Electronic Supporting Information for

Distorted copper(II) radicals with sterically hindered salens: Electronic structure and aerobic oxidation of alcohols

R. Kunert, C. Philouze, F. Berthiol, O. Jarjayes, T. Storr, F. Thomas

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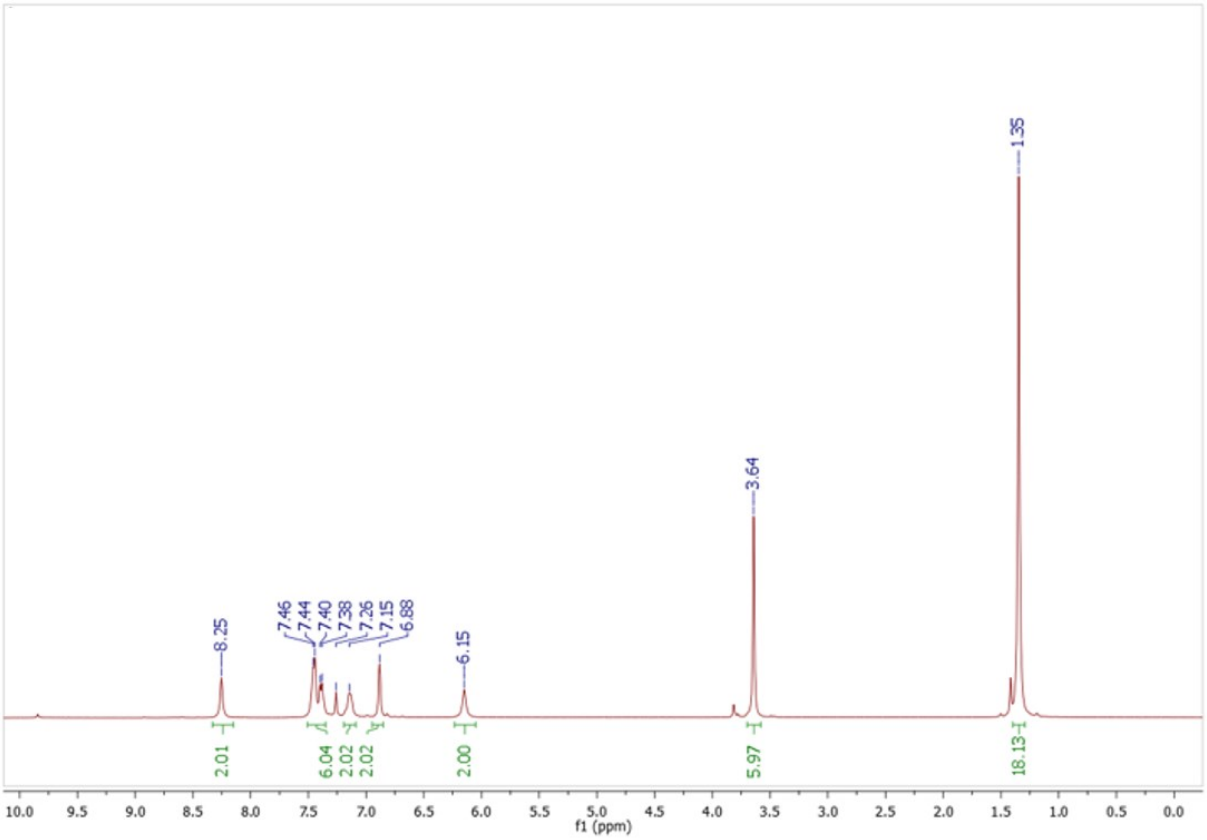

Figure S1. ^{1}H NMR spectrum of $\mathbf{H_2L^{bp,OMe}}$

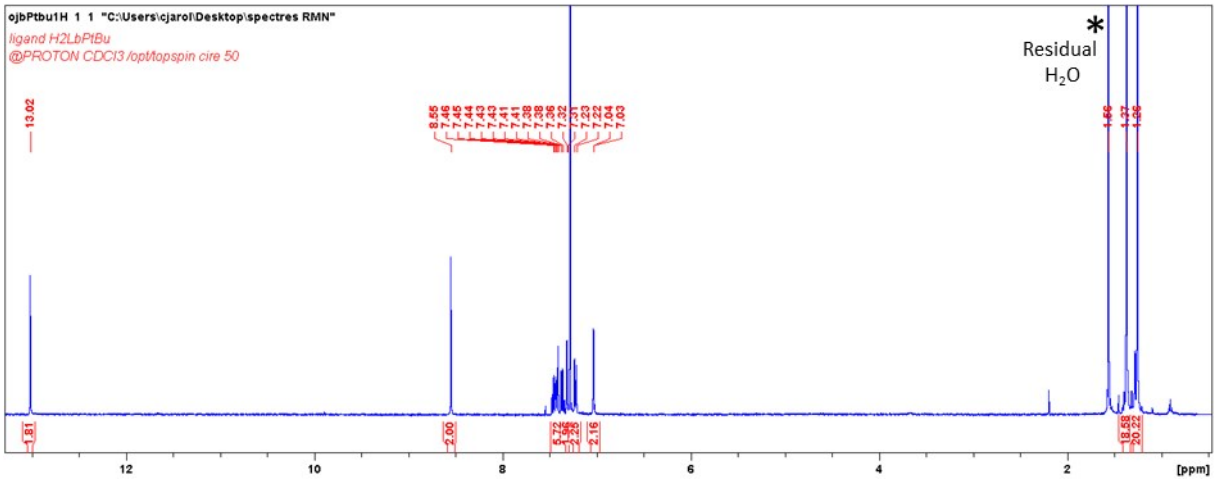

Figure S2. ^{1}H NMR spectrum of $\mathbf{H_2L^{bp,tBu}}$

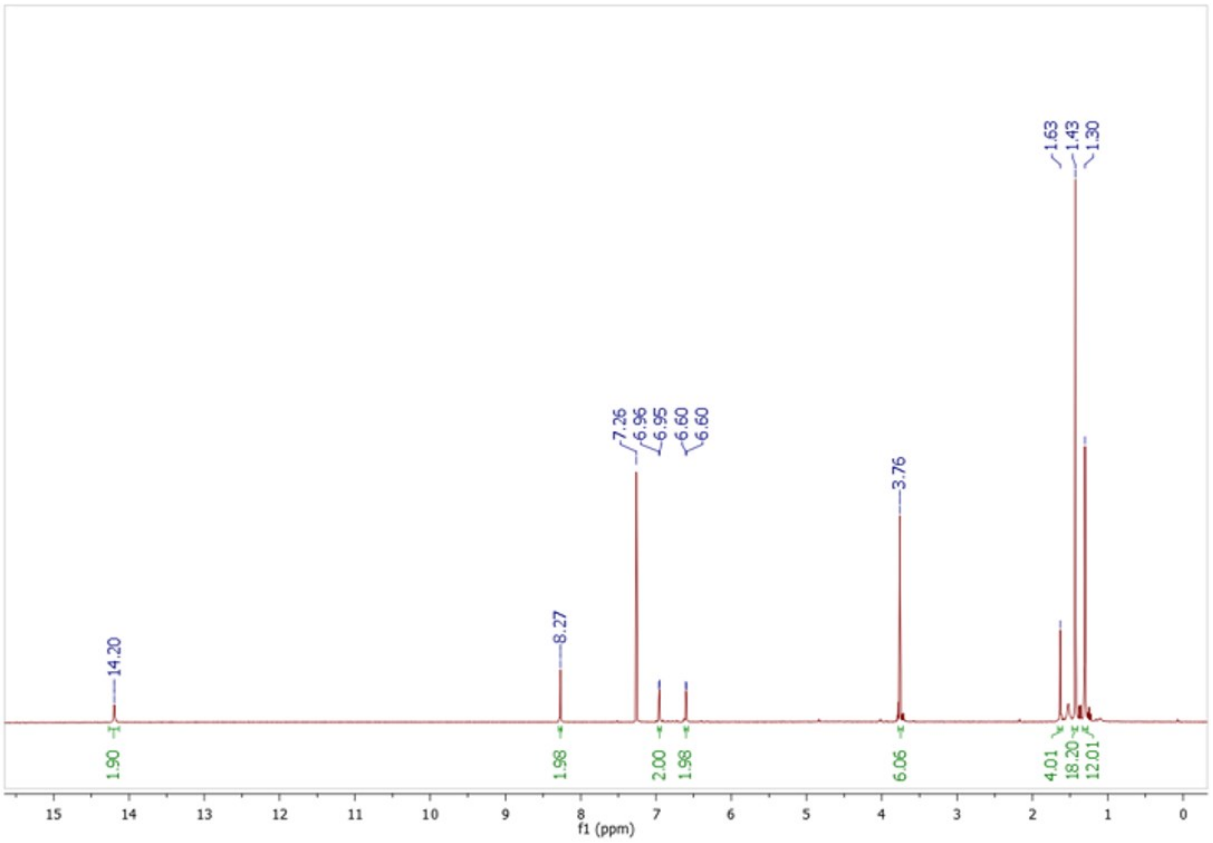

Figure S3. ^{1}H NMR spectrum of **$H_2L^{pu,OMe}$**

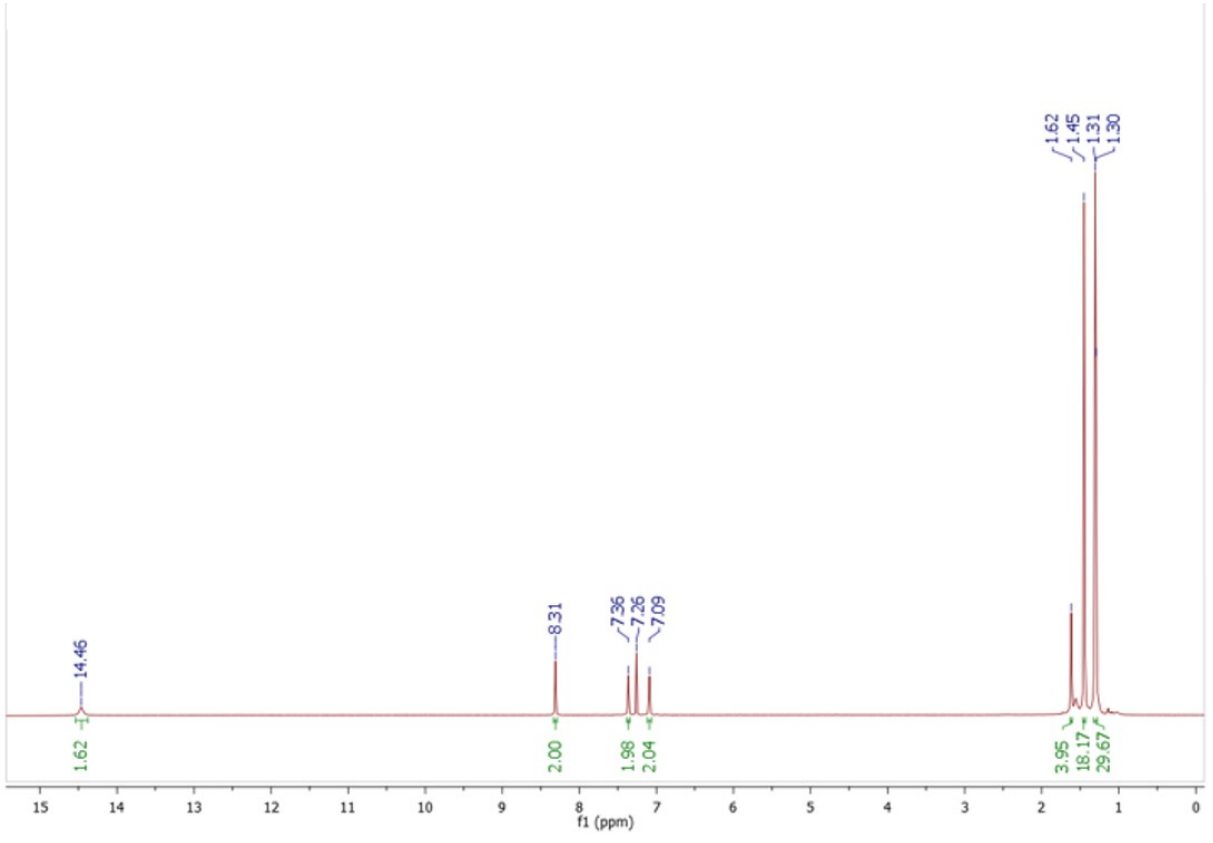

Figure S4. ^{1}H NMR spectrum of $H_2L^{pu,tBu}$

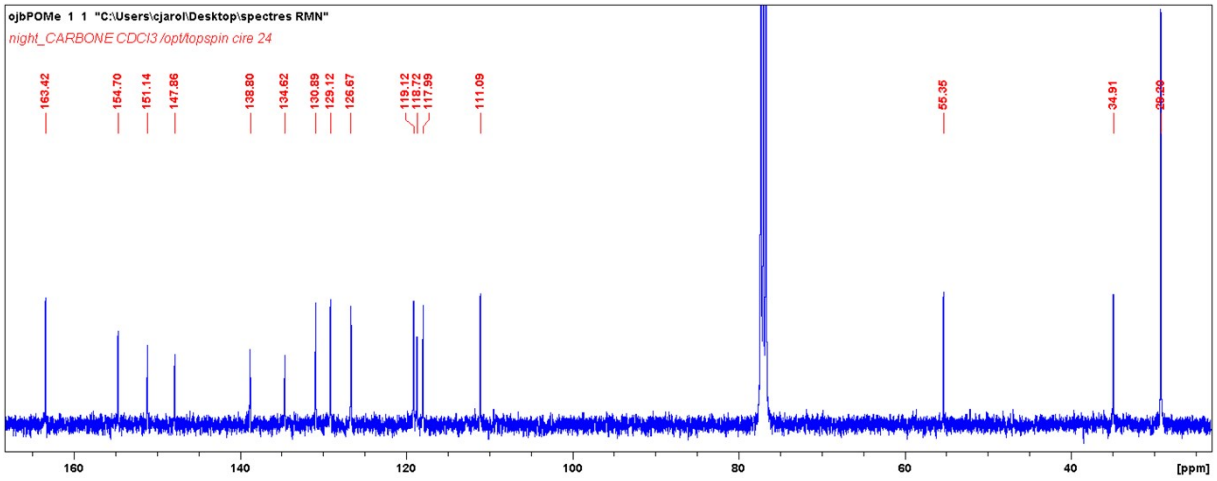

Figure S5. ^{13}C NMR spectrum of $H_2L^{bp,OMe}$

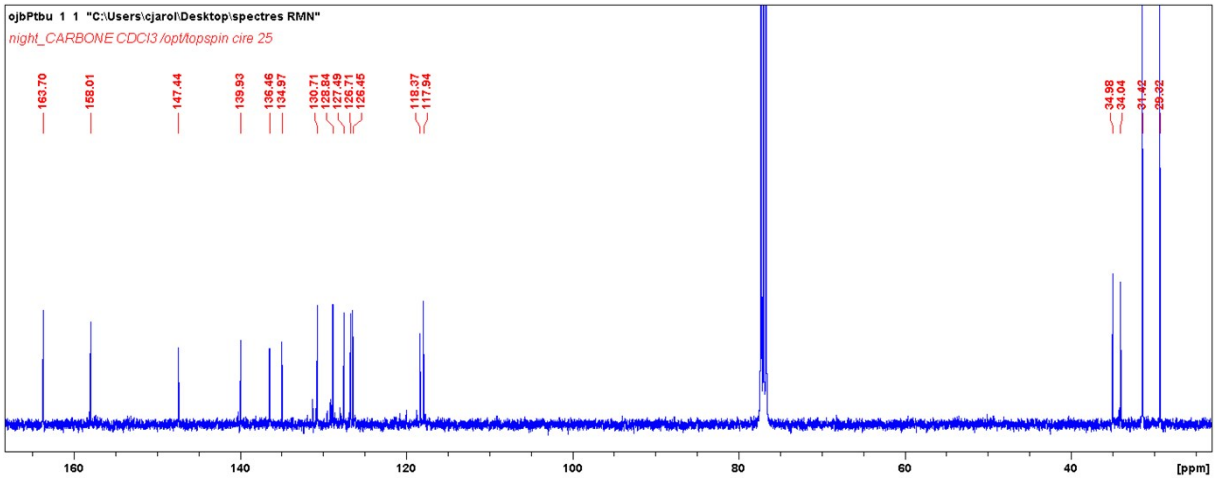

Figure S6. ^{13}C NMR spectrum of $H_2L^{bp,tBu}$

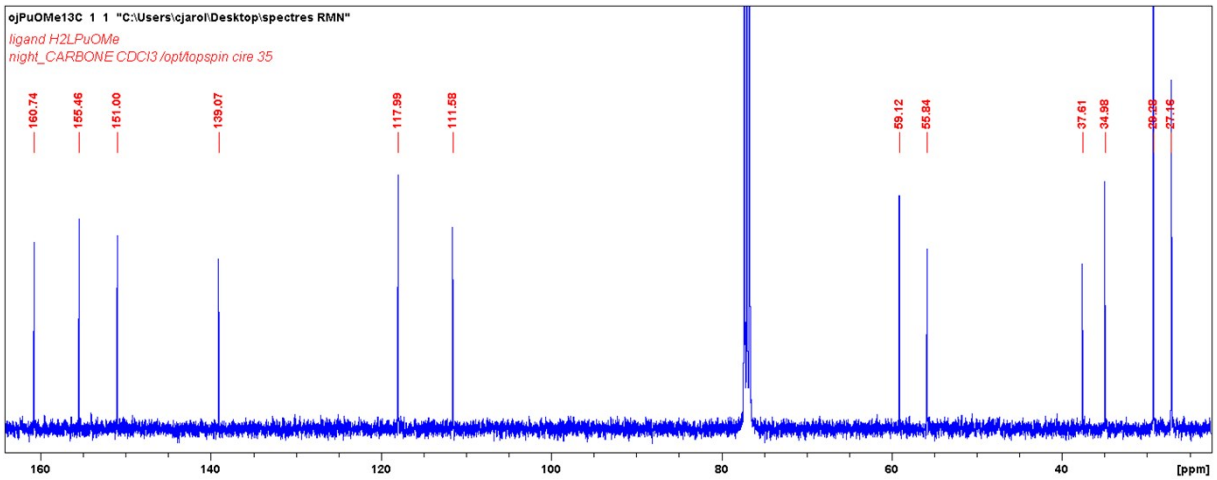

Figure S7. ^{13}C NMR spectrum of $H_2L^{pu,OMe}$

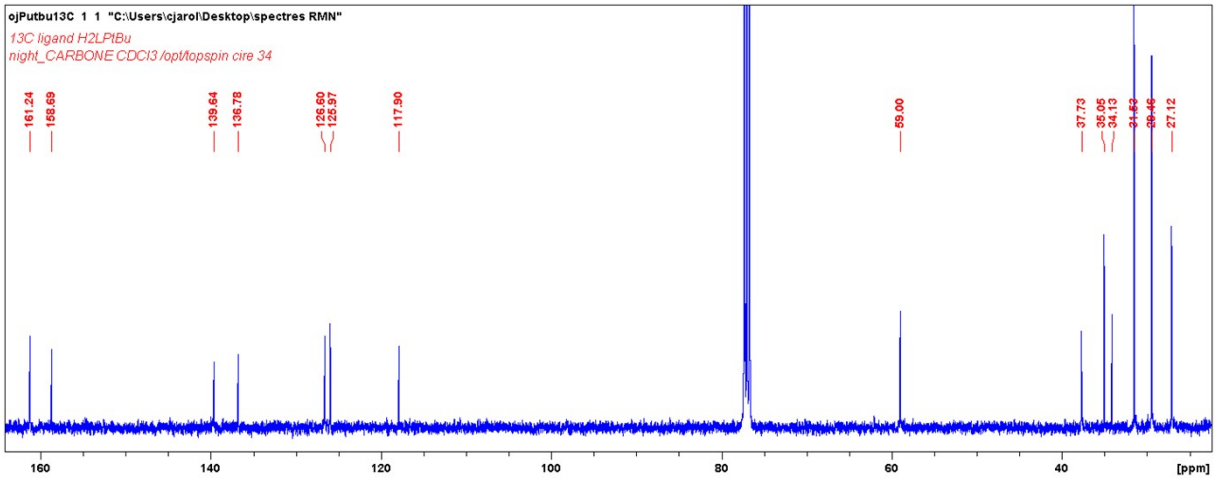

Figure S8. ^{13}C NMR spectrum of $H_2L^{pu,tBu}$

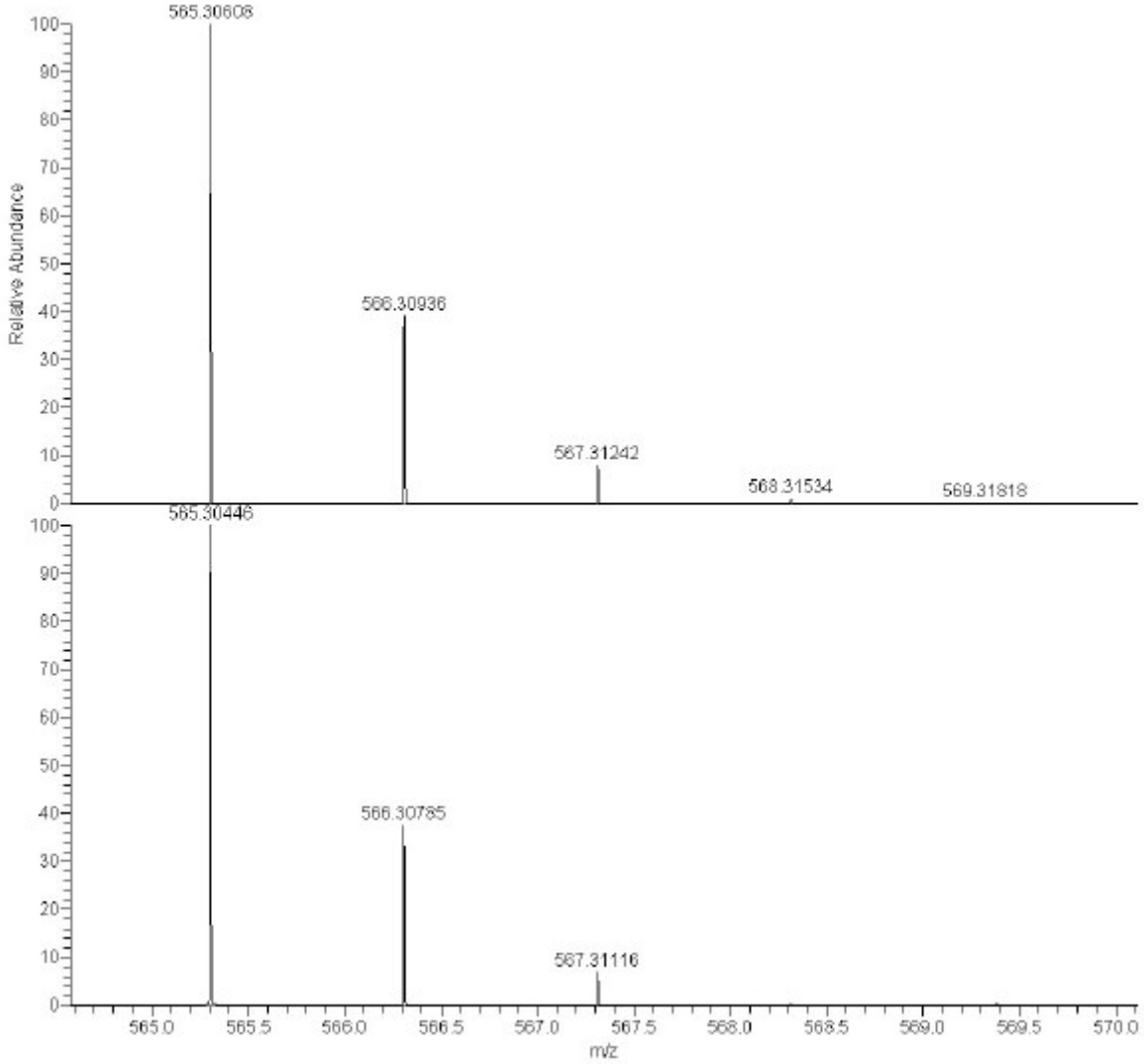

Figure S9. ESI-MS of $\mathbf{H_2L^{bp,OMe}}$

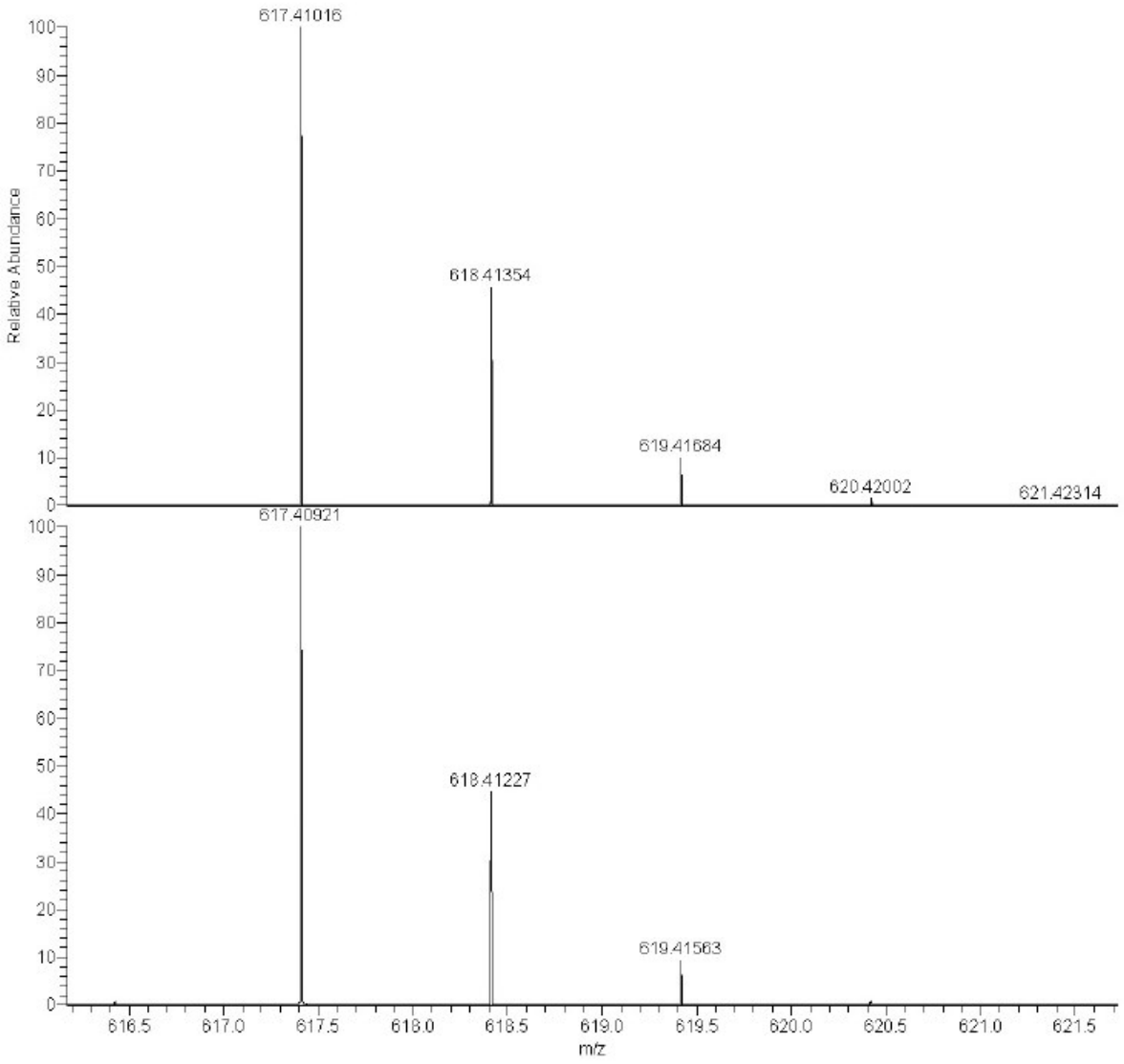

Figure S10. ESI-MS of $H_2L^{bp,tBu}$

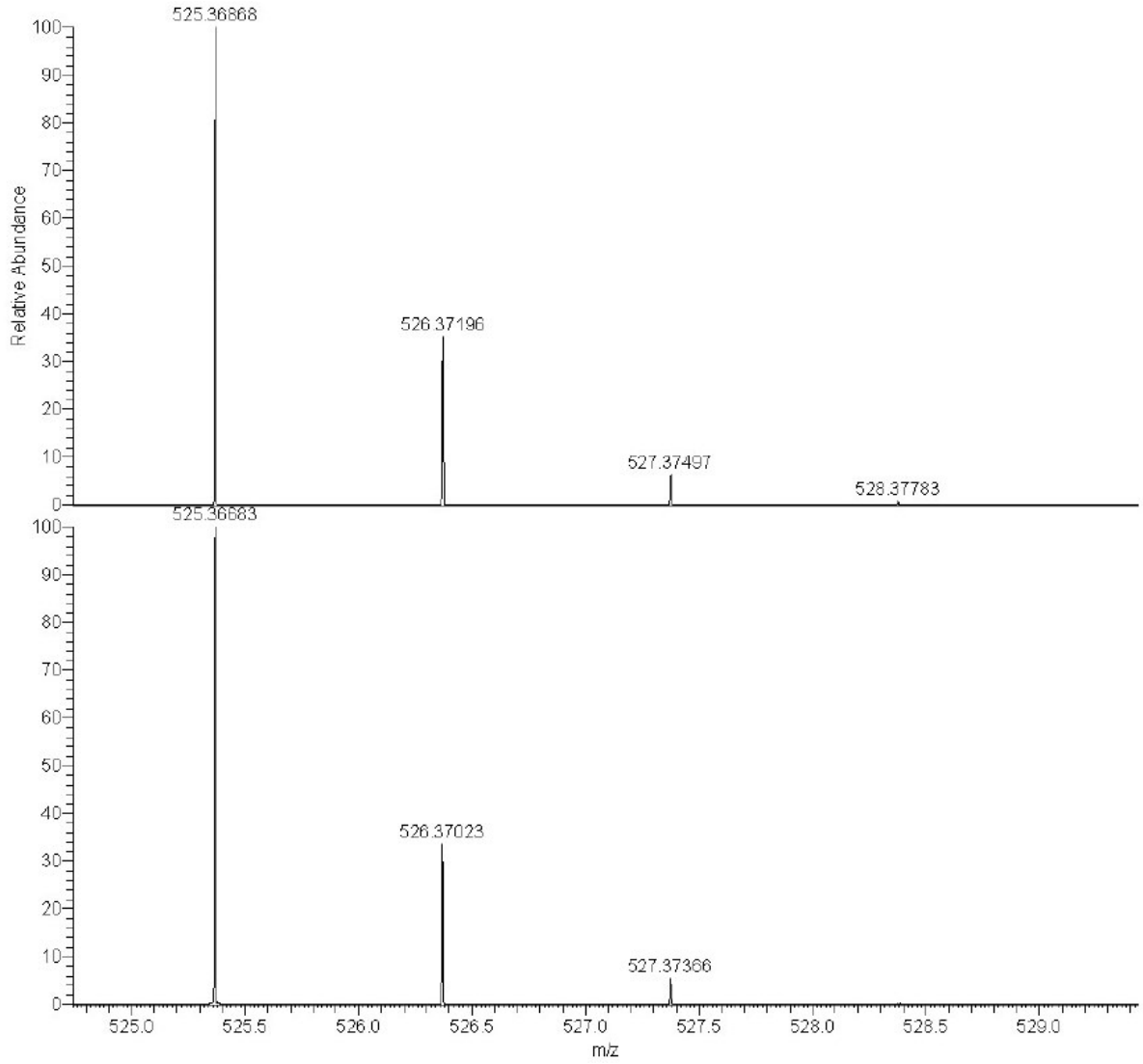

Figure S11. ESI-MS of $H_2L^{pu,OMe}$

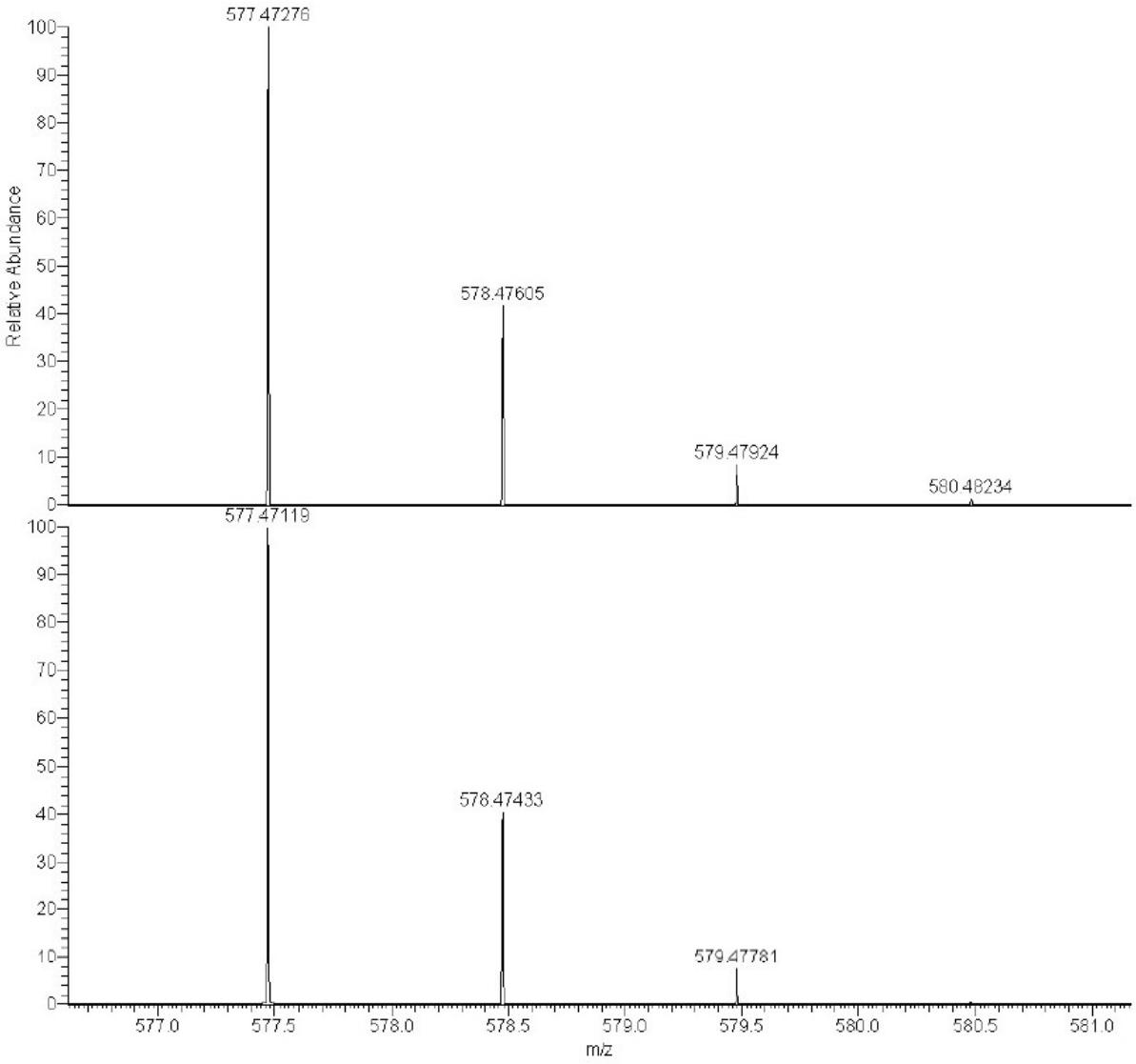

Figure S12. ESI-MS of $\mathbf{H_2L^{pu,tBu}}$

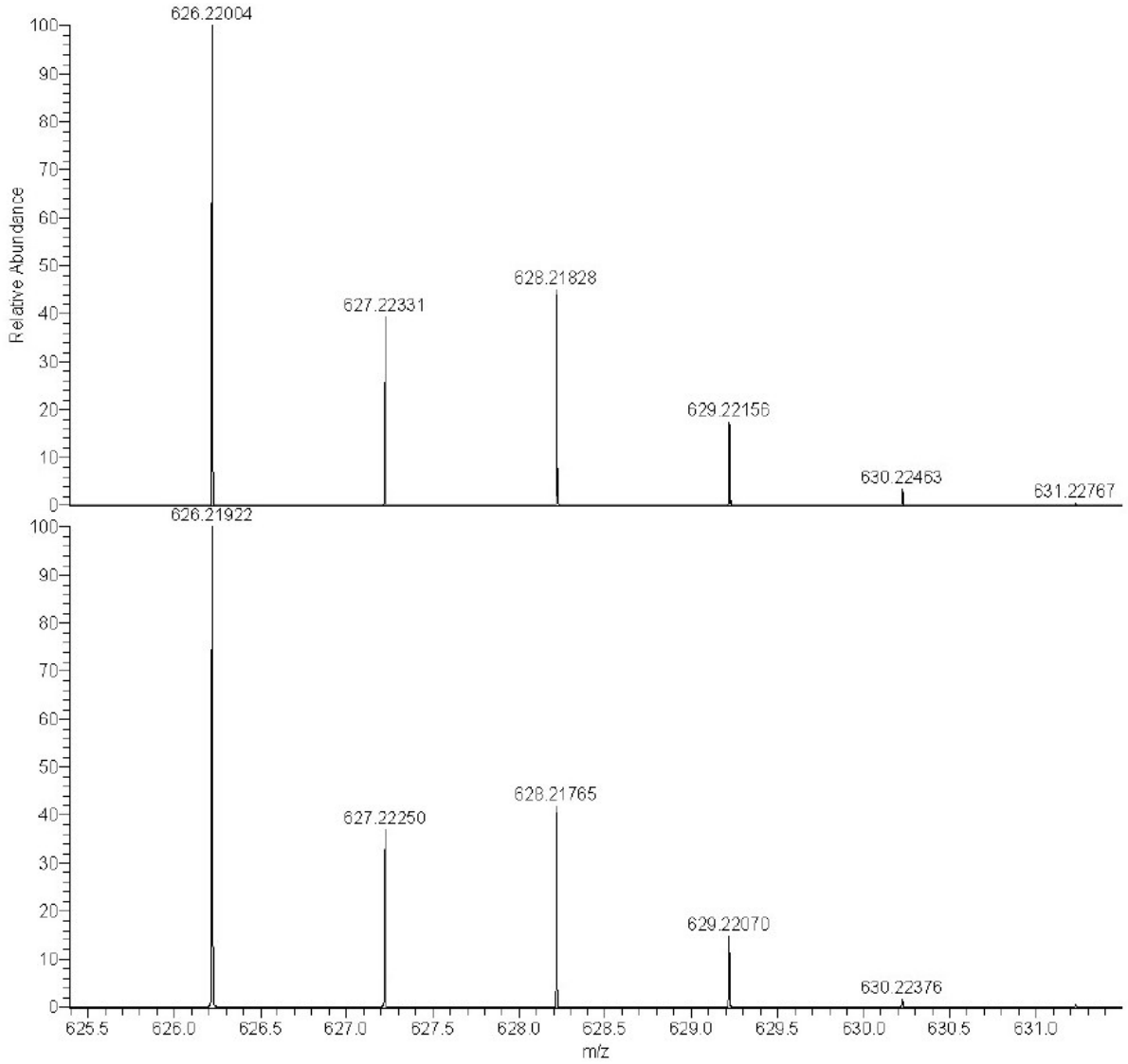

Figure S13. ESI-MS of **CuL^{bp,OMe}**

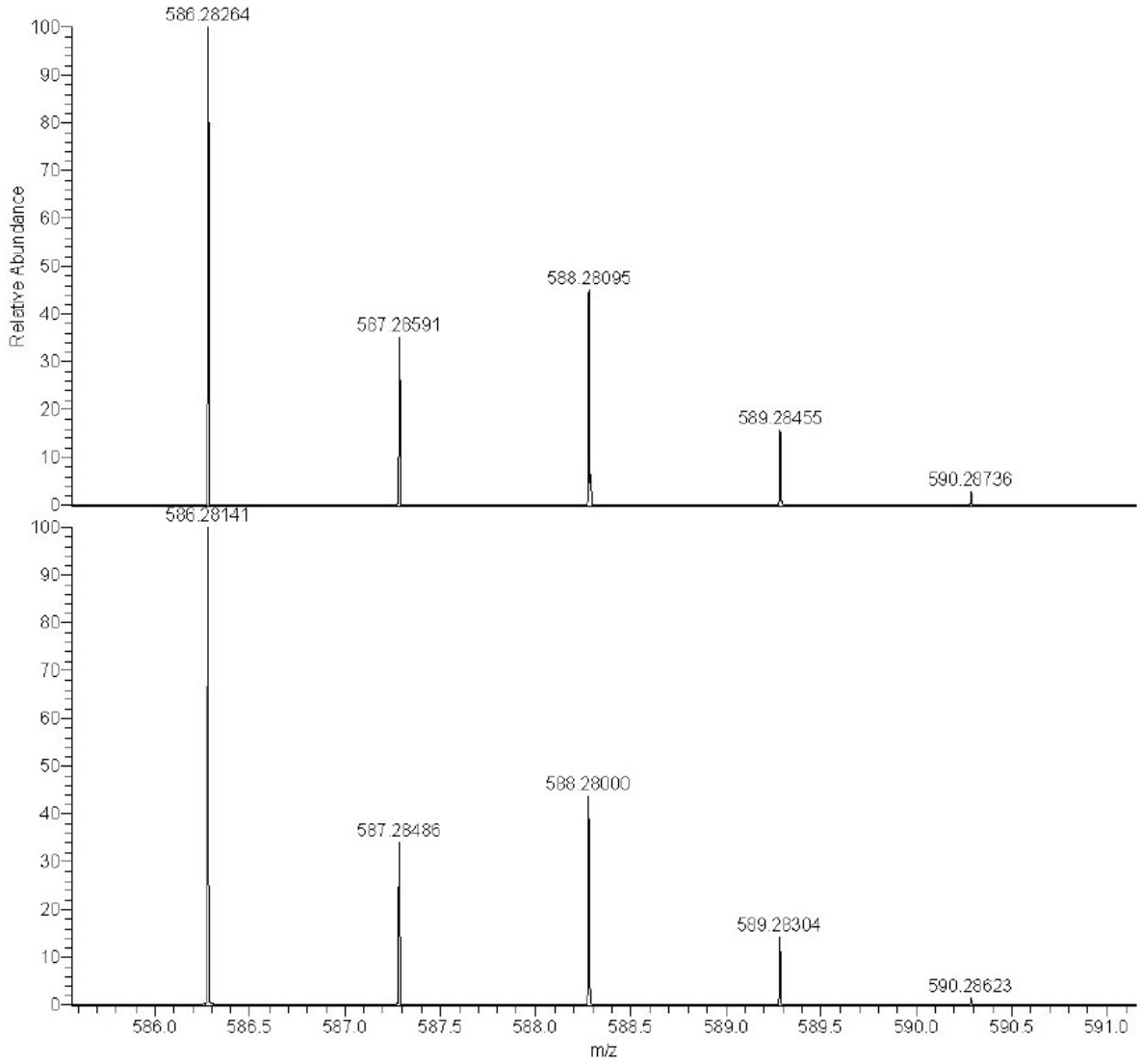

Figure S14. ESI-MS of **CuL^{pu,OMe}**

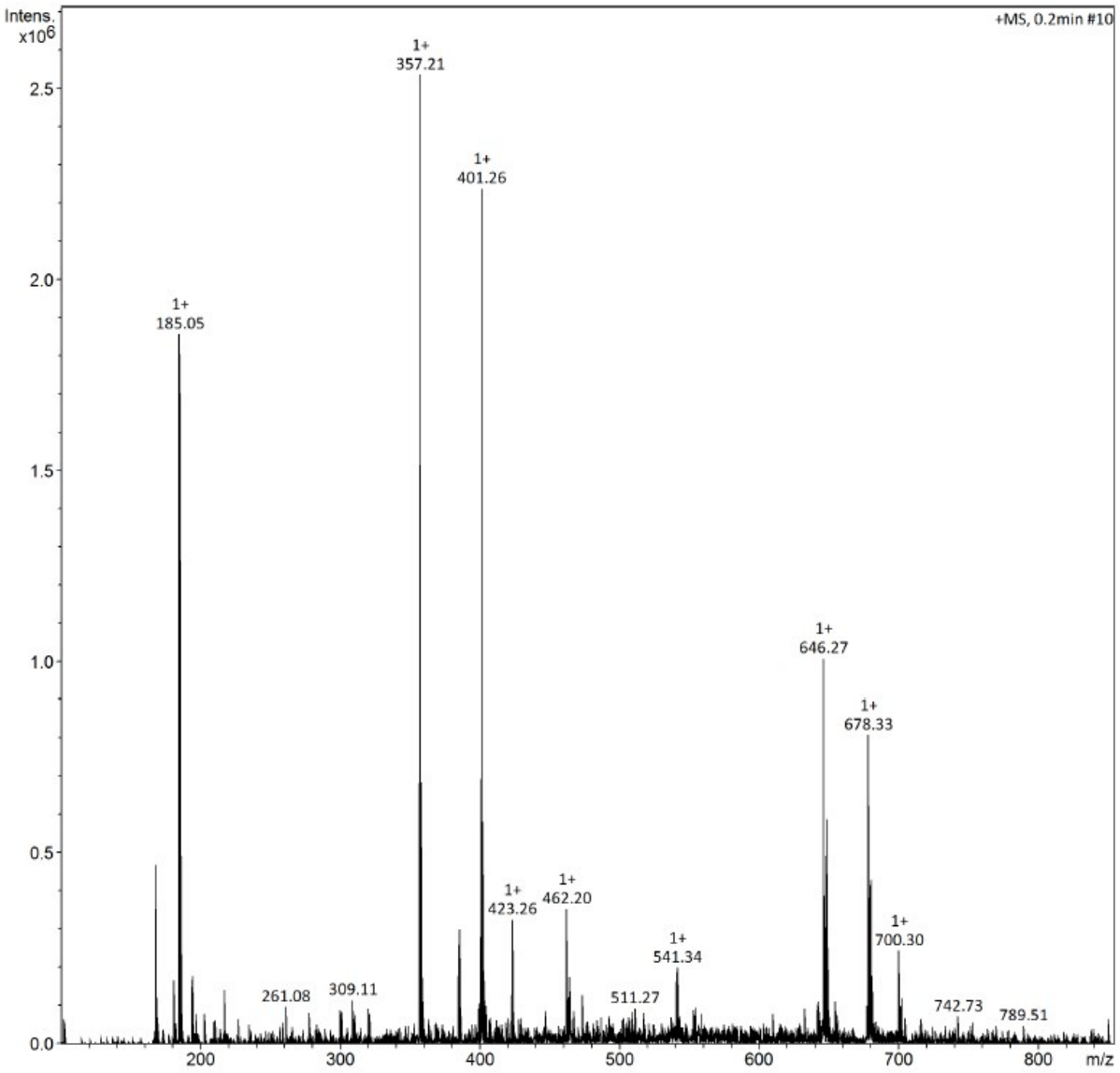

Figure S15. ESI-MS of **CuL^{bp,tBu}**

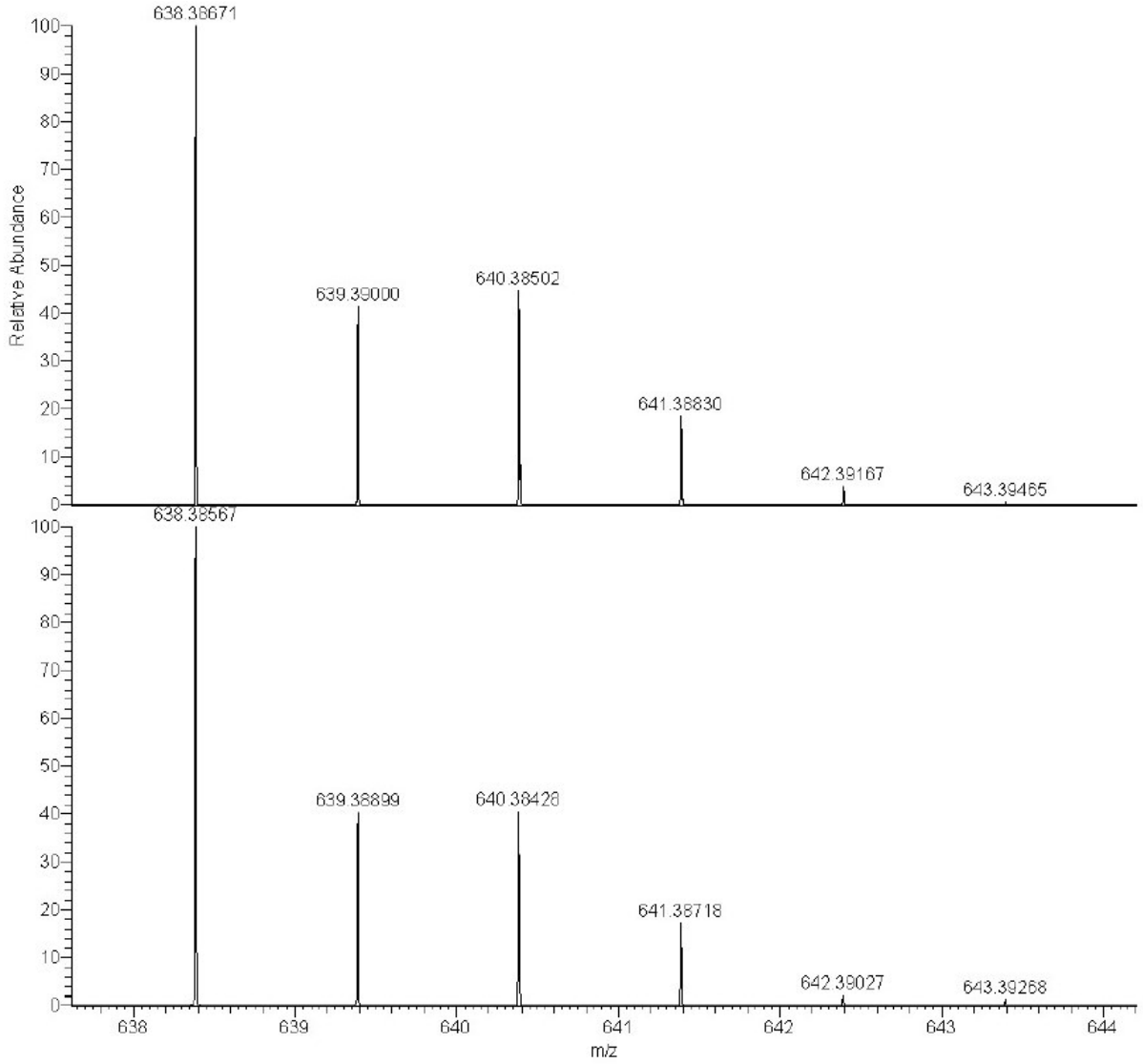

Figure S16. ESI-MS of **CuL^{pu,tBu}**

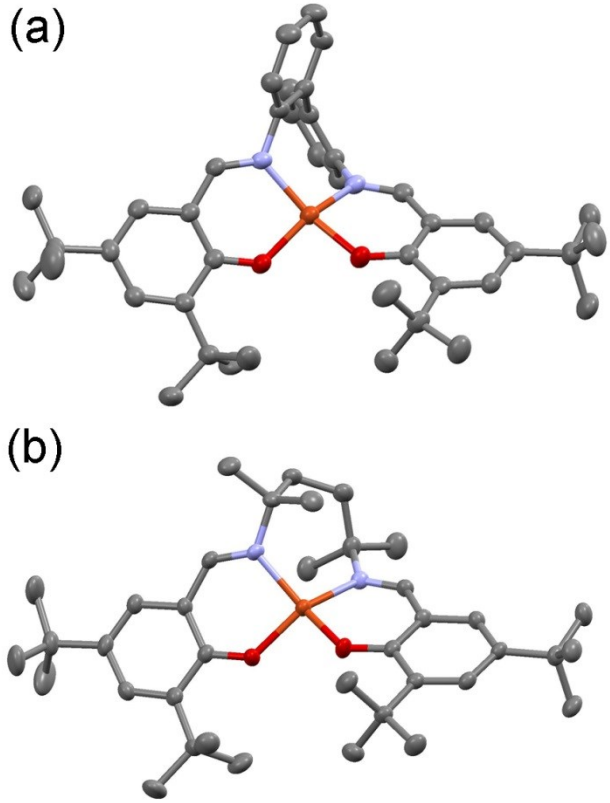

Figure S17. Structures of (a) **CuL^{bp,tBu}** and (b) **CuL^{pu,tBu}**. The hydrogen atoms are omitted for clarity.

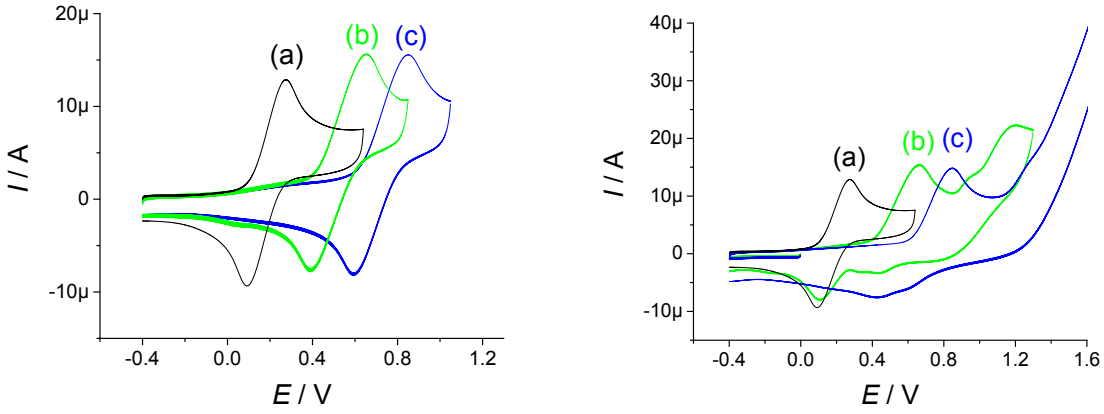

Figure S18. Cyclic voltammetry curves of 0.44 mM CH_2Cl_2 solutions (containing 0.1 M TBAP as supporting electrolyte) of (a) ferrocene, (b) $H_2L^{pu,OMe}$ and (c) $H_2L^{pu,tBu}$ at a carbon electrode. The potentials are referenced vs. the $AgNO_3$ 0.01 M/CH_3CN electrode. *T* = 298 K, scan rate = 0.1 V/sec.

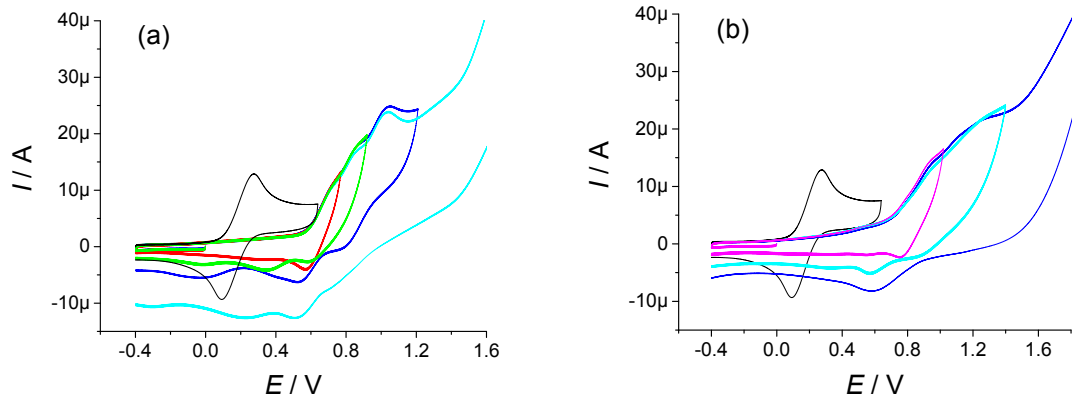

Figure S19. Cyclic voltammetry curves of 0.44 mM CH_2Cl_2 solutions (containing 0.1 M TBAP as supporting electrolyte) of (a) $H_2L^{bp,OMe}$ and (c) $H_2L^{bp,tBu}$ at a carbon electrode. The black curve corresponds to ferrocene. The potentials are referenced vs. the $AgNO_3$ 0.01 M/CH_3CN electrode. *T* = 298 K, scan rate = 0.1 V/sec.

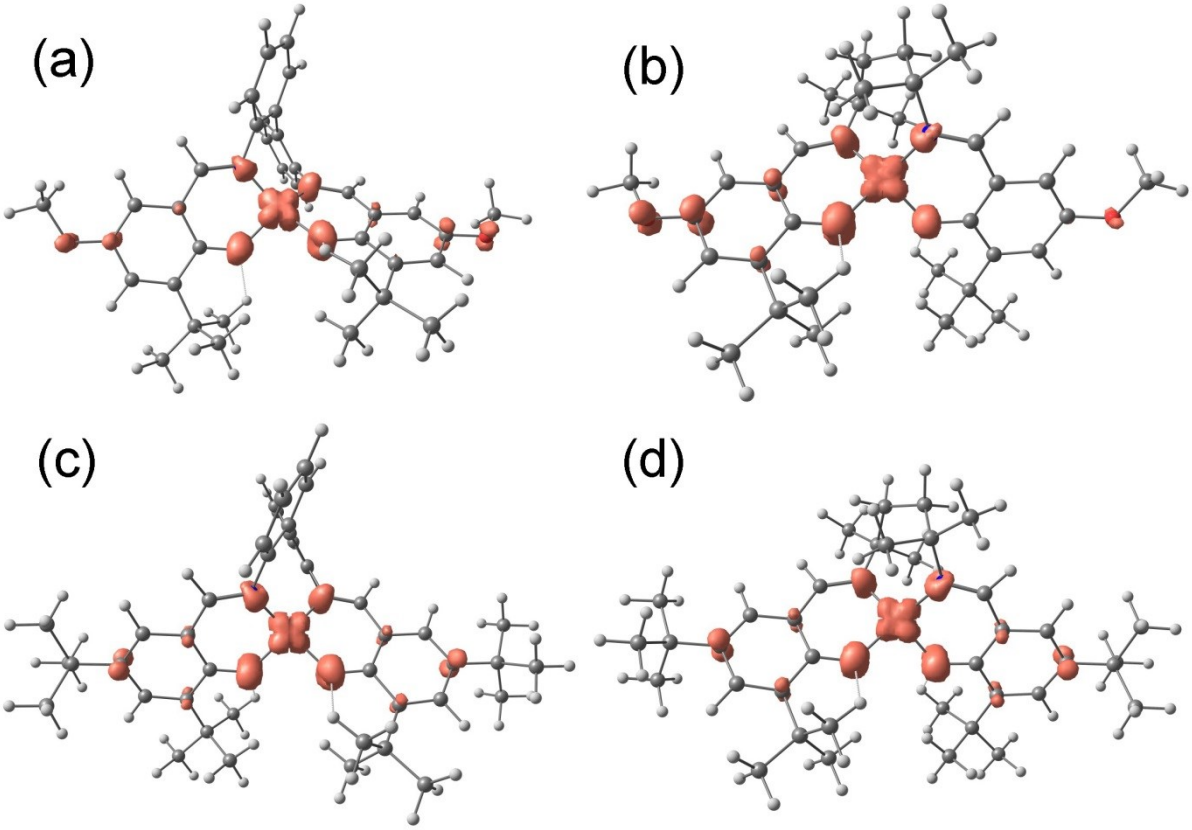

Figure S20. Spin density plot of the triplets: (a) **[CuL^{bp,OMe}]$^+$**, (b) **[CuL^{pu,OMe}]$^+$**, (c) **[CuL^{bp,tBu}]$^+$** and (d) **[CuL^{pu,tBu}]$^+$**.

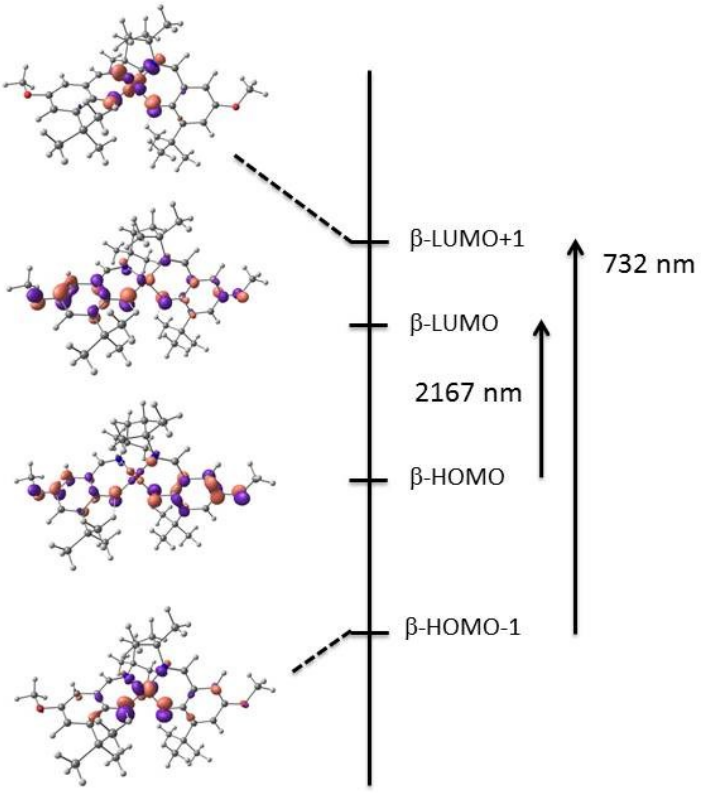

Figure S21. TDDFT-assignment of the low energy band for triplet **[CuL^{pu,OMe}]$^{+}$** (BLYP/TZVP/SCRF).

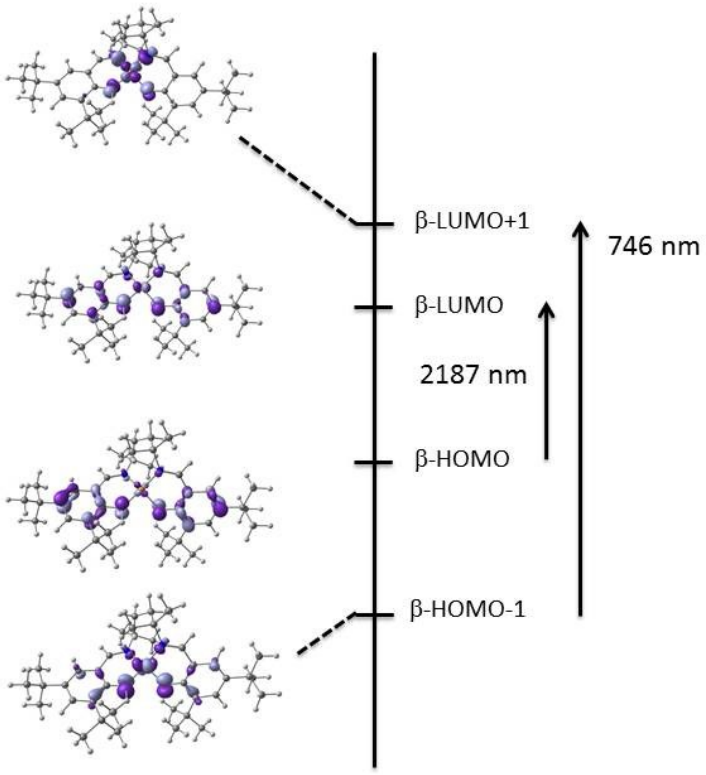

Figure S22. TDDFT-assignment of the low energy band for triplet **[CuL^{pu,tBu}]$^{+}$** (BLYP/TZVP/SCRF).

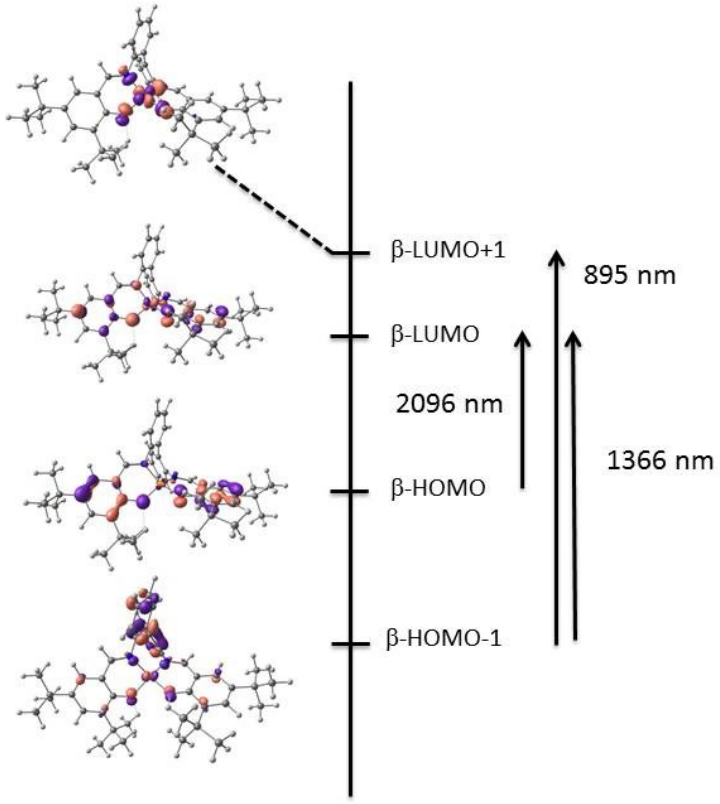

Figure S23. TDDFT-assignment of the low energy band for triplet **[CuL^{bp,tBu}]$^{+}$** (BLYP/TZVP/SCRF).

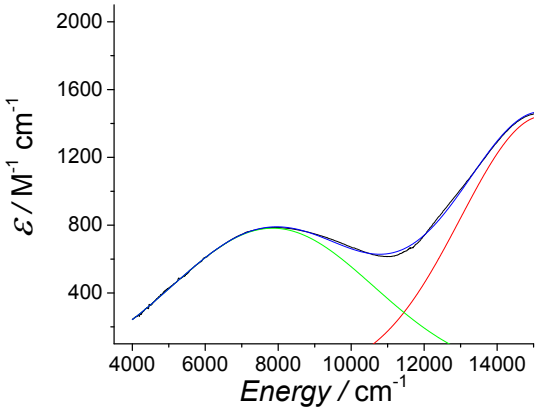

Figure S24. Deconvolution of the low energy region of the absorption spectrum of **[CuL^{bp,OMe}]$^{+}$**; black spectrum: experimental; Blue spectrum: sum of the subspectra.

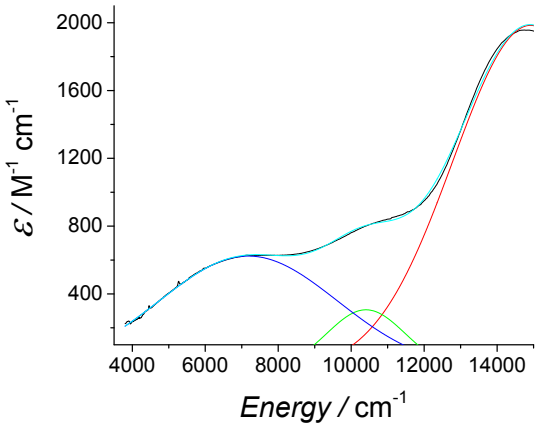

Figure S25. Deconvolution of the low energy region of the absorption spectrum of **[CuL^{pu,OMe}]$^{+}$**; black spectrum: experimental; Cyan spectrum: sum of the subspectra.

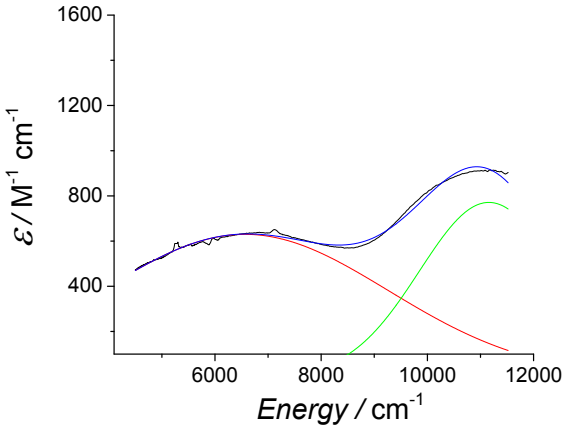

Figure S26. Deconvolution of the low energy region of the absorption spectrum of **[CuL^{bp,tBu}]$^{+}$**; black spectrum: experimental; Blue spectrum: sum of the subspectra.

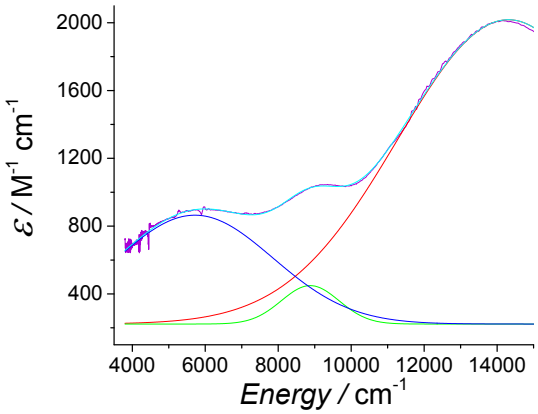

Figure S27. Deconvolution of the low energy region of the absorption spectrum of **[CuL^{pu,tBu}]$^{+}$** ; black spectrum: experimental; Cyan spectrum: sum of the subspectra.

Table S1. Coordination sphere within the neutral complexes (in Å)

Complex	**Bond**	**Exp.** [a]	**(*S* = 1/2)** [b]
CuL^{bp,OMe}	Cu-O	1.895(3) / 1.880(3)	1.901 / 1.901
	Cu-N	1.946(5) / 1.953(4)	1.939 / 1.939
CuL^{pu,OMe}	Cu-O	1.892(2) / 1.892(2)	1.905 / 1.905
	Cu-N	1.972(3) / 1.972(3)	1.961 / 1.961
CuL^{bp,tBu}	Cu-O	1.885(2) / 1.894(2)	1.902 / 1.902
	Cu-N	1.959(3) / 1.951(3)	1.940 / 1.940
CuL^{pu,tBu}	Cu-O	1.896(1) / 1.896(1)	1.906 / 1.906
	Cu-N	1.958(1) / 1.958(1)	1.962 / 1.962

[a] From the crystal structures.

[b] From a B3LYP/6-31g*/SCRF calculation.

Table S2. Coordination sphere within the oxidized complexes (in Å)

Complex	**Bond**	**Exp.** [a]	**(*S* = 1)** [b]	**(*S* = 0)** [b]
[CuL^{bp,OMe}]$^{+}$	Cu-O	1.926(2)/1.926(2)	1.897 / 1.898	1.871 / 1.871
	Cu-N	1.965(3)/1.965(3)	1.933 / 1.933	1.892 / 1.892
[CuL^{pu,OMe}]$^{+}$	Cu-O	1.904(3)/1.911(3)	1.883 / 1.928	1.882 / 1.882
	Cu-N	1.957(3)/1.954(3)	1.946 / 1.962	1.920 / 1.920
[CuL^{bp,tBu}]$^{+}$	Cu-O		1.896 / 1.896	1.856 / 1.856
	Cu-N		1.933 / 1.933	1.881 / 1.881
[CuL^{pu,tBu}]$^{+}$	Cu-O		1.903 / 1.903	1.869 / 1.869
	Cu-N		1.953 / 1.953	1.910 / 1.910

[a] From the crystal structures.

[b] From a B3LYP/6-31g*/SCRF calculation.

Table S3. Distortion within the coordination sphere in the complexes

Complex	Exp. τ_4[a]	Calc. τ_4 [b]	**Complex**	Exp. τ_4[a]	Calc. τ_4 [b]
CuL^{bp,OMe}	0.36	0.49	**[CuL^{bp,OMe}]$^+$**	0.21	0.47
CuL^{pu,OMe}	0.46	0.56	**[CuL^{pu,OMe}]$^+$**	0.43	0.55
CuL^{bp,tBu}	0.40	0.49	**[CuL^{bp,tBu}]$^+$**		0.47
CuL^{pu,tBu}	0.54	0.55	**[CuL^{pu,tBu}]$^+$**		0.55

[a] From the crystal structures.

[b] From a B3LYP/6-31g*/SCRF/CH_2Cl_2 calculation.

XYZ coordinates :

Triplet **[CuL^{bp,OMe}]$^{+}$**

Cu	-0.014247000	0.208282000	-0.025909000
O	1.337911000	-1.021494000	0.380381000
O	-1.318661000	-1.066561000	-0.440529000
N	1.152213000	1.477459000	-0.810079000
N	-1.227488000	1.428125000	0.778343000
C	2.613523000	-0.937534000	0.155017000
C	-3.253846000	0.165469000	0.236927000
C	-4.649508000	0.221165000	0.349313000
H	-5.141761000	1.130557000	0.678949000
O	-6.754985000	-0.762879000	0.180033000
C	5.429350000	-0.666936000	-0.055863000
C	-2.591618000	-1.046802000	-0.183751000
C	0.584077000	2.620760000	-1.466528000
C	-0.032843000	3.657206000	-0.740279000
C	3.227433000	0.299615000	-0.256658000
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C	4.824779000	-1.905574000	0.279049000
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H	3.478652000	-5.514560000	1.058925000
H	4.633263000	-4.334540000	1.686261000
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H	0.644078000	5.643780000	3.411581000
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H	-4.355228000	-4.860544000	0.093196000
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H	-8.381603000	0.371310000	0.544982000
H	-7.051187000	1.265333000	-0.241060000

Singlet **[CuL^{bp,OMe}]$^{+}$**

Cu	-0.000146000	0.218265000	-0.001234000
O	1.330527000	-1.037734000	0.391252000
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C	5.423196000	-0.759715000	-0.066936000
C	-2.606088000	-0.976772000	-0.155864000
C	0.629730000	2.607589000	-1.464734000
C	0.037638000	3.661159000	-0.742637000
C	3.239684000	0.249149000	-0.254001000
O	6.774236000	-0.801891000	-0.105867000
C	4.796991000	-1.989746000	0.261376000
H	5.464466000	-2.823770000	0.439538000
C	2.482192000	1.370803000	-0.713471000
H	3.060021000	2.223450000	-1.075261000
C	0.206546000	3.748707000	-3.558513000
H	0.271367000	3.772826000	-4.641985000
C	-0.375397000	4.805846000	-2.858992000
H	-0.770994000	5.664926000	-3.392113000
C	-3.431128000	-2.154533000	-0.342842000
C	-2.481009000	1.372187000	0.714406000
H	-3.058111000	2.224781000	1.077504000
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H	5.083669000	1.285675000	-0.672908000
C	-2.809356000	-3.523511000	-0.670448000
C	0.705950000	2.649135000	-2.861218000
H	1.159192000	1.816380000	-3.390047000
C	3.429240000	-2.156900000	0.343006000
C	-0.627343000	2.608499000	1.463065000
C	-0.034123000	3.661297000	0.740746000
C	0.460794000	4.756130000	1.465265000

H	0.922176000	5.574536000	0.920588000
C	-0.456290000	4.756284000	-1.467383000
H	-0.916845000	5.575275000	-0.922886000
C	-5.423883000	-0.756872000	0.071416000
C	3.878172000	-4.627068000	0.799125000
H	4.463667000	-4.744583000	-0.119723000
H	3.382155000	-5.582759000	0.998619000
H	4.568144000	-4.436174000	1.628834000
C	-0.703700000	2.650554000	2.859528000
H	-1.157776000	1.818379000	3.388552000
C	-4.798716000	-1.986892000	-0.258821000
H	-5.466837000	-2.820487000	-0.436532000
C	0.379833000	4.806162000	2.856851000
H	0.776243000	5.664989000	3.389774000
C	-3.881756000	-4.624148000	-0.800755000
H	-4.466172000	-4.742308000	0.118695000
H	-3.386365000	-5.579849000	-1.001763000
H	-4.572678000	-4.432208000	-1.629433000
C	-1.857302000	-3.931603000	0.480365000
H	-1.059715000	-3.201217000	0.623884000
H	-1.397349000	-4.900674000	0.254349000
H	-2.411371000	-4.033482000	1.421029000
C	-2.041019000	-3.462609000	-2.013792000
H	-2.715997000	-3.190145000	-2.833848000
H	-1.618238000	-4.448369000	-2.240548000
H	-1.226657000	-2.737114000	-1.980640000
C	2.806383000	-3.525864000	0.668518000
C	7.484037000	0.392981000	-0.440843000
H	7.238995000	0.723062000	-1.456785000
H	8.541241000	0.133844000	-0.385261000
H	7.261831000	1.194419000	0.272702000
C	2.036434000	-3.465862000	2.010985000
H	2.710578000	-3.194625000	2.832133000
H	1.612791000	-4.451599000	2.236225000
H	1.222538000	-2.739858000	1.977582000
C	-0.203244000	3.749802000	3.556589000
H	-0.268129000	3.774254000	4.640050000
C	1.855617000	-3.932532000	-0.483868000
H	1.058421000	-3.201784000	-0.627725000
H	1.395078000	-4.901667000	-0.259325000
H	2.410831000	-4.033722000	-1.423929000
C	-7.483613000	0.396494000	0.449132000
H	-7.237040000	0.725914000	1.464929000
H	-8.541039000	0.137964000	0.394895000
H	-7.262002000	1.198242000	-0.264256000

Triplet **[CuL^{bp,tBu}]$^{+}$**

Cu	0.000006000	0.306467000	-0.000003000
O	-1.348775000	-0.997904000	-0.273175000
O	1.348779000	-0.997864000	0.273326000
N	-1.205731000	1.562604000	0.840068000
N	1.205725000	1.562511000	-0.840233000
C	-2.630466000	-0.902951000	-0.148304000
C	3.238933000	0.232611000	-0.507300000
C	4.632213000	0.289005000	-0.687016000
H	5.042083000	1.154607000	-1.195123000
C	6.993921000	-0.687670000	-0.389557000
C	-5.469651000	-0.718127000	0.222761000
C	2.630473000	-0.902921000	0.148429000
C	-0.634754000	2.695740000	1.496516000
C	-0.018109000	3.717850000	0.743816000

C	-3.238934000	0.232660000	0.507288000
C	-6.993921000	-0.687616000	0.389568000
C	-4.854716000	-1.815757000	-0.437534000
H	-5.506963000	-2.597738000	-0.803333000
C	-2.480039000	1.342118000	1.006524000
H	-3.046825000	2.087296000	1.568786000
C	-0.158501000	3.875424000	3.561075000
H	-0.207445000	3.924386000	4.644554000
C	0.446051000	4.899145000	2.831211000
H	0.873186000	5.757852000	3.340069000
C	3.493051000	-1.958134000	0.643983000
C	2.480037000	1.342010000	-1.006656000
H	3.046820000	2.087128000	-1.569000000
C	-4.632212000	0.289077000	0.686974000
H	-5.042092000	1.154736000	1.194977000
C	2.909656000	-3.187730000	1.363443000
C	-0.699481000	2.778359000	2.893416000
H	-1.162023000	1.968217000	3.449208000
C	-3.493042000	-1.958222000	-0.643750000
C	0.634750000	2.695577000	-1.496802000
C	0.018110000	3.717771000	-0.744213000
C	-7.663457000	-0.731506000	-1.006813000
H	-7.370517000	0.135104000	-1.610119000
H	-8.753720000	-0.716291000	-0.895748000
H	-7.399490000	-1.636538000	-1.563879000
C	-0.507671000	4.816396000	-1.440836000
H	-0.978517000	5.613739000	-0.873642000
C	0.507673000	4.816548000	1.440322000
H	0.978524000	5.613829000	0.873043000
C	5.469653000	-0.718156000	-0.222721000
C	-4.012481000	-4.152853000	-1.844111000
H	-4.600265000	-4.557561000	-1.012543000
H	-3.544581000	-5.000250000	-2.356352000
H	-4.697650000	-3.676729000	-2.554847000
C	0.699472000	2.778043000	-2.893711000
H	1.162011000	1.967840000	-3.449416000
C	-7.442137000	-1.920527000	1.213728000
H	-7.165561000	-2.863019000	0.729973000
H	-8.531996000	-1.913676000	1.329701000
H	-6.993064000	-1.908306000	2.213239000
C	4.854722000	-1.815710000	0.437705000
H	5.506970000	-2.597660000	0.803568000
C	-0.446052000	4.898841000	-2.831734000
H	-0.873185000	5.757493000	-3.340685000
C	4.012461000	-4.152713000	1.844482000
H	4.600176000	-4.557498000	1.012903000
H	3.544543000	-5.000057000	2.356794000
H	4.697694000	-3.676590000	2.555157000
C	1.994465000	-3.973479000	0.391443000
H	1.166933000	-3.359265000	0.033688000
H	1.578985000	-4.849692000	0.903128000
H	2.563759000	-4.328994000	-0.475546000
C	2.104984000	-2.745491000	2.611643000
H	2.747882000	-2.206947000	3.317948000
H	1.710163000	-3.630243000	3.124625000
H	1.265619000	-2.100959000	2.345467000
C	-2.909652000	-3.187905000	-1.363060000
C	-7.475311000	0.582008000	1.116801000
H	-7.061639000	0.655828000	2.129024000
H	-8.566218000	0.558151000	1.208397000
H	-7.210423000	1.492565000	0.567475000
C	7.663478000	-0.731564000	1.006813000
H	7.370576000	0.135064000	1.610114000

H	8.753740000	-0.716388000	0.895733000
H	7.399488000	-1.636579000	1.563896000
C	-2.104850000	-2.745806000	-2.611227000
H	-2.747655000	-2.207267000	-3.317620000
H	-1.710048000	-3.630619000	-3.124116000
H	-1.265461000	-2.101313000	-2.345028000
C	0.158494000	3.875038000	-3.561488000
H	0.207436000	3.923882000	-4.644973000
C	-1.994594000	-3.973645000	-0.390925000
H	-1.167035000	-3.359472000	-0.033163000
H	-1.579153000	-4.849936000	-0.902506000
H	-2.563977000	-4.329039000	0.476055000
C	7.442109000	-1.920588000	-1.213720000
H	7.165538000	-2.863076000	-0.729955000
H	8.531965000	-1.913748000	-1.329721000
H	6.993012000	-1.908370000	-2.213220000
C	7.475317000	0.581944000	-1.116803000
H	7.061566000	0.655802000	-2.128990000
H	8.566215000	0.558037000	-1.208486000
H	7.210518000	1.492504000	-0.567439000

Singlet **[CuL^{bp,tBu}]$^{+}$**

Cu	0.000010000	0.336515000	0.000036000
O	1.305976000	-0.946710000	0.302603000
O	-1.305945000	-0.946730000	-0.302530000
N	1.171624000	1.584114000	-0.780120000
N	-1.171628000	1.584108000	0.780145000
C	2.594552000	-0.868204000	0.114850000
C	-3.228801000	0.362327000	0.265502000
C	-4.637495000	0.457520000	0.349668000
H	-5.061178000	1.408706000	0.651765000
C	-6.981672000	-0.576921000	0.139146000
C	5.447993000	-0.627387000	-0.077297000
C	-2.594528000	-0.868215000	-0.114834000
C	0.607862000	2.720245000	-1.454800000
C	0.030913000	3.787409000	-0.741072000
C	3.228813000	0.362323000	-0.265548000
C	6.981684000	-0.576940000	-0.139316000
C	4.795192000	-1.846881000	0.246324000
H	5.425826000	-2.705245000	0.440067000
C	2.473609000	1.482200000	-0.714524000
H	3.045759000	2.331770000	-1.090811000
C	0.171319000	3.835317000	-3.558320000
H	0.224260000	3.844902000	-4.642537000
C	-0.393260000	4.906397000	-2.866440000
H	-0.786059000	5.762062000	-3.406942000
C	-3.421770000	-2.030529000	-0.319370000
C	-2.473610000	1.482206000	0.714493000
H	-3.045768000	2.331785000	1.090747000
C	4.637504000	0.457504000	-0.349778000
H	5.061180000	1.408679000	-0.651919000
C	-2.805117000	-3.402205000	-0.653303000
C	0.668494000	2.739728000	-2.852203000
H	1.110000000	1.896840000	-3.374654000
C	3.421790000	-2.030515000	0.319394000
C	-0.607872000	2.720232000	1.454838000
C	-0.030924000	3.787403000	0.741121000
C	7.561186000	-0.954367000	1.246035000
H	7.230346000	-0.247830000	2.015697000
H	8.656637000	-0.932122000	1.211898000
H	7.259861000	-1.959805000	1.558640000

C	0.461704000	4.876658000	1.472598000
H	0.910667000	5.706398000	0.934859000
C	-0.461716000	4.876670000	-1.472538000
H	-0.910679000	5.706404000	-0.934790000
C	-5.447980000	-0.627372000	0.077175000
C	3.881222000	-4.494880000	0.818540000
H	4.480482000	-4.626052000	-0.089636000
H	3.387284000	-5.449670000	1.027668000
H	4.558253000	-4.286281000	1.654700000
C	-0.668505000	2.739701000	2.852242000
H	-1.110012000	1.896807000	3.374684000
C	7.491123000	-1.582365000	-1.200496000
H	7.187966000	-2.610065000	-0.974253000
H	8.586390000	-1.560968000	-1.240251000
H	7.109370000	-1.329187000	-2.196113000
C	-4.795171000	-1.846881000	-0.246369000
H	-5.425800000	-2.705255000	-0.440098000
C	0.393245000	4.906371000	2.866500000
H	0.786042000	5.762031000	3.407011000
C	-3.881281000	-4.494878000	-0.818374000
H	-4.480550000	-4.625966000	0.089808000
H	-3.387392000	-5.449704000	-1.027449000
H	-4.558302000	-4.286287000	-1.654545000
C	-1.874032000	-3.836457000	0.504980000
H	-1.071660000	-3.115955000	0.669881000
H	-1.419919000	-4.806945000	0.272623000
H	-2.442725000	-3.945499000	1.436102000
C	-2.014511000	-3.329125000	-1.982991000
H	-2.674851000	-3.045011000	-2.811061000
H	-1.588845000	-4.312526000	-2.215035000
H	-1.198708000	-2.605995000	-1.928293000
C	2.805110000	-3.402161000	0.653411000
C	7.499762000	0.824511000	-0.513060000
H	7.153115000	1.137986000	-1.504510000
H	8.594599000	0.815238000	-0.535740000
H	7.190744000	1.581906000	0.216402000
C	-7.561138000	-0.954196000	-1.246262000
H	-7.230256000	-0.247588000	-2.015842000
H	-8.656588000	-0.931929000	-1.212158000
H	-7.259828000	-1.959610000	-1.558961000
C	2.014509000	-3.328969000	1.983094000
H	2.674861000	-3.044836000	2.811147000
H	1.588797000	-4.312336000	2.215194000
H	1.198738000	-2.605803000	1.928352000
C	-0.171333000	3.835283000	3.558369000
H	-0.224277000	3.844859000	4.642586000
C	1.873991000	-3.836432000	-0.504835000
H	1.071661000	-3.115890000	-0.669773000
H	1.419823000	-4.806879000	-0.272414000
H	2.442670000	-3.945563000	-1.435955000
C	-7.491146000	-1.582458000	1.200203000
H	-7.187958000	-2.610130000	0.973870000
H	-8.586415000	-1.561084000	1.239909000
H	-7.109442000	-1.329373000	2.195863000
C	-7.499753000	0.824494000	0.513022000
H	-7.153185000	1.137839000	1.504542000
H	-8.594592000	0.815242000	0.535610000
H	-7.190656000	1.581973000	-0.216318000

Singlet **[CuL^{pu,OMe}]$^{+}$**

Cu	-0.000006000	-0.626107000	0.000120000
O	-1.300790000	0.662437000	-0.436445000
N	-1.207046000	-1.811582000	0.906975000
C	-2.574566000	0.651202000	-0.209025000
C	-0.702622000	-3.077302000	1.561624000
C	-3.228019000	-0.535180000	0.278622000
C	-2.734434000	3.166092000	-0.883595000
C	-2.497029000	-1.652997000	0.799889000
H	-3.137189000	-2.443081000	1.187432000
C	-3.379249000	1.829657000	-0.478864000
C	-5.394442000	0.498259000	0.023737000
C	-0.580204000	-4.205185000	0.502732000
H	-0.491140000	-5.143682000	1.063245000
H	-1.537013000	-4.269702000	-0.030201000
C	-4.748833000	1.692070000	-0.390397000
H	-5.402608000	2.521794000	-0.629373000
C	-4.633876000	-0.600811000	0.384204000
H	-5.091732000	-1.505693000	0.766162000
C	0.627253000	-2.756301000	2.262324000
H	1.391420000	-2.380065000	1.581895000
H	1.022542000	-3.662340000	2.732460000
H	0.469690000	-2.008750000	3.046923000
C	-1.906398000	3.008696000	-2.182984000
H	-1.089485000	2.296439000	-2.059258000
H	-1.481017000	3.978621000	-2.466566000
H	-2.542567000	2.667858000	-3.008648000
O	-6.744830000	0.565778000	0.059890000
C	-1.680975000	-3.565716000	2.656486000
H	-1.970924000	-2.748696000	3.324919000
H	-1.173457000	-4.327903000	3.254258000
H	-2.584464000	-4.030287000	2.249955000
C	-1.833671000	3.646283000	0.279834000
H	-2.432299000	3.825952000	1.180605000
H	-1.343053000	4.587860000	0.007538000
H	-1.060143000	2.914124000	0.516747000
C	-3.790502000	4.259668000	-1.142382000
H	-4.453055000	4.004149000	-1.977227000
H	-3.278730000	5.192206000	-1.402538000
H	-4.406890000	4.458651000	-0.258459000
C	-7.474329000	-0.588740000	0.481657000
H	-7.272826000	-1.442380000	-0.175364000
H	-8.526934000	-0.313911000	0.414483000
H	-7.228075000	-0.852261000	1.516616000
O	1.300932000	0.662205000	0.436863000
N	1.206981000	-1.811593000	-0.906810000
C	2.574663000	0.651094000	0.209189000
C	0.702415000	-3.077158000	-1.561687000
C	3.228069000	-0.535300000	-0.278548000
C	2.734573000	3.165998000	0.883667000
C	2.496957000	-1.653070000	-0.799828000
H	3.137076000	-2.443131000	-1.187494000
C	3.379331000	1.829554000	0.478871000
C	5.394491000	0.498137000	-0.023944000
C	0.579793000	-4.205191000	-0.502964000
H	0.490591000	-5.143590000	-1.063621000
H	1.536587000	-4.269937000	0.029966000
C	4.748911000	1.691962000	0.390243000
H	5.402762000	2.521653000	0.629129000
C	4.633876000	-0.600954000	-0.384315000
H	5.091692000	-1.505824000	-0.766357000
C	-0.627359000	-2.755851000	-2.262429000
H	-1.391565000	-2.379726000	-1.581983000
H	-1.022680000	-3.661737000	-2.732834000

H	-0.469652000	-2.008115000	-3.046822000
C	1.906749000	3.008646000	2.183188000
H	1.089874000	2.296314000	2.059640000
H	1.481338000	3.978561000	2.466759000
H	2.543072000	2.667926000	3.008783000
O	6.744854000	0.565657000	-0.060271000
C	1.680774000	-3.565545000	-2.656542000
H	1.970912000	-2.748469000	-3.324824000
H	1.173181000	-4.327555000	-3.254476000
H	2.584152000	-4.030331000	-2.250012000
C	1.833600000	3.646103000	-0.279649000
H	2.432073000	3.825723000	-1.180531000
H	1.343010000	4.587690000	-0.007331000
H	1.060047000	2.913910000	-0.516364000
C	3.790657000	4.259596000	1.142217000
H	4.453426000	4.004065000	1.976886000
H	3.278924000	5.192113000	1.402529000
H	4.406821000	4.458620000	0.258148000
C	7.474347000	-0.588918000	-0.481894000
H	7.272791000	-1.442498000	0.175184000
H	8.526960000	-0.314121000	-0.414694000
H	7.228148000	-0.852509000	-1.516852000

Triplet **[CuL^{pu,OMe}]$^{+}$**

Cu	-0.013570000	-0.554722000	-0.025161000
O	-1.323410000	0.760081000	-0.343947000
N	-1.175064000	-1.745759000	0.984365000
C	-2.611530000	0.688655000	-0.179580000
C	-0.626706000	-2.991849000	1.626215000
C	-3.207315000	-0.407096000	0.529867000
C	-2.892025000	2.929460000	-1.478773000
C	-2.446988000	-1.494642000	1.089827000
H	-3.057270000	-2.190375000	1.662243000
C	-3.470889000	1.733693000	-0.698456000
C	-5.413886000	0.541772000	0.237070000
C	-0.542856000	-4.109294000	0.547346000
H	-0.427897000	-5.052765000	1.095103000
H	-1.522269000	-4.171160000	0.057374000
C	-4.829361000	1.615504000	-0.476863000
H	-5.516914000	2.364460000	-0.850246000
C	-4.604579000	-0.460519000	0.741096000
H	-5.018810000	-1.295735000	1.294275000
C	0.741067000	-2.651806000	2.243000000
H	1.447556000	-2.253892000	1.512564000
H	1.187367000	-3.552615000	2.676963000
H	0.622078000	-1.913341000	3.043221000
C	-2.121021000	2.430052000	-2.725476000
H	-1.289921000	1.778835000	-2.449739000
H	-1.720249000	3.287194000	-3.279915000
H	-2.787796000	1.877606000	-3.398495000
O	-6.766004000	0.602884000	0.361095000
C	-1.524200000	-3.520163000	2.766240000
H	-1.766595000	-2.731136000	3.485828000
H	-0.979783000	-4.303868000	3.300536000
H	-2.455094000	-3.969281000	2.405331000
C	-1.947710000	3.740031000	-0.558488000
H	-2.497104000	4.145154000	0.299661000
H	-1.520776000	4.584004000	-1.113731000
H	-1.130021000	3.122309000	-0.184958000
C	-3.995977000	3.886572000	-1.971685000
H	-4.699257000	3.391163000	-2.650854000

H	-3.532436000	4.712152000	-2.522667000
H	-4.564462000	4.323488000	-1.142971000
C	-7.427305000	-0.448296000	1.063089000
H	-7.265394000	-1.415059000	0.571622000
H	-8.488807000	-0.200150000	1.039553000
H	-7.086964000	-0.504883000	2.103897000
O	1.336140000	0.791171000	0.263612000
N	1.202424000	-1.764519000	-0.977993000
C	2.609490000	0.714382000	0.147617000
C	0.656665000	-3.018669000	-1.610570000
C	3.220115000	-0.397207000	-0.551360000
C	2.866896000	2.948130000	1.474684000
C	2.462754000	-1.500300000	-1.110463000
H	3.077795000	-2.183395000	-1.692482000
C	3.465120000	1.762346000	0.699786000
C	5.410424000	0.567038000	-0.211577000
C	0.573153000	-4.117372000	-0.511421000
H	0.459967000	-5.067777000	-1.047114000
H	1.553090000	-4.170712000	-0.021353000
C	4.821440000	1.645085000	0.500397000
H	5.508919000	2.387321000	0.885707000
C	4.604245000	-0.447716000	-0.735665000
H	5.038481000	-1.279852000	-1.277373000
C	-0.711022000	-2.684178000	-2.230327000
H	-1.419963000	-2.285545000	-1.503051000
H	-1.152017000	-3.589935000	-2.658851000
H	-0.593808000	-1.951426000	-3.036022000
C	2.057341000	2.434415000	2.692146000
H	1.222468000	1.801695000	2.386930000
H	1.655714000	3.289207000	3.248518000
H	2.699172000	1.862969000	3.373110000
O	6.746784000	0.619642000	-0.316259000
C	1.557561000	-3.561932000	-2.739393000
H	1.794373000	-2.786727000	-3.475825000
H	1.017423000	-4.358883000	-3.257772000
H	2.490823000	-3.999488000	-2.369849000
C	1.953241000	3.772858000	0.534528000
H	2.526973000	4.176885000	-0.307727000
H	1.526189000	4.617668000	1.087336000
H	1.134228000	3.170416000	0.139773000
C	3.962608000	3.891645000	2.009918000
H	4.646377000	3.381855000	2.698149000
H	3.487801000	4.708906000	2.562687000
H	4.551570000	4.340955000	1.202529000
C	7.443641000	-0.425120000	-1.010734000
H	7.281740000	-1.390301000	-0.520519000
H	8.497627000	-0.155480000	-0.957455000
H	7.125466000	-0.474662000	-2.056861000

Triplet **[CuL^{pu,tBu}]$^{+}$**

Cu	0.000003000	0.647912000	0.000003000
O	-1.324156000	-0.687612000	0.289662000
N	-1.189363000	1.853880000	-0.972445000
C	-2.606433000	-0.607694000	0.167359000
C	-0.643116000	3.102166000	-1.615324000
C	-3.212504000	0.504488000	-0.520191000
C	-2.875156000	-2.855388000	1.452204000
C	-2.457301000	1.599173000	-1.082065000
H	-3.073236000	2.291695000	-1.652025000
C	-3.464475000	-1.649660000	0.698586000
C	-5.443637000	-0.434459000	-0.187409000

C	-0.557583000	4.213339000	-0.529820000
H	-0.441366000	5.158502000	-1.074168000
H	-1.537400000	4.274285000	-0.040549000
C	-4.828458000	-1.512144000	0.501254000
H	-5.478869000	-2.280910000	0.897409000
C	-4.604717000	0.555608000	-0.691995000
H	-5.019085000	1.402169000	-1.228190000
C	0.722693000	2.763304000	-2.236966000
H	1.434860000	2.371517000	-1.509031000
H	1.162489000	3.665009000	-2.675282000
H	0.602754000	2.023052000	-3.035400000
C	-2.063419000	-2.373115000	2.680984000
H	-1.228147000	-1.734627000	2.388825000
H	-1.662530000	-3.240398000	3.218765000
H	-2.703505000	-1.814935000	3.374642000
C	-6.969281000	-0.401863000	-0.343482000
C	-1.546151000	3.632802000	-2.749179000
H	-1.788314000	2.847122000	-3.472509000
H	-1.005380000	4.420521000	-3.281019000
H	-2.476859000	4.078077000	-2.383042000
C	-1.964374000	-3.667938000	0.498616000
H	-2.539950000	-4.056140000	-0.349990000
H	-1.537318000	-4.523462000	1.035272000
H	-1.145485000	-3.059782000	0.112089000
C	-3.972758000	-3.807083000	1.969817000
H	-4.653580000	-3.310762000	2.670841000
H	-3.499508000	-4.637897000	2.503936000
H	-4.565620000	-4.237354000	1.154833000
C	-7.627741000	-0.395642000	1.058906000
H	-7.362481000	-1.282306000	1.644056000
H	-8.718875000	-0.379722000	0.956361000
H	-7.326406000	0.489670000	1.630176000
C	-7.430400000	-1.659297000	-1.122078000
H	-6.989559000	-1.682782000	-2.125005000
H	-8.521168000	-1.651205000	-1.229469000
H	-7.153856000	-2.586139000	-0.609089000
C	-7.451491000	0.844824000	-1.108896000
H	-7.177391000	1.772250000	-0.593289000
H	-8.543293000	0.823420000	-1.189964000
H	-7.046711000	0.882153000	-2.126688000
O	1.324157000	-0.687616000	-0.289655000
N	1.189373000	1.853876000	0.972451000
C	2.606435000	-0.607702000	-0.167352000
C	0.643132000	3.102165000	1.615330000
C	3.212510000	0.504479000	0.520194000
C	2.875135000	-2.855396000	-1.452193000
C	2.457311000	1.599166000	1.082069000
H	3.073249000	2.291688000	1.652028000
C	3.464470000	-1.649671000	-0.698581000
C	5.443640000	-0.434470000	0.187399000
C	0.557601000	4.213337000	0.529827000
H	0.441387000	5.158500000	1.074174000
H	1.537418000	4.274281000	0.040556000
C	4.828455000	-1.512154000	-0.501260000
H	5.478864000	-2.280921000	-0.897418000
C	4.604724000	0.555598000	0.691990000
H	5.019097000	1.402158000	1.228182000
C	-0.722677000	2.763308000	2.236976000
H	-1.434848000	2.371524000	1.509043000
H	-1.162468000	3.665015000	2.675293000
H	-0.602739000	2.023056000	3.035410000
C	2.063324000	-2.373104000	-2.680916000
H	1.228063000	-1.734629000	-2.388694000

H	1.662410000	-3.240379000	-3.218692000
H	2.703365000	-1.814904000	-3.374598000
C	6.969284000	-0.401875000	0.343461000
C	1.546172000	3.632796000	2.749184000
H	1.788333000	2.847114000	3.472513000
H	1.005406000	4.420518000	3.281025000
H	2.476881000	4.078067000	2.383044000
C	1.964413000	-3.667977000	-0.498576000
H	2.540036000	-4.056185000	0.349995000
H	1.537346000	-4.523499000	-1.035228000
H	1.145532000	-3.059842000	-0.111999000
C	3.972719000	-3.807068000	-1.969886000
H	4.653498000	-3.310727000	-2.670937000
H	3.499449000	-4.637876000	-2.503997000
H	4.565630000	-4.237350000	-1.154943000
C	7.627734000	-0.395656000	-1.058933000
H	7.362470000	-1.282321000	-1.644079000
H	8.718870000	-0.379737000	-0.956395000
H	7.326396000	0.489655000	-1.630202000
C	7.430409000	-1.659308000	1.122055000
H	6.989574000	-1.682791000	2.124985000
H	8.521177000	-1.651216000	1.229438000
H	7.153860000	-2.586150000	0.609069000
C	7.451501000	0.844813000	1.108869000
H	7.177398000	1.772239000	0.593263000
H	8.543304000	0.823409000	1.189930000
H	7.046728000	0.882144000	2.126664000

Singlet **[CuL^{pu,tBu}]$^{+}$**

Cu	-0.000001000	0.718238000	-0.000010000
O	-1.284130000	-0.587169000	0.373217000
N	-1.190594000	1.910804000	-0.898439000
C	-2.567019000	-0.559356000	0.171196000
C	-0.674263000	3.171022000	-1.560625000
C	-3.215857000	0.632532000	-0.295350000
C	-2.740510000	-3.063286000	0.854738000
C	-2.482250000	1.745614000	-0.810082000
H	-3.115093000	2.533374000	-1.212912000
C	-3.377407000	-1.723340000	0.443708000
C	-5.419895000	-0.381277000	-0.051961000
C	-0.569565000	4.310097000	-0.514111000
H	-0.465553000	5.242701000	-1.081651000
H	-1.536466000	4.383038000	-0.000929000
C	-4.751807000	-1.567655000	0.355958000
H	-5.370478000	-2.419985000	0.606456000
C	-4.624014000	0.695800000	-0.394336000
H	-5.063737000	1.616248000	-0.761691000
C	0.662575000	2.844788000	-2.245197000
H	1.427425000	2.491514000	-1.553764000
H	1.052329000	3.744401000	-2.731680000
H	0.516170000	2.080131000	-3.015331000
C	-1.908948000	-2.902645000	2.151422000
H	-1.088635000	-2.194838000	2.021611000
H	-1.485993000	-3.872004000	2.440722000
H	-2.541257000	-2.553259000	2.976530000
C	-6.953445000	-0.356604000	-0.122954000
C	-1.643044000	3.640206000	-2.672869000
H	-1.921476000	2.814025000	-3.334667000
H	-1.131141000	4.397130000	-3.273415000
H	-2.552467000	4.105950000	-2.281588000
C	-1.843856000	-3.560433000	-0.304879000

H	-2.444170000	-3.742067000	-1.204169000
H	-1.360495000	-4.503952000	-0.025759000
H	-1.064178000	-2.836801000	-0.547779000
C	-3.800932000	-4.150286000	1.124726000
H	-4.459776000	-3.887247000	1.960271000
H	-3.292125000	-5.083258000	1.389406000
H	-4.421144000	-4.353348000	0.244311000
C	-7.534218000	-0.655739000	1.281158000
H	-7.223344000	-1.636847000	1.654955000
H	-8.629697000	-0.647694000	1.241759000
H	-7.214633000	0.099770000	2.007913000
C	-7.443127000	-1.434171000	-1.121049000
H	-7.061088000	-1.237295000	-2.129143000
H	-8.538475000	-1.432175000	-1.165549000
H	-7.125072000	-2.440737000	-0.830025000
C	-7.491039000	1.010547000	-0.585335000
H	-7.195521000	1.816721000	0.095745000
H	-8.585545000	0.982796000	-0.609294000
H	-7.146112000	1.265712000	-1.593800000
O	1.284135000	-0.587161000	-0.373242000
N	1.190586000	1.910805000	0.898425000
C	2.567024000	-0.559344000	-0.171224000
C	0.674248000	3.171017000	1.560616000
C	3.215856000	0.632544000	0.295334000
C	2.740527000	-3.063278000	-0.854759000
C	2.482243000	1.745620000	0.810069000
H	3.115082000	2.533380000	1.212905000
C	3.377417000	-1.723326000	-0.443733000
C	5.419897000	-0.381266000	0.051979000
C	0.569548000	4.310097000	0.514106000
H	0.465533000	5.242697000	1.081650000
H	1.536448000	4.383042000	0.000926000
C	4.751815000	-1.567643000	-0.355950000
H	5.370491000	-2.419974000	-0.606437000
C	4.624011000	0.695812000	0.394338000
H	5.063729000	1.616260000	0.761703000
C	-0.662592000	2.844773000	2.245179000
H	-1.427437000	2.491499000	1.553740000
H	-1.052354000	3.744381000	2.731665000
H	-0.516187000	2.080113000	3.015309000
C	1.909248000	-2.902736000	-2.151637000
H	1.088935000	-2.194882000	-2.022076000
H	1.486315000	-3.872108000	-2.440927000
H	2.541747000	-2.553463000	-2.976646000
C	6.953446000	-0.356595000	0.122999000
C	1.643021000	3.640200000	2.672866000
H	1.921455000	2.814017000	3.334661000
H	1.131112000	4.397118000	3.273415000
H	2.552443000	4.105952000	2.281592000
C	1.843600000	-3.560242000	0.304724000
H	2.443716000	-3.741817000	1.204160000
H	1.360236000	-4.503760000	0.025606000
H	1.063919000	-2.836534000	0.547385000
C	3.800939000	-4.150373000	-1.124408000
H	4.460000000	-3.887447000	-1.959817000
H	3.292131000	-5.083331000	-1.389133000
H	4.420928000	-4.353409000	-0.243829000
C	7.534242000	-0.655747000	-1.281101000
H	7.223370000	-1.636858000	-1.654892000
H	8.629720000	-0.647707000	-1.241682000
H	7.214672000	0.099754000	-2.007870000
C	7.443109000	-1.434151000	1.121115000
H	7.061053000	-1.237263000	2.129200000

H	8.538456000	-1.432156000	1.165633000
H	7.125058000	-2.440720000	0.830097000
C	7.491034000	1.010561000	0.585372000
H	7.195530000	1.816728000	-0.095722000
H	8.585540000	0.982808000	0.609351000
H	7.146091000	1.265739000	1.593828000

Doublet **[CuL^{pu,OMe}]**

Cu	-0.000083000	-0.526485000	-0.000303000
O	-1.332428000	0.796665000	-0.320917000
N	-1.186477000	-1.745728000	0.975006000
C	-2.624202000	0.700390000	-0.164623000
C	-0.647445000	-2.994888000	1.608129000
C	-3.219852000	-0.411526000	0.510415000
C	-2.928957000	2.967103000	-1.407954000
C	-2.463298000	-1.503477000	1.059194000
H	-3.081076000	-2.214627000	1.606687000
C	-3.498100000	1.741176000	-0.664939000
C	-5.443369000	0.508643000	0.215140000
C	-0.559066000	-4.111703000	0.528469000
H	-0.446681000	-5.058394000	1.072689000
H	-1.537169000	-4.169774000	0.034366000
C	-4.860442000	1.603136000	-0.462606000
H	-5.549657000	2.356156000	-0.826656000
C	-4.629554000	-0.487673000	0.700786000
H	-5.034929000	-1.345361000	1.227156000
C	0.721592000	-2.665855000	2.229541000
H	1.423557000	-2.254745000	1.502584000
H	1.169104000	-3.572357000	2.651772000
H	0.602468000	-1.938160000	3.039955000
C	-2.137733000	2.512646000	-2.658557000
H	-1.312958000	1.853004000	-2.385211000
H	-1.728596000	3.386808000	-3.180683000
H	-2.793220000	1.980130000	-3.358907000
O	-6.812942000	0.553261000	0.322771000
C	-1.546067000	-3.529484000	2.745923000
H	-1.793627000	-2.740691000	3.464421000
H	-1.002377000	-4.313075000	3.282086000
H	-2.476329000	-3.978825000	2.382868000
C	-2.003273000	3.766888000	-0.459931000
H	-2.567055000	4.145656000	0.401548000
H	-1.577806000	4.629440000	-0.988479000
H	-1.185173000	3.146181000	-0.092562000
C	-4.038078000	3.924702000	-1.888647000
H	-4.728464000	3.439014000	-2.588188000
H	-3.579599000	4.771150000	-2.412636000
H	-4.622692000	4.331960000	-1.055672000
C	-7.449434000	-0.521665000	0.997658000
H	-7.266163000	-1.479451000	0.492476000
H	-8.518505000	-0.302307000	0.978270000
H	-7.113296000	-0.598129000	2.040335000
O	1.332638000	0.796272000	0.321794000
N	1.186427000	-1.745653000	-0.975068000
C	2.624346000	0.700274000	0.164885000
C	0.647362000	-2.995000000	-1.607913000
C	3.219931000	-0.411623000	-0.510356000
C	2.929128000	2.966861000	1.408221000
C	2.463348000	-1.503723000	-1.058795000
H	3.081211000	-2.215274000	-1.605663000
C	3.498249000	1.741089000	0.664930000
C	5.443421000	0.508859000	-0.215744000

C	0.559192000	-4.111680000	-0.528131000
H	0.446944000	-5.058448000	-1.072247000
H	1.537310000	-4.169557000	-0.034032000
C	4.860592000	1.603273000	0.462153000
H	5.549783000	2.356455000	0.825890000
C	4.629558000	-0.487612000	-0.701085000
H	5.034950000	-1.345168000	-1.227654000
C	-0.721796000	-2.666094000	-2.229104000
H	-1.423677000	-2.255028000	-1.502037000
H	-1.169306000	-3.572657000	-2.651210000
H	-0.602876000	-1.938438000	-3.039583000
C	2.138472000	2.512037000	2.659051000
H	1.313864000	1.852105000	2.385881000
H	1.729131000	3.385996000	3.181366000
H	2.794361000	1.979722000	3.359177000
O	6.812894000	0.553654000	-0.324164000
C	1.545787000	-3.529656000	-2.745847000
H	1.793484000	-2.740801000	-3.464226000
H	1.001883000	-4.313042000	-3.282097000
H	2.475958000	-3.979293000	-2.382934000
C	2.002794000	3.766402000	0.460642000
H	2.566046000	4.145330000	-0.401120000
H	1.577353000	4.628826000	0.989407000
H	1.184729000	3.145424000	0.093642000
C	4.038136000	3.924758000	1.888564000
H	4.728938000	3.439237000	2.587809000
H	3.579587000	4.771013000	2.412804000
H	4.622294000	4.332259000	1.055390000
C	7.449187000	-0.521909000	-0.998083000
H	7.265633000	-1.479292000	-0.492204000
H	8.518325000	-0.302857000	-0.978776000
H	7.113201000	-0.599180000	-2.040771000

Doublet **[CuL^{pu,tBu}]**

Cu	0.000011000	0.617293000	-0.000001000
O	-1.329132000	-0.710984000	0.319935000
N	-1.191282000	1.839266000	-0.967704000
C	-2.620701000	-0.612978000	0.176275000
C	-0.655680000	3.088479000	-1.604130000
C	-3.220204000	0.503734000	-0.490289000
C	-2.925656000	-2.879435000	1.408943000
C	-2.468155000	1.597186000	-1.042819000
H	-3.090869000	2.308861000	-1.584282000
C	-3.496429000	-1.646993000	0.675859000
C	-5.475073000	-0.402284000	-0.184216000
C	-0.561720000	4.205625000	-0.525449000
H	-0.452095000	5.152122000	-1.070570000
H	-1.537321000	4.263929000	-0.026501000
C	-4.861746000	-1.495252000	0.481126000
H	-5.516145000	-2.269809000	0.862939000
C	-4.627670000	0.575352000	-0.661429000
H	-5.022369000	1.442330000	-1.182899000
C	0.709791000	2.759166000	-2.233011000
H	1.415942000	2.348441000	-1.509880000
H	1.155057000	3.665409000	-2.658172000
H	0.586147000	2.031188000	-3.042522000
C	-2.123513000	-2.434780000	2.656310000
H	-1.298588000	-1.776190000	2.380623000
H	-1.712735000	-3.312562000	3.171286000
H	-2.772049000	-1.903686000	3.364267000
C	-7.005121000	-0.358520000	-0.338384000

C	-1.560850000	3.622028000	-2.737129000
H	-1.812901000	2.832392000	-3.453136000
H	-1.020172000	4.404888000	-3.277449000
H	-2.488866000	4.071895000	-2.369056000
C	-2.008766000	-3.678737000	0.451783000
H	-2.579187000	-4.051075000	-0.408253000
H	-1.582964000	-4.545763000	0.972965000
H	-1.190306000	-3.059844000	0.082048000
C	-4.031610000	-3.838508000	1.894681000
H	-4.715591000	-3.356428000	2.603116000
H	-3.569090000	-4.687927000	2.410450000
H	-4.624026000	-4.241869000	1.065177000
C	-7.670888000	-0.369027000	1.058741000
H	-7.406519000	-1.264740000	1.631320000
H	-8.763483000	-0.347522000	0.961817000
H	-7.364327000	0.505548000	1.644500000
C	-7.484222000	-1.592916000	-1.139243000
H	-7.044108000	-1.601315000	-2.143304000
H	-8.576005000	-1.580279000	-1.246434000
H	-7.210188000	-2.531698000	-0.645811000
C	-7.475449000	0.905853000	-1.081775000
H	-7.190560000	1.820390000	-0.548785000
H	-8.567897000	0.899738000	-1.168485000
H	-7.063434000	0.958899000	-2.096237000
O	1.329150000	-0.710984000	-0.319942000
N	1.191308000	1.839258000	0.967706000
C	2.620720000	-0.612973000	-0.176293000
C	0.655705000	3.088462000	1.604148000
C	3.220230000	0.503737000	0.490268000
C	2.925607000	-2.879427000	-1.408942000
C	2.468183000	1.597184000	1.042809000
H	3.090898000	2.308857000	1.584274000
C	3.496434000	-1.646997000	-0.675876000
C	5.475089000	-0.402306000	0.184202000
C	0.561741000	4.205621000	0.525482000
H	0.452112000	5.152111000	1.070614000
H	1.537341000	4.263935000	0.026534000
C	4.861753000	-1.495272000	-0.481136000
H	5.516150000	-2.269837000	-0.862936000
C	4.627697000	0.575344000	0.661406000
H	5.022403000	1.442318000	1.182877000
C	-0.709764000	2.759139000	2.233028000
H	-1.415916000	2.348425000	1.509892000
H	-1.155030000	3.665375000	2.658203000
H	-0.586118000	2.031148000	3.042527000
C	2.123622000	-2.434751000	-2.656402000
H	1.298751000	-1.776048000	-2.380821000
H	1.712785000	-3.312514000	-3.171363000
H	2.772281000	-1.903773000	-3.364333000
C	7.005137000	-0.358558000	0.338376000
C	1.560879000	3.621996000	2.737152000
H	1.812933000	2.832349000	3.453146000
H	1.020202000	4.404847000	3.277485000
H	2.488893000	4.071869000	2.369082000
C	2.008522000	-3.678551000	-0.451822000
H	2.578805000	-4.050885000	0.408308000
H	1.582677000	-4.545569000	-0.972981000
H	1.190092000	-3.059531000	-0.082229000
C	4.031479000	-3.838676000	-1.894528000
H	4.715585000	-3.356729000	-2.602932000
H	3.568892000	-4.688063000	-2.410288000
H	4.623768000	-4.242070000	-1.064950000
C	7.670909000	-0.369095000	-1.058746000

H	7.406526000	-1.264811000	-1.631314000
H	8.763504000	-0.347607000	-0.961817000
H	7.364366000	0.505478000	-1.644517000
C	7.484218000	-1.592948000	1.139255000
H	7.044097000	-1.601329000	2.143314000
H	8.576000000	-1.580322000	1.246454000
H	7.210178000	-2.531734000	0.645834000
C	7.475477000	0.905819000	1.081751000
H	7.190603000	1.820352000	0.548746000
H	8.567925000	0.899691000	1.168468000
H	7.063456000	0.958886000	2.096209000

Doublet **[CuL^{pb,OMe}]**

Cu	-0.000052000	0.173406000	-0.000128000
O	1.356324000	-1.122074000	0.311125000
O	-1.356282000	-1.122282000	-0.310607000
N	1.207478000	1.441751000	-0.832649000
N	-1.207591000	1.441766000	0.832631000
C	2.645731000	-1.020416000	0.141985000
C	-3.246340000	0.112502000	0.502823000
C	-4.655095000	0.186353000	0.710011000
H	-5.058158000	1.060057000	1.210603000
O	-6.830051000	-0.888777000	0.397967000
C	5.464526000	-0.832314000	-0.270152000
C	-2.645715000	-1.020529000	-0.141733000
C	0.649190000	2.578787000	-1.488166000
C	0.025081000	3.602941000	-0.744725000
C	3.246321000	0.112686000	-0.502523000
O	6.830036000	-0.888611000	-0.398095000
C	4.879566000	-1.944249000	0.380820000
H	5.568312000	-2.713303000	0.710425000
C	2.488137000	1.222153000	-0.984511000
H	3.056694000	1.978601000	-1.532888000
C	0.187618000	3.765911000	-3.558130000
H	0.248409000	3.815856000	-4.641473000
C	-0.426070000	4.788132000	-2.834626000
H	-0.850115000	5.647221000	-3.346166000
C	-3.520370000	-2.081074000	-0.598836000
C	-2.488185000	1.221972000	0.984826000
H	-3.056701000	1.978294000	1.533418000
C	4.655049000	0.186562000	-0.709791000
H	5.058096000	1.060322000	-1.210294000
C	-2.954289000	-3.326653000	-1.310468000
C	0.721038000	2.667467000	-2.885009000
H	1.189568000	1.858049000	-3.437320000
C	3.520415000	-2.081025000	0.598828000
C	-0.649319000	2.578818000	1.488106000
C	-0.025234000	3.602965000	0.744626000
C	0.499520000	4.700647000	1.444214000
H	0.977743000	5.495394000	0.878674000
C	-0.499708000	4.700574000	-1.444364000
H	-0.977959000	5.495333000	-0.878866000
C	-5.464526000	-0.832458000	0.270180000
C	4.065604000	-4.303398000	1.746195000
H	4.637422000	-4.687387000	0.893516000
H	3.610111000	-5.163768000	2.249421000
H	4.767353000	-3.842850000	2.451407000
C	-0.721148000	2.667567000	2.884952000
H	-1.189617000	1.858148000	3.437310000
C	7.470607000	0.203175000	-1.043166000

H	7.121915000	0.319297000	-2.077879000
H	8.537030000	-0.028864000	-1.045054000
H	7.304023000	1.143758000	-0.501684000
C	-4.879526000	-1.944313000	-0.380919000
H	-5.568265000	-2.713312000	-0.710665000
C	0.425882000	4.788273000	2.834470000
H	0.849899000	5.647399000	3.345971000
C	-4.065287000	-4.303329000	-1.746636000
H	-4.637080000	-4.687620000	-0.894076000
H	-3.609684000	-5.163514000	-2.250080000
H	-4.767062000	-3.842672000	-2.451748000
C	-2.013462000	-4.092941000	-0.349679000
H	-1.191618000	-3.459866000	-0.013139000
H	-1.593252000	-4.970923000	-0.856354000
H	-2.564542000	-4.445403000	0.530927000
C	-2.181901000	-2.908229000	-2.585340000
H	-2.848204000	-2.397936000	-3.291774000
H	-1.779240000	-3.797461000	-3.086244000
H	-1.353512000	-2.239936000	-2.345808000
C	2.954479000	-3.326737000	1.310331000
C	2.182209000	-2.908626000	2.585379000
H	2.848534000	-2.398359000	3.291812000
H	1.779739000	-3.797998000	3.086186000
H	1.353698000	-2.240402000	2.346077000
C	-0.187765000	3.766059000	3.558020000
H	-0.248548000	3.816042000	4.641362000
C	2.013618000	-4.092933000	0.349496000
H	1.191692000	-3.459870000	0.013128000
H	1.593500000	-4.971024000	0.856057000
H	2.564639000	-4.445214000	-0.531220000
C	-7.470619000	0.202688000	1.043638000
H	-7.121713000	0.318391000	2.078316000
H	-8.537014000	-0.029469000	1.045609000
H	-7.304227000	1.143505000	0.502504000

Doublet **[CuL^{pb,tBu}]**

Cu	-0.000002000	0.290712000	-0.000007000
O	-1.350867000	-1.009881000	-0.317871000
O	1.350859000	-1.009887000	0.317846000
N	-1.215666000	1.561626000	0.819333000
N	1.215664000	1.561627000	-0.819337000
C	-2.641319000	-0.906031000	-0.168618000
C	3.248580000	0.231392000	-0.464496000
C	4.656410000	0.300274000	-0.646078000
H	5.051115000	1.182634000	-1.140404000
C	7.026082000	-0.665609000	-0.376868000
C	-5.497456000	-0.699190000	0.210022000
C	2.641314000	-0.906027000	0.168622000
C	-0.663975000	2.698638000	1.481022000
C	-0.032775000	3.723202000	0.744353000
C	-3.248581000	0.231382000	0.464512000
C	-7.026083000	-0.665618000	0.376900000
C	-4.879516000	-1.808309000	-0.427145000
H	-5.532040000	-2.598460000	-0.778459000
C	-2.497403000	1.342142000	0.955384000
H	-3.073724000	2.098255000	1.496290000
C	-0.222966000	3.884400000	3.556051000
H	-0.294488000	3.933768000	4.638760000
C	0.397401000	4.907240000	2.839189000
H	0.816107000	5.766159000	3.355395000
C	3.515901000	-1.958914000	0.629950000

C	2.497403000	1.342149000	-0.955375000
H	3.073726000	2.098265000	-1.496275000
C	-4.656410000	0.300260000	0.646108000
H	-5.051113000	1.182617000	1.140440000
C	2.944885000	-3.211383000	1.327833000
C	-0.749461000	2.786169000	2.877064000
H	-1.223476000	1.976434000	3.424209000
C	-3.515905000	-1.958920000	-0.629941000
C	0.663973000	2.698638000	-1.481029000
C	0.032769000	3.723201000	-0.744363000
C	-7.703294000	-0.722634000	-1.013457000
H	-7.410608000	0.137755000	-1.626525000
H	-8.795023000	-0.708844000	-0.906967000
H	-7.435297000	-1.631960000	-1.562522000
C	-0.484770000	4.820626000	-1.449662000
H	-0.968450000	5.615790000	-0.889383000
C	0.484763000	4.820629000	1.449650000
H	0.968439000	5.615793000	0.889369000
C	5.497456000	-0.699173000	-0.209984000
C	-4.050809000	-4.189205000	-1.774975000
H	-4.635690000	-4.568742000	-0.929060000
H	-3.588676000	-5.052766000	-2.266787000
H	-4.741753000	-3.732481000	-2.493380000
C	0.749462000	2.786167000	-2.877071000
H	1.223482000	1.976433000	-3.424214000
C	-7.485408000	-1.881295000	1.217162000
H	-7.208551000	-2.831500000	0.747661000
H	-8.576069000	-1.874547000	1.334622000
H	-7.035549000	-1.857541000	2.216586000
C	4.879512000	-1.808299000	0.427166000
H	5.532033000	-2.598459000	0.778467000
C	-0.397405000	4.907236000	-2.839200000
H	-0.816113000	5.766153000	-3.355409000
C	4.050829000	-4.189208000	1.774934000
H	4.635761000	-4.568660000	0.929016000
H	3.588708000	-5.052821000	2.266665000
H	4.741726000	-3.732509000	2.493401000
C	2.019066000	-3.977073000	0.351828000
H	1.199166000	-3.345700000	0.007278000
H	1.594976000	-4.859154000	0.848362000
H	2.582635000	-4.323423000	-0.523398000
C	2.153784000	-2.803887000	2.594923000
H	2.808659000	-2.294962000	3.313045000
H	1.747379000	-3.697095000	3.085871000
H	1.326100000	-2.137143000	2.348490000
C	-2.944882000	-3.211369000	-1.327854000
C	-7.500969000	0.615421000	1.088227000
H	-7.079488000	0.701721000	2.096475000
H	-8.592341000	0.601383000	1.186036000
H	-7.230424000	1.516575000	0.525913000
C	7.703302000	-0.722402000	1.013494000
H	7.410593000	0.138067000	1.626438000
H	8.795029000	-0.708593000	0.906995000
H	7.435339000	-1.631656000	1.562694000
C	-2.153789000	-2.803831000	-2.594934000
H	-2.808671000	-2.294895000	-3.313041000
H	-1.747372000	-3.697021000	-3.085905000
H	-1.326113000	-2.137083000	-2.348484000
C	0.222967000	3.884396000	-3.556060000
H	0.294491000	3.933763000	-4.638769000
C	-2.019046000	-3.977067000	-0.351870000
H	-1.199157000	-3.345686000	-0.007306000
H	-1.594940000	-4.859126000	-0.848429000

H	-2.582606000	-4.323450000	0.523348000
C	7.485412000	-1.881415000	-1.216941000
H	7.208545000	-2.831546000	-0.747295000
H	8.576074000	-1.874689000	-1.334392000
H	7.035561000	-1.857813000	-2.216373000
C	7.500955000	0.615324000	-1.088396000
H	7.079530000	0.701427000	-2.096684000
H	8.592332000	0.601315000	-1.186139000
H	7.230336000	1.516566000	-0.526257000

Excitation energies and oscillator strengths:

Triplet **[CuL^{bp,OMe}]$^{+}$**

```
Excited State   1:  3.003-A      0.5850 eV 2119.25 nm  f=0.1134  <S**2>=2.004
    162B -> 165B       0.13156
    163B -> 164B       1.06904
    163B <- 164B      -0.41177
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -3445.46114855
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  3.005-A      0.6478 eV 1913.84 nm  f=0.0014  <S**2>=2.007
    162B -> 164B       0.10603
    163B -> 165B       0.99295

 Excited State   3:  3.004-A      1.0968 eV 1130.43 nm  f=0.0191  <S**2>=2.006
    162B -> 164B       0.98797

 Excited State   4:  3.006-A      1.4422 eV  859.70 nm  f=0.0428  <S**2>=2.009
    161B -> 165B      -0.16608
    162B -> 165B       0.97357
    163B -> 164B      -0.13971

 Excited State   5:  3.004-A      1.4473 eV  856.65 nm  f=0.0002  <S**2>=2.006
    161B -> 164B       0.99101

 Excited State   6:  3.005-A      1.4994 eV  826.90 nm  f=0.0054  <S**2>=2.008
    160B -> 164B       0.99406

 Excited State   7:  3.005-A      1.6136 eV  768.39 nm  f=0.0088  <S**2>=2.007
    159B -> 164B       0.99334

 Excited State   8:  3.005-A      1.7512 eV  707.99 nm  f=0.0002  <S**2>=2.007
    158B -> 164B       0.98402
    160B -> 165B      -0.10038

 Excited State   9:  3.009-A      1.8446 eV  672.13 nm  f=0.0400  <S**2>=2.013
    165A -> 166A      -0.14158
    157B -> 164B       0.16781
    159B -> 165B      -0.18022
    161B -> 165B       0.93604
    162B -> 165B       0.12347

 Excited State  10:  3.006-A      1.8535 eV  668.92 nm  f=0.0071  <S**2>=2.009
    156B -> 164B      -0.12057
    157B -> 164B      -0.13876
    160B -> 165B       0.96896

 Excited State  11:  3.005-A      1.8555 eV  668.19 nm  f=0.0447  <S**2>=2.008
    157B -> 164B       0.96525
    160B -> 165B       0.13102
    161B -> 165B      -0.16391

 Excited State  12:  3.029-A      1.9717 eV  628.83 nm  f=0.0341  <S**2>=2.044
    165A -> 166A      -0.29650
    159B -> 165B       0.92364
    161B -> 165B       0.10951
    163B -> 167B      -0.10579

 Excited State  13:  3.496-A      2.0471 eV  605.66 nm  f=0.0008  <S**2>=2.805
    164A -> 166A      -0.23372
    165A -> 167A       0.69286
    163B -> 166B       0.66459

 Excited State  14:  3.412-A      2.0560 eV  603.03 nm  f=0.0370  <S**2>=2.660
    164A -> 167A      -0.20876
    165A -> 166A       0.60902
    158B -> 165B       0.30290
    159B -> 165B       0.25359
    161B -> 165B       0.15707
    163B -> 167B       0.61238

 Excited State  15:  3.041-A      2.0944 eV  591.99 nm  f=0.0044  <S**2>=2.061
    164A -> 167A      -0.10346
    165A -> 166A      -0.16112
```

```
   154B -> 164B       0.26526
   155B -> 164B       0.27924
   158B -> 165B       0.85710
   163B -> 167B      -0.24241

Excited State  16:  3.009-A      2.1078 eV  588.21 nm  f=0.0077  <S**2>=2.013
   154B -> 164B      -0.14255
   155B -> 164B       0.95036
   158B -> 165B      -0.20831

Excited State  17:  3.008-A      2.1771 eV  569.50 nm  f=0.0064  <S**2>=2.012
   164A -> 166A      -0.17379
   156B -> 164B       0.55730
   157B -> 165B       0.79641

Excited State  18:  3.548-A      2.1990 eV  563.81 nm  f=0.0063  <S**2>=2.896
   164A -> 166A       0.49969
   164A -> 167A       0.49667
   165A -> 166A       0.42466
   165A -> 167A       0.34428
   154B -> 164B      -0.15473
   157B -> 165B       0.11207
   158B -> 165B       0.11511
   163B -> 166B      -0.23009
   163B -> 167B      -0.28396

Excited State  19:  3.537-A      2.2009 eV  563.33 nm  f=0.0054  <S**2>=2.878
   164A -> 166A       0.51545
   164A -> 167A      -0.48668
   165A -> 166A      -0.31564
   165A -> 167A       0.44994
   154B -> 164B       0.14720
   157B -> 165B       0.12427
   158B -> 165B      -0.10055
   163B -> 166B      -0.24422
   163B -> 167B       0.25933

Excited State  20:  3.023-A      2.2309 eV  555.75 nm  f=0.0095  <S**2>=2.035
   164A -> 167A       0.23293
   165A -> 166A       0.15139
   152B -> 165B       0.10877
   154B -> 164B       0.90839
   158B -> 165B      -0.23596

Excited State  21:  3.007-A      2.2415 eV  553.13 nm  f=0.0014  <S**2>=2.011
   164A -> 166A       0.22259
   153B -> 165B      -0.16250
   156B -> 164B       0.75176
   157B -> 165B      -0.50480
   160B -> 165B       0.10965
   163B -> 166B       0.19946

Excited State  22:  3.010-A      2.3576 eV  525.90 nm  f=0.0045  <S**2>=2.015
   163A -> 167A       0.14171
   153B -> 164B       0.96286

Excited State  23:  3.171-A      2.3591 eV  525.56 nm  f=0.0059  <S**2>=2.263
   163A -> 166A       0.60273
   164A -> 166A       0.38817
   165A -> 167A      -0.23413
   152B -> 164B      -0.50377
   153B -> 164B      -0.11429
   154B -> 165B       0.13069
   157B -> 165B       0.14592
   163B -> 166B       0.33016

Excited State  24:  3.053-A      2.3804 eV  520.84 nm  f=0.0003  <S**2>=2.080
   163A -> 166A       0.47313
   164A -> 166A       0.16728
   152B -> 164B       0.78670
   153B -> 165B      -0.15152
   154B -> 165B      -0.18310
   155B -> 165B      -0.13963
   157B -> 165B       0.15930

Excited State  25:  3.204-A      2.3848 eV  519.88 nm  f=0.0108  <S**2>=2.317
   163A -> 167A       0.74772
```

```
   164A -> 167A       0.42567
   165A -> 166A      -0.24549
   152B -> 165B      -0.12382
   156B -> 165B      -0.17686
   158B -> 165B       0.16401
   163B -> 167B       0.30190

 Excited State  26:  3.014-A      2.4555 eV  504.93 nm  f=0.0056  <S**2>=2.021
   163A -> 167A       0.24449
   151B -> 164B       0.11329
   155B -> 165B      -0.33540
   156B -> 165B       0.88033

 Excited State  27:  3.011-A      2.4559 eV  504.85 nm  f=0.0011  <S**2>=2.017
   163A -> 166A       0.16644
   155B -> 165B       0.91217
   156B -> 165B       0.32117

 Excited State  28:  3.015-A      2.5282 eV  490.40 nm  f=0.0430  <S**2>=2.022
   163A -> 166A      -0.39154
   164A -> 166A       0.28066
   165A -> 167A      -0.18882
   152B -> 164B       0.29320
   153B -> 165B       0.12427
   154B -> 165B       0.62831
   155B -> 165B       0.16161
   156B -> 164B      -0.16103
   157B -> 165B       0.11886
   163B -> 166B       0.36223

 Excited State  29:  3.024-A      2.5573 eV  484.83 nm  f=0.0402  <S**2>=2.035
   163A -> 167A       0.54780
   164A -> 167A      -0.37377
   165A -> 166A       0.27979
   151B -> 164B      -0.37591
   153B -> 164B      -0.11502
   156B -> 165B      -0.15634
   163B -> 167B      -0.49429

 Excited State  30:  3.013-A      2.6678 eV  464.74 nm  f=0.1181  <S**2>=2.020
   163A -> 166A       0.41624
   164A -> 166A      -0.22589
   165A -> 167A       0.23830
   149B -> 164B      -0.11232
   150B -> 164B       0.25923
   153B -> 165B       0.24313
   154B -> 165B       0.61860
   157B -> 165B      -0.10296
   163B -> 166B      -0.35499
```

Triplet **[CuL^{bp,tBu}]$^{+}$**

```
Excited State   1:  3.004-A      0.5915 eV 2096.24 nm  f=0.1084  <S**2>=2.005
    178B -> 181B       0.13128
    179B -> 180B       1.04685
    179B <- 180B      -0.35609
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -3530.78375913
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  3.006-A      0.8018 eV 1546.36 nm  f=0.0001  <S**2>=2.008
    178B -> 180B       0.26203
    179B -> 181B       0.96448

 Excited State   3:  3.005-A      0.9075 eV 1366.15 nm  f=0.0292  <S**2>=2.007
    178B -> 180B       0.95986
    179B -> 181B      -0.25827

 Excited State   4:  3.005-A      1.2156 eV 1019.93 nm  f=0.0070  <S**2>=2.008
    177B -> 180B       0.99573

 Excited State   5:  3.005-A      1.2298 eV 1008.14 nm  f=0.0001  <S**2>=2.008
    176B -> 180B       0.99427
```

```
Excited State   6:  3.005-A      1.3606 eV  911.27 nm  f=0.0103  <S**2>=2.008
   175B -> 180B       0.99264

Excited State   7:  3.007-A      1.3858 eV  894.65 nm  f=0.0283  <S**2>=2.011
   175B -> 181B       0.12165
   176B -> 181B       0.13727
   178B -> 181B       0.97332
   179B -> 180B      -0.12663

Excited State   8:  3.005-A      1.5385 eV  805.86 nm  f=0.0024  <S**2>=2.008
   174B -> 180B       0.99717

Excited State   9:  3.005-A      1.6526 eV  750.24 nm  f=0.0126  <S**2>=2.008
   173B -> 180B       0.98812

Excited State  10:  3.006-A      1.7126 eV  723.95 nm  f=0.0094  <S**2>=2.010
   177B -> 181B       0.98933

Excited State  11:  3.007-A      1.7639 eV  702.91 nm  f=0.0205  <S**2>=2.010
   175B -> 181B      -0.34447
   176B -> 181B       0.92645

Excited State  12:  3.006-A      1.8892 eV  656.27 nm  f=0.0016  <S**2>=2.008
   172B -> 180B       0.96360
   175B -> 181B      -0.22832

Excited State  13:  3.007-A      1.9452 eV  637.39 nm  f=0.1303  <S**2>=2.010
   181A -> 182A      -0.13078
   172B -> 180B       0.25536
   173B -> 180B      -0.10953
   174B -> 181B      -0.11847
   175B -> 181B       0.86925
   176B -> 181B       0.27324
   178B -> 181B      -0.13633
   179B -> 180B       0.15239
   179B <- 180B      -0.11270

Excited State  14:  3.006-A      2.0335 eV  609.70 nm  f=0.0071  <S**2>=2.009
   169B -> 180B       0.14452
   170B -> 180B       0.64696
   174B -> 181B       0.71465
   175B -> 181B       0.12820
   176B -> 181B       0.12248

Excited State  15:  3.006-A      2.0874 eV  593.95 nm  f=0.0302  <S**2>=2.009
   169B -> 180B      -0.15236
   170B -> 180B       0.74027
   174B -> 181B      -0.63962

Excited State  16:  3.006-A      2.1507 eV  576.48 nm  f=0.0104  <S**2>=2.010
   168B -> 180B       0.11321
   169B -> 181B      -0.10227
   171B -> 180B       0.58525
   173B -> 181B       0.78588

Excited State  17:  3.005-A      2.1670 eV  572.14 nm  f=0.0011  <S**2>=2.008
   169B -> 180B       0.97049
   174B -> 181B      -0.20935

Excited State  18:  3.006-A      2.1900 eV  566.13 nm  f=0.0078  <S**2>=2.009
   168B -> 180B       0.36557
   169B -> 181B      -0.17082
   171B -> 180B       0.67979
   173B -> 181B      -0.58281

Excited State  19:  3.057-A      2.3234 eV  533.64 nm  f=0.0001  <S**2>=2.086
   179A -> 182A       0.12618
   181A -> 183A       0.27212
   168B -> 180B       0.83785
   170B -> 181B      -0.26492
   171B -> 180B      -0.29519
   173B -> 181B       0.10414
   179B -> 182B      -0.13518

Excited State  20:  3.428-A      2.3506 eV  527.45 nm  f=0.0005  <S**2>=2.688
   179A -> 182A      -0.15184
   180A -> 182A       0.18393
```

```
   181A -> 183A      -0.62912
   168B -> 180B       0.28875
   171B -> 180B      -0.10018
   172B -> 181B       0.18049
   179B -> 182B       0.63717

 Excited State  21:  3.442-A      2.3568 eV  526.06 nm  f=0.0152  <S**2>=2.711
   179A -> 183A       0.15582
   180A -> 183A      -0.14739
   181A -> 182A       0.70731
   179B -> 183B      -0.65465

 Excited State  22:  3.041-A      2.4001 eV  516.57 nm  f=0.0032  <S**2>=2.061
   172B -> 181B       0.97446
   179B -> 182B      -0.20614

 Excited State  23:  3.054-A      2.4365 eV  508.86 nm  f=0.0030  <S**2>=2.082
   180A -> 182A       0.92627
   181A -> 183A       0.28710
   169B -> 181B      -0.18780
   170B -> 181B      -0.11607

 Excited State  24:  3.104-A      2.4487 eV  506.33 nm  f=0.0005  <S**2>=2.158
   180A -> 183A       0.92062
   181A -> 182A       0.32115
   171B -> 181B      -0.11729
   179B -> 183B       0.11149

 Excited State  25:  3.005-A      2.4955 eV  496.83 nm  f=0.0004  <S**2>=2.008
   167B -> 180B       0.99679

 Excited State  26:  3.661-A      2.5426 eV  487.63 nm  f=0.0075  <S**2>=3.101
   179A -> 182A       0.61916
   180A -> 182A       0.18953
   181A -> 183A      -0.55900
   170B -> 181B       0.14069
   179B -> 182B      -0.47270

 Excited State  27:  3.624-A      2.5495 eV  486.32 nm  f=0.0120  <S**2>=3.033
   179A -> 183A       0.55351
   180A -> 183A       0.21172
   181A -> 182A      -0.50284
   171B -> 181B      -0.34836
   179B -> 183B      -0.51013

 Excited State  28:  3.017-A      2.5652 eV  483.34 nm  f=0.0014  <S**2>=2.026
   179A -> 182A       0.14455
   180A -> 182A      -0.14670
   161B -> 180B       0.14297
   165B -> 180B       0.62589
   168B -> 180B      -0.16433
   169B -> 181B      -0.35814
   170B -> 181B      -0.60441

 Excited State  29:  3.005-A      2.5803 eV  480.51 nm  f=0.0004  <S**2>=2.008
   166B -> 180B       0.99757

 Excited State  30:  3.073-A      2.6064 eV  475.69 nm  f=0.0018  <S**2>=2.110
   179A -> 183A       0.29940
   180A -> 183A       0.15886
   181A -> 182A      -0.13361
   168B -> 181B      -0.22432
   171B -> 181B       0.88731
```

Triplet **[CuL^{pu,OMe}]$^{+}$**

```
Excited State   1:  3.003-A      0.5722 eV 2166.96 nm  f=0.1046  <S**2>=2.005
   154B -> 157B       0.15243
   155B -> 156B       1.06546
   155B <- 156B      -0.40299
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -3297.79409147
 Copying the excited state density for this state as the 1-particle RhoCI density.
```

```
Excited State   2:  3.004-A      0.7103 eV 1745.40 nm  f=0.0022  <S**2>=2.006
   154B -> 156B       0.14666
   155B -> 157B       0.98539

Excited State   3:  3.004-A      1.2476 eV  993.80 nm  f=0.0019  <S**2>=2.006
   151B -> 156B      -0.17693
   154B -> 156B       0.97128
   155B -> 157B      -0.12993

Excited State   4:  3.005-A      1.5852 eV  782.13 nm  f=0.0033  <S**2>=2.008
   153B -> 156B       0.99259

Excited State   5:  3.004-A      1.6941 eV  731.84 nm  f=0.1230  <S**2>=2.007
   152B -> 156B      -0.16718
   153B -> 157B      -0.11538
   154B -> 157B       0.95271
   155B -> 156B      -0.18222
   155B <- 156B       0.13403

Excited State   6:  3.006-A      1.7071 eV  726.28 nm  f=0.0037  <S**2>=2.009
   152B -> 156B       0.97060
   154B -> 157B       0.17074

Excited State   7:  3.005-A      1.9136 eV  647.92 nm  f=0.0064  <S**2>=2.007
   150B -> 156B       0.85979
   151B -> 156B      -0.39000
   151B -> 157B      -0.12616
   152B -> 157B       0.11083
   153B -> 157B      -0.22762

Excited State   8:  3.005-A      1.9411 eV  638.73 nm  f=0.0055  <S**2>=2.007
   149B -> 156B      -0.10140
   150B -> 156B       0.38598
   151B -> 156B       0.87006
   154B -> 156B       0.14361

Excited State   9:  3.004-A      1.9640 eV  631.28 nm  f=0.0236  <S**2>=2.007
   150B -> 156B       0.22736
   152B -> 157B       0.13025
   153B -> 157B       0.95085

Excited State  10:  3.005-A      2.0837 eV  595.03 nm  f=0.0407  <S**2>=2.007
   149B -> 156B       0.10354
   150B -> 156B      -0.14089
   151B -> 157B       0.19529
   152B -> 157B       0.94351

Excited State  11:  3.523-A      2.1936 eV  565.21 nm  f=0.0044  <S**2>=2.853
   156A -> 158A      -0.35744
   157A -> 158A      -0.25534
   157A -> 159A       0.47141
   151B -> 157B       0.47918
   155B -> 158B       0.51484
   155B -> 159B      -0.21704

Excited State  12:  3.218-A      2.2058 eV  562.09 nm  f=0.0028  <S**2>=2.339
   156A -> 158A      -0.28834
   156A -> 159A      -0.13711
   157A -> 158A       0.64833
   149B -> 156B       0.25097
   150B -> 157B      -0.34450
   151B -> 157B       0.23670
   152B -> 157B      -0.10977
   155B -> 158B       0.19423
   155B -> 159B       0.40645

Excited State  13:  3.267-A      2.2477 eV  551.61 nm  f=0.0029  <S**2>=2.418
   155A -> 158A      -0.11772
   157A -> 158A      -0.12893
   157A -> 159A      -0.21094
   146B -> 157B       0.10848
   147B -> 156B       0.10266
   150B -> 156B       0.11206
   151B -> 157B       0.73765
   152B -> 157B      -0.14609
   155B -> 158B      -0.53439
```

```
Excited State  14:  3.054-A      2.2741 eV  545.21 nm  f=0.0033  <S**2>=2.082
   157A -> 158A      -0.35289
   146B -> 156B       0.12932
   149B -> 156B       0.66480
   150B -> 157B      -0.52245
   155B -> 159B      -0.31822

Excited State  15:  3.373-A      2.3119 eV  536.29 nm  f=0.0006  <S**2>=2.594
   156A -> 158A       0.61401
   156A -> 159A       0.15015
   157A -> 158A       0.39235
   157A -> 159A       0.50590
   148B -> 156B       0.15631
   150B -> 157B      -0.16764
   155B -> 159B      -0.31093

Excited State  16:  3.007-A      2.3288 eV  532.41 nm  f=0.0071  <S**2>=2.010
   156A -> 158A      -0.13965
   157A -> 158A      -0.13140
   157A -> 159A      -0.12051
   147B -> 156B       0.18403
   148B -> 156B       0.74828
   149B -> 156B      -0.43868
   149B -> 157B      -0.10374
   150B -> 157B      -0.34084
   155B -> 158B      -0.11915

Excited State  17:  3.070-A      2.3561 eV  526.22 nm  f=0.0003  <S**2>=2.105
   156A -> 158A       0.13396
   156A -> 159A      -0.31597
   147B -> 156B       0.21162
   148B -> 156B       0.50604
   149B -> 156B       0.45004
   150B -> 157B       0.55043
   155B -> 159B       0.16866

Excited State  18:  3.256-A      2.3853 eV  519.79 nm  f=0.0010  <S**2>=2.401
   156A -> 158A      -0.30104
   156A -> 159A       0.78350
   157A -> 158A       0.22181
   157A -> 159A      -0.15493
   148B -> 156B       0.20925
   149B -> 156B       0.20952
   150B -> 157B       0.24671
   155B -> 159B      -0.20539

Excited State  19:  3.141-A      2.4727 eV  501.42 nm  f=0.0655  <S**2>=2.217
   155A -> 158A       0.27114
   156A -> 158A       0.13595
   156A -> 159A       0.12332
   157A -> 159A      -0.26604
   147B -> 156B       0.79661
   148B -> 156B      -0.19596
   149B -> 157B       0.12770
   150B -> 157B      -0.10909
   155B -> 158B       0.29429

Excited State  20:  3.274-A      2.5333 eV  489.42 nm  f=0.0093  <S**2>=2.429
   155A -> 158A       0.55321
   155A -> 159A       0.24213
   156A -> 158A       0.31100
   156A -> 159A       0.29722
   157A -> 158A      -0.17534
   157A -> 159A      -0.13563
   146B -> 156B       0.15222
   146B -> 157B       0.11580
   147B -> 156B      -0.39710
   148B -> 156B       0.11564
   148B -> 157B       0.16151
   155B -> 158B       0.17224
   155B -> 159B       0.31154

Excited State  21:  3.296-A      2.5633 eV  483.69 nm  f=0.0105  <S**2>=2.466
   155A -> 158A      -0.35908
   155A -> 159A       0.51818
   156A -> 159A       0.22906
   157A -> 158A      -0.19162
```

```
   157A -> 159A       0.35159
   146B -> 156B       0.18937
   146B -> 157B      -0.13767
   147B -> 156B       0.22626
   147B -> 157B       0.13198
   149B -> 157B      -0.21724
   155B -> 159B       0.40751

Excited State  22:  3.050-A      2.6265 eV  472.06 nm  f=0.0045  <S**2>=2.075
   155A -> 158A      -0.13728
   155A -> 159A      -0.35287
   146B -> 156B       0.88665
   150B -> 157B       0.14429

Excited State  23:  3.023-A      2.6851 eV  461.75 nm  f=0.0009  <S**2>=2.034
   155A -> 158A      -0.17164
   156A -> 158A      -0.11850
   157A -> 159A       0.12869
   146B -> 157B       0.29860
   148B -> 157B       0.26563
   149B -> 157B       0.83753
   151B -> 157B      -0.18653

Excited State  24:  3.027-A      2.7314 eV  453.93 nm  f=0.0263  <S**2>=2.041
   155A -> 158A       0.56912
   156A -> 158A      -0.31503
   156A -> 159A      -0.12116
   157A -> 159A       0.28161
   141B -> 156B       0.11213
   145B -> 156B       0.11535
   146B -> 156B       0.12097
   147B -> 156B       0.12287
   147B -> 157B      -0.25492
   148B -> 156B      -0.11580
   148B -> 157B       0.28371
   149B -> 157B      -0.11689
   151B -> 157B      -0.11755
   155B -> 158B      -0.42901

Excited State  25:  3.016-A      2.7467 eV  451.39 nm  f=0.0149  <S**2>=2.024
   155A -> 158A      -0.28596
   155A -> 159A       0.17831
   157A -> 159A      -0.20221
   146B -> 156B      -0.11387
   146B -> 157B       0.17259
   147B -> 157B      -0.48054
   148B -> 157B       0.61246
   149B -> 157B      -0.26552
   155B -> 158B       0.21005
   155B -> 159B      -0.17063

Excited State  26:  3.052-A      2.8045 eV  442.10 nm  f=0.0068  <S**2>=2.078
   155A -> 159A       0.57153
   157A -> 159A      -0.10210
   145B -> 156B      -0.41943
   146B -> 156B       0.22358
   147B -> 157B      -0.36305
   148B -> 157B      -0.39938
   149B -> 157B       0.14382
   155B -> 159B      -0.26457

Excited State  27:  3.015-A      2.8545 eV  434.35 nm  f=0.0216  <S**2>=2.023
   155A -> 159A       0.36648
   156A -> 159A      -0.11342
   157A -> 158A       0.12388
   157A -> 159A      -0.13970
   145B -> 156B       0.75349
   147B -> 157B       0.29246
   149B -> 157B       0.10068
   150B -> 157B       0.13191
   155B -> 159B      -0.28258

Excited State  28:  3.010-A      2.9009 eV  427.39 nm  f=0.0298  <S**2>=2.015
   141B -> 156B       0.15138
   146B -> 157B       0.87813
   147B -> 157B       0.10821
   148B -> 157B      -0.23852
```

```
   149B -> 157B      -0.26674
   151B -> 157B      -0.10402

 Excited State  29:  3.005-A      2.9473 eV  420.67 nm  f=0.0020  <S**2>=2.007
   144B -> 156B       0.98561
   147B -> 157B      -0.10298

 Excited State  30:  3.008-A      3.0213 eV  410.36 nm  f=0.0632  <S**2>=2.012
   155A -> 159A       0.14215
   156A -> 159A      -0.13388
   157A -> 158A       0.12398
   139B -> 156B       0.10489
   140B -> 156B      -0.13417
   142B -> 156B      -0.21980
   143B -> 156B       0.35324
   144B -> 156B       0.13274
   144B -> 157B      -0.13524
   145B -> 156B      -0.39218
   147B -> 157B       0.56344
   148B -> 157B       0.32693
   150B -> 157B       0.10244
   155B -> 159B      -0.18611
```

Triplet **[CuL^{pu,tBu}]$^{+}$**

```
Excited State   1:  3.004-A      0.5668 eV 2187.28 nm  f=0.1008  <S**2>=2.006
   170B -> 173B       0.15798
   171B -> 172B       1.05833
   171B <- 172B      -0.38465
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -3383.11713056
 Copying the excited state density for this state as the 1-particle RhoCI density.

 Excited State   2:  3.005-A      0.8231 eV 1506.32 nm  f=0.0003  <S**2>=2.008
   170B -> 172B       0.18580
   171B -> 173B       0.98043

 Excited State   3:  3.005-A      1.0590 eV 1170.82 nm  f=0.0036  <S**2>=2.007
   166B -> 172B      -0.14313
   170B -> 172B       0.97084
   171B -> 173B      -0.17360

 Excited State   4:  3.005-A      1.3145 eV  943.23 nm  f=0.0026  <S**2>=2.008
   169B -> 172B       0.99610

 Excited State   5:  3.005-A      1.3796 eV  898.70 nm  f=0.0060  <S**2>=2.008
   168B -> 172B       0.99573

 Excited State   6:  3.005-A      1.6606 eV  746.64 nm  f=0.0802  <S**2>=2.008
   167B -> 172B       0.11038
   168B -> 173B       0.31393
   170B -> 173B       0.92942
   171B -> 172B      -0.16363
   171B <- 172B       0.11864

 Excited State   7:  3.005-A      1.7868 eV  693.87 nm  f=0.0094  <S**2>=2.008
   166B -> 173B      -0.11505
   167B -> 172B       0.97759
   170B -> 173B      -0.14087

 Excited State   8:  3.005-A      1.8250 eV  679.37 nm  f=0.0003  <S**2>=2.008
   169B -> 173B       0.99725

 Excited State   9:  3.005-A      1.8904 eV  655.86 nm  f=0.0039  <S**2>=2.008
   164B -> 172B      -0.15347
   165B -> 173B      -0.13811
   166B -> 172B       0.95940
   170B -> 172B       0.11153

 Excited State  10:  3.006-A      1.9655 eV  630.81 nm  f=0.1257  <S**2>=2.008
   162B -> 173B       0.10317
   167B -> 172B      -0.10485
   168B -> 173B       0.93523
   170B -> 173B      -0.28093
   171B -> 172B       0.15098
```

```
   171B <- 172B      -0.11515

Excited State  11:  3.005-A      2.1023 eV  589.75 nm  f=0.0007  <S**2>=2.008
   165B -> 172B       0.99409

Excited State  12:  3.007-A      2.2031 eV  562.78 nm  f=0.0012  <S**2>=2.010
   162B -> 172B       0.10614
   164B -> 172B       0.86570
   166B -> 172B       0.11238
   167B -> 173B      -0.45965

Excited State  13:  3.011-A      2.3610 eV  525.14 nm  f=0.0087  <S**2>=2.016
   172A -> 175A      -0.10635
   173A -> 174A       0.20229
   164B -> 173B       0.17432
   166B -> 173B       0.94090
   167B -> 172B       0.10702

Excited State  14:  3.007-A      2.3654 eV  524.16 nm  f=0.0033  <S**2>=2.010
   172A -> 174A      -0.13852
   162B -> 172B      -0.28952
   164B -> 172B       0.45468
   165B -> 173B      -0.19913
   167B -> 173B       0.79224

Excited State  15:  3.547-A      2.5050 eV  494.94 nm  f=0.0264  <S**2>=2.895
   171A -> 174A       0.15821
   172A -> 175A       0.31380
   173A -> 174A      -0.53319
   163B -> 172B      -0.39428
   164B -> 173B       0.12592
   166B -> 173B       0.12228
   171B -> 174B       0.61915

Excited State  16:  3.170-A      2.5138 eV  493.22 nm  f=0.0005  <S**2>=2.263
   171A -> 175A      -0.10816
   172A -> 174A      -0.58364
   173A -> 175A       0.18442
   162B -> 172B       0.65333
   165B -> 173B       0.19438
   167B -> 173B       0.15688
   171B -> 175B      -0.33878

Excited State  17:  3.027-A      2.5241 eV  491.19 nm  f=0.0032  <S**2>=2.040
   161B -> 172B       0.82209
   163B -> 172B      -0.54215
   171B -> 174B      -0.13291

Excited State  18:  3.116-A      2.5418 eV  487.78 nm  f=0.0286  <S**2>=2.177
   172A -> 175A       0.10628
   173A -> 174A      -0.15919
   161B -> 172B       0.55833
   163B -> 172B       0.72645
   171B -> 174B       0.32225

Excited State  19:  3.264-A      2.5557 eV  485.13 nm  f=0.0008  <S**2>=2.414
   172A -> 174A       0.39982
   173A -> 175A      -0.25910
   159B -> 172B      -0.10430
   162B -> 172B       0.63848
   167B -> 173B       0.27317
   171B -> 175B       0.51731

Excited State  20:  3.081-A      2.5778 eV  480.97 nm  f=0.0009  <S**2>=2.123
   171A -> 174A       0.18635
   172A -> 175A       0.46675
   173A -> 174A       0.72554
   164B -> 173B      -0.24341
   171B -> 174B       0.37156

Excited State  21:  3.007-A      2.6158 eV  473.99 nm  f=0.0002  <S**2>=2.011
   173A -> 175A      -0.10926
   160B -> 172B       0.99180

Excited State  22:  3.049-A      2.6232 eV  472.64 nm  f=0.0003  <S**2>=2.074
   172A -> 174A       0.37903
   173A -> 175A       0.87908
```

```
   160B -> 172B       0.11317
   165B -> 173B       0.20005
   167B -> 173B       0.11216

Excited State  23:  3.085-A      2.6971 eV  459.70 nm  f=0.0005  <S**2>=2.130
   171A -> 174A      -0.18629
   172A -> 175A       0.33382
   173A -> 174A       0.19600
   162B -> 173B       0.29855
   164B -> 173B       0.81406
   166B -> 173B      -0.17860
   171B -> 174B      -0.10888

Excited State  24:  3.010-A      2.7236 eV  455.22 nm  f=0.0001  <S**2>=2.015
   159B -> 172B       0.97853
   171B -> 175B       0.11080

Excited State  25:  3.418-A      2.7353 eV  453.27 nm  f=0.0001  <S**2>=2.671
   171A -> 175A       0.36229
   172A -> 174A      -0.35590
   157B -> 172B       0.38921
   162B -> 172B      -0.18038
   165B -> 173B       0.56018
   171B -> 175B       0.46198

Excited State  26:  3.007-A      2.7457 eV  451.56 nm  f=0.0028  <S**2>=2.010
   158B -> 172B       0.99461

Excited State  27:  3.407-A      2.7797 eV  446.04 nm  f=0.0090  <S**2>=2.652
   171A -> 174A       0.60954
   172A -> 175A      -0.59721
   173A -> 174A       0.17948
   155B -> 172B       0.14059
   162B -> 173B       0.10698
   164B -> 173B       0.29802
   166B -> 173B      -0.15103
   171B -> 174B       0.27717

Excited State  28:  3.281-A      2.8014 eV  442.58 nm  f=0.0079  <S**2>=2.441
   171A -> 175A      -0.40865
   172A -> 174A       0.28378
   173A -> 175A      -0.17361
   157B -> 172B       0.75526
   165B -> 173B       0.17534
   171B -> 175B      -0.32294

Excited State  29:  3.072-A      2.8617 eV  433.26 nm  f=0.0123  <S**2>=2.110
   171A -> 175A       0.27089
   172A -> 174A      -0.13328
   173A -> 175A       0.16033
   154B -> 172B       0.15658
   156B -> 172B       0.61050
   157B -> 172B       0.41004
   165B -> 173B      -0.50418
   171B -> 175B       0.10992

Excited State  30:  3.029-A      2.9033 eV  427.04 nm  f=0.0082  <S**2>=2.044
   171A -> 175A      -0.19513
   154B -> 172B      -0.28353
   156B -> 172B       0.77506
   157B -> 172B      -0.28469
   165B -> 173B       0.35300
```