.38
		203	1.45	0.63
		213	3	1.11
		223	6.45	2.05
		233	-	3.04
50	2.5	193	0.99	0.75
		203	2.25	1.31
		213	4.75	2.28
		223	10	3.9
		233	-	6.1
75	3.75	193	1.35	1.11
		203	3	2.01
		213	6.2	3.4
		223	12.8	5.8
		233	-	9.3
100	5.0	193	1.68	1.50
		203	3.7	2.66
		213	7.55	4.5
		223	15	7.8
		233	-	12.6

[a] Conditions: $[\mathbf{1}]_0$ = 0.25 mM (after mixing), neat THF or THF/MeCN (v/v 160:1, [MeCN] = 0.12 M after mixing). Standard deviation in the values of the rate constants is within 5%. These data are plotted in Figure 6.

Table S5. Rate constants for pathways A and B for the oxygenation of **1**.

T (K)	k_A (M^{-1} s^{-1})[a]	k_A (M^{-1} s^{-1})[b]	k_B (s^{-1})[b]
193	299 ± 4	283 ± 5	0.275 ± 0.002
203	531 ± 6	600 ± 13	0.725 ± 0.043
213	903 ± 9	1208 ± 52	1.60 ± 0.18
223	1560 ± 19	2276 ± 171	3.95 ± 0.59
233	2494 ± 30	-	-

[a] Values obtained from experiments performed in THF/MeCN as the slopes of the linear fits shown in Figure 8a. [b] Values obtained from experiments performed in neat THF, with k_A being the slope and k_B the y intercept of the linear fits in Figure 8b.

Table S6. Calculated Cu-O1/O2 distances (Å) for points along the reaction coordination for the associative oxygenation mechanism (pathway A, Figure S5).

	singlet		triplet	
Cu-dioxygen midpoint distance	Cu–O1	Cu–O2	Cu–O1	Cu–O2
2.50	2.393	2.911	2.402	2.811
2.35	2.282	2.463	2.259	2.577
2.20	2.103	2.389	2.133	2.387
2.05	2.003	2.170	2.053	2.143
2.04	n/a	n/a	2.023	2.288
1.96	1.920	2.086	n/a	n/a
1.88	1.877	2.017	n/a	n/a

Table S7. Calculated relative values for components of enthalpies, entropies, and free energies along the two reaction pathways.

ΔDFT refers to the energy difference from the DFT calculations, ΔCASPT2 to the difference in CASPT2 corrections to the singlet DFT energies, ΔZPE to the difference in zero point energies, and $\Delta H_{thermal}$ and $\Delta S_{thermal}$ to the thermal contributions to the enthalpy and entropy, respectively. $\Delta G_{solvation}$ refers to the difference in solvation free energies in THF.

ΔS_{ssc} refers to the standard state correction to the translational entropy (pertinent to reactions in solution) due to a change in concentration from the gas phase to the 1 M standard-state solution concentration.[i] ΔS_{ssc} is computed as follows:

$$\Delta S_{ssc} = R \ln (Q°_{ss}/Q°) \quad (a)$$

where $Q°_{ss}$ and Q° are the reaction quotients evaluated with species at their standard-state solution and gas phase concentrations, respectively. Gas phase concentration can be computed from the ideal gas law to be 1 mol / 24.466 L at 298 K and 1 mol / 18.299 L at 223 K. The concentration of neat THF, which can be computed from its density,[ii,iii] is 12.20 M at 298 K and 13.24 M at 223 K.

Total _H values are computed as shown:

$$\Delta H_{total} = \Delta DFT + \Delta CASPT2 + \Delta ZPE + \Delta H_{thermal} + \Delta G_{solvation} \quad (b)$$

Adding $\Delta G_{solvation}$ to the computed total enthalpy change is not technically proper and leads to an energy that is not an enthalpy change in a rigorous sense. However, the free energy of solvation computed via the continuum solvation model[iv,v] cannot be resolved into enthalpic and entropic terms. This detail is therefore neglected for the sake of simplicity, and the $_H_{total}$ then represents a solvation-corrected enthalpy change.

Total ΔS values are computed as shown:

$$\Delta S_{total} = \Delta S_{thermal} + \Delta S_{ssc} \quad (c)$$

Total ΔG values are computed as shown:

$$\Delta G_{total} = \Delta H_{total} - T\Delta S_{total} \quad (d)$$

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[i] Cramer, C. J. *Essentials of Computational Chemistry. Theories and Models*.; John Wiley & Sons, Ltd.: West Sussex, England, 2002.

[ii] Carvajal, C.; Tolle, K. J.; Smid, J.; Szwarc, M. *J. Am. Chem. Soc.* **1965**, *87*, 5548.

[iii] Metz, D. J.; Glines, A. *J. Phys. Chem.* **1967**, *71*, 1158.

[iv] Marten, B.; Kim, K.; Cortis, C.; Friesner, R. A.; Murphy, R. B.; Ringnalda, M. N.; Sitkoff, D.; Honig, B. *J. Phys. Chem.* **1996**, *100*, 11775.

[v] Tannor, D. J.; Marten, B.; Murphy, R. B.; Friesner, R. A.; Sitkoff, D.; Nicholls, A.; Ringnalda, M. N.; Goddard, W. A., III; Honig, B. *J. Am. Chem. Soc.* **1994**, *116*, 11875.

(a) associative bimolecular pathway A

species[a]	ΔDFT[b]	ΔCASPT2[b]	ΔZPE[b]	$\Delta H_{thermal}$[b]		$\Delta G_{solvation}$[b]		$\Delta S_{thermal}$[c]		ΔS_{ssc}[c]	
				223K	298K	223K	298K	223K	298K	223K	298K
$L^1Cu(MeCN)$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	12.1	0.0	0.4	-2.1	-2.4	4.6	4.7	-140.2	-141.5	32.3	26.5
2	60.9	-76.0	4.9	-3.0	-3.1	0.7	1.2	-161.3	-161.9	32.3	26.5
3	59.1	-72.3	5.1	-3.2	-3.4	-9.0	-7.8	-159.7	-160.6	32.3	26.5
L^1CuO_2	44.9	-68.5	5.3	-3.6	-4.6	-23.7	-21.2	-19.1	-22.8	0.0	0.0

[a] All energy comparisons are for stochiometrically equivalent species. [b] Units kJ mol^{-1}. [c] Units J K^{-1} mol^{-1}.

(b) solvolytic pathway B

species[a]	ΔDFT[b]	ΔCASPT2[b]	ΔZPE[b]	$\Delta H_{thermal}$[b]		$\Delta G_{solvation}$[b]		$\Delta S_{thermal}$[c]		ΔS_{ssc}[c]	
				223K	298K	223K	298K	223K	298K	223K	298K
$L^1Cu(MeCN)$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	14.2	0.0	-0.2	1.0	1.8	12.1	11.5	-162.0	-158.9	61.0	47.4
$L^1Cu(THF)$	20.8	0.0	-0.6	-0.6	-1.1	-3.3	-2.6	-24.1	-26.0	28.7	20.8
t.s. A	20.8	0.0	3.1	-1.5	-1.3	-12.1	-11.1	-165.3	-164.8	61.0	47.4
5	109.0	-118.6	3.1	-1.5	-1.3	-12.1	-11.1	-165.3	-164.8	61.0	47.4
t.s. B	113.1	-113.0	3.1	-1.5	-1.3	-10.1	-20.1	-165.3	-164.8	61.0	47.4
6	113.1	-113.0	2.1	-1.9	-2.5	-22.2	-20.1	-1.1	-3.3	0.0	0.0
7	121.8	-104.3	0.8	-3.1	-4.2	-26.0	-19.7	-14.9	-19.4	0.0	0.0
L^1CuO_2	44.9	-68.5	5.3	-3.6	-4.6	-23.7	-21.2	-19.1	-22.8	0.0	0.0

[a] All energy comparisons are for stochiometrically equivalent species. [b] Units kJ mol^{-1}. [c] Units J K^{-1} mol^{-1}.

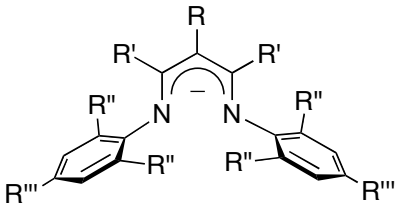
Table S8. Mulliken charge populations for species along the pathways shown in Figure 12 (223K, in THF).

species	Cu	L^1	MeCN	THF	O1	O2
Associative Bimolecular Pathway A						
$L^1Cu(MeCN)$	0.34	-0.44	0.10	na	0.00	0.00
1	0.36	-0.36	0.12	na	-0.07	-0.05
2	0.55	-0.16	0.16	na	-0.28	-0.27
3	0.59	-0.17	0.16	na	-0.29	-0.29
L^1CuO_2	0.68	-0.08	0.00	na	-0.30	-0.30
Solvolytic Pathway B						
$L^1Cu(MeCN)$	0.34	-0.44	0.10	0.00	0.00	0.00
4	0.28	-0.47	0.08	0.11	0.00	0.00
$L^1Cu(THF)$	0.27	-0.42	0.00	0.15	0.00	0.00
5	0.49	-0.21	0.00	0.14	-0.23	-0.19
6	0.52	-0.09	0.00	0.00	-0.24	-0.19
7	0.56	-0.08	0.00	0.00	-0.27	-0.21
L^1CuO_2	0.68	-0.08	0.00	na	-0.30	-0.30

Table S9. Bond distances (Å) determined by X-ray crystallography between Cu and the N atoms of coordinated β-diketiminate ligands in complexes reported in the literature. The β-diketiminate ligands are identified according to the drawing at the bottom of the table (next page). All references are listed at the end of the Supporting Information (p. S51).

	Cu-N1	Cu-N2	ref
3-Coordinate Cu(I) Complexes			
$Ph(H_2L^{iPr2})Cu(MeCN)$	1.964(2)	1.950(2)	7, 9
$[3,5\text{-}(CF_3)_2C_6H_3(H_2L^{iPr2})Cu(MeCN)]$	1.908(3)	1.977(3)	9
$[Cl(Me_2L^{Me2})Cu(CNC_6H_3Me_2)]$	1.931(2)	1.954(2)	9
$H(Me_2L^{iPr2})Cu(CNC_6H_3Me_2)$	1.9284(17)	1.9616(17)	10
$H(Me_2L^{iPr2})Cu(MeCN)$	1.9404(16)	1.9425(17)	**Error! Bookmark not defined.**
$H(tBu_2L^{iPr2})Cu(MeCN)$	1.931(2)	1.936(2)	**Error! Bookmark not defined.**
$H(Me_2L^{iPr2})Cu(pyridine)$	1.9467(16)	1.9467(16)	11
$H(Me_2L^{iPr2})Cu(S\text{-}THP)$	1.904(3)	1.900(3)	11
$H(Me_2L^{iPr2})Cu(N\text{-}THP)$	1.955(4)	1.926(3)	11
$NO_2(H_2L^{Me2Me})Cu(NO_2\text{-}R)$	1.992(2)	1.991(2)	12
$H(Me_2L^{Me2})Cu(CH_2CH_2)$	1.917(2)	1.908(2)	13
$H(Me_2L^{Me2})Cu(CH_2CHPh)$	1.913(3)	1.915(3)	13
$H(CF_3L^{3,5\text{-}CF3})Cu(C_6H_6)$	1.952(3)	1.954(3)	14
3-Coordinate Cu(II) Complexes			
$H(Me_2L^{iPr2})CuCl$	1.869(2)	1.870(2)	15
$Cl(Me_2L^{iPr2})CuCl$	1.869(2)	1.864(2)	10
$H(Me_2L^{iPr2})Cu(OC_6H_4OMe)$	1.864(2)	1.888(2)	10
$H(Me_2L^{iPr2})Cu(OC_6H_3Me_2)$	1.8825(17)	1.8946(17)	10
$H(Me_2L^{iPr2})Cu(OC_6H_4tBu)$	1.869(3)	1.896(3)	10
$Cl(Me_2L^{iPr2})Cu(OC_6H_4tBu)$	1.858(2)	1.8959(17)	10
$H(Me_2L^{iPr2})Cu(SCPh_2CH_2OMe)$	1.900(4)	1.908(4)	16
$H(Me_2L^{iPr2})Cu(SCPh_3)$	1.923(2)	1.921(2)	15
$H(Me_2L^{iPr2})Cu(SC_6H_3Me_2)$	1.8945(15)	1.908(2)	17
4-Coordinate Cu(II) Complexes			
$H(Me_2L^{iPr2})Cu(SCPh_2CH_2SMe)$	1.987(3)	1.952(3)	16
$[Cl(Me_2L^{Me2})CuCl]_2$	1.9223(15)	1.9194(15)	9
$[H(Me_2L^{Et2})CuCl]_2$	1.9297(18)	1.9295(19)	9
$(Ph,H(L^{iPr2})Cu)_2(\mu\text{-}S_2)]$	1.880(5)	1.922(5)	18
$[H(Me_2L^{Et2}Cu)_2(\mu\text{-}S_2)]$	1.9065(18)	1.9101(18)	18
$*[\{NO_2(H_2L^{Me2Me})Cu\}_2\text{-}(\mu\text{-}OH)_2]$	1.940(2)	1.934(2)	9
$(H_2L^{Me2})Cu\}_2\text{-}(\mu\text{-}OH)_2$	1.9446(11)	1.9373(11)	13

$H(Me_2L^{Me2Me})Cu(OAc)$	1.913(3)	1.917(3)	19
$(H(CF_3L^{3,5\text{-}CF3})Cu(\mu\text{-}OH,\mu\text{-}$	1.919(3) (Cu1)	1.934(3) (Cu1)	14
$OPh)Cu(H(CF_3L^{OPh,\ 3,5\text{-}CF3})$	1.911(3) (Cu2)	1.917(3) (Cu2)	
$[H(Me_2L)]_2Cu$	1.95(1)	1.98(1)	20
(2 independent molecules)	1.97(1)	1.96(1)	
	1.97(1)	1.97(1)	
	1.97(1)	1.95(1)	
$[COH(H_2L^{3,5\text{-}Me})]_2Cu$	1.950(4)	1.953(4)	21
4-Coordinate Cu(III) Complexes			
$[(Me_2L^{iPr2}Cu)\ (\mu\text{-}O)_2)(tmpdaCu)]^{1+}$	1.888(2)	1.897(2)	22
$(Me_2L^{Et2}Cu)_2(\mu\text{-}O)_2$	1.881(3)	1.902(3)	23



$R(R'_2L^{R"2R'''})^-$

Table S9. Atomic coordinates for calculated structures.

1) L^1Cu

Cu	-.3566942169	-.9484658246	.1137053697
N	-2.1429757196	-.3351432479	-.1332197838
N	.9441010298	.4418059103	.2053808489
C	-3.5247330055	1.6889378897	-.2663964247
C	-2.1727732249	1.0029371977	-.1605078088
C	-1.0372735612	1.8552918289	-.1074114800
C	.3588927779	1.6333227853	.0316354073
C	1.2441772938	2.8682845008	-.0128441847
C	-3.3087807310	-1.1513239129	-.2033069899
C	-3.8613796165	-1.4987003631	-1.4577860121
C	-4.9504945281	-2.3778102526	-1.4867535582
C	-5.4815828254	-2.9109052936	-.3161647748
C	-4.9094961498	-2.5841624515	.9114357135
C	-3.8189986780	-1.7130404778	.9924788403
C	-3.2248522955	-1.0187915767	-2.7583611676
C	-4.2488313049	-.5915448795	-3.8217227968
C	-2.2791071606	-2.1035204916	-3.3126530599
C	-3.1287941618	-1.4374376544	2.3243899657
C	-1.9989195545	-2.4629242336	2.5538228311
C	-4.0798960680	-1.4128536736	3.5299357650
C	2.3504055834	.2699050676	.3580505741
C	3.1061788942	-.1773629389	-.7536586945
C	4.4714612771	-.4260223209	-.5799081769
C	5.0832973985	-.2517400960	.6591372705
C	4.3232928532	.1580790124	1.7507404979
C	2.9540681820	.4203974264	1.6278606149
C	2.4158017989	-.4648817013	-2.0829165696
C	1.8813948681	-1.9121511829	-2.0976193674
C	3.2975884327	-.2121728203	-3.3149551956
C	2.1193354560	.7546005604	2.8595640450
C	2.7900839800	1.7679739578	3.8005158415
C	1.7579654079	-.5402281904	3.6156026384
H	-3.4331335786	2.7698597978	-.1556365780
H	-4.2069473201	1.3125136075	.5015942043
H	-3.9949535313	1.4791050955	-1.2326916706
H	-1.2921633364	2.9046984525	-.1914332982
H	.6715974673	3.7609331495	-.2662990222
H	2.0424771852	2.7411616401	-.7505633666
H	1.7339586860	3.0338225147	.9518754790
H	-5.3835829004	-2.6571255063	-2.4426342552
H	-6.3290143218	-3.5889000320	-.3596954545
H	-5.3162059259	-3.0186960485	1.8191436827
H	-2.6078014051	-.1465079406	-2.5269492406
H	-3.7355946698	-.1626371469	-4.6888611221
H	-4.9426157883	.1599782168	-3.4313696762

H	-4.8431330521	-1.4374244027	-4.1832766490
H	-1.7800593423	-1.7573644590	-4.2249994129
H	-2.8316146374	-3.0186140894	-3.5532546944
H	-1.5076210685	-2.3613972119	-2.5800540103
H	-2.6607942113	-.4504936118	2.2547040556
H	-1.4488666567	-2.2478481923	3.4763604950
H	-1.2762974343	-2.4531004011	1.7244605389
H	-2.4034316454	-3.4789484904	2.6203920997
H	-3.5400115352	-1.0905538173	4.4263187373
H	-4.4992405801	-2.4017592859	3.7442742490
H	-4.9132642817	-.7222090443	3.3676990565
H	5.0658123137	-.7644226547	-1.4227737686
H	6.1452736558	-.4478633741	.7753878828
H	4.8014321795	.2670134735	2.7195842551
H	1.5501692369	.2006862257	-2.1553014031
H	1.3277741354	-2.1205343878	-3.0195482298
H	1.2030087111	-2.0977220827	-1.2511866283
H	2.7038766218	-2.6315471166	-2.0171981064
H	2.7048225551	-.3207831116	-4.2291309678
H	4.1261041110	-.9256560324	-3.3808727780
H	3.7225175903	.7963078425	-3.3025206664
H	1.1794937154	1.1961083272	2.5174528476
H	2.1011292628	2.0494624251	4.6038884888
H	3.0811547854	2.6789814325	3.2676619226
H	3.6882769669	1.3575642845	4.2739212093
H	1.1149687550	-.3239124903	4.4764527121
H	2.6601709362	-1.0422950982	3.9823490326
H	1.2273922296	-1.2400449169	2.9622534527

2) $L^1Cu(MeCN)$

Cu	-.0847660797	.1859183417	-.1187602309
N	1.4594872211	1.3954195222	-.3316803781
N	-1.5558435182	1.5033157152	-.2616209739
N	-.1841501837	-1.7235961622	.1736976756
C	-.2483098120	-2.8683944333	.3516731526
C	-.3304545399	-4.3042643579	.5771934100
C	2.4884382163	3.5997490562	-.6916926956
C	1.2748119524	2.7012334600	-.5205763916
C	.0117717395	3.3314338758	-.5714896980
C	-1.2892364693	2.7950030615	-.4463765361
C	-2.4414712891	3.7815121287	-.5376295599
C	2.7631968680	.8183368486	-.2943571145
C	3.4087097184	.6206425916	.9505615729
C	4.6341224033	-.0544488148	.9744341799
C	5.2222750091	-.5298069633	-.1943768061
C	4.5772107473	-.3344576588	-1.4134066577
C	3.3505640092	.3337366412	-1.4891959686

C	2.7664235681	1.0780196036	2.2570310559
C	3.7246523687	1.8962673465	3.1393074600
C	2.1974947726	-.1235041609	3.0369385072
C	2.6317994019	.4702055590	-2.8283623255
C	1.9262271044	-.8491199381	-3.1996880799
C	3.5527547428	.9332384173	-3.9687794432
C	-2.8904910046	1.0225547427	-.1162666558
C	-3.4665302271	.9260169907	1.1745659548
C	-4.7285778062	.3371839578	1.3068627382
C	-5.4205317579	-.1512685741	.2013162540
C	-4.8442718541	-.0549126697	-1.0625485150
C	-3.5842224271	.5250349911	-1.2463284655
C	-2.7068178248	1.3881281933	2.4147801890
C	-2.1163663797	.1817496300	3.1712083471
C	-3.5587155364	2.2562852772	3.3557671984
C	-2.9615920445	.5655362808	-2.6389047425
C	-3.8967512213	1.1852555846	-3.6911567309
C	-2.5022401697	-.8392457291	-3.0755479179
H	-1.3117320866	-4.6776432792	.2709261988
H	-.1842138694	-4.5203736625	1.6392453114
H	.4439279057	-4.8191294125	.0016141153
H	2.1947545277	4.6407058695	-.8340635426
H	3.0885007573	3.2860585961	-1.5522007238
H	3.1443117734	3.5388437262	.1830157372
H	.0466636124	4.4027083109	-.7270299584
H	-2.0817472422	4.7974888527	-.7065032090
H	-3.0375407202	3.7718432989	.3807729165
H	-3.1215680737	3.5116965036	-1.3522678086
H	5.1338321552	-.2154247245	1.9259217968
H	6.1749079614	-1.0505822747	-.1561050341
H	5.0334467368	-.7144326888	-2.3231195088
H	1.9221484538	1.7229673570	1.9994510565
H	3.1998776505	2.2710784521	4.0249159291
H	4.1309993218	2.7559799868	2.5969629205
H	4.5705560043	1.2953602784	3.4904494755
H	1.6974553819	.2089975555	3.9539059761
H	2.9932245896	-.8222401181	3.3198655520
H	1.4684757031	-.6704051471	2.4310160205
H	1.8518918336	1.2270013829	-2.7075846470
H	1.3655489657	-.7421857742	-4.1354966604
H	1.2250738420	-1.1507312396	-2.4157285514
H	2.6547651287	-1.6578063480	-3.3305599839
H	2.9673131573	1.1156258791	-4.8764318246
H	4.3099579799	.1815848872	-4.2169421092
H	4.0755538114	1.8596085677	-3.7101210368
H	-5.1748736891	.2523902768	2.2939495607
H	-6.4002989239	-.6041446578	.3243295429

H	-5.3809991728	-.4433914205	-1.9239416280
H	-1.8641736089	1.9972535690	2.0768829130
H	-1.5293347792	.5128909753	4.0356601841
H	-1.4611614957	-.4038498112	2.5192427928
H	-2.9107071562	-.4805291023	3.5345516220
H	-2.9443596824	2.6384108730	4.1782966387
H	-4.3839113059	1.6902188916	3.8013360440
H	-3.9903042014	3.1131225191	2.8285805469
H	-2.0679923626	1.1925529708	-2.5805529594
H	-3.3835368574	1.2670863880	-4.6555637302
H	-4.2227423980	2.1873034331	-3.3944771114
H	-4.7942948415	.5772971697	-3.8485539021
H	-2.0167693793	-.8022168949	-4.0575340546
H	-3.3516621405	-1.5286720374	-3.1442593028
H	-1.7876909145	-1.2549764379	-2.3585199139

3) $L^1Cu(THF)$

Cu	.4060881435	-.1235149167	.4858504557
N	1.7237183690	1.3169863213	.7238894790
N	-1.2942097873	.8707261320	.4914129189
C	2.3002719709	3.6887721431	1.0096769643
C	1.2859499250	2.5717224956	.8229758707
C	-.0736843908	2.9573029037	.7711758549
C	-1.2564533288	2.1958356688	.6232165895
C	-2.5645830299	2.9708815573	.6166585705
C	3.1039268500	.9785481757	.8009265913
C	3.6823380085	.6630925164	2.0562830831
C	4.9986304653	.1915644286	2.0919884947
C	5.7441815010	.0327267020	.9261395263
C	5.1700250939	.3522216277	-.3019064834
C	3.8564759031	.8275567330	-.3904568517
C	2.8697784986	.7697462832	3.3434395270
C	3.6390618678	1.4467351350	4.4889977335
C	2.3523070198	-.6146995943	3.7782914318
C	3.2416472141	1.1264344757	-1.7552602111
C	2.9019555168	-.1768288083	-2.5044966754
C	4.1275253406	2.0368835690	-2.6213561635
C	-2.5120916507	.1499421209	.3445483697
C	-3.1615670742	-.3718707735	1.4912380401
C	-4.2736335987	-1.2018266698	1.3163109395
C	-4.7510480417	-1.5162618861	.0462022031
C	-4.1111083897	-.9924683031	-1.0746559232
C	-2.9944171248	-.1576274633	-.9521915549
C	-2.6245734842	-.0899697320	2.8912656733
C	-1.7865234902	-1.2777395095	3.4047616440
C	-3.7268173196	.2740098088	3.8994232620
C	-2.2826361848	.3595310782	-2.1992714896

C	-3.2463851591	.9809661056	-3.2259286381
C	-1.4347544944	-.7530406540	-2.8500396228
H	1.8181088211	4.6675487901	1.0149565340
H	3.0511505107	3.6726007125	.2127983767
H	2.8440134883	3.5660412056	1.9532108439
H	-.2385817667	4.0237539559	.8645105050
H	-2.3936715259	4.0431961575	.7248215280
H	-3.2181330235	2.6393170716	1.4307394034
H	-3.1148163874	2.7981799127	-.3144263520
H	5.4482870581	-.0601874561	3.0484259475
H	6.7654172695	-.3341723037	.9749394568
H	5.7522237602	.2276218365	-1.2108399616
H	1.9913449523	1.3834933807	3.1285781293
H	2.9820262087	1.5891480130	5.3537840764
H	4.0220335984	2.4267574745	4.1880235773
H	4.4908831654	.8454773516	4.8237907143
H	1.7399325215	-.5366138438	4.6838404342
H	3.1838179995	-1.2967093145	3.9885103115
H	1.7357400949	-1.0620699877	2.9926988829
H	2.2989922764	1.6521147506	-1.5819623902
H	2.4346774568	.0407671260	-3.4718238022
H	2.2050525183	-.7911272411	-1.9262372330
H	3.8043697866	-.7706099126	-2.6913398928
H	3.6109718313	2.2951431474	-3.5522666407
H	5.0699111861	1.5503583915	-2.8943024930
H	4.3727412496	2.9676533444	-2.1005915773
H	-4.7743091353	-1.6127044138	2.1885955355
H	-5.6167817973	-2.1621268740	-.0689866968
H	-4.4848305564	-1.2389033387	-2.0645310695
H	-1.9496133380	.7666575948	2.8164931860
H	-1.3679298576	-1.0625350951	4.3940317812
H	-.9538875227	-1.4879395692	2.7263915179
H	-2.3974493549	-2.1837509466	3.4854103896
H	-3.2814489188	.5710049196	4.8548071161
H	-4.3944597096	-.5701660964	4.1017999710
H	-4.3414079308	1.1049410566	3.5376117487
H	-1.5900265570	1.1436738938	-1.8794926268
H	-2.6822664577	1.4246655595	-4.0534694848
H	-3.8603027118	1.7675822507	-2.7730945275
H	-3.9250518962	.2356206017	-3.6572205603
H	-.8926812189	-.3703695438	-3.7225810633
H	-2.0674139778	-1.5848216094	-3.1840662675
H	-.6969806305	-1.1485059736	-2.1434655659
C	1.9611737463	-2.8398437811	.4036400743
O	.7121350439	-2.1514786533	.1801907862
C	-.3137245041	-3.1669810599	.1753034765
C	1.8435488939	-4.1374154832	-.4130226636

C	.3117368472	-4.3392149098	-.5931288387
H	2.0680950578	-3.0440323577	1.4766950617
H	2.7620989482	-2.1709861238	.0878661262
H	-1.1982426364	-2.7328852797	-.2893429307
H	-.5506939533	-3.4389970146	1.2115943521
H	2.3165253839	-4.9745895460	.1062020348
H	2.3336815311	-4.0278895477	-1.3833339316
H	.0409973693	-4.2903706669	-1.6505599156
H	-.0343106964	-5.3000774391	-.2040538868

4) L^1CuO_2 side-on singlet

Cu	-.5758635651	-.5834236022	.0138496438
O	.1762387641	-2.2476472803	-.3865500627
O	-1.1777005354	-2.3189886612	-.3138871007
N	.8194449426	.7032326449	.2263509595
N	-2.0850856479	.5385699780	.3326851982
C	1.7246025666	2.9474128940	.6526827409
C	.5659826254	1.9794276976	.5146153160
C	-.7242778094	2.5014975336	.7071267402
C	-1.9571582723	1.8320355900	.6269944377
C	-3.2037747255	2.6544801764	.8858608956
C	2.1651049221	.2441474512	.0250621731
C	2.8873052804	-.2740816224	1.1219947780
C	4.1924022009	-.7274530326	.8990846160
C	4.7652091895	-.6832733689	-.3685337581
C	4.0274905262	-.1955084582	-1.4438128410
C	2.7193140991	.2700114296	-1.2744136551
C	2.2631048398	-.3972270764	2.5082129261
C	3.1339207510	.2238757262	3.6140111306
C	1.9357770380	-1.8715533544	2.8194907971
C	1.9080277891	.7250619328	-2.4831666200
C	1.4577475615	-.4957347417	-3.3114199014
C	2.6529903690	1.7453735654	-3.3609494204
C	-3.3790013479	-.0813641741	.2742682799
C	-3.9285534575	-.6507564366	1.4444403559
C	-5.1842268827	-1.2613103365	1.3532939045
C	-5.8719137478	-1.3216484561	.1441313723
C	-5.3005492110	-.7818092914	-1.0048094412
C	-4.0474670405	-.1601956187	-.9676578631
C	-3.1634079923	-.6679213942	2.7640776811
C	-2.6181245450	-2.0828519204	3.0466526765
C	-3.9937665759	-.1477080623	3.9494637355
C	-3.4120731190	.3580846023	-2.2540233516
C	-4.3418659616	1.2894267165	-3.0503112131
C	-2.9279451741	-.8202620589	-3.1228415080
H	1.3648781726	3.9472328913	.8994553135
H	2.3020353940	2.9996528932	-.2754902791

H	2.4169883747	2.6186943574	1.4340460179
H	-.7755307126	3.5546492085	.9467725579
H	-2.9443296412	3.6933832484	1.0941891586
H	-3.7657337522	2.2543227834	1.7355253229
H	-3.8767253540	2.6244509296	.0232573104
H	4.7642930904	-1.1301894690	1.7296793747
H	5.7800855536	-1.0389317837	-.5207933439
H	4.4713575832	-.1857543951	-2.4347237826
H	1.3157322819	.1496380738	2.4951773428
H	2.6156077419	.1721822163	4.5774278206
H	3.3591520564	1.2755914392	3.4081308763
H	4.0866318546	-.3039860095	3.7263627844
H	1.4153837808	-1.9553856310	3.7803059674
H	2.8510576156	-2.4706842777	2.8793682093
H	1.3032775412	-2.3044097213	2.0390171245
H	1.0038646608	1.2161767497	-2.1118752177
H	.8018545788	-.1840976774	-4.1321435307
H	.9210551111	-1.2169495046	-2.6882748384
H	2.3219547069	-1.0094499879	-3.7471025307
H	1.9998346046	2.0982669750	-4.1660818117
H	3.5412898690	1.3090015338	-3.8292769391
H	2.9763743181	2.6170584984	-2.7822931523
H	-5.6237099890	-1.7082546550	2.2399139646
H	-6.8457499647	-1.8001086803	.0949587003
H	-5.8299242269	-.8551950773	-1.9500983128
H	-2.3010199057	-.0032592653	2.6570441313
H	-1.9961216680	-2.0817707917	3.9489211657
H	-2.0191439213	-2.4472880236	2.2072990394
H	-3.4388280524	-2.7913974610	3.2044834073
H	-3.3769876489	-.1098510267	4.8536395288
H	-4.8488159113	-.7968483219	4.1645820329
H	-4.3797071846	.8598524731	3.7618607304
H	-2.5293224652	.9416143869	-1.9769348890
H	-3.8180179539	1.6879416458	-3.9256987549
H	-4.6792713735	2.1368832067	-2.4443380539
H	-5.2317657094	.7646495011	-3.4130172853
H	-2.3964655181	-.4531091402	-4.0081392372
H	-3.7745793739	-1.4256003833	-3.4654422780
H	-2.2576503836	-1.4742979327	-2.5577068941

5) L^1CuO_2 side-on triplet

Cu	-.5737837235	-.6010130188	.0219552473
O	.1681039121	-2.4613926505	-.3839657700
O	-1.1324312075	-2.5279637244	-.3152140814
N	.8421810809	.7112239409	.2200482177
N	-2.1099885563	.5413824331	.3362336967
C	1.7205135492	2.9676824886	.6369459492

C	.5723123158	1.9852987951	.5034939678
C	-.7256473765	2.4973633335	.6897117647
C	-1.9665613209	1.8369827550	.6160850202
C	-3.2040450327	2.6766679921	.8695012617
C	2.1874699867	.2592724253	.0217578825
C	2.9083299453	-.2792634324	1.1119052527
C	4.1983830510	-.7693287419	.8793095856
C	4.7655264423	-.7390983918	-.3913838760
C	4.0367078228	-.2208326304	-1.4584856810
C	2.7437966161	.2826713847	-1.2788481673
C	2.2988920989	-.3784887471	2.5072343906
C	3.1796174199	.2772765229	3.5854087315
C	1.9923123040	-1.8450959836	2.8680565355
C	1.9510243670	.7901089111	-2.4802789146
C	1.5007895177	-.3851539403	-3.3706208080
C	2.7200646946	1.8360633147	-3.3055703840
C	-3.4033651815	-.0721650609	.2784889788
C	-3.9553715296	-.6463474395	1.4466184119
C	-5.1922658598	-1.2925860619	1.3483658890
C	-5.8677926696	-1.3810314939	.1342000413
C	-5.3032385066	-.8253510386	-1.0104489784
C	-4.0684780801	-.1685528410	-.9654000396
C	-3.2139414766	-.6196039394	2.7802295791
C	-2.6733360990	-2.0196485509	3.1327234195
C	-4.0718576012	-.0612095044	3.9287861223
C	-3.4516498706	.3813871110	-2.2482954506
C	-4.3970615109	1.3331502688	-3.0019021937
C	-2.9842611096	-.7654933286	-3.1657442829
H	1.3547820278	3.9660430345	.8797385583
H	2.2956429656	3.0213742839	-.2926797184
H	2.4174172438	2.6488298453	1.4179495453
H	-.7769335446	3.5530117924	.9223965189
H	-2.9380271898	3.7166014888	1.0627083880
H	-3.7652123139	2.2933166306	1.7273310972
H	-3.8814482078	2.6404371919	.0108859445
H	4.7641463879	-1.1888079582	1.7062891641
H	5.7680799193	-1.1248181686	-.5512661958
H	4.4767095388	-.2138615102	-2.4515290729
H	1.3464309273	.1587812565	2.4917410111
H	2.6793443906	.2403846108	4.5590736608
H	3.3869704972	1.3266543668	3.3520259915
H	4.1416177268	-.2354143745	3.6903116401
H	1.4902345000	-1.9060037915	3.8401028493
H	2.9120410057	-2.4372208300	2.9267389438
H	1.3471023623	-2.3114756667	2.1173666566
H	1.0474557307	1.2754556933	-2.1011277464
H	.8658772916	-.0286423270	-4.1894635403

H	.9378661600	-1.1266017294	-2.7957484152
H	2.3640754369	-.8964003038	-3.8105046934
H	2.0855757559	2.2254386764	-4.1089421720
H	3.6143454256	1.4096993433	-3.7722153133
H	3.0390675779	2.6812342140	-2.6870337350
H	-5.6284854293	-1.7429780521	2.2352565440
H	-6.8264347972	-1.8883508027	.0788355890
H	-5.8254183942	-.9109027244	-1.9590717252
H	-2.3510411335	.0427239994	2.6667679475
H	-2.0788924617	-1.9832843751	4.0525274180
H	-2.0435810989	-2.4163450303	2.3308227253
H	-3.4934596051	-2.7288802683	3.2892012865
H	-3.4771557824	.0092264434	4.8458146659
H	-4.9317852308	-.7040296911	4.1443321964
H	-4.4542522894	.9380756189	3.6965848858
H	-2.5646634882	.9568434425	-1.9689120855
H	-3.8923660889	1.7534963721	-3.8784304077
H	-4.7200700721	2.1646431426	-2.3671127801
H	-5.2957228431	.8175690567	-3.3566389697
H	-2.4766043649	-.3683423046	-4.0519283644
H	-3.8337562359	-1.3677986234	-3.5058844805
H	-2.2936657153	-1.4351629148	-2.6444058550

6) L^1CuO_2 end-on singlet

Cu	-.9423573291	-.6007871627	.1056138644
O	-.7945812617	-3.3092063659	.6387233586
O	-.8018423473	-2.1306868433	1.1400556720
N	.5507774409	.2902579528	-.7569843158
N	-2.3454579617	.5995343359	-.4432107677
C	1.6311096499	2.1208255474	-1.9832189288
C	.4031511500	1.4481973901	-1.3984030308
C	-.8301872639	2.1012864483	-1.5799802570
C	-2.1093381004	1.7014583680	-1.1520420918
C	-3.2778046780	2.5911604723	-1.5304443228
C	1.8211718904	-.3453804551	-.6071531944
C	2.5768300809	-.1056917764	.5653939243
C	3.7940321732	-.7745146191	.7208138540
C	4.2559680774	-1.6661904488	-.2444798781
C	3.4900743920	-1.9116744134	-1.3801824791
C	2.2633082382	-1.2698879917	-1.5838636495
C	2.0566478305	.8069433422	1.6702226410
C	3.0909740664	1.8528935251	2.1195101426
C	1.5600489862	-.0256970363	2.8691711611
C	1.4262763997	-1.6087979153	-2.8129324824
C	.8649283317	-3.0409982977	-2.7153707702
C	2.2051317058	-1.4180018332	-4.1269775754
C	-3.6634788941	.2042174120	-.0586012711

C	-4.1729936385	.6017805252	1.2008755661
C	-5.4434131080	.1515248849	1.5742430268
C	-6.1904371629	-.6751671039	.7393106485
C	-5.6655322803	-1.0783203604	-.4860368806
C	-4.3999875540	-.6577550758	-.9062923129
C	-3.3426550431	1.4432035107	2.1639309741
C	-2.7530363200	.5567669019	3.2795138906
C	-4.1257165250	2.6247194956	2.7600569676
C	-3.8043441371	-1.1790693142	-2.2091091330
C	-4.7907772284	-1.1357139298	-3.3885103407
C	-3.2504077135	-2.6055055808	-2.0124954495
H	1.3686144529	3.0618764928	-2.4680078104
H	2.1176707287	1.4715446992	-2.7172147302
H	2.3711051496	2.3212693765	-1.2023136061
H	-.7899313262	3.0327200068	-2.1291697251
H	-2.9439743039	3.4514888444	-2.1117376756
H	-3.7961418485	2.9508022263	-.6358457984
H	-4.0147668523	2.0344909393	-2.1175246370
H	4.3862454818	-.6014487515	1.6146142739
H	5.2044079615	-2.1767478995	-.1055329506
H	3.8458696633	-2.6229592834	-2.1198780999
H	1.1958301056	1.3514773416	1.2720759682
H	2.6477104248	2.5304350583	2.8571059015
H	3.4457343250	2.4552596247	1.2768354922
H	3.9650291347	1.3873425737	2.5869277320
H	1.1125822123	.6236585563	3.6300621369
H	2.3888330066	-.5697946838	3.3355501240
H	.8127849016	-.7653011275	2.5663504299
H	.5731554891	-.9250609854	-2.8343750144
H	.2224514100	-3.2590599590	-3.5758729910
H	.2773326354	-3.1803985116	-1.8030177409
H	1.6743461060	-3.7794900890	-2.7062683819
H	1.5517470338	-1.6073339267	-4.9853464648
H	3.0516997732	-2.1089298813	-4.2004416680
H	2.5988086034	-.4004580248	-4.2197880464
H	-5.8514680831	.4461492667	2.5365215938
H	-7.1752868732	-1.0137654816	1.0474339239
H	-6.2461326999	-1.7388764985	-1.1225661618
H	-2.5024695646	1.8593255421	1.6008129557
H	-2.1091090421	1.1462136482	3.9417563308
H	-2.1577328576	-.2649886574	2.8689555609
H	-3.5490951230	.1134220346	3.8876824081
H	-3.4634329477	3.2458690538	3.3723356298
H	-4.9453913473	2.2892850969	3.4040936142
H	-4.5553659988	3.2574268343	1.9766299632
H	-2.9588498445	-.5354791104	-2.4687275071
H	-4.2808874076	-1.4219453631	-4.3142998449

H	-5.2094756286	-.1337264065	-3.5278190704
H	-5.6257460309	-1.8306058923	-3.2510368453
H	-2.7739075455	-2.9623613753	-2.9324051129
H	-4.0577800889	-3.3016438359	-1.7591812410
H	-2.5108117937	-2.6578721154	-1.2076741099

7) L^1CuO_2 end-on triplet

Cu	-.9525798912	-.6980306113	-.0280093359
O	-1.0239781749	-3.5917464299	.3124613461
O	-.9747805089	-2.4372421603	.8076578858
N	.5968542129	.2491365252	-.7328598537
N	-2.3988284141	.5136154998	-.4817688378
C	1.6214187784	2.1202435189	-1.9526134946
C	.4120685928	1.3962360655	-1.3881442996
C	-.8419704913	2.0097086803	-1.5924239920
C	-2.1316625544	1.6211780847	-1.1742282971
C	-3.2763088141	2.5493006059	-1.5384276677
C	1.9030911407	-.3026519665	-.5332569269
C	2.6179612495	.0208491251	.6461032804
C	3.8677281112	-.5716718275	.8545598554
C	4.4060129941	-1.4671531313	-.0656470021
C	3.6851705326	-1.7906278649	-1.2111184919
C	2.4303487106	-1.2260716505	-1.4670551980
C	2.0325353956	.9480232192	1.7069199778
C	2.9968717787	2.0754718061	2.1139057575
C	1.5826584075	.1411217732	2.9405378311
C	1.6522643312	-1.6499911063	-2.7093738027
C	1.1972269725	-3.1189376655	-2.6017803268
C	2.4473375737	-1.4241336932	-4.0082396991
C	-3.7226321438	.1875415315	-.0502137934
C	-4.1427816296	.5914396582	1.2398533434
C	-5.4102681202	.1995772800	1.6825432264
C	-6.2466592680	-.5748847272	.8823356688
C	-5.8156477778	-.9755820929	-.3790332591
C	-4.5563312975	-.6105224707	-.8680516326
C	-3.2143797737	1.3790366025	2.1593747019
C	-2.5488697884	.4394404764	3.1845099680
C	-3.9120495345	2.5521918923	2.8673302222
C	-4.0928577107	-1.1158022557	-2.2310207318
C	-5.0943275037	-.7996064346	-3.3555346345
C	-3.7918217231	-2.6270885698	-2.1827928245
H	1.3284559513	3.0430295682	-2.4547096743
H	2.1562596736	1.4871717611	-2.6670590039
H	2.3332908686	2.3645837218	-1.1581237339
H	-.8071808763	2.9352244217	-2.1525124142
H	-2.9178544140	3.4199655803	-2.0888538726
H	-3.7978336386	2.8929262126	-.6395515633

H	-4.0188710989	2.0290270712	-2.1513793527
H	4.4260689020	-.3322700215	1.7552493544
H	5.3788919752	-1.9156884906	.1135353981
H	4.1008920506	-2.5021496974	-1.9189038478
H	1.1412727633	1.4176246187	1.2822202692
H	2.5071682807	2.7577796232	2.8170322468
H	3.3204017586	2.6592492858	1.2460882636
H	3.8947008042	1.6870232646	2.6063630097
H	1.1058619956	.7948060818	3.6794826141
H	2.4360838874	-.3483795904	3.4225861317
H	.8675948954	-.6404199036	2.6644829709
H	.7517111788	-1.0319357344	-2.7639028976
H	.5920354871	-3.3985609310	-3.4714053857
H	.6005067272	-3.2892895003	-1.7010136570
H	2.0575596569	-3.7960353640	-2.5609290817
H	1.8348523592	-1.6819817657	-4.8789464266
H	3.3480544062	-2.0461443920	-4.0435948138
H	2.7612829287	-.3807154279	-4.1130869487
H	-5.7464538869	.4996234713	2.6706768201
H	-7.2280953256	-.8688235938	1.2431057514
H	-6.4667564591	-1.5903197953	-.9936727822
H	-2.4163347396	1.8002020116	1.5418771176
H	-1.8349948078	.9877123381	3.8093349117
H	-2.0108196403	-.3763678241	2.6910583729
H	-3.2982099179	-.0139087367	3.8428156648
H	-3.1808230218	3.1404842881	3.4318626691
H	-4.6718498514	2.2102247353	3.5779669082
H	-4.4019610945	3.2185039662	2.1500611933
H	-3.1567459323	-.6049112679	-2.4735055357
H	-4.6851979948	-1.1061944907	-4.3241061601
H	-5.3185206668	.2707772751	-3.4057089073
H	-6.0417045316	-1.3312982028	-3.2177993851
H	-3.4049499659	-2.9744598255	-3.1474241001
H	-4.6978509814	-3.2002340720	-1.9569421106
H	-3.0520091980	-2.8663727539	-1.4133735202

8) $L^1Cu(MeCN)O_2$ singlet

Cu	.1577571631	-.1654760858	.2178537395
O	.9547298945	-.0717367463	2.0643901217
O	-.3762707985	-.2040804045	2.0158847828
N	-1.4682837132	-.8239633774	-.6474051982
N	1.4520567628	-.4628170224	-1.1970139272
N	.1893759914	2.1361146462	.3676162589
C	.9240899878	2.6179347068	1.1272751491
C	1.8576824639	3.1714839412	2.0948868979
C	-2.6191208883	-2.0916276715	-2.4158274979
C	-1.3744410486	-1.4657079032	-1.8105991184

C	-.1825109214	-1.6466988779	-2.5355585161
C	1.1162039080	-1.1760952345	-2.2671824230
C	2.1630184288	-1.5363519873	-3.3070340671
C	-2.7100469280	-.7338897287	.0663719988
C	-3.1386075028	-1.8013140836	.8944572092
C	-4.3500363638	-1.6638538301	1.5820242628
C	-5.1260729717	-.5154008476	1.4673808973
C	-4.6863093064	.5293856851	.6611839417
C	-3.4779438894	.4511142733	-.0394782025
C	-2.3276370148	-3.0810335483	1.0840686875
C	-3.1405386850	-4.3408593558	.7270385897
C	-1.7839163307	-3.1911708701	2.5222602415
C	-3.0427401647	1.6227914910	-.9134646415
C	-3.0771381364	2.9567798487	-.1486970672
C	-3.8925775702	1.7125125023	-2.1959281529
C	2.7274487252	.1579527292	-1.0138062786
C	3.6135293478	-.3891820170	-.0479277629
C	4.8028875355	.2908840705	.2277024523
C	5.1242349447	1.4807678703	-.4219909188
C	4.2561238203	1.9975808398	-1.3778835716
C	3.0516400318	1.3574478481	-1.6984530245
C	3.3129090151	-1.7157488771	.6443828215
C	3.7516181527	-1.7593476369	2.1159083406
C	3.9335065311	-2.8917271702	-.1365502744
C	2.1681733397	1.9636760070	-2.7883127839
C	2.8805387185	1.9226672053	-4.1563861856
C	1.7366475230	3.4102182155	-2.4817830020
H	2.8692944117	3.1437238707	1.6809640501
H	1.8222913084	2.5562439005	2.9967221231
H	1.5923071449	4.2028162753	2.3402796375
H	-2.4849573688	-2.2516036302	-3.4868342259
H	-3.5008204714	-1.4698079664	-2.2539273668
H	-2.8191908803	-3.0615736275	-1.9493654320
H	-.2812261841	-2.2174356333	-3.4509994104
H	2.0977294350	-2.6039390404	-3.5348577596
H	3.1741951829	-1.3064620403	-2.9725064388
H	1.9743438324	-.9944662056	-4.2386863137
H	-4.6884088293	-2.4733775798	2.2219894038
H	-6.0651865436	-.4330859742	2.0069550658
H	-5.2916403120	1.4266183968	.5743156921
H	-1.4656416287	-3.0375808057	.4123568063
H	-2.5054743134	-5.2312600063	.7846219282
H	-3.5614037276	-4.2885821350	-.2819719236
H	-3.9743792446	-4.4884108792	1.4215796470
H	-1.1693786074	-4.0923585596	2.6287673529
H	-2.6034324591	-3.2601062757	3.2465343050
H	-1.1764257670	-2.3186976579	2.7694796549

H	-2.0074413720	1.4452589969	-1.2113097591
H	-2.6574297383	3.7554105369	-.7687226659
H	-2.4901606523	2.8962623957	.7709227264
H	-4.0986680338	3.2494061960	.1152611286
H	-3.5530893622	2.5426415019	-2.8248244342
H	-4.9484220713	1.8818855649	-1.9582607475
H	-3.8291872536	.7950750639	-2.7890236306
H	5.4898206272	-.1163074256	.9621582371
H	6.0526484179	1.9952130721	-.1911381140
H	4.5169793499	2.9182684884	-1.8917972308
H	2.2294680812	-1.8514675056	.6346820674
H	3.3921467149	-2.6846152711	2.5774268654
H	3.3323635034	-.9223583265	2.6785457423
H	4.8417167744	-1.7470030035	2.2247514178
H	3.6866021627	-3.8429713776	.3469518106
H	5.0250656977	-2.8043867514	-.1730049826
H	3.5663475331	-2.9326208373	-1.1656680520
H	1.2584689316	1.3623297430	-2.8609788548
H	2.2027267213	2.2595721651	-4.9481866949
H	3.2302861633	.9185123785	-4.4090087961
H	3.7524717615	2.5860065007	-4.1629936189
H	1.1209843212	3.7963190934	-3.3013888376
H	2.6018171634	4.0746113991	-2.3816465988
H	1.1497586893	3.4662282979	-1.5648734589

9) $L^1Cu(MeCN)O_2$ triplet

Cu	.1100524030	-.3261469344	.3044722603
O	.9744796841	-.6221789337	2.4023761395
O	-.2897138096	-.4104652000	2.2857864060
N	-1.6228824951	-.9819351765	-.4331249566
N	1.2862514117	-.7798489020	-1.2302564032
N	.8009259368	1.8178975294	.7534060647
C	1.7422557182	2.3692669038	1.1452246962
C	2.9426445733	3.0405634269	1.6197760159
C	-2.9782299492	-2.1670144948	-2.1216157576
C	-1.6579863148	-1.6268972969	-1.5948124123
C	-.5311852380	-1.8822668577	-2.4034980855
C	.8127589039	-1.4954029855	-2.2500758666
C	1.7356404559	-1.9400037582	-3.3744654962
C	-2.7920370915	-.8064545935	.3698864884
C	-3.2577232825	-1.8516135385	1.2044867822
C	-4.3742031611	-1.6112624432	2.0130298703
C	-5.0221628815	-.3811033035	2.0112270700
C	-4.5469012516	.6424242032	1.1974903235
C	-3.4292411177	.4584582461	.3778177240
C	-2.5687426684	-3.2121480165	1.2773874680
C	-3.5366979570	-4.3739772081	.9854090755

C	-1.8871114427	-3.4232669883	2.6422773592
C	-2.9461083420	1.6017261062	-.5092165983
C	-2.7387807935	2.9065308349	.2781297640
C	-3.8999728301	1.8261096016	-1.6982897715
C	2.6116514565	-.2495674028	-1.2090219131
C	3.5676908996	-.8195467893	-.3277334878
C	4.8262107179	-.2195477269	-.2192820174
C	5.1544166488	.9174906970	-.9549612756
C	4.2146020608	1.4646618051	-1.8230800844
C	2.9390132175	.9025823158	-1.9716093692
C	3.2555589315	-2.0924060858	.4515043989
C	3.8689578225	-2.1173803747	1.8594108375
C	3.6865022556	-3.3409143182	-.3431349467
C	1.9651573684	1.5478484160	-2.9570253657
C	2.5179442024	1.5136253886	-4.3951851608
C	1.6063172962	2.9954125229	-2.5712513250
H	3.7643898488	2.8336050597	.9303249674
H	3.2034992008	2.6660437248	2.6108580224
H	2.7766206273	4.1221133582	1.6747809219
H	-2.9523425473	-2.2409638523	-3.2098556536
H	-3.8185222390	-1.5374878904	-1.8270088775
H	-3.1673038842	-3.1691748567	-1.7235291884
H	-.7361923834	-2.4531662586	-3.3016866372
H	1.5659954392	-2.9981502822	-3.5914388213
H	2.7880402211	-1.7937534516	-3.1334564030
H	1.5131834023	-1.3832198691	-4.2897928032
H	-4.7386797978	-2.4036548224	2.6600659447
H	-5.8896719457	-.2190181832	2.6436257777
H	-5.0530631795	1.6029257722	1.1982554814
H	-1.7849389768	-3.2322791155	.5161013734
H	-2.9934102806	-5.3241687832	.9524400139
H	-4.0532865307	-4.2442043897	.0306128767
H	-4.3017103063	-4.4622907032	1.7629826367
H	-1.3574720901	-4.3824559175	2.6601242111
H	-2.6248156299	-3.4345255538	3.4516885213
H	-1.1715305703	-2.6261460807	2.8530997018
H	-1.9749594132	1.3118255048	-.9172686234
H	-2.3208232095	3.6786331231	-.3747040304
H	-2.0477287107	2.7565009092	1.1110328318
H	-3.6791790389	3.2936810178	.6820124652
H	-3.5289317896	2.6282481885	-2.3450783297
H	-4.9013980669	2.1087382984	-1.3528531774
H	-4.0003632789	.9211713085	-2.3069473847
H	5.5658962128	-.6513273023	.4469680849
H	6.1406910026	1.3641475378	-.8617948282
H	4.4765109502	2.3427787220	-2.4073436142
H	2.1701616906	-2.1409029088	.5693725029

H	3.4965378835	-2.9864439149	2.4100340912
H	3.6026231624	-1.2225331560	2.4271561781
H	4.9611588361	-2.1964834173	1.8324665299
H	3.4275495783	-4.2524235645	.2056195099
H	4.7692521731	-3.3432198548	-.5099640419
H	3.1970663101	-3.3850314866	-1.3190058118
H	1.0365747464	.9720881149	-2.9396336752
H	1.7693551392	1.8896223988	-5.0999417159
H	2.7957601514	.5012465765	-4.6993790746
H	3.4087491404	2.1439136402	-4.4934799889
H	.9168182758	3.4227791679	-3.3067995949
H	2.4955754257	3.6355415117	-2.5447136280
H	1.1235359297	3.0372881757	-1.5937738736

10) $L^1Cu(THF)O_2$ singlet

Cu	-.4799839783	-.1330957360	.8210020594
N	-.5611574404	.1297236932	-1.1408442228
N	-.2027136320	-2.0819399649	.9114604208
C	-1.1102421273	-.7555053442	-3.3683648877
C	-.8444593541	-.9389209951	-1.8838573894
C	-.9101109441	-2.2670649513	-1.3998734321
C	-.5503260620	-2.8110111991	-.1462292086
C	-.5642683967	-4.3245709618	-.0329335805
C	-.3085073098	1.4130683290	-1.7260336834
C	-1.3398981734	2.3737523044	-1.8697889691
C	-1.0169919338	3.6259227575	-2.4074570770
C	.2798650647	3.9456338933	-2.7908932648
C	1.2869681071	2.9994453632	-2.6363211629
C	1.0230595122	1.7322384005	-2.1046426859
C	-2.7842600262	2.1048755599	-1.4618598179
C	-3.7358647602	2.1317046528	-2.6727434635
C	-3.2652137723	3.1078802292	-.3976858325
C	2.1815502374	.7480161698	-1.9539966032
C	3.2585727004	1.2878981130	-.9945624940
C	2.8045693271	.3884504966	-3.3163455765
C	.3123818628	-2.6630015135	2.1105270050
C	-.5385166949	-2.8049754945	3.2370246221
C	.0053394323	-3.2995845086	4.4286780057
C	1.3518676772	-3.6353874017	4.5302091292
C	2.1815140851	-3.4723192185	3.4240947588
C	1.6888372277	-2.9916788151	2.2052077986
C	-2.0123187842	-2.4106305299	3.2005078754
C	-2.3226747334	-1.2872329564	4.2088177248
C	-2.9337968263	-3.6217603992	3.4381878376
C	2.6543926892	-2.7966345463	1.0392512911
C	3.3961650324	-4.0938044312	.6683853702
C	3.6597851179	-1.6691787229	1.3398213957

C	.8623048368	2.4884689003	1.8858516963
O	1.0241124300	1.0554532067	1.9780363225
C	1.2483111728	.7871227311	3.3780505671
C	1.9201456165	3.0634966461	2.8396757624
C	2.1862532651	1.9095423051	3.8455691940
H	-1.2627936797	-1.7156411261	-3.8629892401
H	-.2784040114	-.2391013916	-3.8547382168
H	-1.9987015066	-.1370582612	-3.5252181502
H	-1.2022349923	-2.9999084919	-2.1413583724
H	-.9484255256	-4.7858066062	-.9441331534
H	-1.1851682643	-4.6396404839	.8118069491
H	.4415631319	-4.7133642429	.1535476237
H	-1.8025298636	4.3662144758	-2.5234497992
H	.5042487689	4.9244528381	-3.2042688900
H	2.3018433773	3.2473797014	-2.9331940514
H	-2.8311804560	1.1112558364	-1.0114310779
H	-4.7590162014	1.9050851382	-2.3536110694
H	-3.4514387909	1.4017157722	-3.4368979746
H	-3.7471180637	3.1192262084	-3.1494444390
H	-4.2637584210	2.8325074698	-.0481170131
H	-3.3164513809	4.1253857294	-.8013999501
H	-2.5964761487	3.1049674226	.4640991040
H	1.7873483693	-.1736590896	-1.5182419898
H	4.0902760518	.5793689260	-.9153805497
H	2.8507174384	1.4384027149	.0085621785
H	3.6666298732	2.2416298818	-1.3468208472
H	3.5865207366	-.3684287417	-3.1894507531
H	3.2611112231	1.2636095758	-3.7918822924
H	2.0583011260	-.0121312050	-4.0098895407
H	-.6407195871	-3.4170253370	5.2944085876
H	1.7536072080	-4.0157425736	5.4650866212
H	3.2356814823	-3.7218664877	3.5072628152
H	-2.2364916417	-2.0147654086	2.2065553542
H	-3.3713922919	-.9861254312	4.1264665494
H	-1.7118411109	-.4019613080	4.0120618561
H	-2.1389059133	-1.6090905380	5.2411676294
H	-3.9834167864	-3.3220427260	3.3432864088
H	-2.7950150663	-4.0428346567	4.4424898084
H	-2.7434426523	-4.4227131580	2.7138314800
H	2.0711742386	-2.4859223790	.1684577668
H	4.0201086420	-3.9353345676	-.2174687967
H	2.7016444538	-4.9103707170	.4500139734
H	4.0533345997	-4.4282779246	1.4779099441
H	4.3434249720	-1.5274745303	.4958369785
H	4.2648159216	-1.9030905437	2.2227784975
H	3.1438802410	-.7218976323	1.5187865597
H	-.1556519931	2.7511875215	2.1972693199

H	.9960998269	2.7625786944	.8385994189
H	1.6632791867	-.2173556438	3.4578994524
H	.2869977322	.8231572879	3.9062731262
H	1.5606188939	3.9723321290	3.3284847292
H	2.8329238609	3.3170990705	2.2955784001
H	3.2281540392	1.5860885330	3.7945688846
H	1.9768316253	2.1969447785	4.8792103871
O	-3.0229347881	.4399058036	1.4708207128
O	-1.8680205715	1.0052077105	1.5331324161

11) $L^1Cu(THF)O_2$ triplet

Cu	-.4633119138	-.0803750419	.8114780982
N	-.5053993723	.1443929458	-1.1687234015
N	-.2241600312	-2.0615068395	.9563827126
C	-1.0393338739	-.7823972764	-3.3857799993
C	-.8000621546	-.9351467372	-1.8926918213
C	-.8956043037	-2.2493647708	-1.3761845406
C	-.5553588538	-2.7863676778	-.1099389810
C	-.5323281660	-4.3031466486	-.0205834408
C	-.2375196317	1.4072728492	-1.7855093383
C	-1.2541256749	2.3878104196	-1.9043754295
C	-.9309067038	3.6335518414	-2.4544444286
C	.3604549841	3.9321647233	-2.8761818780
C	1.3579416123	2.9725990971	-2.7356549611
C	1.0892534814	1.7115606560	-2.1908262127
C	-2.6803312049	2.1431655121	-1.4233245775
C	-3.7049843305	2.2403321176	-2.5689099653
C	-3.0565404171	3.1175662191	-.2901379832
C	2.2405685950	.7206773278	-2.0308760643
C	3.3072617804	1.2658272799	-1.0631137733
C	2.8775625446	.3469523390	-3.3813070004
C	.2915316119	-2.6620395126	2.1462432374
C	-.5493531421	-2.8386423263	3.2736167332
C	.0042616247	-3.3369694056	4.4582015664
C	1.3560567084	-3.6507909417	4.5547960224
C	2.1772728089	-3.4634374459	3.4471985925
C	1.6739168232	-2.9729468077	2.2366693771
C	-2.0357111631	-2.5022644550	3.2323605134
C	-2.4142567093	-1.4652284815	4.3058379266
C	-2.9089769876	-3.7629230867	3.3710573356
C	2.6387705229	-2.7477050189	1.0745392724
C	3.4126796469	-4.0237896296	.6968826969
C	3.6188245258	-1.6007540082	1.3874432591
C	.7784362222	2.6340919254	1.8510378188
O	.8043753539	1.1994500149	2.0055861771
C	1.1318767156	.9524263228	3.3881061038
C	1.9436393047	3.1473658366	2.7174719928

C	2.2267368593	1.9805644825	3.7053516512
H	-1.2527923034	-1.7441867904	-3.8547359386
H	-.1689002344	-.3394752726	-3.8795666227
H	-1.8810755490	-.1076610166	-3.5733076164
H	-1.1832366816	-2.9938792986	-2.1084091811
H	-1.1316568388	-4.7495061495	-.8166248537
H	-.9052166956	-4.6517282399	.9455357034
H	.4929361070	-4.6771856785	-.1228214614
H	-1.7090339948	4.3858375280	-2.5505190554
H	.5888719525	4.9043611521	-3.3033644682
H	2.3708367097	3.2063056355	-3.0523972131
H	-2.7274879594	1.1292241826	-1.0180173500
H	-4.7110791533	2.0104534702	-2.2020048643
H	-3.4737458263	1.5428454535	-3.3798973698
H	-3.7301698862	3.2481188831	-2.9979279587
H	-4.0493244773	2.8806786128	.1065887797
H	-3.0738983795	4.1536528446	-.6459085085
H	-2.3427334978	3.0572649631	.5359866996
H	1.8367059500	-.1936636887	-1.5896958802
H	4.1289064115	.5508256252	-.9500660963
H	2.8784161926	1.4441527001	-.0730796468
H	3.7329689164	2.2075866539	-1.4253750579
H	3.6670622173	-.3993054068	-3.2394725462
H	3.3283655061	1.2186271157	-3.8675956407
H	2.1392931636	-.0716710619	-4.0716215746
H	-.6388262352	-3.4798306886	5.3221924935
H	1.7664057531	-4.0352038859	5.4840803493
H	3.2355265611	-3.6979315226	3.5232869776
H	-2.2486629145	-2.0608593397	2.2566658550
H	-3.4650706237	-1.1762480988	4.2022977973
H	-1.8085391103	-.5594831609	4.2117991470
H	-2.2729609555	-1.8614695588	5.3173141369
H	-3.9706375945	-3.5023519914	3.3032109142
H	-2.7462644045	-4.2567097257	4.3356221397
H	-2.6892647255	-4.4906798267	2.5839280615
H	2.0528580781	-2.4439165526	.2037281511
H	4.0284034175	-3.8472522134	-.1916044333
H	2.7368613103	-4.8569086880	.4809818209
H	4.0824649280	-4.3434351503	1.5022589776
H	4.3102057523	-1.4448393495	.5527323248
H	4.2161841147	-1.8220787825	2.2784865984
H	3.0836485178	-.6631938936	1.5593697082
H	-.1882901798	3.0139726590	2.2076387480
H	.8766336277	2.8474477384	.7856821782
H	1.4441079677	-.0892190422	3.4708383834
H	.2370385017	1.1111353216	4.0054044462
H	1.6730491623	4.0725917916	3.2318817645

H	2.8220838982	3.3554819539	2.1025396580
H	3.2143900812	1.5513538306	3.5191563885
H	2.1916615050	2.2951215815	4.7511850967
O	-3.2680772717	.2227559807	1.4295668825
O	-2.1461847741	.6880295506	1.7314163743

12) $L^1Cu(MeCN) + O_2$ _ $L^1Cu(MeCN)O_2$ transition state (triplet)

Cu	.0302214877	-.2060247890	.2058033768
O	1.3523390677	-.7073063027	2.8482206530
O	.1629877822	-.4845022200	2.5877214167
N	-1.6304395864	-1.1579120161	-.2076788085
N	1.2827903287	-.9762524961	-1.2031202955
N	.9773991607	1.4961825850	.7674899669
C	1.8648887236	2.2337022910	.8669962013
C	3.0083664214	3.1264491016	.9695432610
C	-2.9468497904	-2.7023705880	-1.6143725308
C	-1.6432581856	-2.0253524889	-1.2214871255
C	-.5182675565	-2.4022762299	-1.9875695452
C	.8045535120	-1.9111709179	-2.0191566907
C	1.6837757863	-2.4867452114	-3.1206644403
C	-2.8280348787	-.8028329357	.4922288533
C	-3.3529815247	-1.6290669629	1.5194076050
C	-4.4932198621	-1.1995155774	2.2090604376
C	-5.1113040518	.0112797082	1.9165517713
C	-4.5773766769	.8239441207	.9210776113
C	-3.4380206870	.4454805540	.2045078525
C	-2.7046439338	-2.9489322943	1.9320577064
C	-3.6688086335	-4.1441546099	1.8069221672
C	-2.1613115978	-2.8679911647	3.3719808862
C	-2.8907947970	1.3792174904	-.8708939188
C	-2.5720882804	2.7755443307	-.3096702146
C	-3.8413021511	1.4723555410	-2.0784619142
C	2.5527338023	-.3707493128	-1.3993866223
C	3.6269918782	-.7056443542	-.5308465130
C	4.8415680716	-.0241984138	-.6646872175
C	5.0113358329	.9821739689	-1.6135039693
C	3.9468255606	1.3190434295	-2.4457410895
C	2.7122461049	.6624661454	-2.3582868390
C	3.4715133022	-1.8014218366	.5186677304
C	4.2369875167	-1.5128547912	1.8201521624
C	3.8793740722	-3.1812047969	-.0352092740
C	1.5671380977	1.1080120420	-3.2650762473
C	1.9579787676	1.0819912116	-4.7536863922
C	1.0481935118	2.5041755250	-2.8692543925
H	3.6487483701	2.9819064742	.0942604670
H	3.5793713229	2.8921649007	1.8698628561
H	2.6763192589	4.1673545070	1.0186938545

H	-2.9062964879	-3.0435916395	-2.6498009905
H	-3.7992481313	-2.0310256763	-1.4945237379
H	-3.1314268964	-3.5765369403	-.9822303749
H	-.7244932601	-3.1632285407	-2.7313925014
H	1.4176757518	-3.5277799578	-3.3181474491
H	2.7431915953	-2.4344924851	-2.8656873557
H	1.5423469949	-1.9280613697	-4.0528011237
H	-4.9001808417	-1.8275141634	2.9968492999
H	-5.9965509315	.3217814436	2.4636781754
H	-5.0535880443	1.7740927484	.6951704355
H	-1.8525547207	-3.1260823950	1.2699051769
H	-3.1456005126	-5.0808413717	2.0283651832
H	-4.0996314492	-4.2236951089	.8051139157
H	-4.5002025721	-4.0577782299	2.5146286946
H	-1.6193351940	-3.7839724521	3.6331290982
H	-2.9745378293	-2.7439009594	4.0952323650
H	-1.4852902632	-2.0187412351	3.4760213929
H	-1.9508523011	.9514142068	-1.2299406505
H	-2.1007817979	3.3970299922	-1.0805488073
H	-1.8860142747	2.7087760433	.5408521063
H	-3.4761959062	3.2944415355	.0273877136
H	-3.4179078067	2.1201134861	-2.8550144174
H	-4.8137945517	1.8859919036	-1.7887671922
H	-4.0174495107	.4870994901	-2.5199146163
H	5.6711792312	-.2836786115	-.0145084225
H	5.9657353126	1.4931396295	-1.7061124718
H	4.0745240167	2.1099776695	-3.1798359641
H	2.4070314473	-1.8538405996	.7671456876
H	3.9602659261	-2.2452003924	2.5846995171
H	4.0037812092	-.5186824953	2.2126558802
H	5.3224693939	-1.5812778343	1.6846895267
H	3.7433971823	-3.9542656306	.7293915239
H	4.9335474835	-3.1851385666	-.3375803145
H	3.2776282575	-3.4610239385	-.9036215255
H	.7389602912	.4089295961	-3.1281683747
H	1.0894899058	1.3138731981	-5.3795613658
H	2.3398916481	.1005952118	-5.0507388357
H	2.7337246631	1.8211424943	-4.9818055659
H	.2132519267	2.8013370977	-3.5134608893
H	1.8335064037	3.2624570983	-2.9696644284
H	.6956999496	2.5144316015	-1.8344292011

13) $L^1Cu(MeCN)O_2$ _ MeCN + L^1CuO_2 side-on transition state (singlet)

Cu	.3381430028	-.7590304881	.2614660450
O	1.0870493980	-2.5145105658	.1436155360
O	-.2604026255	-2.5576882216	.1213862439
N	-1.2135105217	.3674529457	-.0814106718

N	1.7601913191	.5256533976	-.0507763797
N	.2938901730	-1.0194363263	2.5462843661
C	.4237400036	-1.9868532157	3.1715268352
C	.5829438396	-3.2323891033	3.9081512308
C	-2.2758510683	2.5009299983	-.6955182155
C	-1.0607283110	1.6658944653	-.3310639091
C	.1773316032	2.3357918961	-.3622130468
C	1.4778074903	1.8049861401	-.2872997078
C	2.6148878134	2.7770818081	-.5471493541
C	-2.5017461402	-.2585962917	-.2049707726
C	-2.8937496919	-.7728505629	-1.4694300937
C	-4.1565904708	-1.3636710028	-1.5915122745
C	-5.0211436207	-1.4557955495	-.5051482730
C	-4.6124358177	-.9699639685	.7327911653
C	-3.3543828454	-.3820659409	.9152895433
C	-1.9813614063	-.7312615681	-2.6953176427
C	-2.6379645785	-.0161473634	-3.8921707880
C	-1.5306579736	-2.1492256054	-3.0997907268
C	-2.9461836122	.0913353018	2.3059205745
C	-3.0900017091	-1.0422705860	3.3389676735
C	-3.7521716156	1.3236979058	2.7574579923
C	3.1045207898	.0299767195	-.1498927113
C	3.5356089266	-.4974907466	-1.3968946895
C	4.8446828109	-.9778863621	-1.5069204775
C	5.7172908796	-.9562999636	-.4226798374
C	5.2707182032	-.4658993622	.7994837379
C	3.9666054903	.0158520936	.9690192806
C	2.6248889051	-.5620316162	-2.6223229508
C	2.4200583569	-2.0142931016	-3.0960566409
C	3.1471414055	.3182900268	-3.7748313960
C	3.5128757149	.4478635276	2.3580542777
C	4.2740750917	1.6871933655	2.8647651533
C	3.6704159613	-.7105953178	3.3620501916
H	1.5858611838	-3.2864742349	4.3418339111
H	.4506968734	-4.0705243940	3.2178659509
H	-.1620754908	-3.3018618491	4.7042628760
H	-2.0551467609	3.5647791748	-.5992730910
H	-3.1409209787	2.2561655335	-.0777912657
H	-2.5630794678	2.3038703748	-1.7345350027
H	.1212361040	3.3987611822	-.5568590405
H	2.2340690535	3.7285109275	-.9241487885
H	3.3207761541	2.3671360916	-1.2745600066
H	3.1808533085	2.9668127129	.3703564571
H	-4.4644270528	-1.7590266082	-2.5555360010
H	-6.0009788390	-1.9106785357	-.6214251044
H	-5.2828301473	-1.0539385766	1.5832883124
H	-1.0855298896	-.1626187109	-2.4294175672

H	-1.9326797409	.0510919429	-4.7279559914
H	-2.9551905118	1.0001208144	-3.6362463544
H	-3.5205185572	-.5571301410	-4.2509385473
H	-.8319841652	-2.1007527084	-3.9429972713
H	-2.3864260033	-2.7596367143	-3.4109368477
H	-1.0364210795	-2.6494599557	-2.2634831542
H	-1.8903112589	.3693038058	2.2663378550
H	-2.6734886941	-.7320183809	4.3037824990
H	-2.5677906142	-1.9430423414	3.0062531622
H	-4.1398537935	-1.3067888602	3.5042979805
H	-3.4322271096	1.6444523502	3.7549750651
H	-4.8238422693	1.0997471970	2.8052888890
H	-3.6190179279	2.1695673539	2.0768865265
H	5.1823091587	-1.3794268957	-2.4582715538
H	6.7323728339	-1.3284485467	-.5280989016
H	5.9457416458	-.4690011544	1.6505671925
H	1.6450750224	-.1722950386	-2.3335572316
H	1.7160215458	-2.0423720357	-3.9361971825
H	2.0168632247	-2.6266702756	-2.2850073248
H	3.3604728905	-2.4626444098	-3.4376412031
H	2.4557049710	.2844334306	-4.6244133692
H	4.1250466064	-.0269237499	-4.1296487560
H	3.2543520661	1.3648797139	-3.4710100291
H	2.4489968529	.6937407781	2.3007786715
H	3.9082263263	1.9823080961	3.8543820172
H	4.1500395415	2.5439122131	2.1959072945
H	5.3484156711	1.4867737949	2.9482973055
H	3.2298748810	-.4432251199	4.3294282329
H	4.7274688904	-.9407628368	3.5393785154
H	3.1911668229	-1.6191262871	2.9880930231

14) $L^1Cu(MeCN)$ _ $L^1Cu(THF)$ transition state

Cu	.0577095027	-.3892489947	-.2069169816
N	-1.5111258653	-.4082985136	1.0365785583
N	-.8581112387	-.3951643618	-1.9886683665
C	-3.9398920960	-.6641081069	1.4138766663
C	-2.7111805112	-.6443727502	.5143981458
C	-2.9714569459	-.8463098576	-.8626297959
C	-2.1673107928	-.6314183381	-2.0083121324
C	-2.9173800226	-.6411662426	-3.3336471872
C	-1.3213019828	-.0150378480	2.3894069205
C	-.7837950603	-.9450060297	3.3196246194
C	-.5076767134	-.5222280072	4.6232310800
C	-.7296591388	.7927216524	5.0238708041
C	-1.2355396235	1.7050325122	4.1037333495
C	-1.5395277663	1.3308631334	2.7890181755
C	-.5157077211	-2.3900435462	2.9132340700

C	-1.6768615460	-3.3165122677	3.3210757690
C	.8148289088	-2.9213030653	3.4753636640
C	-2.0582319169	2.3947926328	1.8250549304
C	-.9871904493	3.4676889406	1.5481713668
C	-3.3534924306	3.0552703789	2.3321544889
C	-.1316251531	.0040717074	-3.1433149256
C	.7349417932	-.9249055791	-3.7778436755
C	1.5183788194	-.5005675432	-4.8547304769
C	1.4779037080	.8153368238	-5.3085703374
C	.6404527085	1.7262319244	-4.6727656030
C	-.1720697963	1.3496566676	-3.5961584188
C	.8055301716	-2.3728253435	-3.3053936322
C	2.2479439085	-2.9053888964	-3.2434187912
C	-.0677293703	-3.2955232014	-4.1770101802
C	-1.0397332758	2.4109111765	-2.9229023837
C	-1.9917439567	3.1002771810	-3.9173928443
C	-.1766376205	3.4598949466	-2.1961468963
C	2.2515830359	1.3008767491	1.5068208662
O	1.6584170440	1.2166467306	.2016246257
C	2.7480812992	1.3552266214	-.7246739683
C	3.2738515976	2.4422968704	1.3918076388
C	3.6548058816	2.4422933389	-.1157223283
C	2.2665153763	-2.7792564489	.2625591931
N	1.6614313045	-1.7988376008	.1226956913
C	2.9911739604	-4.0320887986	.4304782360
H	-4.6887627480	-1.3577813796	1.0235943353
H	-4.4023011046	.3289622521	1.4490538336
H	-3.6934772060	-.9459394668	2.4394189314
H	-4.0077768778	-1.0748441159	-1.0870924234
H	-3.7669836691	-1.3267302032	-3.2874495795
H	-2.2736386097	-.9279486522	-4.1671711104
H	-3.3142288861	.3561623367	-3.5551520218
H	-.1079849847	-1.2323439473	5.3413228732
H	-.5071823836	1.1026741185	6.0409641647
H	-1.3986406383	2.7350657779	4.4102974740
H	-.4497331707	-2.4030753570	1.8216246151
H	-1.4822813904	-4.3482227404	3.0045389346
H	-2.6180072765	-2.9974702181	2.8652642564
H	-1.8129599304	-3.3170371104	4.4087832444
H	1.0416792892	-3.9137711236	3.0651637485
H	.7881882131	-3.0328209891	4.5649407061
H	1.6444720277	-2.2506016016	3.2303081965
H	-2.2796553644	1.9060483222	.8734417416
H	-1.3675298978	4.2186700256	.8466571794
H	-.0892612466	3.0232558081	1.1113416615
H	-.7008546118	3.9889328821	2.4689999438
H	-3.7479784401	3.7496053770	1.5820207004

H	-3.1787696577	3.6278095494	3.2496103566
H	-4.1273020713	2.3130298431	2.5501241623
H	2.1736777322	-1.2112570348	-5.3500852363
H	2.0947676176	1.1272036334	-6.1465783210
H	.6153260817	2.7565018814	-5.0180565365
H	.3973208644	-2.3927486488	-2.2909773817
H	2.2655874915	-3.9021569549	-2.7847572832
H	2.8910764679	-2.2426896686	-2.6553735068
H	2.6949813501	-3.0094592350	-4.2382585681
H	-.0252213295	-4.3291247759	-3.8136574796
H	.2745353033	-3.2898964607	-5.2185090339
H	-1.1142782275	-2.9789391515	-4.1663752631
H	-1.6499185768	1.9142639846	-2.1647850464
H	-2.6601823320	3.7903642690	-3.3906394425
H	-2.6071606394	2.3739068054	-4.4564887651
H	-1.4408007331	3.6830504222	-4.6636824340
H	-.8094060020	4.2191614161	-1.7229500429
H	.4944155916	3.9732584587	-2.8941648640
H	.4288226731	2.9945769510	-1.4146080598
H	2.7413738619	.3451435714	1.7444956926
H	1.4483814908	1.4765153897	2.2236025684
H	2.3244999932	1.6059415703	-1.6981376969
H	3.2749910130	.3937986358	-.8044850424
H	4.1350483840	2.2837457209	2.0469097559
H	2.8135321054	3.3937169453	1.6713871039
H	3.4508212873	3.4169980512	-.5666534619
H	4.7119291391	2.2165404744	-.2806924949
H	2.3859616914	-4.7192308526	1.0290119003
H	3.9428672401	-3.8553516995	.9402477043
H	3.1853514922	-4.4781078928	-.5486086823

15) L^1CuO_2 end-on singlet _ L^1CuO_2 side-on singlet transition state

Cu	-1.0101241724	-.5478095149	.1887209534
O	-.9045348756	-2.9824519006	.5563341077
O	-.4128340112	-1.9639623879	1.2023700419
N	.5550664308	.2692470984	-.6689859108
N	-2.3728440878	.6110186823	-.4561218110
C	1.6531046729	2.0948615822	-1.8875991865
C	.4138433125	1.4244757435	-1.3211781064
C	-.8114400416	2.0834944992	-1.5489352583
C	-2.1117348155	1.6968274253	-1.1776445986
C	-3.2628821077	2.5702485156	-1.6313618390
C	1.8315056938	-.3645797913	-.5329179565
C	2.6590800144	-.0661729273	.5752624642
C	3.8896441310	-.7219704300	.6808656005
C	4.2953437276	-1.6577957663	-.2669869855
C	3.4563127428	-1.9649862344	-1.3337902848

C	2.2134940765	-1.3399214025	-1.4853443162
C	2.2183762488	.8949557859	1.6737842929
C	3.2489777006	2.0042216340	1.9456657790
C	1.8934890749	.1214819860	2.9672279996
C	1.3101059278	-1.7390469062	-2.6483871518
C	.8688303941	-3.2103613141	-2.5314302932
C	1.9707035904	-1.4726755691	-4.0136439369
C	-3.6905184953	.1790089449	-.1089924139
C	-4.1907621919	.4866360066	1.1816695645
C	-5.4390674471	-.0230193745	1.5500806343
C	-6.1763070149	-.8232199184	.6813953399
C	-5.6637760417	-1.1364550403	-.5745435864
C	-4.4190674122	-.6556606366	-.9935438517
C	-3.3943754031	1.3395880005	2.1632659743
C	-2.8752295570	.4851344343	3.3365019899
C	-4.1943041751	2.5484182164	2.6747258828
C	-3.8520329703	-1.0952819665	-2.3396875017
C	-4.8089726111	-.8077563109	-3.5090726003
C	-3.4637325363	-2.5866156817	-2.3024103542
H	1.3884646869	2.9862748137	-2.4574056481
H	2.2050695119	1.4104898060	-2.5374206696
H	2.3366053691	2.3837440397	-1.0834193595
H	-.7434594894	3.0055129833	-2.1109538319
H	-2.9015318706	3.4791673588	-2.1137773408
H	-3.8986682423	2.8460067946	-.7846794382
H	-3.8982968750	2.0306342700	-2.3410172553
H	4.5375159804	-.5029475221	1.5246688902
H	5.2557438542	-2.1550500740	-.1667016048
H	3.7665046348	-2.7107581191	-2.0602269496
H	1.2953688053	1.3787947528	1.3418396016
H	2.8664450929	2.7017990160	2.6983586666
H	3.4779914480	2.5755352137	1.0402923452
H	4.1909536712	1.5960258060	2.3265823718
H	1.4890784280	.7963675712	3.7299980874
H	2.7948021408	-.3470744092	3.3777486601
H	1.1656313676	-.6726092068	2.7794878520
H	.4084442071	-1.1227081829	-2.5956345583
H	.1725464172	-3.4644895395	-3.3386578023
H	.3746470074	-3.3991558762	-1.5735779315
H	1.7258600169	-3.8888917467	-2.6067059555
H	1.2823142263	-1.7276674244	-4.8266097181
H	2.8760597625	-2.0745270175	-4.1462335101
H	2.2521300620	-.4209325923	-4.1281304696
H	-5.8379434479	.2058179708	2.5340947755
H	-7.1427593909	-1.2127128364	.9870998239
H	-6.2348976021	-1.7793709121	-1.2380350033
H	-2.5182831569	1.7231925013	1.6344406208

H	-2.2764803390	1.0956250938	4.0217217879
H	-2.2482141650	-.3397042783	2.9830750736
H	-3.7016761892	.0495706165	3.9084497278
H	-3.5698477737	3.1686884462	3.3264210223
H	-5.0681683187	2.2372170355	3.2567871353
H	-4.5500833020	3.1730652430	1.8491845509
H	-2.9346472180	-.5270781051	-2.5179480277
H	-4.3369134636	-1.0778608913	-4.4596881873
H	-5.0846169859	.2507194772	-3.5562461866
H	-5.7342241469	-1.3877234708	-3.4263213616
H	-2.9907442489	-2.8831728108	-3.2453352140
H	-4.3466982275	-3.2184467793	-2.1559267271
H	-2.7651225878	-2.7978222570	-1.4869007011

Table S10. 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^1Cu

31.58	52.48	53.94	55.09	70.29	93.30
98.85	99.80	122.27	134.76	151.39	211.64
219.21	248.16	268.45	295.42	339.24	351.39
426.22	427.26	440.41	462.35	498.21	523.96
541.67	550.54	560.41	625.84	629.81	644.06
675.89	696.11	716.98	717.34	760.80	766.57
770.96	841.98	842.29	846.48	859.27	916.33
917.82	948.30	954.69	965.33	966.24	992.26
993.12	1000.69	1005.43	1034.65	1046.39	1048.25
1050.30	1055.32	1059.15	1091.73	1092.01	1181.05
1184.52	1189.06	1189.21	1216.61	1262.50	1278.70
1292.81	1294.48	1321.12	1340.22	1340.69	1418.27
1418.56	1450.34	1480.22	1480.95	1488.01	1493.13
1494.27	1505.16	1516.38	1518.36	1552.38	1575.61
1625.29	1625.63	1634.57	1635.24	3057.13	3057.86
3115.40	3115.59	3154.22	3155.40	3177.09	3177.24
3187.64	3187.72	3197.08	3197.20	3202.89	3205.60
3205.66	3210.42	3210.49			

2) $L^1Cu(MeCN)$

22.69	30.04	37.42	45.68	54.22	56.41
56.73	71.27	90.52	106.88	113.07	119.55
128.47	130.83	144.23	172.50	191.32	214.80
218.10	266.61	267.76	297.94	310.85	357.31
381.98	391.17	427.74	427.87	445.71	467.28
498.91	523.27	541.27	551.23	553.07	625.13
628.32	649.01	662.41	691.99	719.13	719.61
753.33	760.99	770.60	840.47	843.15	845.55
845.86	913.82	914.79	952.90	954.97	961.19
964.20	964.59	987.87	988.02	1002.41	1003.01
1038.00	1047.24	1049.77	1050.78	1055.18	1055.41
1057.31	1060.35	1091.33	1091.46	1179.38	1184.88
1186.93	1186.96	1209.45	1251.41	1290.65	1291.16
1298.88	1314.46	1340.99	1341.30	1417.11	1418.40
1418.57	1467.53	1476.59	1478.87	1479.60	1479.66
1493.02	1493.37	1493.93	1505.26	1515.46	1523.44
1567.34	1602.72	1622.97	1623.09	1634.49	1634.97

2363.55 3052.44 3052.75 3058.68 3109.02 3109.32
3137.92 3139.43 3147.63 3148.37 3167.72 3168.44
3175.25 3176.48 3188.01 3188.13 3193.28 3193.80
3200.62 3201.28 3204.83

3) $L^1Cu(THF)$

(-41.97)   11.23   15.38   32.27   35.77   50.85
  51.06   53.58   65.73   70.39   85.63   108.96
 113.53   116.32   126.27   131.14   144.79   162.19
 215.23   218.56   219.41   263.99   268.30   290.28
 310.99   353.53   426.33   427.48   443.61   463.05
 498.52   520.43   537.31   547.94   552.68   625.57
 629.43   645.61   646.03   662.70   665.14   692.26
 718.96   719.36   751.30   758.77   768.53   812.08
 836.33   841.01   846.21   846.45   862.15   907.72
 912.29   913.23   925.44   950.35   951.32   956.60
 965.10   965.55   965.73   988.25   988.64   997.64
1002.76 1036.24 1046.93 1047.46 1049.84 1055.15
1059.37 1060.15 1074.15 1090.59 1091.02 1150.76
1178.39 1184.31 1187.03 1187.08 1208.83 1225.92
1230.88 1252.99 1267.59 1272.96 1288.46 1289.49
1295.16 1318.21 1318.79 1327.44 1340.53 1340.99
1372.23 1403.36 1418.60 1418.86 1466.98 1478.68
1479.49 1492.52 1493.81 1494.76 1501.80 1503.67
1514.79 1518.77 1520.02 1522.97 1537.86 1563.95
1599.64 1620.99 1621.19 1633.00 1633.85 3035.80
3040.52 3048.13 3049.54 3078.23 3087.67 3104.23
3105.68 3118.16 3136.03 3144.99 3146.08 3152.29
3160.29 3169.56 3170.25 3176.70 3177.24 3188.37
3188.52 3193.62 3193.83 3201.77 3202.17 3203.26

4) L^1CuO_2 side-on singlet

   9.06   53.22   55.96   58.36   71.31   81.92
  86.45   113.91   134.31   135.40   149.97   154.29
 184.21   197.02   215.16   217.17   252.33   275.39
 306.93   338.30   367.70   423.03   425.40   434.01
 468.94   470.55   494.31   501.06   532.27   550.63
 556.64   561.23   625.78   628.54   666.29   675.83
 695.17   716.75   717.65   760.85   769.11   778.76
 841.63   841.83   864.27   866.63   922.01   923.33
 965.10   965.23   966.69   976.46   995.52   995.96
1006.31 1007.32 1048.90 1049.94 1052.10 1054.73
1062.12 1064.48 1092.77 1093.03 1103.92 1182.14
1185.71 1190.73 1190.80 1218.00 1252.39 1297.85
1298.59 1302.60 1313.64 1339.84 1340.11 1421.94
1422.23 1456.08 1481.44 1481.95 1491.55 1492.33

1493.55 1507.21 1516.18 1521.90 1572.88 1606.80
1628.98 1629.71 1634.90 1635.59 3058.17 3058.41
3119.16 3119.35 3152.93 3153.37 3178.95 3179.05
3189.18 3189.25 3200.81 3200.93 3212.66 3213.04
3215.44 3215.68 3228.54

5) L^1CuO_2 side-on triplet

25.21 55.75 56.27 58.15 70.88 73.13
76.40 107.74 117.73 118.96 119.71 138.47
144.98 166.68 208.26 216.57 217.95 271.06
291.49 299.43 334.09 347.05 381.77 426.51
426.90 437.87 466.05 500.06 528.84 549.66
553.06 555.01 626.11 629.09 658.81 670.70
694.75 720.06 720.67 762.76 766.34 775.49
847.34 847.50 856.62 857.52 922.13 923.30
962.11 967.04 967.07 969.83 995.05 995.12
1004.96 1005.73 1045.66 1050.45 1050.79 1052.19
1059.36 1063.18 1093.33 1093.58 1182.94 1186.91
1190.09 1190.12 1215.23 1235.10 1257.69 1294.66
1295.68 1307.78 1308.63 1341.37 1341.58 1420.81
1420.90 1459.70 1480.95 1481.29 1492.08 1492.87
1493.40 1507.71 1516.82 1521.75 1573.01 1605.35
1627.51 1627.72 1635.70 1635.92 3058.69 3058.87
3118.83 3118.97 3153.57 3154.24 3175.31 3175.55
3182.16 3182.43 3192.81 3192.85 3197.94 3198.07
3205.83 3206.03 3217.50

6) L^1CuO_2 end-on singlet

25.85 30.56 51.69 54.12 55.04 63.73
70.59 91.06 99.96 115.85 131.91 139.31
147.34 200.44 206.39 215.48 232.46 248.26
267.87 298.77 322.16 366.61 419.30 425.41
431.53 459.37 467.87 497.33 525.95 542.71
544.66 552.46 627.04 628.81 656.38 667.57
693.99 716.53 717.38 761.24 765.29 774.52
842.17 842.37 850.70 855.21 918.84 919.97
958.27 968.81 969.07 969.69 997.33 997.75
1005.04 1006.00 1044.63 1049.21 1049.53 1050.66
1057.70 1062.03 1093.03 1093.37 1179.07 1185.12
1191.18 1191.33 1212.12 1252.85 1290.12 1293.12
1293.83 1306.31 1311.00 1340.23 1340.33 1419.09
1419.74 1453.11 1480.95 1481.62 1491.48 1492.41
1492.64 1502.80 1513.21 1518.73 1569.73 1606.10
1624.31 1624.57 1633.64 1633.94 3057.41 3059.65
3116.86 3119.93 3154.58 3155.12 3177.60 3179.16
3186.64 3189.37 3200.08 3200.85 3210.45 3211.10
3214.16 3214.44 3220.62

7) L^1CuO_2 end-on triplet

```
   5.14    34.38    51.57    54.76    55.14    62.18
  71.31    91.46   107.89   113.32   126.33   132.25
 139.53   168.44   180.01   211.77   218.61   232.17
 269.59   297.66   322.25   337.19   363.80   425.65
 426.26   438.31   465.13   497.83   524.94   543.84
 552.37   553.04   627.86   630.05   654.26   668.50
 693.67   718.13   719.05   762.90   764.13   774.25
 842.86   843.46   850.22   853.71   917.26   918.04
 956.48   962.02   964.69   965.57   993.81   994.42
1004.48  1005.36  1041.72  1049.33  1049.91  1051.01
1057.88  1062.05  1091.84  1092.04  1180.04  1185.04
1189.80  1190.04  1212.29  1248.57  1291.72  1293.48
1297.33  1311.21  1336.67  1339.47  1339.58  1419.87
1420.05  1456.01  1480.69  1481.20  1492.33  1492.65
1493.32  1504.58  1514.59  1519.98  1567.33  1598.14
1625.71  1625.78  1634.70  1634.82  3057.36  3058.89
3116.77  3118.66  3153.21  3153.84  3174.92  3176.51
3183.70  3186.09  3198.06  3198.60  3208.61  3209.10
3211.72  3212.19  3215.34
```

8) $L^1Cu(MeCN)O_2$ singlet

```
<-100.06>  25.87    28.86    34.87    44.31    48.52
  54.17    58.89    66.81    68.93    71.98    74.65
  87.90   119.93   124.19   134.04   156.42   188.63
 191.23   197.66   200.81   229.03   241.14   270.36
 301.48   326.06   339.32   375.14   396.99   399.95
 422.25   426.31   433.67   455.63   470.66   501.75
 524.34   537.98   546.30   560.21   623.97   626.94
 648.07   670.07   698.14   713.35   714.58   762.52
 762.59   772.87   839.27   839.44   848.72   855.45
 917.12   918.65   941.23   954.84   966.04   966.19
 967.21   992.40   993.57  1004.45  1005.24  1038.26
1045.29  1050.11  1052.28  1053.67  1055.90  1059.59
1069.62  1092.07  1093.36  1144.20  1179.77  1186.04
1190.04  1190.37  1208.34  1244.37  1284.44  1289.66
1303.19  1310.94  1340.29  1341.03  1408.26  1408.92
1414.50  1466.06  1473.07  1479.31  1479.90  1483.30
1486.76  1497.49  1499.33  1503.74  1510.72  1520.54
1569.40  1613.51  1622.42  1626.95  1633.39  1635.04
2363.54  3062.18  3063.44  3065.70  3122.63  3131.19
3145.00  3156.05  3160.04  3167.54  3176.60  3176.99
3187.29  3190.88  3200.07  3203.18  3205.12  3214.81
3216.96  3217.66  3221.92
```

9) $L^1Cu(MeCN)O_2$ triplet

<-107.51>	<-49.53>	(-8.99)	29.43	35.24	42.96
52.15	53.10	59.63	65.37	69.74	71.89
79.24	102.69	120.37	125.03	132.00	141.95
150.69	165.93	181.26	191.31	211.50	238.68
270.36	302.08	309.93	340.29	359.72	389.19
391.82	424.49	428.18	438.77	457.52	501.88
523.57	539.96	541.64	561.04	625.75	628.68
642.00	665.53	696.92	715.52	717.45	761.09
762.89	771.12	840.14	842.81	843.65	846.34
915.67	917.23	942.77	950.76	959.46	961.77
964.72	987.91	989.15	1002.69	1005.06	1032.40
1044.15	1049.59	1051.51	1052.31	1057.21	1061.57
1067.25	1090.69	1092.53	1179.22	1185.12	1188.30
1189.14	1207.64	1241.12	1271.72	1284.30	1291.77
1304.55	1310.98	1339.75	1340.78	1408.20	1412.27
1415.17	1470.64	1476.79	1478.77	1480.65	1481.36
1486.98	1498.59	1500.92	1504.46	1512.35	1520.62
1571.81	1613.08	1620.84	1628.01	1631.69	1637.44
2379.29	3059.25	3062.13	3063.14	3122.41	3130.29
3136.52	3160.92	3162.72	3166.95	3171.16	3177.55
3186.13	3186.65	3197.26	3199.36	3201.16	3211.42
3214.24	3214.48	3218.24			

10) $L^1Cu(THF)O_2$ singlet

(-35.86)	10.73	21.56	31.25	36.79	42.46
48.39	54.26	59.39	62.01	67.18	83.17
84.23	90.91	100.25	109.38	115.72	124.50
130.10	140.22	150.00	186.06	206.90	214.90
237.74	268.46	295.48	300.48	313.06	357.55
405.71	425.69	427.44	441.24	466.50	497.23
523.02	544.30	546.40	553.16	625.57	628.60
646.07	648.53	658.32	663.65	690.79	718.72
721.02	760.87	763.87	772.75	807.58	841.88
846.34	848.21	851.94	863.22	910.71	917.69
921.25	922.59	951.78	955.99	959.38	968.01
969.86	971.64	994.41	995.79	1003.02	1003.69
1040.16	1047.67	1051.30	1053.54	1054.40	1060.58
1060.93	1070.52	1092.13	1092.66	1150.27	1179.83
1187.30	1189.70	1190.41	1206.98	1225.45	1232.90
1238.03	1263.98	1267.67	1274.25	1283.37	1287.15
1292.40	1312.99	1320.77	1326.84	1341.56	1342.35
1371.62	1404.29	1416.63	1419.05	1446.83	1477.82
1478.74	1490.12	1492.80	1494.33	1501.45	1501.71
1512.99	1518.51	1519.19	1520.72	1538.47	1562.21
1587.55	1622.73	1626.84	1632.49	1633.90	3037.48
3052.43	3056.02	3063.60	3078.02	3087.57	3115.94

3117.26 3125.74 3134.65 3147.77 3149.37 3154.03
3156.15 3171.93 3176.26 3179.62 3185.71 3191.99
3195.35 3197.67 3202.05 3203.60 3209.38 3211.46

11) $L^1Cu(THF)O_2$ triplet

(-29.26) (-24.00)   23.95   26.32   32.53   38.25
  47.02   50.65   52.62   56.32   68.68   83.07
  85.57   90.09   108.89   113.21   116.26   120.26
 124.50   132.14   140.87   155.23   204.01   208.65
 211.95   269.84   279.79   286.67   299.33   309.34
 355.98   426.25   426.39   446.75   462.26   497.70
 523.79   540.51   548.20   556.67   626.64   629.56
 642.90   643.96   661.77   670.39   691.85   720.39
 720.85   759.11   763.23   770.83   809.61   839.08
 841.00   848.82   849.18   865.92   908.70   916.95
 917.61   923.15   949.95   952.53   955.41   966.63
 967.03   967.45   991.49   991.66 1002.34 1002.91
1036.74 1047.95 1051.84 1052.88 1053.62 1058.58
1062.33 1075.26 1091.64 1092.11 1152.51 1179.72
1187.17 1188.83 1188.95 1206.83 1225.02 1232.69
1240.36 1264.58 1276.27 1282.40 1285.36 1292.36
1314.00 1318.48 1327.28 1341.33 1341.65 1371.56
1379.80 1404.64 1417.16 1418.58 1452.88 1478.61
1479.36 1488.92 1493.69 1499.82 1501.86 1502.54
1514.35 1519.06 1520.00 1521.23 1538.94 1561.26
1589.08 1623.98 1624.06 1634.87 1635.46 3026.29
3032.72 3051.34 3054.60 3078.48 3088.30 3113.62
3115.99 3118.98 3135.45 3146.10 3147.69 3148.33
3150.69 3170.67 3171.44 3177.84 3178.63 3191.37
3191.58 3195.75 3196.16 3203.25 3203.81 3204.94

12) $L^1Cu(MeCN) + O_2$ _ $L^1Cu(MeCN)O_2$ transition state (triplet)

 -58.23 <-39.14>   25.26   33.63   35.95   46.63
  48.73   52.74   53.83   55.05   62.38   70.79
  74.73   88.67   99.89   120.22   126.86   137.68
 144.49   158.99   185.65   196.73   202.86   214.16
 253.45   271.93   298.95   318.58   356.34   381.78
 395.44   425.96   429.93   442.64   460.16   503.20
 523.73   538.66   541.64   562.08   624.03   627.81
 640.76   661.94   693.87   716.16   717.63   757.48
 765.49   769.82   832.09   839.85   843.02   845.07
 911.99   913.92   947.95   949.84   954.11   962.51
 964.05   984.31   988.68   997.96 1002.99 1031.89
1044.86 1047.41 1051.85 1053.60 1057.46 1058.84
1063.37 1088.92 1091.40 1177.12 1184.46 1186.46
1188.54 1206.53 1243.68 1284.13 1285.75 1295.58
1318.12 1339.36 1339.86 1411.55 1413.16 1414.91

1442.02 1465.96 1475.04 1477.02 1478.59 1479.91
1485.69 1500.38 1501.77 1502.29 1511.71 1519.26
1568.70 1604.09 1618.79 1624.18 1630.32 1635.58
2379.59 3053.13 3059.92 3062.26 3118.98 3127.88
3138.28 3153.45 3154.47 3156.11 3171.33 3171.92
3179.71 3184.53 3194.97 3197.12 3197.64 3208.63
3210.61 3212.28 3216.80

13) $L^1Cu(MeCN)O_2$ _ MeCN + L^1CuO_2 side-on transition state (singlet)

 -32.64   16.13   27.36   28.71   47.97   51.89
  52.31   53.23   60.14   70.88   80.03   102.75
 111.84   119.30   127.05   135.55   151.10   175.92
 189.80   195.96   206.08   215.95   239.29   277.30
 309.12   330.23   361.75   382.59   388.32   420.42
 425.74   427.25   434.27   449.32   467.64   500.60
 531.86   540.51   555.41   558.02   624.71   627.42
 657.47   668.83   692.50   715.57   716.82   757.95
 766.18   777.31   840.61   841.11   852.35   855.30
 919.51   920.56   942.44   961.10   966.06   966.23
 968.59   993.94   994.23 1004.65 1005.51 1045.96
1048.61 1050.98 1052.64 1055.40 1058.82 1062.82
1067.63 1090.46 1091.08 1123.07 1180.44 1186.07
1189.58 1189.73 1210.47 1240.66 1287.35 1288.93
1304.06 1305.78 1338.59 1339.06 1414.28 1416.75
1419.04 1460.33 1476.26 1478.07 1478.77 1481.36
1485.62 1495.73 1500.49 1504.36 1513.87 1523.17
1567.59 1606.75 1625.23 1625.73 1633.94 1635.03
2380.06 3057.88 3058.98 3061.49 3122.45 3128.65
3139.24 3145.70 3147.68 3162.58 3173.18 3173.90
3183.00 3183.30 3197.08 3198.19 3212.02 3214.05
3215.85 3216.40 3217.68

14) $L^1Cu(MeCN)$ _ $L^1Cu(THF)$ transition state

 -27.82   13.76   24.13   32.00   35.36   38.92
  51.07   52.58   55.48   62.36   63.66   66.01
  73.82   78.66   82.06   83.59   85.97   94.85
 104.44   109.07   122.55   134.45   137.16   153.99
 193.23   204.70   205.77   268.63   295.13   303.75
 307.87   354.17   376.70   380.07   426.61   426.76
 442.46   458.47   498.25   519.76   530.61   547.75
 550.17   626.40   629.33   638.04   643.17   660.02
 660.96   694.63   716.62   717.38   754.02   758.86
 767.51   807.46   831.27   834.87   843.64   843.91
 868.16   908.26   910.03   910.91   928.61   940.59
 945.74   947.44   951.33   962.25   962.44   964.68
 985.10   985.18 1001.09 1001.45 1028.46 1042.29
1048.41 1050.86 1051.52 1055.09 1059.38 1059.44

1062.63 1083.99 1090.20 1090.51 1152.09 1176.52
1183.61 1186.95 1187.40 1205.15 1222.02 1230.94
1245.54 1264.49 1276.25 1281.36 1284.10 1294.61
1317.52 1317.62 1324.36 1340.33 1340.68 1366.92
1402.36 1410.61 1411.79 1415.75 1470.21 1478.58
1479.27 1479.82 1480.38 1488.13 1500.14 1500.60
1500.86 1501.62 1512.33 1518.58 1520.91 1523.25
1538.14 1561.05 1606.99 1620.13 1620.44 1633.78
1634.49 2360.35 3010.44 3018.94 3049.81 3050.56
3056.70 3070.10 3080.03 3108.63 3113.41 3114.58
3126.91 3136.33 3141.25 3142.55 3145.95 3146.07
3147.67 3167.12 3167.38 3175.51 3175.87 3184.73
3188.46 3188.90 3194.02 3194.86 3201.29 3201.65

15) L^1CuO_2 end-on singlet _ L^1CuO_2 side-on singlet transition state

-176.12   28.66   52.38   54.05   55.58   58.32
  68.83   69.84   99.38   101.02   105.79   125.54
 145.98   152.97   200.37   214.13   217.98   241.93
 266.13   300.55   324.15   369.65   419.86   425.38
 431.85   463.39   496.59   509.36   527.49   542.75
 547.61   556.00   626.86   628.75   656.00   668.88
 695.91   715.24   716.54   762.37   764.24   774.40
 840.85   841.79   847.18   860.90   917.93   920.83
 959.90   967.38   967.77   970.14   996.21   999.18
1004.56 1005.91 1044.51 1049.18 1049.71 1051.09
1057.90 1061.89 1092.82 1093.90 1178.83 1185.60
1191.16 1192.12 1207.34 1210.77 1250.62 1290.01
1292.42 1298.41 1314.59 1339.67 1340.35 1418.59
1419.69 1452.07 1480.65 1481.55 1489.37 1492.02
1494.18 1501.87 1511.90 1519.29 1567.97 1605.06
1622.65 1625.38 1633.48 1633.69 3057.85 3062.84
3117.49 3124.98 3155.49 3156.42 3176.20 3178.28
3185.27 3186.68 3199.42 3201.39 3211.16 3212.07
3214.99 3215.05 3221.27

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