Electronic Supplementary Information

Direct influence of hydrogen-bonding on the reduction potential of a Cu^{II} Centers

Thorsten Glaser*, Ioannis Liratzis, Olga Kataeva, Roland Fröhlich, Manuel Piacenza, and Stefan Grimme

1. Experimental Section

Both complexes have been synthesized by starting from the respective ligand and copper acetate. However, the template reactions described below resulted in microcrystaline materials of higher yields.

[(H_2**L**^{OH})Cu^{II}]: A solution of $Cu(OAc)_2 \cdot H_2O$ (80 mg, 0.40 mmol) in ethanol (30 mL) was added slowly to a stirred solution of 2-formyl-1,8-naphthalenediol (150 mg, 0.80 mmol) in $CHCl_3$ (10 mL) resulting in a brown suspension. After addition of a solution of 1,3-diaminopropane (30 mg, 0.40 mmol) in $CHCl_3$ (6 mL), the mixture was heated to reflux for 30 minutes. Upon stirring overnight at room temperature, brown microcrystals separated which were washed with diethyl ether and dried in vacuum. Yield: 180 mg (95 %). Single-crystals suitable for single-crystal X-ray diffraction were obtained by slow evaporation of a solution of [(H_2**L**^{OH})Cu^{II}] in CH_2Cl_2. MALDI-TOF MS of [(H_2**L**^{OH})Cu^{II}]: *m*/*z* (%): 475 (100) [(H_2**L**^{OH})Cu^{II}]$^+$; IR (KBr): $\tilde{\nu}$ = 1611 (C=N); elemental analysis calcd for $C_{25}H_{20}N_2O_4Cu$ ([(H_2**L**^{OH})Cu^{II}]) (%): C 63.08, H 4.24, N 5.89; found: C 63.26, H 4.03, N 5.80.

[**L**^{H}Cu^{II}]: A stirred suspension of 2-formyl-1-naphthol (120 mg, 0.70 mmol) in methanol (30 mL) was subsequently treated with a solution of 1,3-diaminopropane (26 mg, 0.35 mmol) in methanol (5 mL) and solid $Cu(OAc)_2 \cdot H_2O$ (70 mg, 0.35 mmol). The resulting olive-green solution was heated to reflux for 30 minutes. Brownish-green microcrystals separated upon cooling. Yield: 100 mg (65 %). Single-crystals suitable for single-crystal X-ray diffraction were obtained by slow evaporation of a solution of [**L**^{H}Cu^{II}] in a CH_2Cl_2/MeOH (3:1) mixture. MALDI-TOF MS of [**L**^{H}Cu^{II}]: *m*/*z* (%): 443 (100) [**L**^{H}Cu^{II}]$^+$; IR (KBr): $\tilde{\nu}$ = 1621 (C=N); elemental analysis calcd for $C_{25}H_{21}N_2O_{2.5}Cu$ ([**L**^{H}Cu^{II}]·0.5H_2O) (%): C 66.29, H 4.67, N 6.18; found: C 66.30, H 4.46, N 5.97.

X-ray crystal structure analysis for [(H_2**L**^{OH})Cu^{II}]: formula $C_{25}H_{20}N_2O_4Cu$, M = 475.97, brown crystal 0.23 × 0.08 × 0.07 mm, a = 22.210(2), b = 10.2458(11), c = 17.7739(19) Å, β = 100.842(2)°, V = 3972.4(7) Å^3, ρ_{calc} = 1.592 g cm^{-3}, μ= 1.14 mm^{-1}, no absorption correction, Z = 8, monoclinic, space group $C2/c$ (No. 15), λ = 0.71073 Å, T = 153 K, ω and φ scans, 18963 reflections collected ($\pm h$, $\pm k$, $\pm l$), [(sinθ)/λ] = 0.65 Å^{-1}, 4547 independent (R_{int} = 0.072) and 3271 observed reflections [$I \geq 2\ \sigma(I)$], 369 refined parameters, R = 0.036, wR^2 = 0.067, max. residual electron density 0.59 (-0.30) e Å^{-3}, hydrogen atoms located from difference Fourier maps and refined independently. X-ray crystal structure analysis for [**L**^{H}Cu^{II}]: formula $C_{25}H_{20}N_2O_2Cu$, M = 443.97, orange crystal 0.40 × 0.20 × 0.06 mm, a = 22.060(1), b = 10.158(1), c = 17.598(1) Å, β = 100.97(1)°, V = 3871.4(5) Å^3, ρ_{calc} = 1.523 g cm^{-3}, μ = 1.15 mm^{-1}, empirical absorption correction ($0.655 \leq T \leq 0.934$), Z = 8, monoclinic, space group $C2/c$ (No. 15), λ = 0.71073 Å, T = 198 K, ω and φ scans, 15324 reflections collected ($\pm h$, $\pm k$, $\pm l$), [(sinθ)/λ] = 0.66 Å^{-1}, 4601 independent (R_{int} = 0.051) and 3542 observed reflections [$I \geq 2\ \sigma(I)$], 271 refined parameters, R = 0.036, wR^2 = 0.094, max. residual electron density 0.37 (-0.40) e Å^{-3}, hydrogen atoms calculated and refined as riding atoms. Data sets were collected with Bruker AXS APEX and Nonius KappaCCD diffractometers, both equipped with rotating anode generators. Programs used: data collection SMART[1] and COLLECT[2], data reduction SAINT[1] and Denzo-SMN[3], absorption correction [4] structure solution SHELXS-97[5], structure refinement SHELXL-97[6]. CCDC 273718 & 273719 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (internat.) +44(1223)336-033, E-mail: deposit@ccdc.cam.ac.uk].

[1] SMART&SAINT, Bruker AXS, **2000**.

[2] COLLECT, Nonius B. V., **1998**.

[3] Z. Otwinowski, W. Minor, *Methods Enzymol.* **1997**, *276*, 307-326.

[4] a) R. H. Blessing, *Acta Cryst.* **1995**, *A51*, 33-37; b) R. H. Blessing, *J. Appl. Cryst.* **1997**, *30*, 421-426.

[5] G. M. Sheldrick, *Acta Cryst.* **1990**, *A46*, 467-473.

[6] SHELXL-97; Sheldrick, G. M.; Universität Göttingen, **1997**

2. Details of Electronic Structure Calculations

[(H_2**L**^{OH})Cu^{II}]

Cartesian Coordinates (Angstroems)

1	c	-4.639234	3.686019	-0.669787
2	c	-3.273619	3.632986	-0.900507
3	c	-2.579281	2.463590	-0.690951
4	c	-3.259576	1.307548	-0.227446
5	c	-4.657100	1.381365	-0.012854
6	c	-5.328857	2.584913	-0.234177
7	c	-5.361171	0.219424	0.418175
8	c	-4.710897	-0.940052	0.604498
9	c	-3.305171	-1.054903	0.406043
10	c	-2.566897	0.071837	0.012407
11	o	-1.290428	0.028501	-0.152102
12	cu	-0.012325	-1.398548	0.104013
13	o	1.317804	-0.022839	0.335340
14	c	2.565450	0.006570	0.022073
15	c	3.226677	-1.119567	-0.493238
16	c	4.594205	-1.013639	-0.880001
17	c	5.280922	0.132204	-0.751245
18	c	4.662281	1.286804	-0.188097
19	c	3.305577	1.223034	0.211192
20	c	5.378504	2.472404	-0.017644
21	c	4.773348	3.565274	0.546432
22	c	3.450817	3.521162	0.957682
23	c	2.713993	2.369309	0.802194
24	c	2.617546	-2.389497	-0.572115
25	n	1.408047	-2.747717	-0.297033
26	c	1.175154	-4.190528	-0.320157
27	c	-0.273897	-4.585405	-0.492545
28	c	-1.172704	-4.086537	0.624448
29	n	-1.482250	-2.676048	0.467046

30	c	-2.717330	-2.327422	0.576352
31	o	1.453139	2.377974	1.231567
32	o	-1.271832	2.465979	-0.944893
33	h	3.293688	-3.178025	-0.888831
34	h	-3.425688	-3.114966	0.813063
35	h	1.531672	-4.612447	0.618434
36	h	1.766040	-4.640314	-1.113975
37	h	-2.093158	-4.663382	0.641207
38	h	-0.678215	-4.243911	1.581250
39	h	-0.656291	-4.236800	-1.447291
40	h	-0.313002	-5.670594	-0.511086
41	h	5.075657	-1.887504	-1.285773
42	h	-5.252946	-1.817424	0.915318
43	h	6.310425	0.195459	-1.053389
44	h	-6.421598	0.289517	0.578770
45	h	2.973758	4.373708	1.403894
46	h	1.053087	1.524126	1.017267
47	h	6.406860	2.513700	-0.327910
48	h	-2.729982	4.492100	-1.246886
49	h	-0.917256	1.594520	-0.719856
50	h	-6.389239	2.633072	-0.064280
51	h	5.330865	4.476378	0.675855
52	h	-5.162404	4.610893	-0.839069

Total energy (BH-LYP/TZVP) = -3015.3232869190 H = -82051.1680897 eV

HOMO-LUMO Separation

HOMO: 245. b 122 a -0.22494391 H = -6.12104 eV

LUMO: 246. a 124 a -0.03090335 H = -0.84092 eV

Gap : +0.19404056 H = +5.28012 eV

Number of MOs= 1484, Electrons= 245.00, Symmetry: c1

Nr.	Orbital	Occupation	Energy
249.	b 124 a		-0.024694 H = -0.672 eV

248. a 125 a		-0.025534 H =	-0.695 eV
247. b 123 a		-0.029967 H =	-0.815 eV
246. a 124 a		-0.030903 H =	-0.841 eV
245. b 122 a	1.000	-0.224944 H =	-6.121 eV
244. a 123 a	1.000	-0.225765 H =	-6.143 eV
243. b 121 a	1.000	-0.227911 H =	-6.202 eV
242. a 122 a	1.000	-0.228183 H =	-6.209 eV

9 a excitation

Total energy: -3015.196451134597

Excitation energy: 0.1268349784028742

Excitation energy / eV: 3.451356845534004

Excitation energy / nm: 359.2333379462104

Excitation energy / cm^(-1): 27837.06004481329

Oscillator strength:

velocity representation: 0.4537133277698157E-01

length representation: 0.4685123855641580E-01

mixed representation: 0.4554017917828262E-01

Dominant contributions:

occ. orbital	energy / eV	virt. orbital	energy / eV	|coeff.|^2*100
122 a beta	-6.12	123 a beta	-0.82	23.4
123 a alpha	-6.14	124 a alpha	-0.84	21.5
122 a alpha	-6.21	125 a alpha	-0.69	12.2
121 a beta	-6.20	124 a beta	-0.67	11.7
122 a alpha	-6.21	124 a alpha	-0.84	10.8
121 a beta	-6.20	123 a beta	-0.82	8.3
123 a alpha	-6.14	125 a alpha	-0.69	4.3

10 a excitation

Total energy: -3015.190109230489

Excitation energy: 0.1331768825112158

Excitation energy / eV: 3.623928910698239

Excitation energy / nm: 342.1265898468734

Excitation energy / cm^(-1): 29228.94710692638

Oscillator strength:

velocity representation: 0.4299978475764270

length representation: 0.4219990662965832

mixed representation: 0.4259661715721701

Dominant contributions:

occ. orbital	energy / eV	virt. orbital	energy / eV	|coeff.|^2*100
123 a alpha	-6.14	125 a alpha	-0.69	26.1
122 a beta	-6.12	124 a beta	-0.67	24.8
122 a alpha	-6.21	124 a alpha	-0.84	22.4
121 a beta	-6.20	123 a beta	-0.82	16.3
121 a beta	-6.20	124 a beta	-0.67	1.4

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$[(H_2\mathbf{L}^{OH})Cu^{I}]^{-}$

Cartesian Coordinates (Angstroems)

1	c	-5.156619	3.567509	-0.612128
2	c	-3.775009	3.655564	-0.710620
3	c	-2.995438	2.533529	-0.520426
4	c	-3.601404	1.286943	-0.219707
5	c	-5.008905	1.218758	-0.132213
6	c	-5.772804	2.378376	-0.329299
7	c	-5.623981	-0.031600	0.148082
8	c	-4.860824	-1.130610	0.324680
9	c	-3.446592	-1.114827	0.262956
10	c	-2.778599	0.104449	-0.013097
11	o	-1.519150	0.206825	-0.096545
12	cu	0.022459	-1.284288	0.281678
13	o	1.629804	0.020413	0.586505
14	c	2.798871	0.000458	0.089401
15	c	3.361140	-1.136411	-0.537639
16	c	4.658827	-1.045739	-1.094715
17	c	5.412190	0.073204	-1.043833
18	c	4.909645	1.234562	-0.397905

19	c	3.614461	1.200934	0.163817
20	c	5.675286	2.406852	-0.308477
21	c	5.173635	3.507015	0.332193
22	c	3.905933	3.493534	0.898476
23	c	3.127342	2.358405	0.824082
24	c	2.719987	-2.414247	-0.612314
25	n	1.572935	-2.765330	-0.186284
26	c	1.253887	-4.172105	-0.264791
27	c	-0.215409	-4.468474	-0.512292
28	c	-1.164709	-4.026638	0.600060
29	n	-1.541594	-2.636850	0.487751
30	c	-2.787235	-2.370732	0.438803
31	o	1.922446	2.382389	1.386818
32	o	-1.676687	2.656940	-0.629424
33	h	3.346298	-3.178748	-1.081844
34	h	-3.482598	-3.208649	0.530227
35	h	1.527631	-4.637482	0.683800
36	h	1.852073	-4.665245	-1.036236
37	h	-2.052911	-4.662469	0.583429
38	h	-0.676100	-4.185860	1.560231
39	h	-0.535242	-4.021758	-1.448936
40	h	-0.307005	-5.547040	-0.626242
41	h	5.056109	-1.925855	-1.575609
42	h	-5.339699	-2.075837	0.527415
43	h	6.395863	0.100670	-1.478016
44	h	-6.696571	-0.085064	0.208103
45	h	3.505103	4.354933	1.400249
46	h	1.511808	1.507836	1.208935
47	h	6.659537	2.423024	-0.742871
48	h	-3.284672	4.585162	-0.934230
49	h	-1.293047	1.770087	-0.448511
50	h	-6.844741	2.316834	-0.257875
51	h	5.766631	4.403796	0.398520
52	h	-5.749494	4.454200	-0.762720

Total energy (BH-LYP/TZVP) = -3015.3783222000 H = -82052.6656767 eV

HOMO-LUMO Separation

HOMO: 123. 123 a -0.10833716 H = -2.94801 eV

LUMO: 124. 124 a +0.09644682 H = +2.62445 eV

Gap : +0.20478398 H = +5.57246 eV

Number of MOs= 742, Electrons= 246.00, Symmetry: c1

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[(H_2**L**^{OH,rot})Cu^{II}]

Cartesian Coordinates (Angstroems)

1	c	4.711716	3.662283	0.685538
2	c	3.366992	3.596784	1.025764
3	c	2.649001	2.437638	0.838977
4	c	3.267981	1.294306	0.278303
5	c	4.643305	1.377627	-0.041891
6	c	5.345023	2.573096	0.163165
7	c	5.326113	0.241174	-0.563854
8	c	4.671763	-0.917060	-0.746702
9	c	3.286317	-1.048034	-0.468791
10	c	2.546155	0.058642	0.016687
11	o	1.307399	-0.009181	0.230405
12	cu	0.009835	-1.387498	-0.093411
13	o	-1.334553	-0.054710	-0.378387
14	c	-2.549010	-0.003125	-0.055829
15	c	-3.218098	-1.112802	0.518505
16	c	-4.565072	-0.989060	0.950739
17	c	-5.249572	0.158627	0.822084
18	c	-4.644796	1.291320	0.202907
19	c	-3.314310	1.215131	-0.270180
20	c	-5.379823	2.474629	0.053674

21	c	-4.822681	3.558468	-0.559625
22	c	-3.524961	3.498681	-1.049954
23	c	-2.777647	2.349691	-0.924341
24	c	-2.608852	-2.379191	0.621380
25	n	-1.403355	-2.744522	0.332977
26	c	-1.167264	-4.184576	0.382033
27	c	0.289523	-4.574130	0.504597
28	c	1.149996	-4.079396	-0.645753
29	n	1.467034	-2.671224	-0.498372
30	c	2.698719	-2.318946	-0.640022
31	o	-1.538203	2.294279	-1.437843
32	o	1.357141	2.382834	1.201523
33	h	-3.279701	-3.158594	0.972699
34	h	3.400973	-3.101556	-0.911873
35	h	-1.560081	-4.631798	-0.530586
36	h	-1.724195	-4.617978	1.209787
37	h	2.067348	-4.660565	-0.695090
38	h	0.619600	-4.236778	-1.583456
39	h	0.704278	-4.214923	1.441816
40	h	0.332944	-5.659222	0.531735
41	h	-5.037000	-1.848784	1.397006
42	h	5.199692	-1.778627	-1.121163
43	h	-6.264885	0.240556	1.164526
44	h	6.372695	0.329205	-0.791424
45	h	-3.097050	4.351563	-1.550135
46	h	-1.324622	3.133259	-1.834354
47	h	-6.388153	2.511438	0.424320
48	h	2.876136	4.455415	1.453131
49	h	1.094825	3.227149	1.555186
50	h	6.388464	2.614416	-0.091981
51	h	-5.387468	4.466934	-0.673288
52	h	5.251067	4.579664	0.842906

Total energy (BH-LYP/TZVP) = -3015.2805172830 H = -82050.0042680 eV

HOMO-LUMO Separation

HOMO: 245. b 122 a -0.21548299 H = -5.86359 eV
LUMO: 246. a 124 a -0.01552373 H = -0.42242 eV
Gap : +0.19995926 H = +5.44117 eV

Number of MOs= 1484, Electrons= 245.00, Symmetry: c1

Nr.	Orbital	Occupation	Energy	
249.	b 124 a		-0.009931 H =	-0.270 eV
248.	a 125 a		-0.010807 H =	-0.294 eV
247.	b 123 a		-0.014609 H =	-0.398 eV
246.	a 124 a		-0.015524 H =	-0.422 eV
245.	b 122 a	1.000	-0.215483 H =	-5.864 eV
244.	a 123 a	1.000	-0.216872 H =	-5.901 eV
243.	b 121 a	1.000	-0.220642 H =	-6.004 eV
242.	a 122 a	1.000	-0.220914 H =	-6.011 eV

9 a excitation

Total energy: -3015.149560104329
Excitation energy: 0.1309571786710959
Excitation energy / eV: 3.563527670124665
Excitation energy / nm: 347.9255824106760
Excitation energy / cm^(-1): 28741.77842635269
Oscillator strength:
velocity representation: 0.6530799258233349E-01
length representation: 0.6954286777226145E-01
mixed representation: 0.6693747381102832E-01
Dominant contributions:

occ. orbital		energy / eV	virt. orbital		energy / eV	|coeff.|^2*100
122 a	beta	-5.86	123 a	beta	-0.40	24.8
123 a	alpha	-5.90	124 a	alpha	-0.42	23.2
122 a	alpha	-6.01	125 a	alpha	-0.29	11.7
121 a	beta	-6.00	124 a	beta	-0.27	10.8
122 a	alpha	-6.01	124 a	alpha	-0.42	9.6
121 a	beta	-6.00	123 a	beta	-0.40	7.5
123 a	alpha	-5.90	125 a	alpha	-0.29	4.4

12 a excitation

Total energy: -3015.142959147430

Excitation energy: 0.1375581355696421

Excitation energy / eV: 3.743148923392101

Excitation energy / nm: 331.2297921988951

Excitation energy / cm^(-1): 30190.52100392774

Oscillator strength:

velocity representation: 0.5012853144278867

length representation: 0.5003717577774971

mixed representation: 0.5008186896350887

Dominant contributions:

occ. orbital	energy / eV	virt. orbital	energy / eV	|coeff.|^2*100
122 a beta	-5.86	124 a beta	-0.27	27.1
123 a alpha	-5.90	125 a alpha	-0.29	25.7
121 a beta	-6.00	123 a beta	-0.40	17.3
122 a alpha	-6.01	124 a alpha	-0.42	17.2
121 a beta	-6.00	124 a beta	-0.27	3.0

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$[(H_2\mathbf{L}^{\mathbf{OH,rot}})Cu^{I}]^{-}$

Cartesian Coordinates (Angstroems)

1	c	5.315142	3.488037	0.632532
2	c	3.939575	3.620077	0.781824
3	c	3.106367	2.534726	0.607251
4	c	3.627133	1.265987	0.265235
5	c	5.031457	1.154449	0.123148
6	c	5.855474	2.279870	0.309623
7	c	5.614092	-0.097168	-0.204664
8	c	4.823018	-1.179322	-0.384775
9	c	3.421076	-1.138179	-0.278490
10	c	2.756711	0.090434	0.057287

11	o	1.529862	0.179328	0.176300
12	cu	-0.042028	-1.213822	-0.344143
13	o	-1.718303	-0.116199	-0.742630
14	c	-2.811209	-0.047750	-0.157384
15	c	-3.353384	-1.128740	0.609574
16	c	-4.576545	-0.973470	1.283733
17	c	-5.304587	0.167021	1.248045
18	c	-4.842842	1.271683	0.489628
19	c	-3.623188	1.179230	-0.224884
20	c	-5.600741	2.457703	0.450047
21	c	-5.175718	3.527134	-0.277494
22	c	-3.985511	3.455876	-0.994048
23	c	-3.225046	2.306294	-0.981424
24	c	-2.722608	-2.411084	0.709403
25	n	-1.622675	-2.802762	0.204239
26	c	-1.289647	-4.195696	0.355390
27	c	0.196683	-4.458234	0.531717
28	c	1.075614	-3.996442	-0.631536
29	n	1.478979	-2.615953	-0.503687
30	c	2.731574	-2.373569	-0.471039
31	o	-2.092262	2.259962	-1.708283
32	o	1.778972	2.693460	0.767602
33	h	-3.306931	-3.131169	1.293664
34	h	3.407676	-3.223548	-0.598497
35	h	-1.609534	-4.722848	-0.545945
36	h	-1.835530	-4.649073	1.189776
37	h	1.954913	-4.642998	-0.691848
38	h	0.521815	-4.120396	-1.560431
39	h	0.553154	-3.991868	1.445058
40	h	0.321048	-5.533125	0.651841
41	h	-4.942922	-1.813026	1.854631
42	h	5.278952	-2.127661	-0.625564
43	h	-6.234301	0.252108	1.781832
44	h	6.683095	-0.165805	-0.299765
45	h	-3.654105	4.297632	-1.580479

46	h	-1.945073	3.116055	-2.096868
47	h	-6.522039	2.500527	1.004356
48	h	3.510622	4.574628	1.041041
49	h	1.605176	3.603175	0.986729
50	h	6.919261	2.166533	0.193826
51	h	-5.755580	4.434073	-0.303143
52	h	5.948057	4.347682	0.773708

Total energy = -3015.3139645350 H = -82050.9144145 eV

HOMO-LUMO Separation

HOMO: 123. 123 a -0.09092884 H = -2.47430 eV

LUMO: 124. 124 a +0.10785696 H = +2.93494 eV

Gap : +0.19878580 H = +5.40924 eV

Number of MOs= 742, Electrons= 246.00, Symmetry: c1

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[($\mathbf{L}^{\mathbf{H}}$)Cu^{II}]

Cartesian Coordinates (Angstroems)

1	c	4.613432	3.829099	0.429954
2	c	3.255067	3.754243	0.750612
3	c	2.593863	2.564088	0.634770
4	c	3.266180	1.415921	0.199992
5	c	4.632279	1.484997	-0.124317
6	c	5.286580	2.719758	0.001605
7	c	5.315937	0.313892	-0.566207
8	c	4.653565	-0.851865	-0.663558
9	c	3.268498	-0.967971	-0.346752
10	c	2.549794	0.164472	0.078998
11	o	1.316948	0.138074	0.364465
12	cu	-0.003137	-1.234242	0.132987
13	n	1.451389	-2.595904	-0.189529

14	c	2.674035	-2.244942	-0.411901
15	o	-1.273007	0.194949	-0.076052
16	c	-2.537452	0.216956	-0.003690
17	c	-3.320808	-0.928128	0.230070
18	c	-4.740026	-0.817561	0.295352
19	c	-5.375283	0.357671	0.142727
20	c	-4.623555	1.544758	-0.099606
21	c	-3.221060	1.480916	-0.174308
22	c	-5.245026	2.791436	-0.269617
23	c	-4.506336	3.916558	-0.504628
24	c	-3.112209	3.846479	-0.579679
25	c	-2.482238	2.645142	-0.416238
26	c	-2.742619	-2.206145	0.382860
27	n	-1.497784	-2.539900	0.371471
28	c	-1.200145	-3.953072	0.528289
29	c	-0.202637	-4.439726	-0.505583
30	c	1.221795	-4.038232	-0.199393
31	h	-3.460820	-3.008463	0.521695
32	h	-2.117473	-4.530808	0.452486
33	h	-0.795653	-4.127293	1.523924
34	h	1.482782	-4.437786	0.779894
35	h	1.888464	-4.507119	-0.918923
36	h	3.367233	-3.040523	-0.669720
37	h	-0.235069	-5.525122	-0.532407
38	h	-0.497306	-4.087422	-1.489721
39	h	-5.309219	-1.714656	0.474725
40	h	-1.412805	2.562904	-0.468896
41	h	5.173584	-1.737916	-0.988131
42	h	1.549862	2.479280	0.871824
43	h	-6.447091	0.418938	0.197727
44	h	-2.540119	4.737518	-0.765915
45	h	-6.318129	2.849296	-0.212935
46	h	6.360683	0.378992	-0.810816
47	h	2.734499	4.633041	1.086277
48	h	6.332272	2.781443	-0.244930

49	h	-5.000174	4.863744	-0.633163
50	h	5.131711	4.767543	0.520849

Total energy (BH-LYP/TZVP) = -2864.8750183970 H = -77957.2600756 eV

HOMO-LUMO Separation

HOMO: 229. b 114 a -0.22547944 H = -6.13561 eV

LUMO: 230. a 116 a -0.02246541 H = -0.61132 eV

Gap : +0.20301403 H = +5.52430 eV

Number of MOs= 1408, Electrons= 229.00, Symmetry: c1

Nr.	Orbital	Occupation	Energy	
233.	b 116 a		-0.016602 H =	-0.452 eV
232.	a 117 a		-0.017380 H =	-0.473 eV
231.	b 115 a		-0.021545 H =	-0.586 eV
230.	a 116 a		-0.022465 H =	-0.611 eV
229.	b 114 a	1.000	-0.225479 H =	-6.136 eV
228.	a 115 a	1.000	-0.226903 H =	-6.174 eV
227.	b 113 a	1.000	-0.231836 H =	-6.309 eV
226.	a 114 a	1.000	-0.232210 H =	-6.319 eV

9 a excitation

Total energy: -2864.741987374411

Excitation energy: 0.1330308455892483

Excitation energy / eV: 3.619955042159133

Excitation energy / nm: 342.5021652548413

Excitation energy / cm^(-1): 29196.89570740900

Oscillator strength:

velocity representation: 0.1870411260227904E-01

length representation: 0.2030898544781044E-01

mixed representation: 0.1909149940461962E-01

Dominant contributions:

occ. orbital		energy / eV	virt. orbital		energy / eV	|coeff.|^2*100
115 a	alpha	-6.17	116 a	alpha	-0.61	29.5
114 a	beta	-6.14	115 a	beta	-0.59	29.5

114 a	alpha	-6.32	117 a	alpha	-0.47	14.0
113 a	beta	-6.31	116 a	beta	-0.45	12.4
114 a	alpha	-6.32	116 a	alpha	-0.61	4.1
113 a	beta	-6.31	115 a	beta	-0.59	3.7

12 a excitation

Total energy: -2864.735247703416
Excitation energy: 0.1397705165842354
Excitation energy / eV: 3.803350899659184
Excitation energy / nm: 325.9868659964519
Excitation energy / cm^(-1): 30676.08251007329
Oscillator strength:
velocity representation: 0.3356977902846983
length representation: 0.3363516239450085
mixed representation: 0.3360161512511329
Dominant contributions:

occ. orbital		energy / eV	virt. orbital		energy / eV	|coeff.|^2*100
114 a	beta	-6.14	116 a	beta	-0.45	26.3
115 a	alpha	-6.17	117 a	alpha	-0.47	26.2
114 a	alpha	-6.32	116 a	alpha	-0.61	20.3
113 a	beta	-6.31	115 a	beta	-0.59	17.5

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$[(\mathbf{L}^{\mathbf{H}})Cu^{I}]^{-}$

Cartesian Coordinates (Angstroems)

1	c	-2.985188	-2.681373	0.407769
2	c	-3.590993	-1.439165	0.203333
3	c	-4.994366	-1.350573	0.162260
4	c	-5.743114	-2.529073	0.329119
5	c	-5.128903	-3.733918	0.528055
6	c	-3.734435	-3.816179	0.568800
7	c	-2.738506	-0.253693	0.037700

8	c	-3.418403	0.982077	-0.177950
9	c	-4.833314	1.010064	-0.198792
10	c	-5.610789	-0.085737	-0.043579
11	o	-1.503527	-0.382895	0.097103
12	cu	0.039887	1.082118	-0.316413
13	n	-1.500183	2.481955	-0.416124
14	c	-1.110691	3.867993	-0.529617
15	c	-0.126572	4.298155	0.557022
16	c	1.334444	4.015338	0.250815
17	n	1.648351	2.613265	0.126869
18	c	2.798638	2.243896	0.527779
19	c	3.410980	0.953984	0.428500
20	c	4.717046	0.825487	0.955781
21	c	5.439741	-0.317328	0.906336
22	c	4.873768	-1.468778	0.296264
23	c	3.573605	-1.401540	-0.238125
24	c	2.788770	-0.163915	-0.194775
25	c	5.569383	-2.688402	0.210479
26	c	5.002597	-3.785027	-0.375151
27	c	3.709209	-3.713938	-0.901398
28	c	3.013378	-2.537609	-0.829919
29	o	1.644131	-0.158683	-0.692976
30	c	-2.749702	2.232756	-0.340803
31	h	-3.434446	3.082846	-0.401748
32	h	-1.992125	4.512699	-0.486157
33	h	-0.647408	4.028007	-1.502327
34	h	1.571541	4.505709	-0.695625
35	h	1.958324	4.493550	1.012560
36	h	3.441560	2.991825	1.004238
37	h	-0.221931	5.373843	0.695144
38	h	-0.409656	3.830173	1.495202
39	h	-5.306780	1.968053	-0.351217
40	h	-1.911085	-2.708338	0.432585
41	h	5.151459	1.698802	1.417898
42	h	2.015782	-2.450067	-1.219626

43	h	-6.684032	-0.015783	-0.069388
44	h	-3.254695	-4.766584	0.725061
45	h	-6.818267	-2.467498	0.297962
46	h	6.432643	-0.367259	1.317474
47	h	3.264330	-4.581336	-1.356939
48	h	6.564987	-2.745158	0.618216
49	h	-5.722200	-4.624040	0.653615
50	h	5.553184	-4.709135	-0.429280

Total energy (BH-LYP/TZVP) = -2864.9144544870 H = -77958.3331868 eV

HOMO-LUMO Separation

HOMO: 115. 115 a -0.09626066 H = -2.61939 eV

LUMO: 116. 116 a +0.10414410 H = +2.83391 eV

Gap : +0.20040477 H = +5.45329 eV

Number of MOs= 704, Electrons= 230.00, Symmetry: c1