Phenolate Hydroxylation in a bis(μ-oxo)dicopper(III) Complex: Lessons from the Guanidine/Amine Series

Sonja Herres–Pawlis[a]*, Pratik Verma[b], Roxana Haase[a], Peng Kang[b], Christopher T. Lyons[c], Erik C. Wasinger[c], Ulrich Flörke[a], Gerald Henkel[a], T. Daniel P. Stack[b]*

[a] Department Chemie, Anorganische Chemie, Universität Paderborn, 33098 Paderborn, Germany
E–mail: shp@mail.uni–paderborn.de

[b] Department of Chemistry, Stanford University, Stanford, California 94305
E–mail: stack@stanford.edu

[c] Department of Chemistry and Biochemistry, California State University, Chico, California 95929–0210

Full Gaussian 03 reference

(1) Frisch, M. J. T., G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; *Gaussian 03, Revision C.02*; Gaussian, Inc.: Wallingford, CT, 2004.

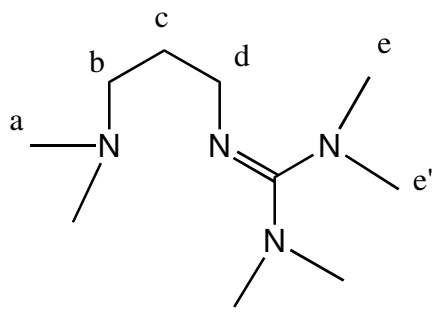
O-H bond strength estimation

The O-H bond strength for FcCOOH was estimated from **Equation S1** based on the thermodynamic cycle developed by Bordwell *et al.* with reduction potentials ($E_{1/2}$ $FcCOOH/Fc^+COOH$) = 0.225 V vs Fc^+/Fc) and acid dissociation constant (pK_a of Fc^+COOH = 4.54) measured in a $MeCN/H_2O$ mixture.[1-3]

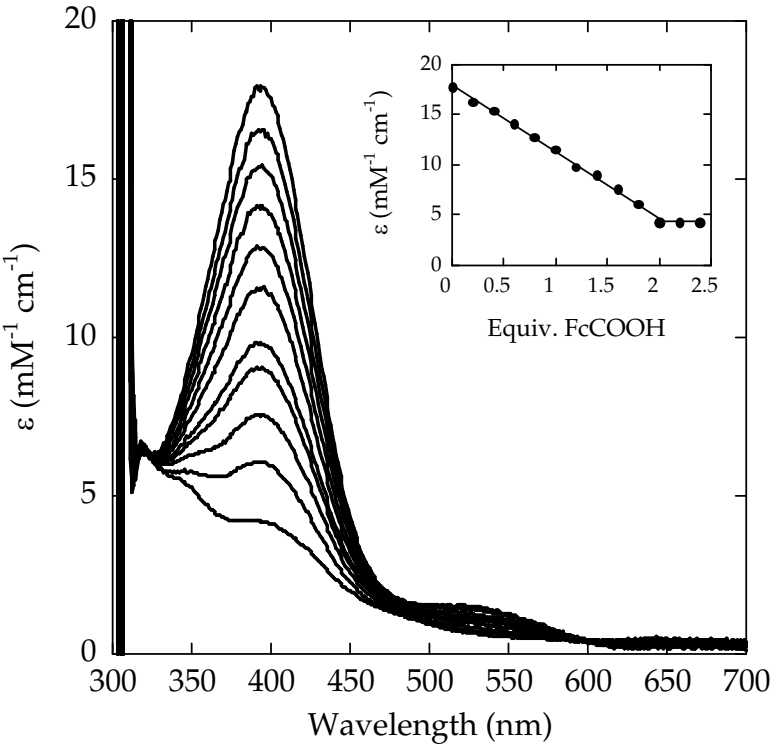
$$BDE(X\text{-}H) = 23.06\ E°(X^-) + 1.37\ pK_a(X\text{-}H) + C \qquad (\mathbf{S1})$$

where, E° is the reduction potential (in volts) versus ferrocene and the constant C is calculated to be 59.5 kcal mol^{-1} in MeCN. Using these data, the BDE for FcCOOH is estimated to be 71 kcal mol^{-1}. A value of 84.1 kcal mol^{-1} is reported for the O-H bond strength of 2,4-di-*tert*-butylphenol.[4]

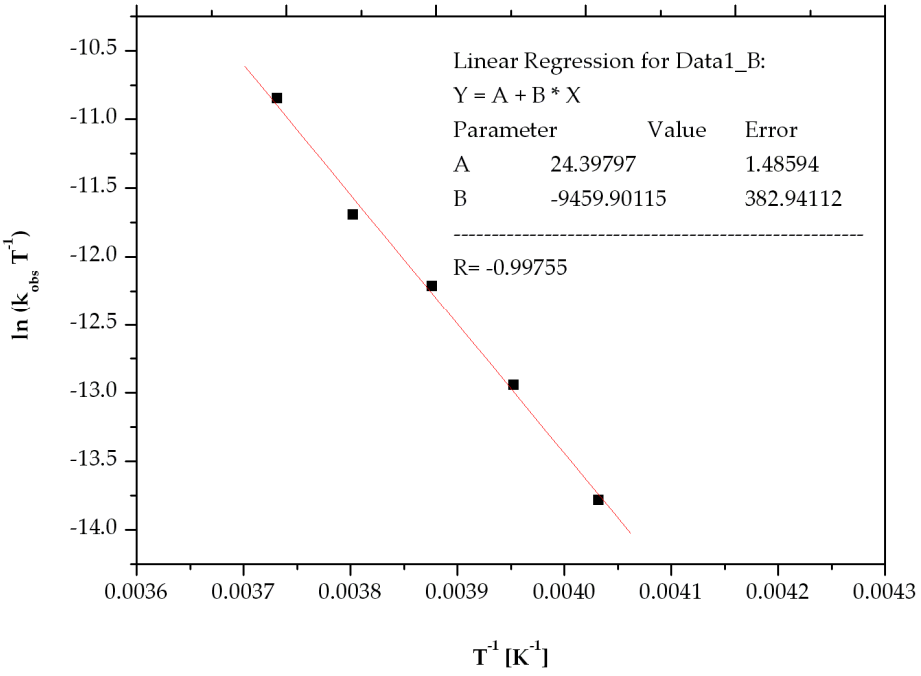
Supporting Information Figures



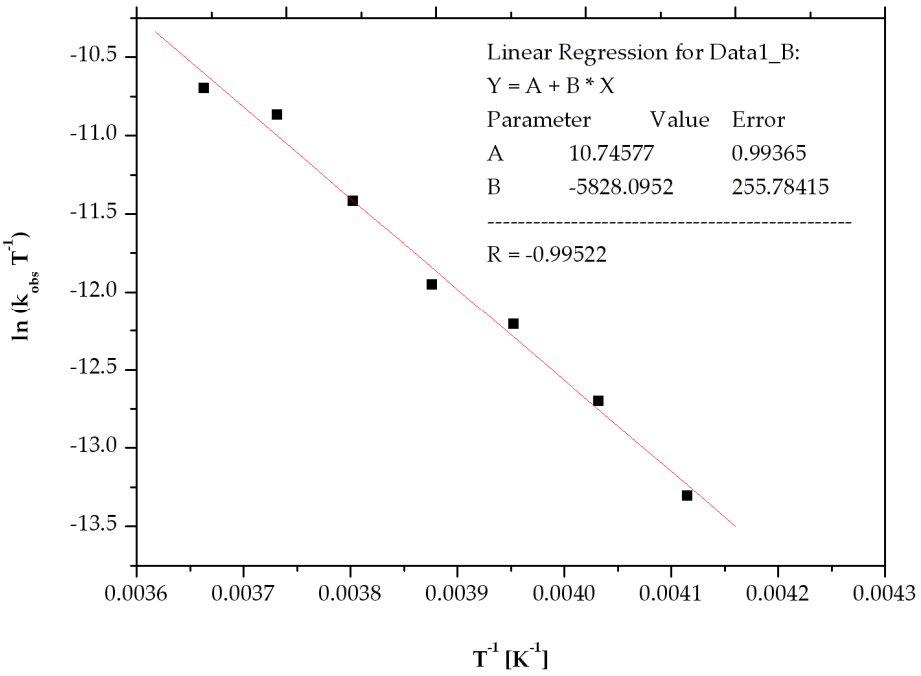
Supporting Figure 1. NMR labeling scheme for **^{2}L**.



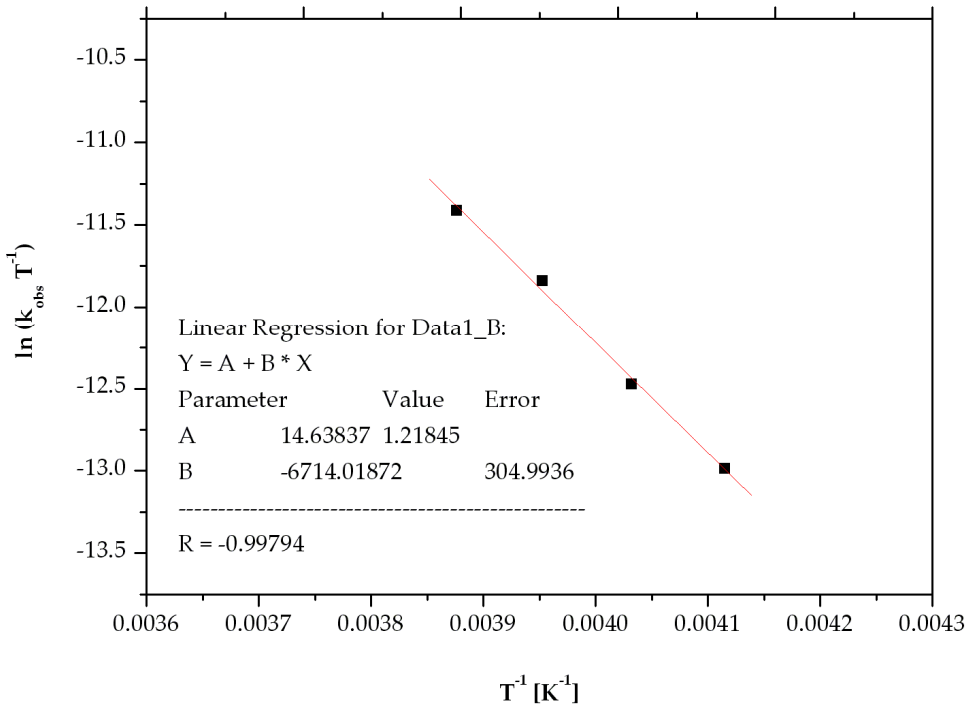
Supporting Figure 2. Titration of **1b** with FcCOOH at 197 K in acetone. The 635 nm absorption feature is from the formed ferrocenium carboxylate product [Inset: extinction coefficient of 400 nm versus the number of equiv of FcCOOH per dimer].



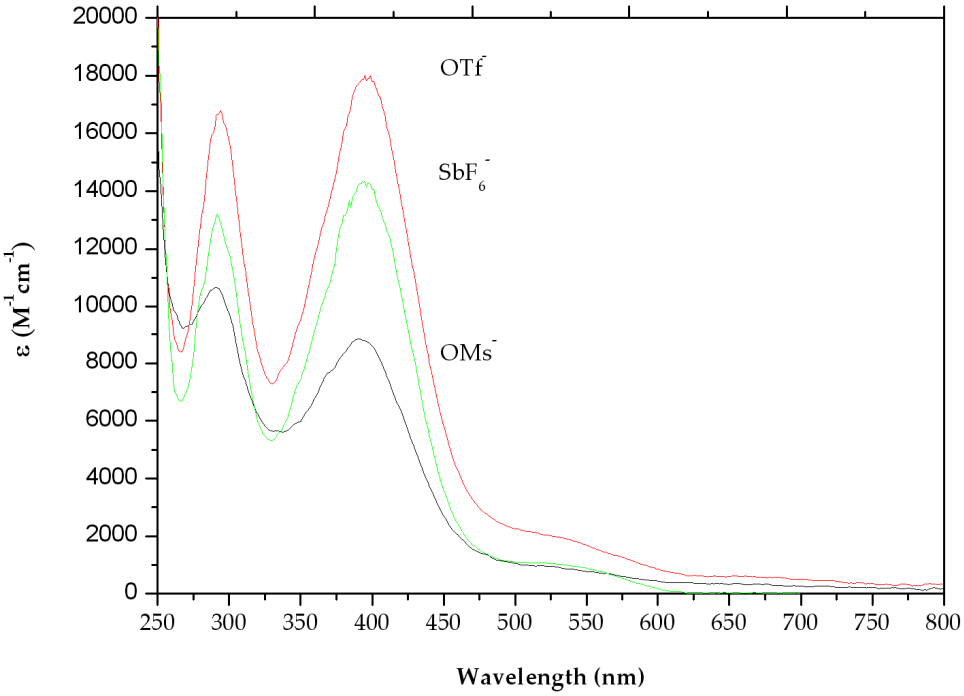
Supporting Figure 3. Eyring plot of **1b.**



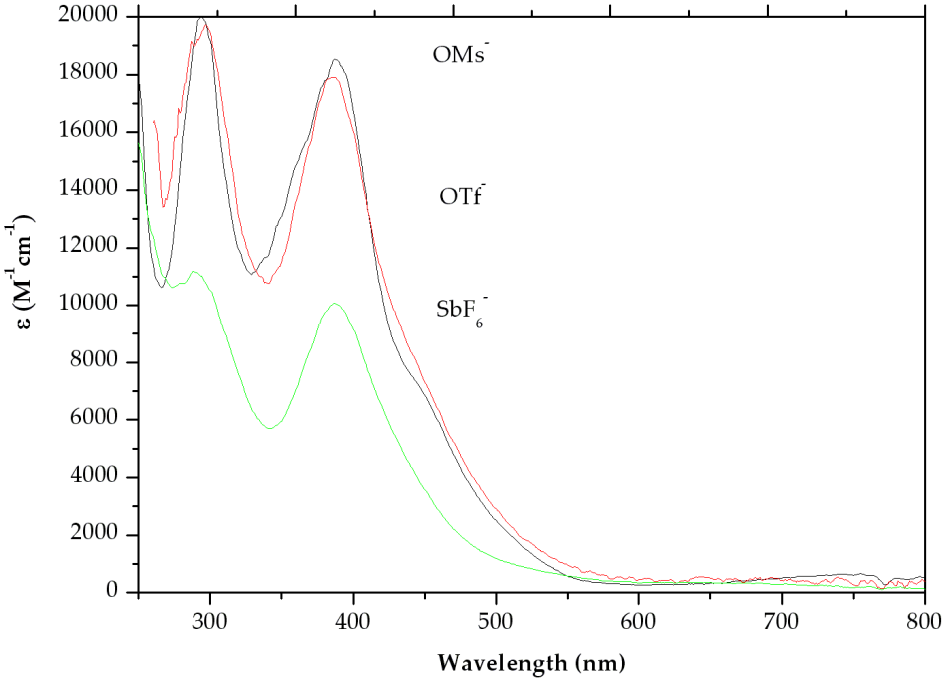
Supporting Figure 4. Eyring plot of **2b.**



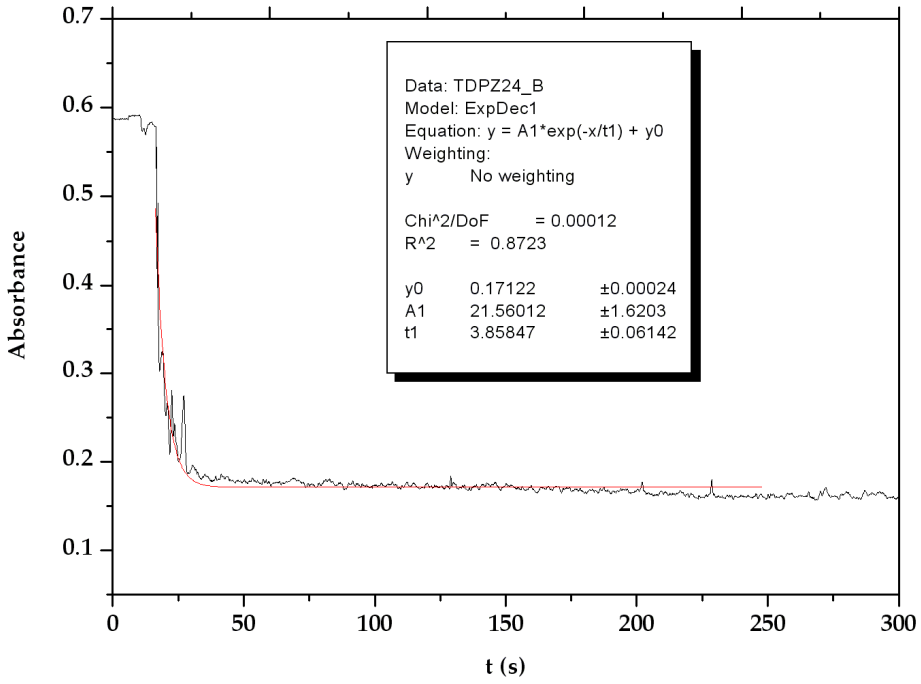
Supporting Figure 5. Eyring plot of **2b•SbF_6.**



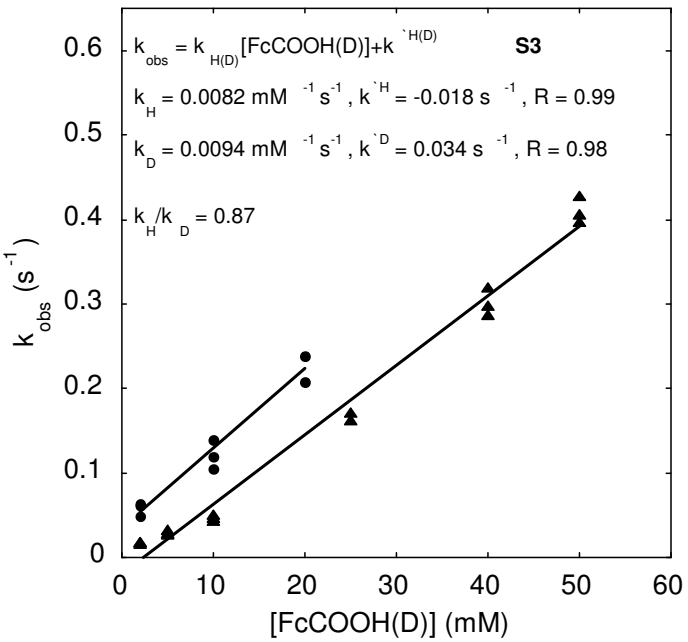
Supporting Figure 6. Solution UV-Vis spectra of **1b** with different counter ions. ([Cu] =1 mM, THF, 197 K). Extinction coefficients reported per Cu-dimer.



Supporting Figure 7. Solution UV-Vis spectra of **2b** with different counter ions. ([Cu] =1 mM, THF, 197 K). Extinction coefficients reported per Cu-dimer.



Supporting Figure 8. Pseudo first order fit of the rate of reaction of **2b** with 2,4-di-*tert*-butylphenolate sodium (195 K, THF, [Cu] = 1.0 mM, [substrate]= 50 mM).



Supporting Figure 9. Linear behavior of k_{obs} for the reaction of **2b** with FcCOOH and FcCOOD concentrations (195 K, THF, [Cu] = 1.0 mM).

Supporting Information Tables

Supporting Table 1. Crystallographic data.

	$[(^2\mathbf{L})Cu^{I}(I)]$	$[(^2\mathbf{L})_2Cu^{II}_2(\mu\text{-}OH)_2]\cdot Cu^{I}I_3$
formula	$C_{10}H_{24}CuIN_4$	$C_{20}H_{50}Cu_3I_3N_8O_2$
fw (g mol^{-1})	390.77	1006.00
space group	P2(1)/c	C2/c
a (Å)	17.775(2)	19.4392(12)
b (Å)	10.7571(12)	11.2206(7)
c (Å)	18.0887(19)	15.2880(9)
α (°)	90	90
β (°)	118.258(2)	93.181(1)
γ (°)	90	90
V (Å^3)	3046.6(6)	3329.5(4)
Z	8	4
μ_{calc} (mm^{-1})	3.445	4.711
F_{000}	1552	1952
δ_{calc} (g cm^{-3})	1.704	2.007
size (mm^3)	0.33 x 0.28 x 0.20	0.41 x 0.37 x 0.20
T (K)	120(2)	120(2)
λ(Mo K_α) (Å)	0.71073	0.71073
θ range(°)	1.30 – 27.88	2.10 – 28.08
Index ranges hkl	–21/23, ±14, ±23	–25/24, ±14, ±20
total no. of data	25371	16306
no. of unique data	7253	4045
no. of param	297	168
R_{int}	0.0309	0.0501
completeness to θ (%)	99.9	99.8
R1 [wR2]	0.0283 [0.0612]	0.0381 [0.0941]
GOF, S	1.036	1.040
ρ_{max} [ρ_{min}] (e Å^{-3})	0.838 [–0.390]	1.392 [–0.868]

Supporting Table 2. Fits to the EXAFS data of **1b**.

Fit #	CN	R(Å)	σ^2 (Å^2)	ΔE_0 (eV)	Error (F)†
1	2 Cu-O (SS)	1.87	0.00160	-5.9	4.00
2	2 Cu-N (SS)	1.89	0.00086	-4.9	4.15
3	2 Cu-O (SS)	1.79	0.00245	-11.6	3.47
	2 Cu-N (SS)	1.81	-0.00030		
4	2 Cu-O (SS)	1.80	0.00227	-11.1	0.86
	2 Cu-N (SS)	1.91	0.00033		
	1 Cu-Cu (SS)	2.82	0.00060		
5	4 Cu-N/O	1.87	0.00413	-9.0	0.92

	1 Cu-Cu	2.83	0.00058		
6	2 C-O (SS)	1.80	0.00151	-10.5	0.80
	2 Cu-N (SS)	1.92	0.00000		
	1 Cu-Cu (SS)	2.83	0.00008		
	4 Cu-N-C (MS)	3.14	-0.0034		

$^{\dagger}F = [\Sigma k^6(\chi_{expt} - \chi_{calc})^2/\Sigma k^6\chi_{expt}^2]^{1/2}$

Pre-edge fit results

Amplitude (Abs)	Energy (eV)	Half-width (eV)	Area[a]
0.015 (0.002)[b]	8980.8 (0.2)[b]	1.4 (0.2)[b]	4.3 (1.0)[b]

[a] Pre-edge area is defined as FWHM*Amplitude*100

[b] Values in parenthesis are standard deviations calculated from all fits to the complex

Supporting Table 3. Fits to the EXAFS data of **2b**.

Fit	Coordination	R (Å)	σ^2 (Å^2)	ΔE_0	Error (F)†
1	4 O	1.82	0.00602	-15.8	2.66
2	2 O	1.82	0.00022	-8.8	2.41
	2 N	1.97	0.00105		
3	2 O	1.80	0.00023	-12.4	0.60
	2 N	1.94	0.00070		
	1 Cu	2.79	0.00185		
4	2 O	1.81	0.00014	-9.7	0.58
	2 N	1.96	0.00057		
	1 Cu	2.79	0.00222		
	5 C (SS)	2.87	0.00869		
5	2 O	1.81	0.00010	-9.7	0.48
	2 N	1.96	0.00042		
	1 Cu	2.80	0.00209		
	5 C (SS)	2.88	0.00758		
	5 C (MS)	3.14	0.00085		

$^{\dagger}F = [\Sigma k^6(\chi_{expt} - \chi_{calc})^2/\Sigma k^6\chi_{expt}^2]^{1/2}$

Energies and areas of the pre-edge features

Peak	Energy	Area
1	8980.5	2.9
2	8983.0	16.2

Supporting Table 4. Gaussian fit parameters to experimental (THF, 193 K, $CF_3SO_3^-$ counter anion, 1 mM Cu) electronic absorption spectrum of **O** complexes (**1b**-**3b**).

	Transition energy (cm^{-1})	Extinction coefficient (M^{-1} cm^{-1})	FWHM	Oscillator strength (f)
1b	40841.4	18800.4	5288.5	0.43

	33323.6	19149.0	5126.8	0.43
	25258.3	27152.5	2846.5	0.34
2b	41000.0[a]	17906.7	5062.8	0.39
	33700.5	15981.6	5895.8	0.41
	25818.8	16608.4	5086.3	0.37
	20938.8	2169.5	4710.0	0.04
3b	41000.0[a]	28000.0	3532.5	0.43
	34077.7	15481.4	5583.9	0.43
	25595.4	16778.5	5490.2	0.40
	18180.0	1326.2	5570.7	0.03

[a]Transition energy fixed in the Gaussian deconvolution.

Supporting Table 5. Free energy (kcal mol^{-1}) for **O** $\rightleftharpoons$ ^{S}**P** equilibrium computed in THF at 193K with B3LYP functional.

Ligand	ΔE_{SCF}[a]	$\Delta\Delta G_{thermal\ correction}$	$\Delta\Delta G_{solvation}$[c]	ΔG[d]
bis-guanidine	-7.55	-3.22	3.16	-7.61
hybrid	-5.26	-3.04	2.17	-6.13
amine	-6.04	-4.12	3.07	-7.09

[a]Electronic energy difference computed with B3LYP/***3z*** in vacuum. [b] Difference in thermal corrections to free energy from frequency calculations computed with B3LYP/***2z***. [c]Difference in free energy of solvation in THF computed with IEF-PCM model with B3LYP/***3z***. [d]$\Delta G = \Delta E_{SCF} + \Delta\Delta G_{thermal\ corrections} + \Delta\Delta G_{solvation}$.

This table shows that B3LYP functional overstabilizes the ^{S}**P** over the **O** to such an extent that it is predicted to be the dominant isomer by > 6 kcal mol^{-1} for each of the three complexes identified as **O** species in this study.

Supporting Table 6. Mulliken atomic charges on selected atoms in **O** complexes computed at B3LYP/***3z***,IEF-PCM/THF level of theory.

Ligand	Cu	O	$N_{guanidine}$	N_{amine}
bis-guanidine	-0.808	+0.147	-0.336	-
hybrid	-0.303	-0.058	-0.518	-0.509
amine	-0.127	-0.244	-	-0.553

Supporting Table 7. Electronic energies computed at BLYP/***3z***, thermal corrections to free energies computed at B3LYP/***2z*** and free energy of solvation computed at BLYP/***3z***,IEF-PCM/THF level of theory.

	E_{SCF}	G_{corr}	$\Delta G_{solvation}$
1b: P	-5114.36044	0.86246	-0.06048
1b: O	-5114.37144	0.86757	-0.06744
$[(^{1}\mathbf{L})_2Cu^{II}Cu^{III}O_2]^{1+}$	-5114.62766	0.86509	0.04849
$[(^{1}\mathbf{L})_2Cu^{II}Cu^{III}O_2H]^{2}$	-5114.98790	0.87450	-0.06583

	E_{SCF}	G_{corr}	$\Delta G_{solvation}$
2b: P	-4659.62006	0.67744	-0.10515
2b: O	-4659.63274	0.68228	-0.10894
$[(^{2}\mathbf{L})_2Cu^{II}Cu^{III}O_2]^{1+}$	-4659.90586	0.67797	0.02084
$[(^{2}\mathbf{L})_2Cu^{II}Cu^{III}O_2H]^{2}$	-4660.24432	0.69005	-0.10468

	E_{SCF}	G_{corr}	$\Delta G_{solvation}$
3b: P	-4204.86111	0.49252	-0.15155
3b: O	-4204.87158	0.49912	-0.15651
$[(^{3}\mathbf{L})_2Cu^{II}Cu^{III}O_2]^{1+}$	-4205.18008	0.49559	-0.01363
$[(^{3}\mathbf{L})_2Cu^{II}Cu^{III}O_2H]^{2}$	-4205.48908	0.50523	-0.15405

All energies are in units of hartrees. All broken symmetry solutions computed at BLYP/***3z*** level of theory for **P** structures collapsed to the restricted values and the energies were used without projection.

Supporting Table 8. Cartesian coordinates of DFT computed structure (B3LYP/***2z***, gas phase).

O: 1b	**O: 2b**	**O: 3b**
Cu -0.0012 0.0141 0.0362	Cu 0.1025 0.0338 0.0270	Cu 0.0309 1.4056 0.0000
Cu 0.0012 -0.0141 2.8083	O -0.2073 -0.1716 1.7774	Cu -0.0309 -1.4056 0.0000
O 1.1407 0.0078 1.4214	N 0.5128 -0.0293 -1.8391	O 0.0000 0.0000 1.1153
O -1.1407 -0.0078 1.4231	N 2.8032 -0.5242 -1.8135	O 0.0000 0.0000 -1.1153
N 1.4416 -0.0566 -1.2580	N 1.4362 -1.5856 -3.3666	N 0.2024 2.6678 -1.5314
N 2.8038 1.7013 -0.5080	N -0.7896 1.8270 -0.0285	N 0.2024 2.6678 1.5314
N 3.8020 -0.1726 -1.4403	C 1.5600 -0.7174 -2.3210	N -0.2024 -2.6678 1.5314
N -1.4436 -0.0808 -1.2570	C 3.1546 0.6735 -1.0616	N -0.2024 -2.6678 -1.5314
N -2.8355 1.6538 -0.5069	H 2.5757 1.5220 -1.4234	C 0.0000 4.1313 1.2637
N -3.8016 -0.2354 -1.4421	H 4.2161 0.8873 -1.2159	C -0.7654 2.2718 -2.6014
N -1.4416 0.0566 4.1025	H 2.9813 0.5392 0.0143	C -0.7654 2.2718 2.6014
N -2.8038 -1.7013 3.3526	C 3.8113 -1.5853 -1.7811	C 0.7654 -2.2718 2.6014
N -3.8020 0.1726 4.2848	H 3.3680 -2.5360 -2.0739	C 0.0000 -4.1313 -1.2637
N 1.4436 0.0808 4.1015	H 4.1964 -1.6767 -0.7599	C -1.5938 -2.4189 2.0221
N 2.8355 -1.6538 3.3514	H 4.6526 -1.3590 -2.4453	C 0.0000 4.1313 -1.2637
N 3.8016 0.2354 4.2866	C 2.4176 -1.6633 -4.4546	C 1.5938 2.4189 2.0221
C 1.2769 -0.9604 -2.4084	H 3.1255 -0.8375 -4.3799	C -1.5938 -2.4189 -2.0221
C 0.0038 -0.6629 -3.1906	H 1.8905 -1.5835 -5.4116	C 0.0000 -4.1313 1.2637
C -1.2637 -0.9816 -2.4075	H 2.9654 -2.6125 -4.4435	C 0.7654 -2.2718 -2.6014
C 2.6524 0.4655 -1.0532	C 0.2836 -2.4785 -3.4950	C 1.5938 2.4189 -2.0221

C 3.9240 2.0382 0.3662
C 1.7440 2.6954 -0.5464
C 4.9238 0.5359 -2.0638
C 3.9632 -1.6206 -1.3448
C -2.6631 0.4212 -1.0530
C -1.7920 2.6652 -0.5423
C -3.9635 1.9723 0.3641
C -3.9398 -1.6856 -1.3468
C -4.9336 0.4551 -2.0675
C -1.2769 0.9604 5.2529
C -0.0038 0.6629 6.0351
C 1.2637 0.9816 5.2521
C -2.6524 -0.4655 3.8977
C -3.9240 -2.0382 2.4784
C -1.7440 -2.6954 3.3909
C -4.9238 -0.5359 4.9083
C -3.9632 1.6206 4.1893
C 2.6631 -0.4212 3.8975
C 1.7920 -2.6652 3.3868
C 3.9635 -1.9723 2.4804
C 3.9398 1.6856 4.1913
C 4.9336 -0.4551 4.9120
H 4.6664 -1.4883 5.1339
H 1.2569 -2.0118 -2.0852
H 2.1344 -0.8481 -3.0780
H -0.0051 0.3846 -3.5148
H 0.0085 -1.2845 -4.0946
H -2.1231 -0.8840 -3.0769
H -1.2259 -2.0325 -2.0842
H 4.5289 1.1531 0.5598
H 3.5300 2.4077 1.3186
H 4.5564 2.8177 -0.0742
H 1.0999 2.5097 -1.4054
H 2.1937 3.6882 -0.6527
H 1.1484 2.6785 0.3745
H 4.6408 1.5651 -2.2847
H 5.1827 0.0370 -3.0047
H 5.8127 0.5366 -1.4216
H 3.1591 -2.0446 -0.7440
H 4.9204 -1.8409 -0.8576
H 3.9675 -2.1016 -2.3304
H -1.1986 2.6574 0.3801
H -2.2576 3.6506 -0.6493
H -1.1428 2.4904 -1.3998
H -4.5541 1.0773 0.5564
H -4.6077 2.7410 -0.0782
H -0.2722 -2.5040 -2.5571
H 0.6462 -3.4896 -3.7112
H -0.3843 -2.1761 -4.3102
C -0.6049 0.2740 -2.7476
H -1.4455 -0.4186 -2.5913
H -0.2745 0.1436 -3.7820
C -1.0968 1.7079 -2.5691
H -1.8823 1.8970 -3.3106
H -0.2903 2.4145 -2.7923
C -1.7140 1.9764 -1.2032
H -2.1265 2.9934 -1.1696
H -2.5462 1.2833 -1.0346
C 0.2888 2.8546 -0.0641
H -0.1500 3.8594 -0.0495
H 0.8880 2.7431 -0.9651
H 0.9259 2.7332 0.8149
C -1.5978 2.0585 1.2014
H -0.9655 1.9393 2.0793
H -2.4072 1.3301 1.2473
H -2.0183 3.0707 1.1722
Cu 0.5455 -1.7661 2.0752
O 0.8553 -1.5606 0.3248
N 0.1352 -1.7029 3.9413
N -2.1552 -1.2081 3.9157
N -0.7882 -0.1466 5.4688
N 1.4375 -3.5593 2.1307
C -0.9120 -1.0148 4.4232
C -2.5066 -2.4057 3.1638
H -1.9278 -3.2542 3.5256
H -3.5681 -2.6196 3.3181
H -2.3333 -2.2714 2.0878
C -3.1633 -0.1470 3.8833
H -2.7200 0.8037 4.1761
H -3.5485 -0.0555 2.8621
H -4.0046 -0.3733 4.5475
C -1.7697 -0.0690 6.5567
H -2.4775 -0.8947 6.4820
H -1.2425 -0.1488 7.5138
H -2.3175 0.8803 6.5456
C 0.3644 0.7462 5.5972
H 0.9201 0.7717 4.6593
H 0.0018 1.7573 5.8134
H 1.0323 0.4439 6.4124
C 1.2529 -2.0062 4.8498
H 2.0934 -1.3136 4.6935
H 0.9225 -1.8758 5.8842
C 0.6652 4.6575 0.0000
C -0.6652 -4.6575 0.0000
H -1.0797 4.3013 1.2021
H 0.3645 4.6748 2.1441
H 0.6043 -2.8968 3.4867
H 0.6161 -1.2246 2.8545
H -0.3645 -4.6748 -2.1441
H -0.3645 -4.6748 2.1441
H 0.6043 -2.8968 -3.4867
H 1.7870 -2.4173 -2.2423
H 0.6161 -1.2246 -2.8545
H 0.3645 4.6748 -2.1441
H -1.0797 4.3013 -1.2021
H 1.7141 1.3533 2.2147
H 2.3219 2.7340 1.2720
H 1.7717 2.9841 2.9438
H -2.3219 -2.7340 -1.2720
H -1.7717 -2.9841 -2.9438
H -1.7141 -1.3533 -2.2147
H -1.7141 -1.3533 2.2147
H -2.3219 -2.7340 1.2720
H -1.7717 -2.9841 2.9438
H -1.7870 2.4173 2.2423
H -0.6043 2.8968 3.4867
H -0.6161 1.2246 2.8545
H -0.6161 1.2246 -2.8545
H -0.6043 2.8968 -3.4867
H -1.7870 2.4173 -2.2423
H 1.7717 2.9841 -2.9438
H 1.7141 1.3533 -2.2147
H 1.7870 -2.4173 2.2423
H 2.3219 2.7340 -1.2720
H 0.5416 5.7466 0.0000
H 1.7476 4.4900 0.0000
H 1.0797 -4.3013 -1.2021
H 1.0797 -4.3013 1.2021
H -1.7476 -4.4900 0.0000
H -0.5416 -5.7466 0.0000

H -3.5783 2.3487 1.3174
H -3.1285 -2.0970 -0.7470
H -3.9373 -2.1663 -2.3327
H -4.8930 -1.9215 -0.8589
H -5.8231 0.4427 -1.4264
H -5.1836 -0.0487 -3.0082
H -4.6664 1.4883 -2.2893
H -1.2569 2.0118 4.9297
H -2.1344 0.8481 5.9225
H 0.0051 -0.3846 6.3593
H -0.0085 1.2845 6.9391
H 2.1231 0.8840 5.9214
H 1.2259 2.0325 4.9287
H -4.5289 -1.1531 2.2847
H -3.5300 -2.4077 1.5260
H -4.5564 -2.8177 2.9187
H -1.0999 -2.5097 4.2499
H -2.1937 -3.6882 3.4972
H -1.1484 -2.6785 2.4700
H -4.6408 -1.5651 5.1292
H -5.1827 -0.0370 5.8492
H -5.8127 -0.5366 4.2661
H -3.1591 2.0446 3.5885
H -4.9204 1.8409 3.7021
H -3.9675 2.1016 5.1750
H 1.1986 -2.6574 2.4645
H 2.2576 -3.6506 3.4938
H 1.1428 -2.4904 4.2443
H 4.5541 -1.0773 2.2881
H 4.6077 -2.7410 2.9228
H 3.5783 -2.3487 1.5271
H 3.1285 2.0970 3.5915
H 3.9373 2.1663 5.1772
H 4.8930 1.9215 3.7035
H 5.8231 -0.4427 4.2709
H 5.1836 0.0487 5.8527
C 1.7448 -3.4402 4.6713
H 2.5303 -3.6293 5.4128
H 0.9382 -4.1467 4.8945
C 2.3620 -3.7086 3.3053
H 2.7745 -4.7257 3.2718
H 3.1941 -3.0155 3.1367
C 0.3591 -4.5869 2.1662
H 0.7980 -5.5917 2.1517
H -0.2400 -4.4753 3.0673
H -0.2780 -4.4655 1.2873
C 2.2458 -3.7908 0.9008
H 1.6135 -3.6715 0.0228
H 3.0551 -3.0623 0.8548
H 2.6662 -4.8029 0.9300

P: 1b

Cu -0.1144 0.0325 1.7719
Cu 0.1144 -0.0325 -1.7719
O -0.0045 0.7539 -0.0142
O 0.0045 -0.7539 0.0142
N -0.3353 1.5604 2.9435
N 1.3363 2.9384 2.0640
N -0.5166 3.9222 3.0781
N -0.3332 -1.4482 3.0028

P: 2b

Cu -0.4749 0.2627 -1.6813
O -0.7231 0.1044 0.1963
N 0.4618 0.1226 -3.3470
N 2.4067 1.2849 -2.7753
N 2.5333 -0.4187 -4.3633
N -2.3130 0.7666 -2.2888
C 1.7761 0.3120 -3.4923
C 1.6836 2.4308 -2.2348

P: 3b

Cu 0.0283 1.7530 0.0000
Cu -0.0283 -1.7530 0.0000
O 0.0000 0.0000 0.7596
O 0.0000 0.0000 -0.7596
N 0.2087 2.9426 -1.5703
N 0.2087 2.9426 1.5703
N -0.2087 -2.9426 1.5703
N -0.2087 -2.9426 -1.5703

N 1.3395 -2.8650 2.1882
N -0.5176 -3.8016 3.2383
N 0.3353 -1.5604 -2.9435
N -1.3363 -2.9384 -2.0640
N 0.5166 -3.9222 -3.0781
N 0.3332 1.4482 -3.0028
N -1.3395 2.8650 -2.1882
N 0.5176 3.8016 -3.2383
C -1.1837 1.3702 4.1330
C -0.8256 0.0949 4.8996
C -1.1842 -1.2085 4.1818
C 0.1341 2.7780 2.6944
C 1.5827 4.0150 1.1080
C 2.3524 1.8954 2.0840
C 0.1868 5.0936 3.6075
C -1.9732 4.0341 3.0375
C 0.1359 -2.6758 2.8075
C 2.3578 -1.8240 2.1660
C 1.5895 -3.9851 1.2848
C -1.9741 -3.9139 3.1961
C 0.1824 -4.9497 3.8205
C 1.1837 -1.3702 -4.1330
C 0.8256 -0.0949 -4.8996
C 1.1842 1.2085 -4.1818
C -0.1341 -2.7780 -2.6944
C -1.5827 -4.0150 -1.1080
C -2.3524 -1.8954 -2.0840
C -0.1868 -5.0936 -3.6075
C 1.9732 -4.0341 -3.0375
C -0.1359 2.6758 -2.8075
C -2.3578 1.8240 -2.1660
C -1.5895 3.9851 -1.2848
C 1.9741 3.9139 -3.1961
C -0.1824 4.9497 -3.8205
H -1.2355 4.7098 -3.9685
H -2.2469 1.3262 3.8546
H -1.0658 2.2264 4.8054
H 0.2408 0.0995 5.1568
H -1.3830 0.1127 5.8446
H -1.0701 -2.0375 4.8880
H -2.2465 -1.1735 3.8988
H 0.6991 4.6454 1.0174
H 1.8070 3.5823 0.1244
H 2.4327 4.6342 1.4171
H 2.2599 1.3087 2.9990
H 3.3409 2.3663 2.0736
H 0.8159 2.6499 -2.8584
H 2.3433 3.3040 -2.2471
H 1.3633 2.2546 -1.1995
C 3.7960 1.1621 -2.3310
H 4.1668 0.1572 -2.5306
H 3.8435 1.3448 -1.2517
H 4.4455 1.8901 -2.8296
C 3.6045 0.1701 -5.1745
H 3.5811 1.2571 -5.0958
H 3.4451 -0.1037 -6.2234
H 4.5931 -0.1946 -4.8722
C 2.3060 -1.8497 -4.5730
H 1.6389 -2.2385 -3.8027
H 3.2655 -2.3739 -4.4989
H 1.8788 -2.0597 -5.5605
C -0.3057 -0.3725 -4.5038
H -0.5539 -1.4370 -4.3845
H 0.3020 -0.2881 -5.4097
C -1.6009 0.4176 -4.7191
H -2.0477 0.0753 -5.6604
H -1.3723 1.4800 -4.8621
C -2.6596 0.2128 -3.6375
H -3.6145 0.6569 -3.9519
H -2.8320 -0.8614 -3.5036
C -2.3510 2.2544 -2.3011
H -3.3509 2.6130 -2.5767
H -1.6276 2.6453 -3.0174
H -2.1027 2.6286 -1.3045
C -3.3172 0.2773 -1.3080
H -3.0920 0.6896 -0.3235
H -3.2776 -0.8134 -1.2575
H -4.3269 0.5842 -1.6093
Cu 0.4749 -0.2627 1.6813
O 0.7231 -0.1044 -0.1963
N -0.4618 -0.1226 3.3470
N -2.4067 -1.2849 2.7753
N -2.5333 0.4187 4.3633
N 2.3130 -0.7666 2.2888
C -1.7761 -0.3120 3.4923
C -1.6836 -2.4308 2.2348
H -0.8159 -2.6499 2.8584
H -2.3433 -3.3040 2.2471
H -1.3633 -2.2546 1.1995
C -3.7960 -1.1621 2.3310
H -4.1668 -0.1572 2.5306
H -3.8435 -1.3448 1.2517
C -0.0050 4.3998 1.2848
C -0.7517 2.5149 -2.6291
C -0.7517 2.5149 2.6291
C 0.7517 -2.5149 2.6291
C 0.0050 -4.3998 -1.2848
C -1.5980 -2.6982 2.0573
C -0.0050 4.3998 -1.2848
C 1.5980 2.6982 2.0573
C -1.5980 -2.6982 -2.0573
C 0.0050 -4.3998 1.2848
C 0.7517 -2.5149 -2.6291
C 1.5980 2.6982 -2.0573
C 0.6496 4.9091 0.0000
C -0.6496 -4.9091 0.0000
H -1.0869 4.5597 1.2251
H 0.3598 4.9721 2.1478
H 0.6129 -3.1168 3.5353
H 0.5843 -1.4636 2.8687
H -0.3598 -4.9721 -2.1478
H -0.3598 -4.9721 2.1478
H 0.6129 -3.1168 -3.5353
H 1.7770 -2.6434 -2.2733
H 0.5843 -1.4636 -2.8687
H 0.3598 4.9721 -2.1478
H -1.0869 4.5597 -1.2251
H 1.7336 1.6283 2.2294
H 2.3251 3.0307 1.3138
H 1.7795 3.2413 2.9925
H -2.3251 -3.0307 -1.3138
H -1.7795 -3.2413 -2.9925
H -1.7336 -1.6283 -2.2294
H -1.7336 -1.6283 2.2294
H -2.3251 -3.0307 1.3138
H -1.7795 -3.2413 2.9925
H -1.7770 2.6434 2.2733
H -0.6129 3.1168 3.5353
H -0.5843 1.4636 2.8687
H -0.5843 1.4636 -2.8687
H -0.6129 3.1168 -3.5353
H -1.7770 2.6434 -2.2733
H 1.7795 3.2413 -2.9925
H 1.7336 1.6283 -2.2294
H 1.7770 -2.6434 2.2733
H 2.3251 3.0307 -1.3138
H 0.5366 5.9996 0.0000
H 1.7318 4.7370 0.0000

H 2.2731 1.2379 1.2090
H 1.2405 4.8595 3.7597
H -0.2512 5.3690 4.5738
H 0.1024 5.9572 2.9364
H -2.3937 3.2124 2.4561
H -2.2439 4.9798 2.5530
H -2.4195 4.0275 4.0392
H 2.2856 -1.2082 1.2606
H 3.3453 -2.2968 2.1841
H 2.2608 -1.1948 3.0517
H 0.7050 -4.6171 1.2170
H 2.4357 -4.5916 1.6279
H 1.8222 -3.5987 0.2841
H -2.3911 -3.1168 2.5791
H -2.4247 -3.8651 4.1946
H -2.2437 -4.8788 2.7503
H 0.1013 -5.8410 3.1862
H -0.2608 -5.1838 4.7953
H 1.2355 -4.7098 3.9685
H 2.2469 -1.3262 -3.8546
H 1.0658 -2.2264 -4.8054
H -0.2408 -0.0995 -5.1568
H 1.3830 -0.1127 -5.8446
H 1.0701 2.0375 -4.8880
H 2.2465 1.1735 -3.8988
H -0.6991 -4.6454 -1.0174
H -1.8070 -3.5823 -0.1244
H -2.4327 -4.6342 -1.4171
H -2.2599 -1.3087 -2.9990
H -3.3409 -2.3663 -2.0736
H -2.2731 -1.2379 -1.2090
H -1.2405 -4.8595 -3.7597
H 0.2512 -5.3690 -4.5738
H -0.1024 -5.9572 -2.9364
H 2.3937 -3.2124 -2.4561
H 2.2439 -4.9798 -2.5530
H 2.4195 -4.0275 -4.0392
H -2.2856 1.2082 -1.2606
H -3.3453 2.2968 -2.1841
H -2.2608 1.1948 -3.0517
H -0.7050 4.6171 -1.2170
H -2.4357 4.5916 -1.6279
H -1.8222 3.5987 -0.2841
H 2.3911 3.1168 -2.5791
H 2.4247 3.8651 -4.1946
H 2.2437 4.8788 -2.7503
H -4.4455 -1.8901 2.8296
C -3.6045 -0.1701 5.1745
H -3.5811 -1.2571 5.0958
H -3.4451 0.1037 6.2234
H -4.5931 0.1946 4.8722
C -2.3060 1.8497 4.5730
H -1.6389 2.2385 3.8027
H -3.2655 2.3739 4.4989
H -1.8788 2.0597 5.5605
C 0.3057 0.3725 4.5038
H 0.5539 1.4370 4.3845
H -0.3020 0.2881 5.4097
C 1.6009 -0.4176 4.7191
H 2.0477 -0.0753 5.6604
H 1.3723 -1.4800 4.8621
C 2.6596 -0.2128 3.6375
H 3.6145 -0.6569 3.9519
H 2.8320 0.8614 3.5036
C 2.3510 -2.2544 2.3011
H 3.3509 -2.6130 2.5767
H 1.6276 -2.6453 3.0174
H 2.1027 -2.6286 1.3045
C 3.3172 -0.2773 1.3080
H 3.0920 -0.6896 0.3235
H 3.2776 0.8134 1.2575
H 4.3269 -0.5842 1.6093
H 1.0869 -4.5597 -1.2251
H 1.0869 -4.5597 1.2251
H -1.7318 -4.7370 0.0000
H -0.5366 -5.9996 0.0000

H -0.1013 5.8410 -3.1862
H 0.2608 5.1838 -4.7953

$[(^{1}\mathbf{L})_2Cu^{II}Cu^{III}O_2]^{1+}$
Cu -0.0000 -0.0424 -1.4391
Cu 0.0002 0.0108 1.4020
O 1.1738 -0.0275 -0.0941
O -1.1733 -0.0448 -0.0936
N 1.4524 -0.1034 -2.7963
N 2.8492 1.6016 -1.9847
N 3.8123 -0.2659 -2.9750
N -1.4516 -0.1276 -2.7959
N -2.8761 1.5543 -1.9843
N -3.8085 -0.3289 -2.9744
N -1.4942 0.1268 2.7679
N -2.8917 -1.5917 1.9962
N -3.8534 0.2459 3.0518
N 1.4927 0.1522 2.7675
N 2.9188 -1.5431 1.9970
N 3.8498 0.3108 3.0512
C 1.2829 -1.0014 -3.9442
C 0.0050 -0.6964 -4.7208
C -1.2674 -1.0229 -3.9437
C 2.6609 0.3791 -2.5693
C 3.8316 1.7707 -0.9175
C 1.7617 2.5642 -1.9216
C 4.9700 0.4475 -3.5031
C 3.9596 -1.7122 -2.8832
C -2.6678 0.3350 -2.5690
C -1.8046 2.5347 -1.9215
C -3.8610 1.7073 -0.9170
C -3.9320 -1.7774 -2.8829
C -4.9779 0.3654 -3.5025
C -1.2938 1.0498 3.8902
C -0.0057 0.7514 4.6578
C 1.2768 1.0719 3.8897
C -2.6998 -0.3696 2.5939
C -3.8918 -1.7404 0.9422
C -1.7803 -2.5227 1.8692
C -4.9717 -0.5018 3.6135
C -4.0526 1.6845 2.9558
C 2.7066 -0.3240 2.5938
C 1.8231 -2.4928 1.8708
C 3.9216 -1.6763 0.9434
C 4.0251 1.7525 2.9547
C 4.9803 -0.4178 3.6136

$[(^{2}\mathbf{L})_2Cu^{II}Cu^{III}O_2]^{1+}$
Cu -0.6398 0.6113 -1.2727
O -1.1274 0.4907 0.4320
N 0.3538 0.9705 -2.9210
N 2.4968 0.9523 -1.9692
N 2.1684 -0.0421 -4.0492
N -2.1370 1.9481 -1.6693
C 1.6310 0.6143 -2.9706
C 2.1498 1.9888 -1.0077
H 1.5618 2.7659 -1.4981
H 3.0752 2.4352 -0.6276
H 1.5774 1.5792 -0.1657
C 3.4613 -0.0190 -1.4549
H 3.5673 -0.8532 -2.1462
H 3.0959 -0.4142 -0.4991
H 4.4390 0.4534 -1.3076
C 3.5145 0.2178 -4.5505
H 3.9216 1.1077 -4.0695
H 3.4707 0.3899 -5.6330
H 4.1921 -0.6271 -4.3690
C 1.4341 -1.1116 -4.7186
H 0.5760 -1.3999 -4.1107
H 2.0908 -1.9841 -4.8225
H 1.0943 -0.8190 -5.7206
C -0.3508 1.2303 -4.1771
H -0.9442 0.3592 -4.4957
H 0.3723 1.4303 -4.9763
C -1.2864 2.4316 -4.0355
H -1.7035 2.6665 -5.0229
H -0.7165 3.3138 -3.7217
C -2.4680 2.1664 -3.1086
H -3.1912 2.9935 -3.1695
H -2.9858 1.2635 -3.4528
C -1.7067 3.2109 -1.0220
H -2.5013 3.9681 -1.0782
H -0.8128 3.5979 -1.5149
H -1.4707 2.9901 0.0201
C -3.3695 1.4651 -0.9931
H -3.1233 1.2516 0.0447
H -3.7034 0.5401 -1.4705
H -4.1658 2.2179 -1.0734
Cu -0.1644 -1.0835 0.8779
O 0.3391 -0.8202 -0.9145

$[(^{3}\mathbf{L})_2Cu^{II}Cu^{III}O_2]^{1+}$
Cu -0.0589 1.4227 0.0000
Cu -0.0157 -1.4009 0.0000
O -0.0404 -0.0645 1.1651
O -0.0404 -0.0645 -1.1651
N 0.1709 2.7527 -1.5569
N 0.1709 2.7527 1.5569
N -0.1521 -2.7345 1.5432
N -0.1521 -2.7345 -1.5432
C 0.0327 4.2087 1.2806
C -0.7874 2.3823 -2.6298
C -0.7874 2.3823 2.6298
C 0.8284 -2.3503 2.5961
C 0.0233 -4.1902 -1.2671
C -1.5246 -2.4721 2.0598
C 0.0327 4.2087 -1.2806
C 1.5447 2.4350 2.0229
C -1.5246 -2.4721 -2.0598
C 0.0233 -4.1902 1.2671
C 0.8284 -2.3503 -2.5961
C 1.5447 2.4350 -2.0229
C 0.7114 4.6946 0.0000
C -0.6569 -4.6955 0.0000
H -1.0398 4.4246 1.2129
H 0.4185 4.7694 2.1457
H 0.6617 -2.9486 3.5015
H 0.7078 -1.2888 2.8008
H -0.3369 -4.7487 -2.1425
H -0.3369 -4.7487 2.1425
H 0.6617 -2.9486 -3.5015
H 1.8420 -2.5323 -2.2289
H 0.7078 -1.2888 -2.8008
H 0.4185 4.7694 -2.1457
H -1.0398 4.4246 -1.2129
H 1.6072 1.3587 2.1861
H 2.2763 2.7147 1.2611
H 1.7804 2.9762 2.9502
H -2.2693 -2.7748 -1.3197
H -1.6991 -3.0344 -2.9864
H -1.6145 -1.4009 -2.2371
H -1.6145 -1.4009 2.2371
H -2.2693 -2.7748 1.3197
H -1.6991 -3.0344 2.9864

H 4.7121 -1.4660 3.7473
H 1.2492 -2.0539 -3.6217
H 2.1394 -0.9046 -4.6208
H -0.0040 0.3559 -5.0305
H 0.0099 -1.3061 -5.6341
H -2.1256 -0.9407 -4.6200
H -1.2157 -2.0745 -3.6210
H 4.5728 0.9736 -0.9522
H 3.3157 1.7225 0.0485
H 4.3402 2.7361 -1.0194
H 1.1413 2.4733 -2.8136
H 2.1895 3.5727 -1.8883
H 1.1496 2.4003 -1.0277
H 4.7165 1.4961 -3.6602
H 5.2641 0.0065 -4.4642
H 5.8340 0.3885 -2.8266
H 3.1319 -2.1332 -2.3128
H 4.8958 -1.9491 -2.3606
H 3.9939 -2.1901 -3.8713
H -1.1897 2.3810 -1.0277
H -2.2489 3.5360 -1.8884
H -1.1829 2.4538 -2.8137
H -4.5889 0.8980 -0.9515
H -4.3855 2.6641 -1.0191
H -3.3442 1.6679 0.0489
H -3.0971 -2.1849 -2.3131
H -3.9590 -2.2555 -3.8712
H -4.8638 -2.0299 -2.3599
H -5.8407 0.2921 -2.8261
H -5.2646 -0.0803 -4.4637
H -4.7416 1.4181 -3.6595
H -1.2518 2.0924 3.5372
H -2.1382 0.9862 4.5865
H 0.0034 -0.2983 4.9764
H -0.0108 1.3660 5.5682
H 2.1223 1.0231 4.5858
H 1.2166 2.1135 3.5364
H -4.6745 -0.9901 1.0506
H -3.4065 -1.6030 -0.0317
H -4.3475 -2.7357 0.9928
H -1.1547 -2.4676 2.7610
H -2.1855 -3.5374 1.7855
H -1.1812 -2.2946 0.9805
H -4.6862 -1.5455 3.7466
H -5.2414 -0.0809 4.5910
H -5.8628 -0.4573 2.9710
N 0.1120 -0.8382 2.8390
N -1.7400 0.4346 3.4776
N 0.3402 0.9320 4.4054
N 0.1485 -3.1379 0.8873
C -0.4041 0.1536 3.5422
C -2.6783 -0.5616 2.9736
H -2.3790 -1.5521 3.3196
H -3.6718 -0.3359 3.3755
H -2.7130 -0.5481 1.8781
C -2.2242 1.8113 3.4003
H -1.4167 2.5090 3.6185
H -2.5867 2.0141 2.3855
H -3.0410 1.9762 4.1125
C -0.1744 1.4096 5.6844
H -1.1291 0.9288 5.9000
H 0.5350 1.1549 6.4821
H -0.3153 2.4991 5.6923
C 1.6847 1.3747 4.0589
H 1.8806 1.1667 3.0059
H 1.7606 2.4585 4.2154
H 2.4567 0.8882 4.6698
C 1.2983 -1.5225 3.3658
H 2.2117 -1.1882 2.8488
H 1.4327 -1.2847 4.4278
C 1.1883 -3.0446 3.2190
H 2.0316 -3.4980 3.7560
H 0.2812 -3.3968 3.7232
C 1.2609 -3.5603 1.7811
H 1.3152 -4.6612 1.7857
H 2.1875 -3.1959 1.3210
C -1.1305 -3.7447 1.3171
H -1.0616 -4.8428 1.3372
H -1.4035 -3.3891 2.3108
H -1.9176 -3.4567 0.6150
C 0.4500 -3.6031 -0.4868
H -0.3484 -3.2840 -1.1561
H 1.3727 -3.1359 -0.8325
H 0.5510 -4.6985 -0.5089
H -1.8075 2.5863 2.2926
H -0.5920 2.9621 3.5432
H -0.6910 1.3155 2.8300
H -0.6910 1.3155 -2.8300
H -0.5920 2.9621 -3.5432
H -1.8075 2.5863 -2.2926
H 1.7804 2.9762 -2.9502
H 1.6072 1.3587 -2.1861
H 1.8420 -2.5323 2.2289
H 2.2763 2.7147 -1.2611
H 0.6510 5.7898 0.0000
H 1.7825 4.4642 0.0000
H 1.0997 -4.3788 -1.1884
H 1.0997 -4.3788 1.1884
H -1.7309 -4.4795 0.0000
H -0.5775 -5.7891 0.0000

H -3.2486 2.1343 2.3731
H -5.0045 1.8895 2.4466
H -4.0878 2.1669 3.9420
H 1.2204 -2.2756 0.9819
H 2.2453 -3.5007 1.7881
H 1.1967 -2.4473 2.7626
H 4.6910 -0.9123 1.0507
H 4.3945 -2.6635 0.9959
H 3.4341 -1.5492 -0.0308
H 3.2135 2.1887 2.3721
H 4.0526 2.2357 3.9407
H 4.9732 1.9731 2.4450
H 5.8707 -0.3589 2.9712
H 5.2428 0.0081 4.5908

$[(^{1}\mathbf{L})_2Cu^{II}Cu^{III}O_2H]^{2+}$
Cu -0.0902 -1.4637 0.1118
Cu 0.0224 1.4142 -0.0560
O -1.2370 -0.0407 0.4358
O 1.0832 -0.1422 -0.1083
N -1.5706 -2.7564 0.2263
N -2.6003 -2.0560 2.2215
N -3.9149 -2.9557 0.5349
N 1.2827 -2.7323 -0.2342
N 2.9656 -2.0758 1.2627
N 3.5605 -2.7987 -0.8636
N 1.4714 2.7035 0.2963
N 3.1414 2.1086 -1.2296
N 3.7647 3.0592 0.8011
N -1.4619 2.7217 -0.2848
N -2.4882 1.8534 -2.1971
N -3.8129 2.9109 -0.5962
C -1.5597 -3.8849 -0.7203
C -0.2389 -4.6467 -0.6829
C 0.9452 -3.8173 -1.1691
C -2.6676 -2.5835 0.9686
C -3.6130 -1.1345 2.7362
C -1.3825 -2.1157 3.0147
C -4.9041 -3.5754 1.4229
C -4.3351 -2.8150 -0.8568
C 2.5745 -2.5093 0.0389
C 2.0957 -2.1783 2.4230
C 4.1090 -1.1855 1.4496
C 3.3875 -2.5547 -2.2941
C 4.8198 -3.4451 -0.4823
C 1.0612 3.8061 1.1821

$[(^{2}\mathbf{L})_2Cu^{II}Cu^{III}O_2H]^{2+}$
Cu -0.5397 0.5680 -1.3123
O -0.9790 0.4105 0.3980
N 0.3692 0.8988 -2.9873
N 2.5029 1.1047 -2.0312
N 2.3069 0.2223 -4.1730
N -2.0656 1.8103 -1.5873
C 1.6991 0.7293 -3.0620
C 2.0971 2.1206 -1.0669
H 1.4169 2.8304 -1.5389
H 2.9874 2.6664 -0.7387
H 1.6167 1.6811 -0.1822
C 3.6795 0.3258 -1.6367
H 3.7866 -0.5484 -2.2775
H 3.5491 -0.0162 -0.6034
H 4.5919 0.9287 -1.6954
C 3.6063 0.7073 -4.6557
H 3.8876 1.6150 -4.1219
H 3.5213 0.9398 -5.7226
H 4.3923 -0.0461 -4.5296
C 1.6996 -0.8311 -4.9881
H 0.8439 -1.2640 -4.4685
H 2.4413 -1.6198 -5.1570
H 1.3720 -0.4563 -5.9646
C -0.3732 1.1941 -4.2206
H -0.9215 0.3104 -4.5776
H 0.3292 1.4759 -5.0104
C -1.3579 2.3398 -4.0056
H -1.8423 2.5646 -4.9634
H -0.8241 3.2497 -3.7101
C -2.4686 1.9915 -3.0255

$[(^{3}\mathbf{L})_2Cu^{II}Cu^{III}O_2H]^{2+}$
Cu -0.1381 1.4950 -0.0331
Cu -0.0188 -1.4564 -0.0820
O 0.0673 -0.0499 1.0004
O -0.3792 -0.0684 -1.2859
N 0.1972 2.8489 -1.5082
N -0.1684 2.6923 1.5932
N 0.2478 -2.6312 1.5159
N -0.1845 -2.8717 -1.5353
C -0.4319 4.1438 1.3307
C -0.5460 2.5299 -2.7619
C -1.2374 2.1891 2.5052
C 1.2611 -2.0467 2.4495
C 0.3304 -4.2468 -1.2167
C -1.0963 -2.5830 2.1723
C -0.0655 4.2915 -1.1910
C 1.1503 2.5264 2.2690
C -1.6394 -2.9591 -1.8635
C 0.6572 -4.0574 1.2755
C 0.5619 -2.4056 -2.7478
C 1.6516 2.6290 -1.7594
C 0.3824 4.7516 0.1925
C -0.0688 -4.7780 0.1507
H -1.4989 4.2434 1.1031
H -0.2494 4.6928 2.2641
H 1.3112 -2.6666 3.3516
H 0.9705 -1.0322 2.7045
H -0.0147 -4.9207 -2.0105
H 0.5153 -4.5907 2.2234
H 0.4463 -3.1383 -3.5545
H 1.6233 -2.3101 -2.5061

C -0.1075 4.6099 0.6045
C -1.4495 3.8808 0.6231
C 2.7556 2.6141 -0.0221
C 4.3598 1.3239 -1.4006
C 2.2073 2.0281 -2.3415
C 4.9240 3.8001 0.3006
C 3.7094 2.8930 2.2503
C -2.5611 2.5069 -0.9915
C -1.3134 1.9471 -3.0540
C -3.5547 0.9913 -2.6978
C -4.2390 2.8546 0.7999
C -4.7763 3.5115 -1.5228
H -4.3104 3.6729 -2.4951
H -1.7352 -3.5363 -1.7490
H -2.3730 -4.5737 -0.4729
H -0.0453 -5.0200 0.3298
H -0.3351 -5.5196 -1.3403
H 1.8149 -4.4729 -1.2696
H 0.7212 -3.4255 -2.1726
H -4.4003 -0.9859 1.9976
H -3.1400 -0.1671 2.9462
H -4.0599 -1.5129 3.6619
H -0.7862 -2.9728 2.7036
H -1.6536 -2.2396 4.0685
H -0.7952 -1.1948 2.9137
H -4.4465 -3.8107 2.3838
H -5.2595 -4.5068 0.9675
H -5.7695 -2.9221 1.5866
H -3.6263 -2.1890 -1.4013
H -5.3202 -2.3342 -0.8840
H -4.4164 -3.7828 -1.3662
H 1.4989 -1.2665 2.5480
H 2.7140 -2.3173 3.3156
H 1.4374 -3.0397 2.3131
H 4.6043 -1.0022 0.4990
H 4.8273 -1.6173 2.1552
H 3.7538 -0.2276 1.8472
H 2.5351 -1.8933 -2.4533
H 3.2430 -3.4840 -2.8588
H 4.2885 -2.0635 -2.6789
H 5.6791 -2.7805 -0.6317
H 4.9663 -4.3370 -1.1025
H 4.7811 -3.7507 0.5634
H 0.7761 3.4223 2.1735
H 1.9013 4.4893 1.3359
H 0.1332 4.9304 -0.4164
H -3.2424 2.7701 -3.0380
H -2.9478 1.0571 -3.3378
C -1.6730 3.1098 -0.9724
H -2.5186 3.8067 -1.0040
H -0.8344 3.5453 -1.5165
H -1.3821 2.9249 0.0620
C -3.2678 1.2879 -0.8670
H -3.0213 1.1669 0.1832
H -3.5487 0.3185 -1.2848
H -4.0983 1.9907 -1.0002
Cu -0.2219 -1.2142 0.9434
O 0.5118 -0.9077 -0.8999
N 0.0561 -0.8440 2.8394
N -1.7264 0.5564 3.4092
N 0.3779 0.9919 4.3049
N -0.0986 -3.2464 1.0389
C -0.4110 0.2180 3.4975
C -2.7533 -0.4338 3.1078
H -2.4332 -1.4136 3.4627
H -3.6734 -0.1583 3.6329
H -2.9642 -0.4873 2.0329
C -2.1823 1.9459 3.4210
H -1.3279 2.6215 3.3897
H -2.8015 2.1279 2.5352
H -2.7833 2.1668 4.3105
C -0.0913 1.5510 5.5764
H -1.0591 1.1232 5.8385
H 0.6256 1.2942 6.3644
H -0.1785 2.6433 5.5350
C 1.7674 1.2924 3.9656
H 1.9595 1.0272 2.9249
H 1.9380 2.3681 4.0886
H 2.4768 0.7595 4.6102
C 1.1671 -1.6032 3.4382
H 2.1202 -1.3774 2.9353
H 1.2889 -1.3140 4.4870
C 0.9258 -3.1148 3.3811
H 1.7238 -3.6058 3.9517
H -0.0091 -3.3621 3.8959
C 0.9682 -3.7202 1.9796
H 0.9070 -4.8161 2.0438
H 1.9290 -3.4758 1.5115
C -1.4388 -3.7123 1.4892
H -1.4639 -4.8074 1.5623
H -1.6777 -3.2859 2.4620
H -2.1964 -3.3930 0.7679
H 0.1849 -1.4386 -3.0709
H 0.4164 4.9015 -1.9668
H -1.1460 4.4446 -1.2851
H 1.3270 1.4662 2.4499
H 1.9526 2.9132 1.6378
H 1.1613 3.0697 3.2217
H -2.2111 -3.2827 -0.9918
H -1.8022 -3.6754 -2.6770
H -2.0124 -1.9874 -2.1913
H -1.3535 -1.5426 2.3640
H -1.8522 -3.0336 1.5258
H -1.0683 -3.1383 3.1165
H -2.2100 2.2700 2.0122
H -1.2588 2.7830 3.4270
H -1.0419 1.1445 2.7421
H -0.3035 1.5167 -3.0815
H -0.2658 3.2303 -3.5582
H -1.6217 2.6162 -2.5851
H 2.0009 3.2518 -2.5922
H 1.8170 1.5786 -2.0100
H 2.2392 -2.0366 1.9642
H 2.2348 2.8789 -0.8708
H 0.2268 5.8362 0.2294
H 1.4590 4.6128 0.3410
H 1.4224 -4.2040 -1.2820
H 1.7316 -4.0508 1.0666
H -1.1547 -4.7880 0.2938
H 0.2382 -5.8294 0.1938
H -1.2718 -0.1361 -1.6663

H -0.2192 5.5185 1.2100
H -2.2390 4.5842 0.3377
H -1.6589 3.5669 1.6566
H 4.9081 1.2692 -0.4617
H 4.0951 0.3056 -1.7113
H 5.0081 1.7642 -2.1668
H 1.5212 2.8749 -2.3025
H 2.7704 2.0768 -3.2790
H 1.6391 1.0900 -2.3117
H 4.8027 4.0106 -0.7623
H 5.0038 4.7538 0.8363
H 5.8591 3.2464 0.4520
H 2.8939 2.2189 2.5163
H 4.6540 2.4565 2.5983
H 3.5675 3.8468 2.7738
H -0.6922 1.0424 -3.0054
H -1.6366 2.0799 -4.0929
H -0.7161 2.8090 -2.7582
H -4.3078 0.8367 -1.9244
H -4.0426 1.4161 -3.5836
H -3.1327 0.0184 -2.9836
H -3.5561 2.2235 1.3711
H -4.2824 3.8463 1.2663
H -5.2432 2.4160 0.8457
H -5.6664 2.8831 -1.6495
H -5.0973 4.4833 -1.1302
H -2.0831 -0.1165 -0.0322
C 0.1697 -3.8494 -0.2918
H -0.5979 -3.5312 -1.0026
H 1.1555 -3.5385 -0.6452
H 0.1503 -4.9451 -0.2308
H 0.5275 -1.5418 -1.6340

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