Supporting Information:

Direct Copper(III) Formation from O_2 and Copper(I) with Histamine Ligation

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Titrations of T_{nBu}, T_{Me3}, and T_{Me2} with decamethylferrocene:

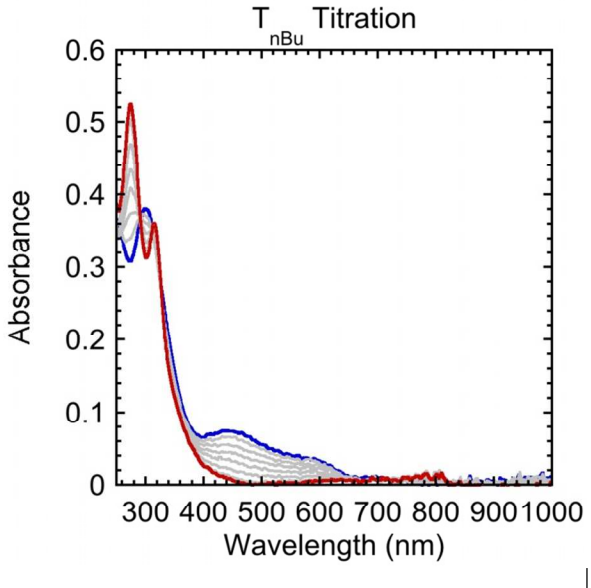


Figure S1. Spectral change of T_{nBu} (blue) with decamethylferrocene (red) at -95°C in 2MeTHF.

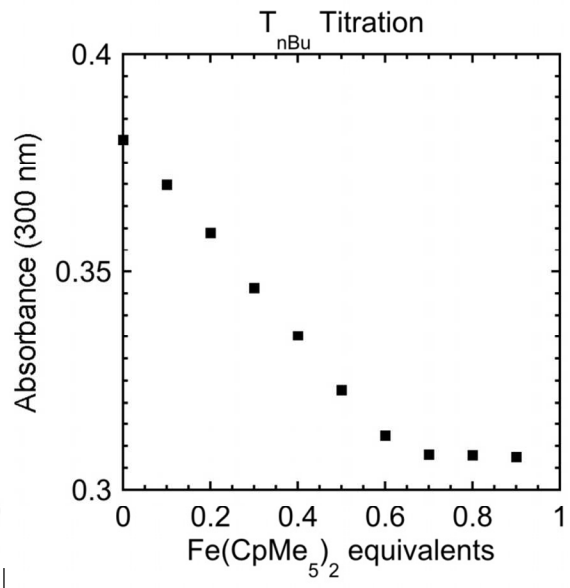


Figure S2. Spectral change of T_{nBu} with decamethylferrocence monitored at 300 nm at -95°C in 2MeTHF.

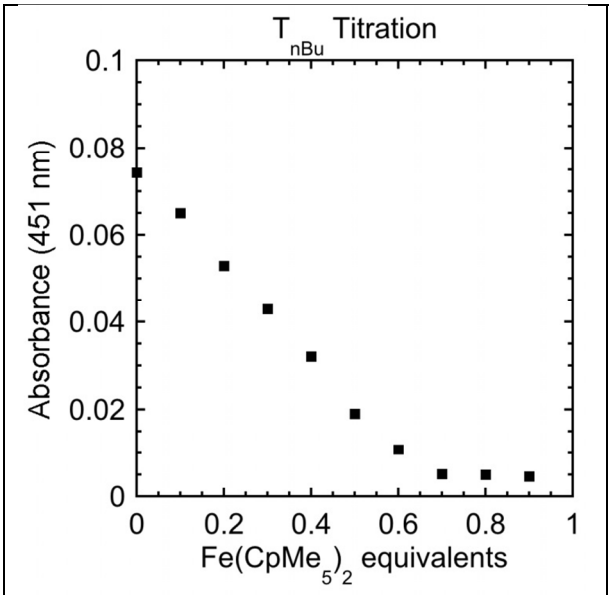


Figure S3. Spectral change of $\mathbf{T_{nBu}}$ with decamethylferrocence monitored at 451 nm at -95°C in 2MeTHF.

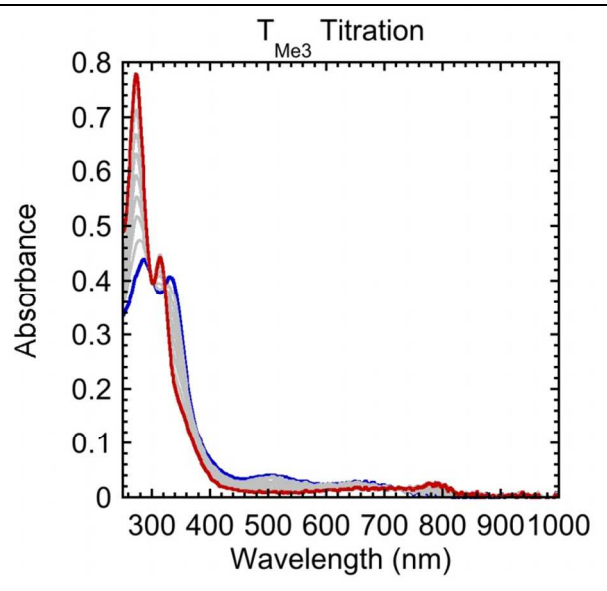


Figure S4. Spectral change of $\mathbf{T_{Me3}}$ (blue) with decamethylferrocence (red) at -95°C in 2MeTHF.

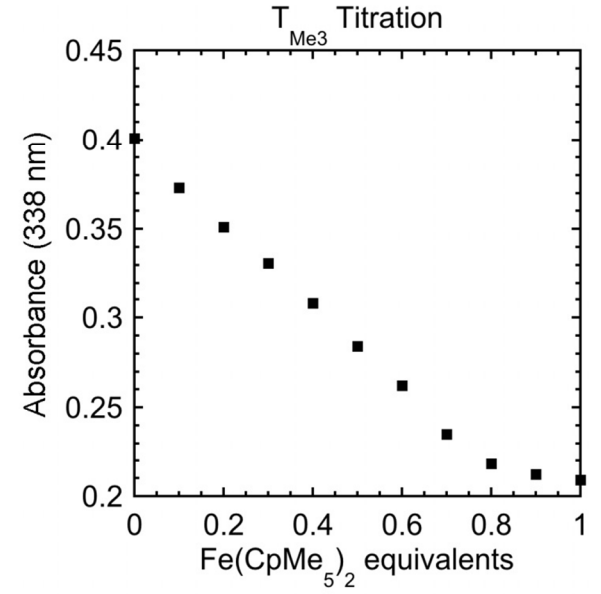


Figure S5. Spectral change of $\mathbf{T_{Me3}}$ with decamethylferrocence monitored at 338 nm at -95°C in 2MeTHF.

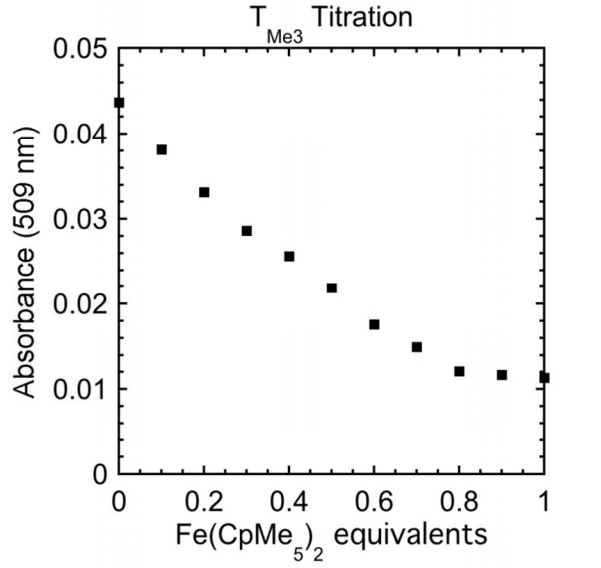


Figure S6. Spectral change of $\mathbf{T_{Me3}}$ with decamethylferrocence monitored at 509 nm at -95°C in 2MeTHF.

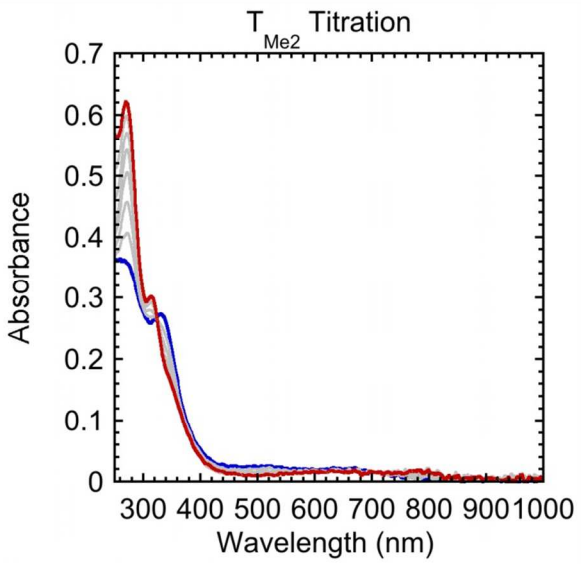


Figure S7. Spectral change of $\mathbf{T_{Me2}}$ (blue) with decamethylferrocence (red) at -95°C in 2MeTHF.

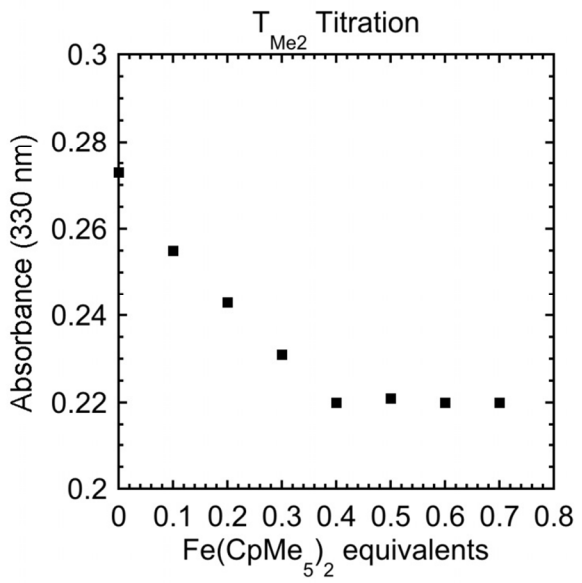


Figure S8. Spectral change of $\mathbf{T_{Me2}}$ with decamethylferrocence monitored at 330 nm at -95°C in 2MeTHF.

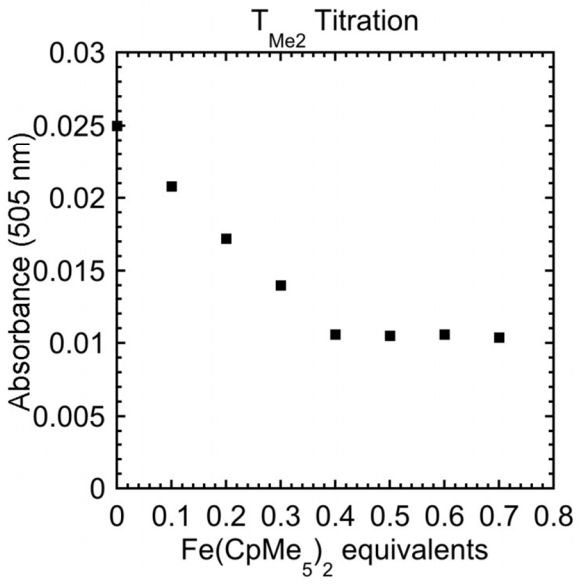


Figure S9. Spectral change of $\mathbf{T_{Me2}}$ with decamethylferrocence monitored at 505 nm at -95°C in 2MeTHF.

O_2 titration with L_{nBu}:

The resulting absorbance (457 nm) versus equivalents plot are shown below. The Cu/O_2 ratio is determined to be the crossing point of the two linear regions (0.334 equivalents of O_2) or Cu/O_2 of 2.975.

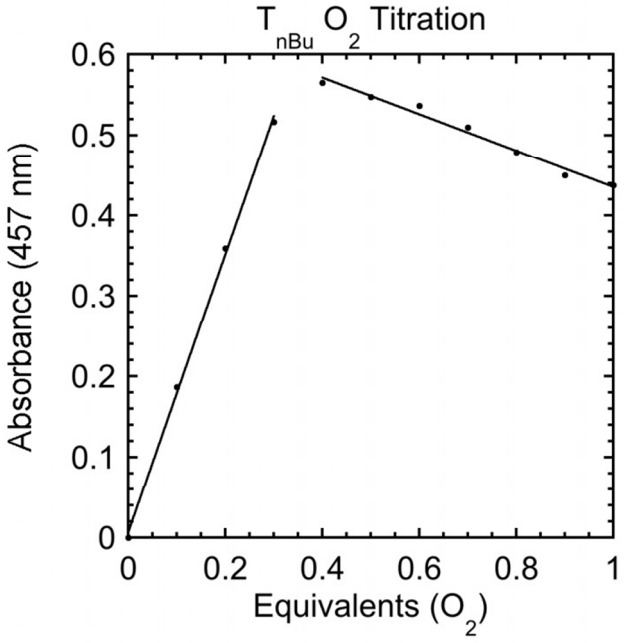


Figure S10. Oxygen titration jobs plot for $\mathbf{T_{nBu}}$ formation. Equations are y=1.723x+.0073; R^2=0.9986 and y=-0.2268x+0.6626; R^2=0.9811.

O_2 titration with L_{Me3}:
The resulting absorbance (510 nm) versus equivalents plot are shown below. The Cu/O_2 ratio is determined to be the crossing point of the two linear regions (0.305 equivalents of O_2) or Cu/O_2 of 3.277.

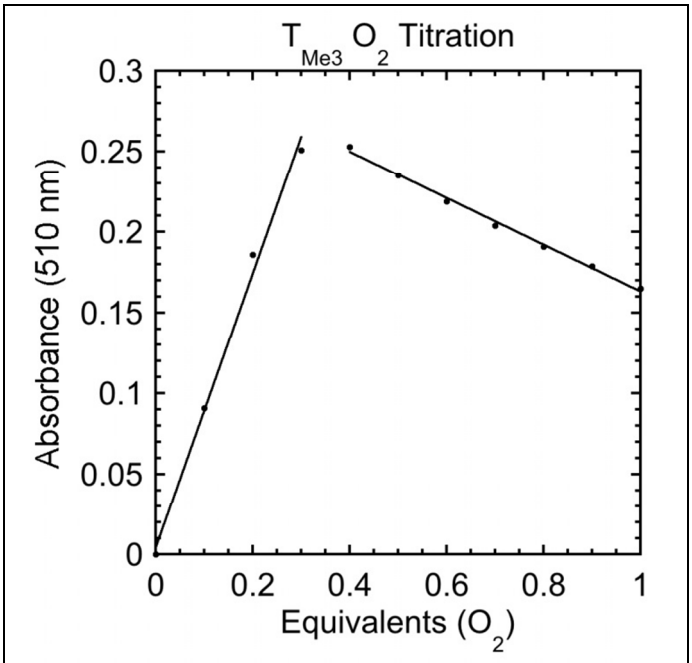


Figure S11. Oxygen titration jobs plot for $\mathbf{T_{nBu}}$ formation. Equations are y=0.848x+.0048; R^2=0.9937 and y=-0.1443x+0.3076; R^2=0.9955.

High-resolution Mass Spectrometry of T_{nBu}:
The resulting $[((\mathbf{L_{nBu}}Cu)_3O_2)(SbF_6)_2]^+$ was observed in the spectrum shown below and full inset of high resolution isotope pattern.

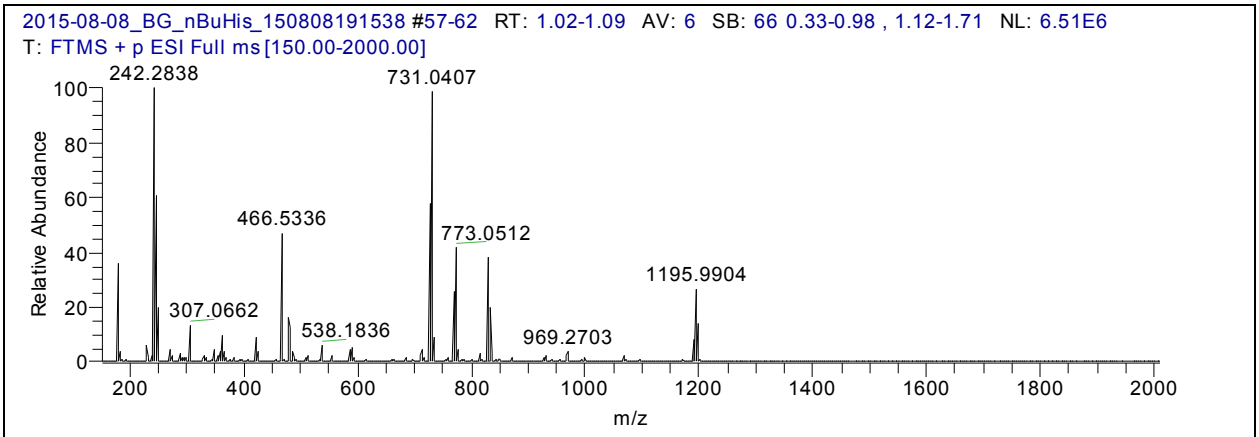


Figure S12. Full mass spectrum of $\mathbf{T_{nBu}}$.

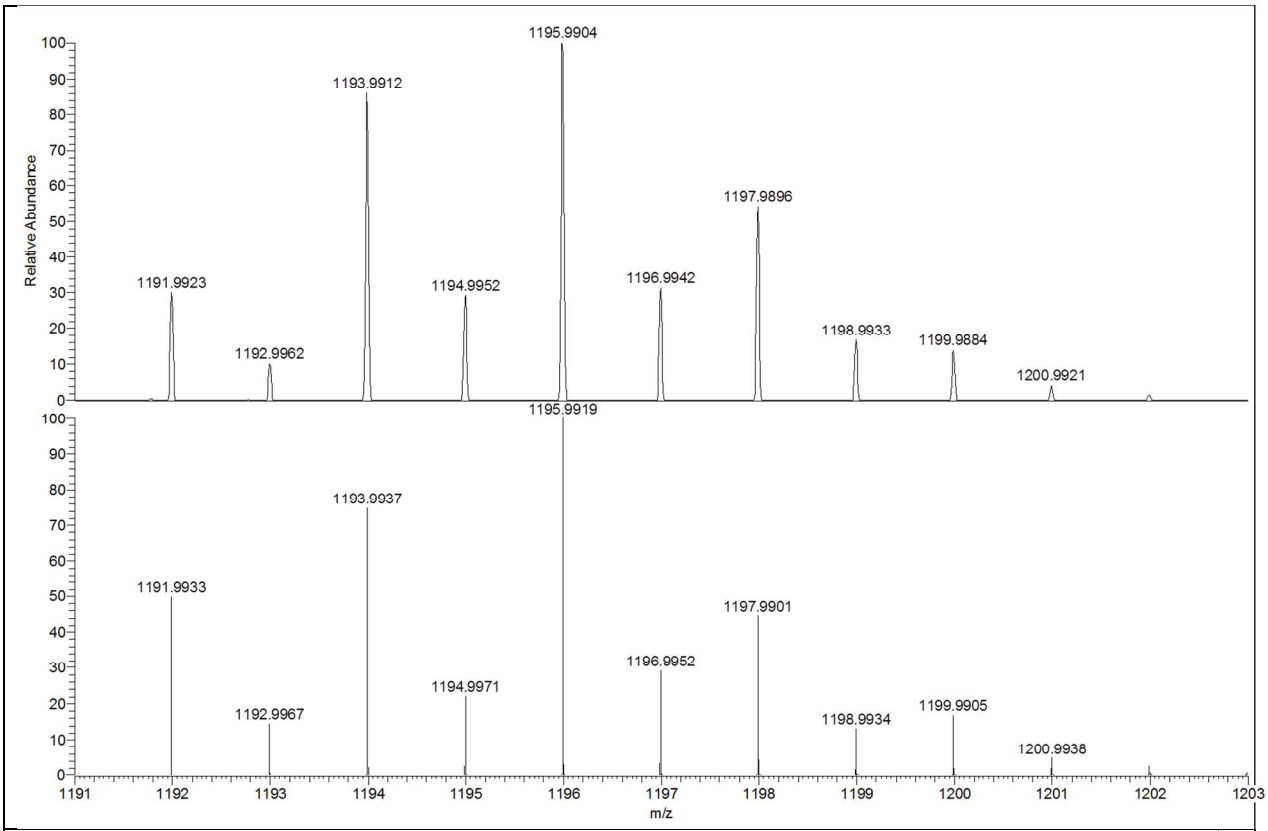


Figure S13. High resolution mass spectrum of $\mathbf{T_{nBu}}$ (observed as $[((\mathbf{L_{nBu}}Cu)_3O_2)(SbF_6)_2]^+$). Experimental spectrum above with theoretical isotope pattern below.

High-resolution Mass Spectrometry of T_{Me3}:

The resulting $[((\mathbf{L_{Me3}}Cu)_3O_2)(SbF_6)_2]^+$ was observed in the spectrum shown below and full inset of high resolution isotope pattern.

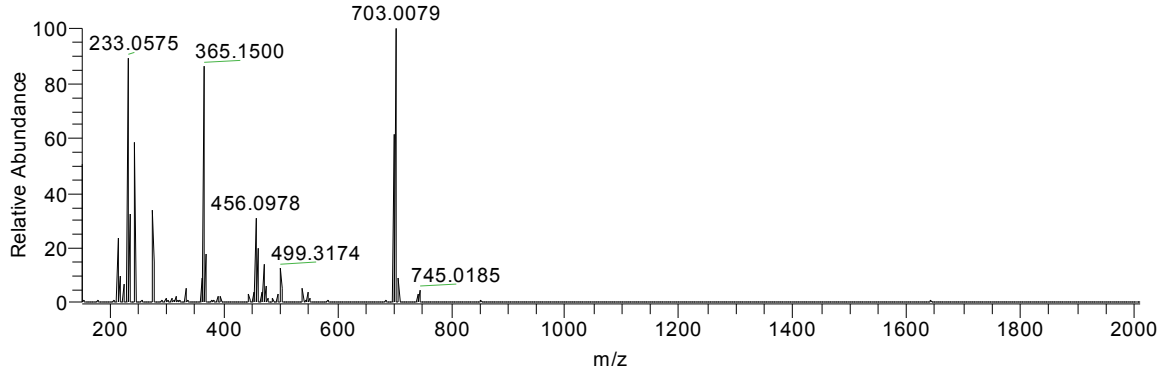


Figure S14. Full mass spectrum of $\mathbf{T_{Me3}}$.

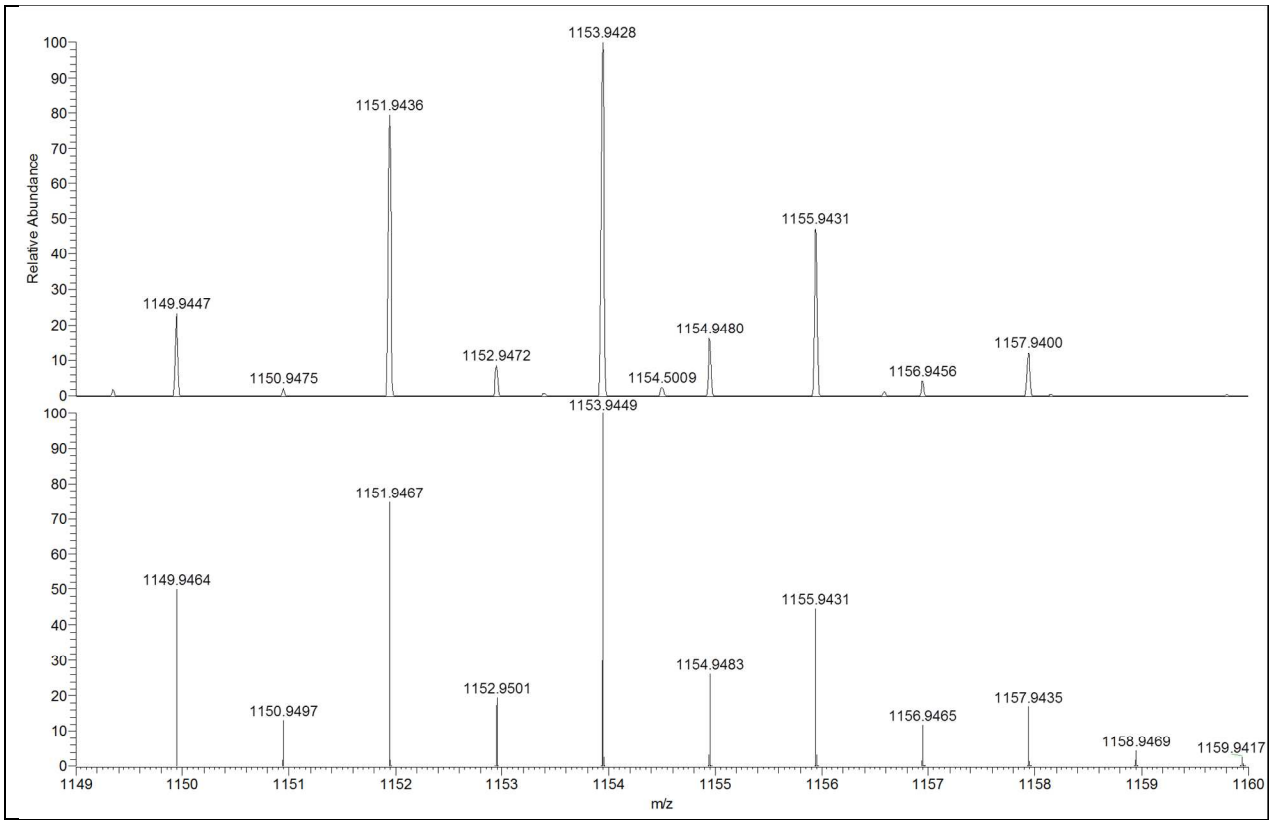


Figure S15. High resolution mass spectrum of $\mathbf{T_{Me3}}$ (observed as $[((\mathbf{L_{Me3}}Cu)_3O_2)(SbF_6)_2]^+$). Experimental spectrum above with theoretical isotope pattern below.

Mixture of T_{nBu} and O_{nBu}:
The mixture is fit by addition of pure optical spectra for independently synthesized $\mathbf{T_{nBu}}$ and $\mathbf{O_{nBu}}$.

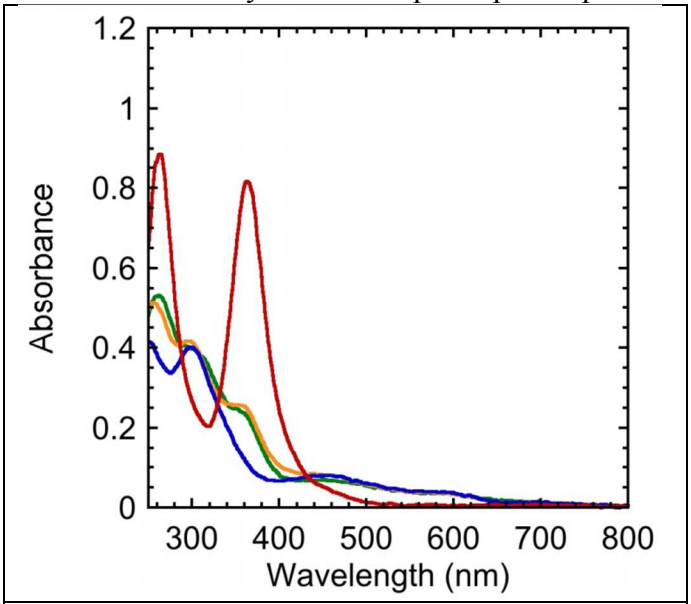


Figure S16. Experimental mixture of $\mathbf{T_{nBu}}$ and $\mathbf{O_{nBu}}$ (Pure $\mathbf{O_{nBu}}$ (red), pure $\mathbf{T_{nBu}}$ (blue), experimental spectrum (green), and fit spectrum (orange)). 5:1 ratio of $\mathbf{T_{nBu}}$:$\mathbf{O_{nBu}}$.

Mixture of T_{Me3} and O_{Me3}:
The mixture is fit by addition of pure optical spectra for independently synthesized $\mathbf{T_{Me3}}$ and $\mathbf{O_{Me3}}$.

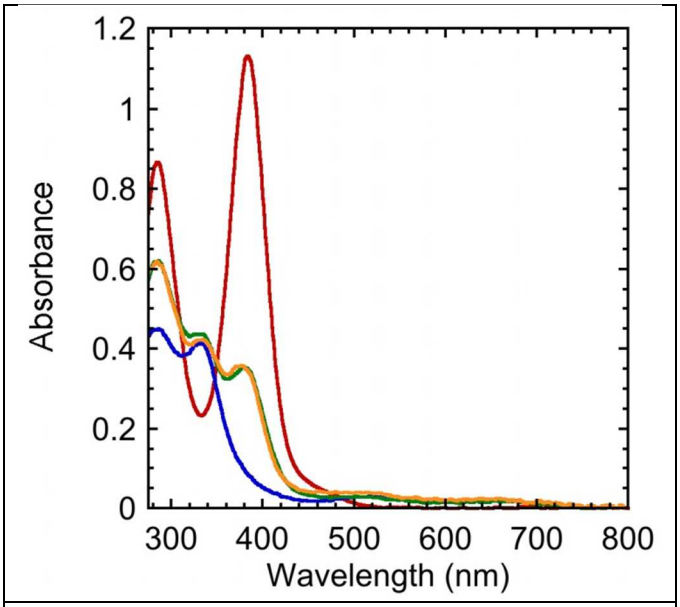


Figure S17. Experimental mixture of $\mathbf{T_{Me3}}$ and $\mathbf{O_{Me3}}$ (Pure $\mathbf{O_{Me3}}$ (red), pure $\mathbf{T_{Me3}}$ (blue), experimental spectrum (green), and fit spectrum (orange)). 3.5:1 ratio of $\mathbf{T_{Me3}}$:$\mathbf{O_{Me3}}$.

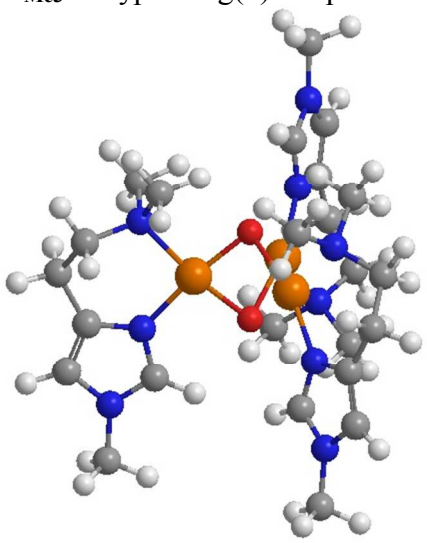
Reactions of T and O with ascorbic acid:
Data for $\mathbf{T_{Me3}}$ was monitored and fit in 300-700 nm range and $\mathbf{T_{nBu}}$ was monitored by single wavelength at 310 nm. Kinetic rates are detailed below (**Table S1**).Data was monitored by single wavelength ($\mathbf{O_{nBu}}$ at 363 nm and $\mathbf{O_{Me3}}$ at 380 nm). Kinetic rates are detailed below (**Table S1**).

Table S1. Ascorbic acid reactivity

Species	[Cu cluster]	[ascorbic acid]	rate
$\mathbf{T_{Me3}}$	0.28 mM	13.9 mM	0.02 min^{-1}
$\mathbf{T_{nBu}}$	0.28 mM	1.4 mM	15 min^{-1}
$\mathbf{O_{Me3}}$	0.028 mM	0.14 mM	> 18 min^{-1}
$\mathbf{O_{nBu}}$	0.028 mM	0.14 mM	> 18 min^{-1}

DFT Calculations:
Geometric Predictions for $\mathbf{T_{Me3}}$ and $\mathbf{T_{nBu}}$:
Geometry optimizations of $\mathbf{T_{Me3}}$ and $\mathbf{T_{nBu}}$ (butyl group was modeled as a methyl group - $\mathbf{T_{Me}}$) were performed in C_1 symmetry at the B3lyp/6-31g(d) level of theory in the gas phase with Gaussian09.[1-3] Optimized calculation structures are tabulated below. Of the multiple *cis/trans* isomers tested, the lowest energy structure has a *trans* relationship of the histamine ligands on the two Cu(II) metal centers.

$\mathbf{T_{Me3}}$ B3lyp/6-31g(d) - triplet

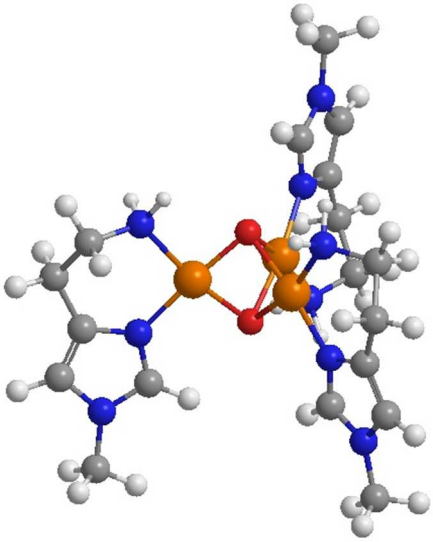


Cu	-0.71457500	1.30973000	-0.61280400
Cu	1.19958100	0.20914300	0.86034300
O	0.76937300	0.12047100	-1.09617900
N	-2.42989500	2.03352900	-0.04890800
N	-0.24733800	2.84445100	-1.86371800
N	3.12900300	0.34250300	0.67827000
Cu	-0.23659100	-1.34976700	-0.75212800
O	-0.68966100	-0.25656700	0.63749600
N	1.13562800	0.42386200	2.88332500
N	0.44203800	-2.32505800	-2.35176500

N	-1.29030200	-2.79653600	-0.09791400
C	-2.10871900	-2.70533000	0.95947800
H	-2.25838600	-1.81422700	1.54441400
C	-3.25503600	1.48549600	0.85131300
H	-3.07897300	0.55835400	1.37145000
C	3.82390500	0.50138900	-0.45525400
H	3.40045200	0.55155200	-1.44548900
C	-0.90547500	4.14498900	-1.49888600
H	-0.53282200	4.42840600	-0.50888500
H	-0.56150000	4.90695000	-2.21060900
C	-1.37641600	-4.10166900	-0.56603500
C	-3.02930800	3.21764100	-0.46187300
C	-0.38734300	-3.50412400	-2.78922400
H	-1.35400900	-3.11109800	-3.11800300
H	0.11145500	-3.93578800	-3.66543100
C	-2.43275300	4.12241800	-1.49584200
H	-2.81654600	3.87422600	-2.49339800
H	-2.76871600	5.14752000	-1.30604700
C	-0.58895400	-4.58834100	-1.73806700
H	-1.12783100	-5.41127700	-2.21933500
H	0.37111600	-5.01402400	-1.42064400
C	4.05720700	0.34256000	1.71246800
C	2.39422800	0.94490300	3.51636200
H	2.49908100	1.99179400	3.21493500
H	2.25622100	0.92719400	4.60532600
C	3.66499300	0.17762000	3.14768100
H	4.47256800	0.55851000	3.78141100
H	3.57002500	-0.88463300	3.40667700
C	-2.26182900	-4.77538500	0.23107900
H	-2.60272700	-5.80010700	0.20154000
C	-4.21383500	3.35577500	0.21245600
H	-4.96590200	4.13035700	0.17665500
C	5.30413000	0.50489600	1.16899000
H	6.27944600	0.55814600	1.63027100
C	6.21521000	0.78884000	-1.17935500
H	5.78103600	0.84870700	-2.17815100
H	6.75218600	1.71489500	-0.96240500
H	6.90667500	-0.05549400	-1.13371000
C	-3.68211800	-4.18372400	2.24388800
H	-4.63571000	-4.47013500	1.79478400
H	-3.30669900	-5.00081500	2.86369400
H	-3.82211800	-3.29611100	2.86178700
C	-5.46789400	1.98846000	1.93609200
H	-6.38818300	1.88288000	1.35712900
H	-5.27570000	1.06486000	2.48352300
H	-5.57303500	2.81275500	2.64491800

N	-4.34115100	2.25400300	1.03312000
N	5.13820900	0.60097700	-0.19792800
N	-2.70835000	-3.88238100	1.18473100
C	1.82619100	-2.74574800	-1.98005700
H	2.28555100	-3.29599100	-2.80930000
H	2.41594900	-1.85479300	-1.76506600
H	1.80878700	-3.38778900	-1.09741500
C	0.51446900	-1.38823100	-3.51371600
H	1.09802300	-0.51698500	-3.22794900
H	0.98327200	-1.89743400	-4.36293100
H	-0.49585200	-1.08531600	-3.79947500
C	-0.64093400	2.41969400	-3.23581100
H	-0.43646900	3.21552200	-3.96262000
H	-0.06381600	1.53575600	-3.50992300
H	-1.70412700	2.17430600	-3.27220000
C	1.22443700	3.06626200	-1.83997600
H	1.50895900	3.83602300	-2.56780100
H	1.53288400	3.39894000	-0.84476100
H	1.72803100	2.13125600	-2.08374300
C	0.03707400	1.37674600	3.20437500
H	-0.89131000	1.02081700	2.75683600
H	-0.09183600	1.46517800	4.29028400
H	0.27736400	2.36596500	2.80410200
C	0.78671100	-0.91282600	3.43945100
H	0.67455500	-0.86045200	4.52947200
H	-0.15160000	-1.24465800	2.99379300
H	1.56594600	-1.64037000	3.20312600

T_{Me} B3lyp/6-31g(d) - triplet



Cu	-0.25484800	1.24283600	-0.80467200
Cu	1.29984800	-0.22190200	0.72269600
O	0.75803600	-0.39164900	-1.18138600

N	-1.35034300	2.72025600	-0.21410700
N	0.43774500	2.17430500	-2.44138900
N	3.19619300	-0.51035700	0.50107300
Cu	-0.64531000	-1.37710100	-0.61563300
O	-0.65525700	-0.06538500	0.63761100
N	1.38083900	0.03308700	2.70912300
N	-0.33773400	-2.63075100	-2.06191500
N	-2.14698000	-2.30308800	0.05548600
C	-2.87912300	-1.90677200	1.10564700
H	-2.67365100	-1.03397000	1.70337300
C	-2.04062900	2.79867700	0.92981000
H	-2.12198700	2.01089900	1.66245200
C	3.85523500	-0.64446500	-0.65686800
H	3.39866100	-0.66102400	-1.63449100
C	0.47667000	3.67329000	-2.41981000
H	1.15175900	3.97671500	-1.61418000
H	0.89063000	4.03999200	-3.36447300
C	-2.74340700	-3.45198900	-0.45753800
C	-1.51096400	3.94238100	-0.86057500
C	-1.51322700	-3.33852400	-2.66077200
H	-2.19633700	-2.57797100	-3.04957600
H	-1.16238700	-3.94545900	-3.50194400
C	-0.92451400	4.24542800	-2.20827000
H	-1.58889000	3.87763800	-3.00518300
H	-0.87769000	5.33085000	-2.34136000
C	-2.18984900	-4.22408900	-1.61810700
H	-2.99876500	-4.77721400	-2.10541400
H	-1.47644800	-4.98510700	-1.26735900
C	4.15310100	-0.54168800	1.51060200
C	2.67808100	0.51139800	3.29173300
H	2.88290200	1.50242500	2.87618800
H	2.57254100	0.61411000	4.37643400
C	3.80985400	-0.46432900	2.96933400
H	4.69842600	-0.15733900	3.52998300
H	3.54715000	-1.46177700	3.35404100
C	-3.84190600	-3.72076700	0.31346300
H	-4.56681500	-4.51982700	0.25555400
C	-2.30258100	4.73615600	-0.07379700
H	-2.66122600	5.74509600	-0.21670600
C	5.38160600	-0.69319900	0.92421800
H	6.37005900	-0.76500000	1.35405800
C	6.22257500	-0.92525600	-1.45673200
H	5.76048000	-0.93996900	-2.44453200
H	6.92677100	-0.09246600	-1.39754900
H	6.75079800	-1.86646100	-1.28938600
C	-4.93999900	-2.65155600	2.33312600

H	-5.92034900	-2.53075500	1.86718100
H	-4.92781800	-3.55965900	2.93965000
H	-4.72786700	-1.78955200	2.96623800
C	-3.47094900	4.46298000	2.15877400
H	-4.46884000	4.70591800	1.78708000
H	-3.54489800	3.67030200	2.90430600
H	-3.02281400	5.34853100	2.61478400
N	-2.62911600	3.99939500	1.04746100
N	5.17466300	-0.75941900	-0.43954100
N	-3.90720800	-2.74494200	1.28938100
H	0.15466800	-2.06758800	-2.76043800
H	0.34612100	-3.32461100	-1.74094200
H	1.13020000	-0.84936600	3.16541000
H	0.63281700	0.67949100	2.96868800
H	1.37614000	1.81068900	-2.62089200
H	-0.11283000	1.88210700	-3.25456000

Marcus theory calculations for $\mathbf{T_{Me3}}$ and $\mathbf{T_{nBu}}$:

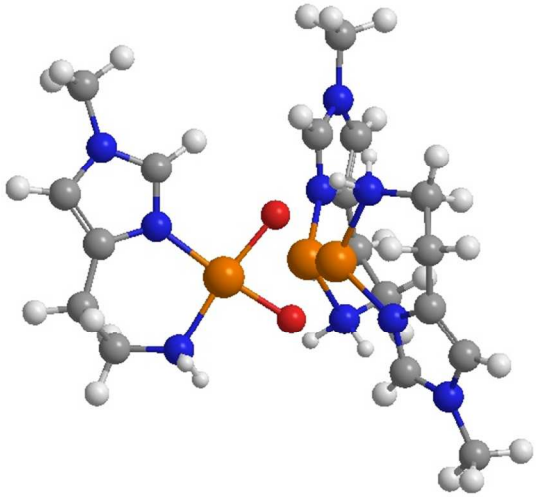
Geometry optimizations of $\mathbf{T_{Me3}}$ and $\mathbf{T_{nBu}}$ (butyl group was modeled as a methyl group) were performed in C_1 symmetry at a m06/TZVP level of theory using an SMD (water) solvation model with Gaussian09 at multiple spin states if possible (only lowest energy structure is tabulate).[4-7] Single point structures were calculated with m06/TZVP level of theory using an SMD (water) solvation model and a 2nd order relativistic correction (DKH2) with Gaussian09.[8] Associate $\mathbf{O_{Me3}}$ and $\mathbf{O_{Me}}$ structures were calculated in either C_1 or C_i (when viable) symmetry. H-atoms are placed at geometrically equivalent positions in the oxidized forms as found in the optimized structures of the reduced form. Optimized structures of all calculated complexes are tabulated below.

Table S2. Marcus theory reorganization energies

	Electron Reduction		H-atom Reduction	
	λ	λ/4	λ	λ/4
$\mathbf{T_{nBu}}$	19.0	4.8	23.1	5.8
$\mathbf{O_{nBu}}$	19.4	4.8	24.5	6.1
$\mathbf{T_{Me3}}$	20.7	5.2	24.8	6.2
$\mathbf{O_{nBu}}$	19.5	4.9	25.3	6.3

Energies are given in kcal/mol.

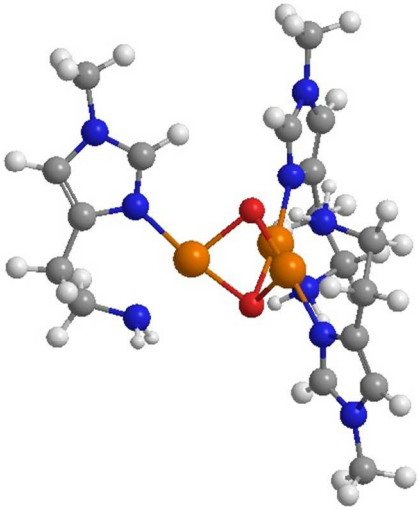
T_{Me} M06/tzvp – triplet



Cu	-0.11524500	1.19175300	-0.85273700
Cu	1.26301000	-0.46322000	0.70804200
O	0.70887900	-0.60361900	-1.20257300
N	-1.01375300	2.83914800	-0.22351100
N	0.79711000	2.10202200	-2.41870800
N	3.18161400	-0.86834800	0.45838700
Cu	-0.85548100	-1.35622900	-0.61972800
O	-0.67998000	-0.02198200	0.62492700
N	1.41455000	-0.27751900	2.72398800
N	-0.79689300	-2.67174200	-2.05859200
N	-2.52849800	-1.98783400	0.07854700
C	-3.21472500	-1.40227800	1.04756900
H	-2.90282200	-0.54016000	1.61511100
C	-1.59534000	3.01339500	0.95034200
H	-1.78894100	2.24591900	1.68446600
C	3.85858400	-0.83747600	-0.67565100
H	3.45020600	-0.63376800	-1.65410900
C	0.97245100	3.56434700	-2.35331700
H	1.63694300	3.78934400	-1.51595600
H	1.45721300	3.92180400	-3.26566100
C	-3.28979900	-3.03374200	-0.39775400
C	-0.95462900	4.07389500	-0.83167900
C	-2.07806100	-3.18780300	-2.56841600
H	-2.65868200	-2.34325000	-2.94449400
H	-1.87823800	-3.85906000	-3.40704000
C	-0.35934400	4.26579900	-2.17740300
H	-1.04962700	3.90653500	-2.95156800
H	-0.22895900	5.33544500	-2.35309900
C	-2.82503800	-3.92848500	-1.48413100
H	-3.68655600	-4.43760200	-1.91860400
H	-2.17074300	-4.71049400	-1.07907900
C	4.08299500	-1.15349000	1.46001900

C	2.75497800	-0.13296600	3.31828000
H	3.16114800	0.83217500	3.00750800
H	2.67750600	-0.12329400	4.40868200
C	3.67112400	-1.25850100	2.88160300
H	4.56514000	-1.25947800	3.50823500
H	3.16410100	-2.21494700	3.06343700
C	-4.44783900	-3.05738800	0.31162000
H	-5.30294900	-3.71142900	0.25630300
C	-1.51605100	4.98705900	0.00614700
H	-1.66630200	6.05034400	-0.08982900
C	5.31280900	-1.29529800	0.89629100
H	6.27732500	-1.51709700	1.32421400
C	6.20903100	-1.13279100	-1.44740200
H	5.76917100	-1.02055000	-2.43623900
H	6.91470100	-0.32101600	-1.27287200
H	6.73548900	-2.08486600	-1.39322500
C	-5.42463600	-1.66065700	2.15831200
H	-6.31431000	-1.34432700	1.61476700
H	-5.66963900	-2.51305800	2.79027400
H	-5.07166200	-0.84062100	2.78004400
C	-2.58140900	4.86625200	2.28521100
H	-3.60204800	5.15450800	2.03459700
H	-2.60191900	4.12179300	3.07846100
H	-2.03480900	5.74302100	2.62974000
N	-1.91544300	4.29918700	1.12866100
N	5.15200400	-1.09740700	-0.45548200
N	-4.37887800	-2.02815800	1.22205900
H	-0.27222700	-2.20332700	-2.79431700
H	-0.21970100	-3.44365900	-1.72454900
H	0.96643100	-1.10420900	3.11575600
H	0.83075200	0.51222500	2.98727600
H	1.70202600	1.64764500	-2.51513200
H	0.27125400	1.86875400	-3.25895500

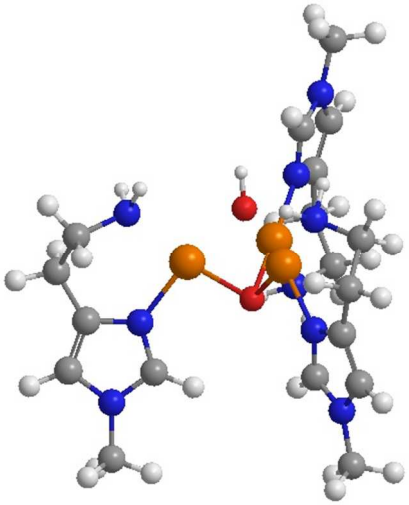
$\mathbf{T_{Me}}$ electron reduced M06/tzvp - quartet



Cu	-0.24668100	1.28775600	-0.70564400
Cu	1.43902700	-0.20411100	0.69022100
O	0.94481000	-0.18960400	-1.21273300
N	-1.65726300	2.60028100	-0.12125300
N	0.39127500	2.51741500	-2.22575100
N	3.42559900	-0.40033900	0.42876900
Cu	-0.54962900	-1.33610200	-0.65995800
O	-0.50539000	0.00869900	0.76704600
N	1.64491400	-0.10733600	2.74101000
N	-0.41511600	-2.51564600	-2.34477300
N	-2.10408200	-2.39630400	0.06200400
C	-2.89177600	-2.05559200	1.06563000
H	-2.77018000	-1.19486200	1.70560900
C	-2.37498500	2.53900600	0.98519500
H	-2.36827400	1.73193400	1.70241100
C	4.06580800	-0.34552900	-0.72418600
H	3.60865800	-0.25818900	-1.69816000
C	0.12048900	3.95937300	-2.11134000
H	0.63004600	4.33263500	-1.21942300
H	0.53207800	4.49431500	-2.97222700
C	-2.63374900	-3.54583900	-0.48375600
C	-1.96892900	3.79719600	-0.72915500
C	-1.58451100	-3.31165700	-2.74868400
H	-2.39657600	-2.62408300	-2.99774900
H	-1.35770000	-3.89239000	-3.64771600
C	-1.36843500	4.22000400	-2.01926700
H	-1.86270400	3.70554600	-2.85373000
H	-1.55971100	5.28597100	-2.16057100
C	-2.00820900	-4.24506400	-1.63361500
H	-2.71685500	-4.97962400	-2.02241600
H	-1.12793200	-4.81033000	-1.30048600
C	4.38724600	-0.49330900	1.41181500

C	2.93703600	0.33500800	3.28846800
H	3.12847300	1.35151600	2.93571300
H	2.89662400	0.36881900	4.38120100
C	4.05040900	-0.59492800	2.85427300
H	4.94780800	-0.38200400	3.43921900
H	3.75890000	-1.62391400	3.10249100
C	-3.75338900	-3.87840600	0.21449800
H	-4.44774300	-4.69630400	0.10678700
C	-2.88456000	4.44592900	0.04100800
H	-3.37581700	5.39847000	-0.07752700
C	5.61160700	-0.49170200	0.81745400
H	6.60747700	-0.55001600	1.22688800
C	6.40946300	-0.38409800	-1.56673700
H	5.92932000	-0.27377200	-2.53697800
H	7.08918700	0.45217200	-1.40640700
H	6.97607500	-1.31490700	-1.54964400
C	-4.94923100	-2.89075300	2.19473200
H	-5.92297300	-2.79271200	1.71518700
H	-4.93159900	-3.80418900	2.78861500
H	-4.78415600	-2.03613900	2.84740500
C	-4.04052800	3.92249500	2.21541600
H	-5.05035100	4.07182400	1.83437300
H	-4.03854800	3.08094500	2.90524800
H	-3.71884500	4.81990600	2.74328700
N	-3.13369500	3.63349500	1.12226200
N	5.39032900	-0.40110000	-0.53697500
N	-3.90021000	-2.92702300	1.19589900
H	1.42643500	-1.02573500	3.12154000
H	0.90130600	0.51082300	3.05204300
H	-0.01193200	2.17320300	-3.09474400
H	1.39162400	2.35459300	-2.29660900
H	-0.14818900	-1.88211500	-3.09270200
H	0.37713100	-3.13981300	-2.20824700

T_{Me} H-atom reduced M06/tzvp – quartet



Cu	0.30685300	-1.38888900	-0.75941700
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O	-0.95555300	0.07097500	-1.34739700
N	1.70121500	-2.59650300	-0.02349700
N	-0.20365100	-2.68189100	-2.24417300
N	-3.42641800	0.29543500	0.44422400
Cu	0.53004900	1.34548700	-0.81262500
O	0.49121100	-0.00074400	0.59195400
N	-1.49253100	0.38670800	2.63710600
N	0.32771400	2.56529400	-2.43073900
N	2.03232800	2.40170500	-0.04914300
C	2.83605700	2.04283000	0.93648900
H	2.77536700	1.12870800	1.50685400
C	2.34762800	-2.44289600	1.11914300
H	2.25766900	-1.60585400	1.79407300
C	-4.14021000	0.02132500	-0.63412900
H	-3.75277200	-0.24595800	-1.60571000
C	0.10124100	-4.10803800	-2.03010100
H	-0.44542400	-4.44462500	-1.14605200
H	-0.24950500	-4.69760000	-2.88125300
C	2.47060700	3.62897500	-0.49761800
C	2.10404200	-3.80334500	-0.55352700
C	1.45795500	3.44424000	-2.77795000
H	2.30904600	2.81482800	-3.04815600
H	1.20430200	4.05002500	-3.65201100
C	1.59030800	-4.31653600	-1.84771200
H	2.11411500	-3.83362400	-2.68280000
H	1.81885700	-5.38168200	-1.91809200
C	1.81271000	4.34829100	-1.61637700
H	2.48012400	5.13944300	-1.96392300
H	0.89798800	4.84478000	-1.26764600
C	-4.32150200	0.56637300	1.45676300

C	-2.74551900	0.06637400	3.34013600
H	-2.96013700	-0.99378700	3.18615000
H	-2.62072500	0.22555800	4.41474600
C	-3.88678300	0.92144800	2.83040000
H	-4.73997900	0.82236000	3.50432700
H	-3.58002600	1.97441400	2.87315200
C	3.55048800	3.99298600	0.24461900
H	4.17872200	4.86856800	0.21171000
C	3.00462300	-4.36341000	0.29844700
H	3.55064900	-5.29209200	0.25487900
C	-5.58084400	0.45219700	0.95569100
H	-6.54877400	0.57836700	1.41374100
C	-6.53350000	-0.15585100	-1.29233600
H	-6.11997600	-0.30497200	-2.28770300
H	-7.07268300	-1.05249900	-0.98719000
H	-7.22173600	0.68808700	-1.31167400
C	4.80108000	2.94990700	2.16339900
H	5.78194200	3.05977300	1.70193800
H	4.64586700	3.75930400	2.87629300
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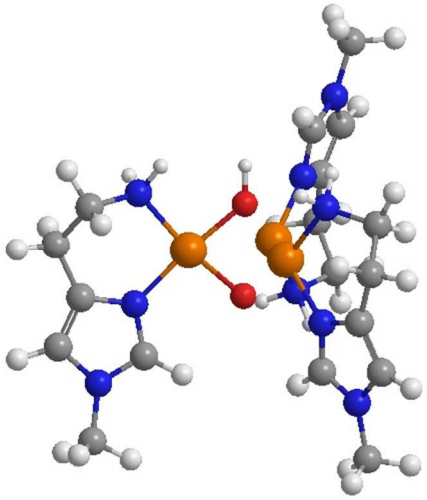
C	4.00699200	-3.68263500	2.50109200
H	5.04583100	-3.76419300	2.18325800
H	3.90234800	-2.82964400	3.16791100
H	3.71935300	-4.59005100	3.03128100
N	3.14862400	-3.48846600	1.34985100
N	-5.44778700	0.11259500	-0.36988300
N	3.76887600	2.97743600	1.14635300
H	-1.50812400	0.09133900	-2.13414800
H	-0.73140900	-0.18704600	2.98934800
H	-1.23635800	1.35319200	2.83198500
H	0.10098000	1.96612800	-3.22030400
H	-0.49568000	3.14326800	-2.27062400
H	0.25565500	-2.37539400	-3.10007900
H	-1.20118300	-2.56240900	-2.40121800

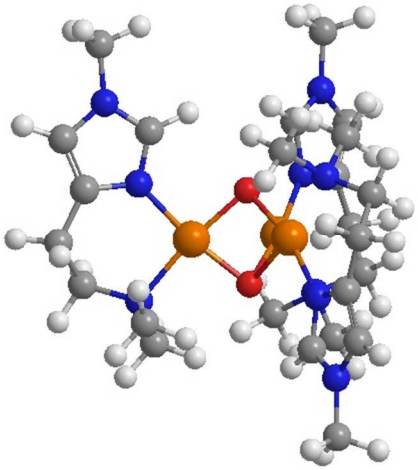
T_{Me} with H-atom – quartet



Cu	-0.11524500	1.19175300	-0.85273700
Cu	1.26301000	-0.46322000	0.70804200
O	0.70887900	-0.60361900	-1.20257300
N	-1.01375300	2.83914800	-0.22351100
N	0.79711000	2.10202200	-2.41870800
N	3.18161400	-0.86834800	0.45838700
Cu	-0.85548100	-1.35622900	-0.61972800
O	-0.67998000	-0.02198200	0.62492700
N	1.41455000	-0.27751900	2.72398800
N	-0.79689300	-2.67174200	-2.05859200
N	-2.52849800	-1.98783400	0.07854700
C	-3.21472500	-1.40227800	1.04756900
H	-2.90282200	-0.54016000	1.61511100
C	-1.59534000	3.01339500	0.95034200
H	-1.78894100	2.24591900	1.68446600
C	3.85858400	-0.83747600	-0.67565100
H	3.45020600	-0.63376800	-1.65410900
C	0.97245100	3.56434700	-2.35331700
H	1.63694300	3.78934400	-1.51595600
H	1.45721300	3.92180400	-3.26566100
C	-3.28979900	-3.03374200	-0.39775400
C	-0.95462900	4.07389500	-0.83167900
C	-2.07806100	-3.18780300	-2.56841600
H	-2.65868200	-2.34325000	-2.94449400
H	-1.87823800	-3.85906000	-3.40704000
C	-0.35934400	4.26579900	-2.17740300
H	-1.04962700	3.90653500	-2.95156800
H	-0.22895900	5.33544500	-2.35309900
C	-2.82503800	-3.92848500	-1.48413100
H	-3.68655600	-4.43760200	-1.91860400
H	-2.17074300	-4.71049400	-1.07907900
C	4.08299500	-1.15349000	1.46001900

C	2.75497800	-0.13296600	3.31828000
H	3.16114800	0.83217500	3.00750800
H	2.67750600	-0.12329400	4.40868200
C	3.67112400	-1.25850100	2.88160300
H	4.56514000	-1.25947800	3.50823500
H	3.16410100	-2.21494700	3.06343700
C	-4.44783900	-3.05738800	0.31162000
H	-5.30294900	-3.71142900	0.25630300
C	-1.51605100	4.98705900	0.00614700
H	-1.66630200	6.05034400	-0.08982900
C	5.31280900	-1.29529800	0.89629100
H	6.27732500	-1.51709700	1.32421400
C	6.20903100	-1.13279100	-1.44740200
H	5.76917100	-1.02055000	-2.43623900
H	6.91470100	-0.32101600	-1.27287200
H	6.73548900	-2.08486600	-1.39322500
C	-5.42463600	-1.66065700	2.15831200
H	-6.31431000	-1.34432700	1.61476700
H	-5.66963900	-2.51305800	2.79027400
H	-5.07166200	-0.84062100	2.78004400
C	-2.58140900	4.86625200	2.28521100
H	-3.60204800	5.15450800	2.03459700
H	-2.60191900	4.12179300	3.07846100
H	-2.03480900	5.74302100	2.62974000
N	-1.91544300	4.29918700	1.12866100
N	5.15200400	-1.09740700	-0.45548200
N	-4.37887800	-2.02815800	1.22205900
H	-0.27222700	-2.20332700	-2.79431700
H	-0.21970100	-3.44365900	-1.72454900
H	0.96643100	-1.10420900	3.11575600
H	0.83075200	0.51222500	2.98727600
H	1.70202600	1.64764500	-2.51513200
H	0.27125400	1.86875400	-3.25895500
H	1.27290793	-0.83982735	-1.94473824

T_{Me3} M06/tzvp – triplet



Cu	0.76344300	-1.18679600	-0.79683800
Cu	-1.11548400	-0.26976700	0.85616100
O	-0.82058200	-0.04413000	-1.09974300
N	2.42818300	-2.05001100	-0.17949800
N	0.30552300	-2.62389200	-2.18840400
N	-3.06811900	-0.52383400	0.76515600
Cu	0.19234600	1.42456400	-0.71250900
O	0.77649800	0.25378100	0.57922800
N	-0.97758500	-0.47263000	2.88933300
N	-0.62596700	2.49220200	-2.19197900
N	1.27775300	2.85738900	-0.01661200
C	2.14133700	2.72326300	0.97922800
H	2.35746100	1.81021200	1.51254600
C	3.17596500	-1.64161700	0.83184200
H	3.05220500	-0.72023900	1.38129600
C	-3.79246000	-0.61810300	-0.33778500
H	-3.42487000	-0.56742500	-1.35201700
C	0.85983300	-3.95433100	-1.84886500
H	0.39474200	-4.26220900	-0.90720300
H	0.53201000	-4.66014300	-2.62458400
C	1.31819000	4.16975400	-0.42611200
C	2.92921100	-3.26631700	-0.58434700
C	0.19797900	3.66046700	-2.59908900
H	1.13768600	3.26503900	-2.99359500
H	-0.33109800	4.14665200	-3.42723900
C	2.36645100	-4.02190400	-1.73014100
H	2.83244300	-3.69451800	-2.66575100
H	2.64078600	-5.07376000	-1.62017800
C	0.46398100	4.68197400	-1.52109800
H	0.96441500	5.53075200	-1.99221500
H	-0.47728700	5.07586800	-1.12475900
C	-3.93403800	-0.64090400	1.82820700

C	-2.12866600	-1.17610000	3.49818000
H	-2.11305600	-2.20223000	3.11944400
H	-1.95501200	-1.22217300	4.58210800
C	-3.48089500	-0.54795800	3.23788900
H	-4.21170900	-1.05474600	3.87225800
H	-3.47965900	0.49673500	3.56690000
C	2.22963000	4.81918700	0.34493100
H	2.55896100	5.84544000	0.34868600
C	3.98996300	-3.57592200	0.20968500
H	4.64930900	-4.42877000	0.22432900
C	-5.19077400	-0.81284100	1.33627900
H	-6.14154500	-0.94321800	1.82770200
C	-6.18260700	-0.89453500	-0.97390200
H	-5.77905500	-1.01846800	-1.97689600
H	-6.80231500	-1.75527200	-0.72665800
H	-6.79083000	0.00918900	-0.93860500
C	3.77018300	4.13250100	2.21304800
H	4.70463700	4.39124000	1.71618200
H	3.47503400	4.94881600	2.87079200
H	3.91133900	3.22815000	2.80065300
C	5.13144000	-2.44104300	2.14474900
H	6.13035700	-2.52811000	1.71867600
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H	4.98007700	-3.23646100	2.87405900
N	4.13706500	-2.53270100	1.09377800
N	-5.08272200	-0.79426200	-0.03424200
N	2.73311200	3.89200400	1.22695500
C	-1.94953100	2.91118200	-1.69700900
H	-2.43293900	3.55754700	-2.43782500
H	-2.56395400	2.02602400	-1.53303700
H	-1.85226500	3.44837200	-0.75384600
C	-0.79695300	1.63939600	-3.38447000
H	-1.44414900	0.79856600	-3.14572700
H	-1.24763100	2.23335600	-4.18644800
H	0.17636700	1.27205100	-3.71245500
C	0.81254500	-2.13534200	-3.47651800
H	0.61618700	-2.86359300	-4.27414400
H	0.31316800	-1.19569800	-3.71961300
H	1.88475200	-1.94601100	-3.42157200
C	-1.15825000	-2.74879900	-2.25782700
H	-1.43630900	-3.52981100	-2.97640900
H	-1.55666100	-3.00736100	-1.27447100
H	-1.59047500	-1.80036800	-2.57519400
C	0.23398500	-1.25620700	3.17292300
H	1.10784200	-0.73209700	2.78654200
H	0.34962600	-1.39966700	4.25480000

H	0.16058700	-2.23269800	2.68991200
C	-0.82373700	0.88091600	3.43984900
H	-0.74974300	0.84391000	4.53438600
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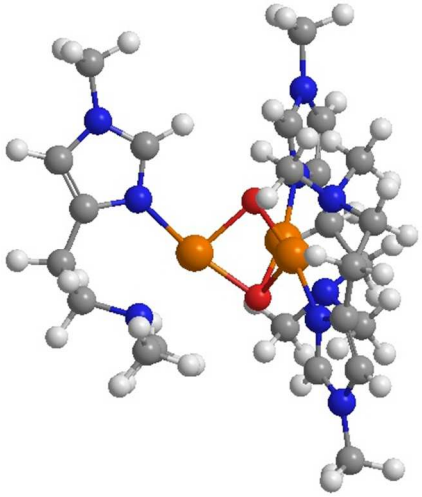
T_{Me3} electron reduced M06/tzvp - quartet



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N	0.15379800	-2.88941100	-1.89573700
N	-3.23857500	-0.18065700	0.59878600
Cu	0.31458600	1.33886400	-0.69242100
O	0.68608700	0.09836000	0.79252300
N	-1.33371300	-0.35638200	2.92594700
N	-0.22581800	2.42199400	-2.41673200
N	1.47086100	2.80233600	0.03642100
C	2.32530900	2.68191700	1.03706300
H	2.45954400	1.80696600	1.65522400
C	3.12447700	-1.80499000	1.02940800
H	2.93050800	-0.97824000	1.69590000
C	-3.89367400	-0.37353800	-0.53209200
H	-3.45210700	-0.49111800	-1.51046100
C	0.94965000	-4.12111100	-1.72055000
H	0.67601600	-4.54963200	-0.75138000
H	0.63999000	-4.83787600	-2.49478400
C	1.63971000	4.06780000	-0.47791500
C	2.99609500	-3.25248600	-0.57500200
C	0.65705900	3.56368500	-2.73212900
H	1.63056200	3.15037900	-3.01361000
H	0.24901600	4.07233900	-3.61765600
C	2.44964600	-3.92228000	-1.77854600

H	2.72461000	-3.36793200	-2.68244100
H	2.92070700	-4.90327100	-1.87524100
C	0.83366500	4.57119100	-1.61529600
H	1.33108600	5.45055000	-2.03143300
H	-0.14330800	4.92182500	-1.26534400
C	-4.18292800	-0.09230300	1.59575200
C	-2.65464400	-0.73503000	3.47115000
H	-2.84217700	-1.77239600	3.17737200
H	-2.58869700	-0.71370800	4.56839700
C	-3.80816400	0.13329600	3.01200700
H	-4.67269300	-0.08998500	3.64142100
H	-3.57887500	1.19054800	3.18342700
C	2.61230100	4.69876000	0.23518300
H	3.03668700	5.68641500	0.15156900
C	4.10772800	-3.55213500	0.15009800
H	4.84616600	-4.33023800	0.04171600
C	-5.41510300	-0.23942600	1.03738100
H	-6.40375100	-0.23660000	1.46760800
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H	-6.94692700	0.18790400	-1.31919600
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H	5.03541600	4.18289800	1.67963300
H	3.84226900	4.91038700	2.77707600
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N	4.17775800	-2.62110200	1.15975300
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H	-1.97017100	3.43590100	-3.07282100
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C	-0.19114200	1.50391600	-3.56178900
H	-0.89655700	0.69089400	-3.39967300
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H	0.81213300	1.08505900	-3.66923500
C	0.28195100	-2.38287200	-3.26651400
H	0.05105100	-3.17331800	-3.99409400
H	-0.41422500	-1.55731600	-3.41405000
H	1.29240900	-2.01470600	-3.45035300
C	-1.25085700	-3.22429500	-1.63321700

H	-1.58272700	-4.04220100	-2.28755800
H	-1.36588700	-3.53817600	-0.59292800
H	-1.87805500	-2.35056700	-1.80680200
C	-0.37333100	-1.40253200	3.30069000
H	0.62435100	-1.12978600	2.95773100
H	-0.35670200	-1.53898700	4.39050600
H	-0.65727000	-2.34709300	2.83127700
C	-0.89528100	0.92734500	3.48631700
H	-0.87709400	0.88560100	4.58397900
H	0.10579900	1.15895300	3.12055100
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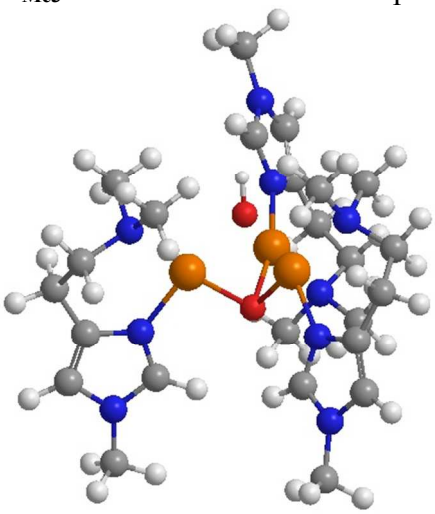
T_{Me3} H-atom reduced M06/tzvp - quartet



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N	0.08365400	-3.02522800	-1.69314500
N	-3.32845800	-0.03788300	0.45104200
Cu	0.43540200	1.38341800	-0.73163600
O	0.54809400	0.08287100	0.70105600
N	-1.45469500	-0.85782500	2.64518400
N	0.48236900	2.36615400	-2.54844000
N	1.38421400	2.79529900	0.27010900
C	1.88293300	2.68834200	1.48961900
H	1.84009000	1.81217000	2.11794700
C	3.16661300	-1.50355700	0.88242200
H	3.00439800	-0.55447300	1.37231100
C	-3.97192000	0.20895700	-0.67822700
H	-3.53091100	0.34757700	-1.65357100
C	0.82754600	-4.24321800	-1.29746900
H	0.54611200	-4.47290600	-0.26494800
H	0.47165700	-5.07105500	-1.92598500

C	1.66759700	4.06672800	-0.17258000
C	2.94803800	-3.25283800	-0.38633200
C	1.43115300	3.50265100	-2.59992700
H	2.44070200	3.08537700	-2.54309700
H	1.32861300	3.97766400	-3.58510200
C	2.33481000	-4.13851500	-1.40648600
H	2.61691700	-3.80935700	-2.41243200
H	2.75198800	-5.14165600	-1.29454400
C	1.24423200	4.53981500	-1.51241500
H	1.83502600	5.41926300	-1.77803100
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C	-4.28130300	-0.14168000	1.43936800
C	-2.78470200	-1.39307200	3.01503300
H	-2.95911600	-2.28115400	2.39929700
H	-2.73041900	-1.72394300	4.06123500
C	-3.93173200	-0.41925400	2.85370500
H	-4.80746600	-0.84392100	3.34964300
H	-3.71330600	0.51161800	3.38812900
C	2.34800200	4.71824900	0.80890300
H	2.74764200	5.71817900	0.86170500
C	4.10256000	-3.40261500	0.31739100
H	4.83987900	-4.18924100	0.32985700
C	-5.50487300	0.04694500	0.87562700
H	-6.49714000	0.03766000	1.29684100
C	-6.31368800	0.54507600	-1.45268400
H	-5.84223200	0.65571300	-2.42703500
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H	-6.83978900	1.46518500	-1.19965000
C	3.11517800	4.10340900	3.12449300
H	4.15876600	4.37144900	2.96313700
H	2.60747200	4.92053500	3.63602800
H	3.06686700	3.20795600	3.74060200
C	5.33001700	-2.00709800	2.00973200
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H	-1.54417800	1.95145200	-2.92623200
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C	0.91578800	1.37326600	-3.54323700
H	0.19837000	0.55469400	-3.59821600
H	0.99797800	1.83586200	-4.53520700

H	1.88977500	0.97025900	-3.25740000
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H	0.00144400	-3.62664900	-3.72485700
H	-0.40552000	-1.92273900	-3.40984300
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H	-1.69830400	-4.14687400	-1.92619700
H	-1.48127300	-3.38574500	-0.32778500
H	-1.93196300	-2.39375200	-1.72831100
C	-0.47747100	-1.94903300	2.76402800
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H	-0.50087600	-2.36881400	3.77782100
H	-0.71781300	-2.73850000	2.04747900
C	-1.06737400	0.24806700	3.52910600
H	-1.12822200	-0.06224300	4.58031400
H	-0.04313100	0.54521300	3.30544600
H	-1.71571100	1.11016800	3.37251300
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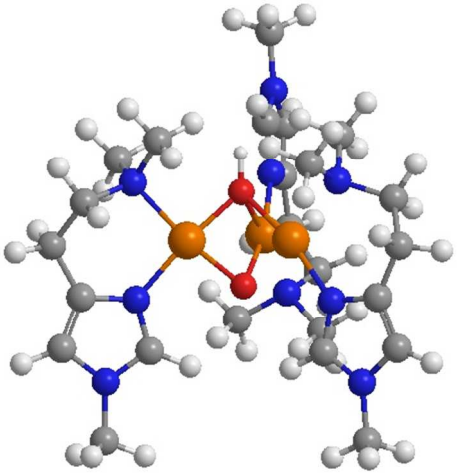
T_{Me3} with H-atom M06/tzvp – quartet



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N	0.30552400	-2.62389200	-2.18840400
N	-3.06811900	-0.52383500	0.76515600
Cu	0.19330203	1.42474252	-0.71150290
O	0.77745503	0.25395952	0.58023410
N	-0.97758500	-0.47263000	2.88933300
N	-0.62501097	2.49238052	-2.19097290
N	1.27870903	2.85756752	-0.01560590
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H	2.35841703	1.81039152	1.51355210
C	3.17596500	-1.64161600	0.83184200

H	3.05220500	-0.72023800	1.38129600
C	-3.79246000	-0.61810400	-0.33778500
H	-3.42487000	-0.56742600	-1.35201700
C	0.85983400	-3.95433100	-1.84886500
H	0.39474300	-4.26220900	-0.90720300
H	0.53201100	-4.66014300	-2.62458400
C	1.31914603	4.16993252	-0.42510590
C	2.92921200	-3.26631600	-0.58434700
C	0.19893503	3.66064552	-2.59808290
H	1.13864203	3.26521752	-2.99258890
H	-0.33014197	4.14683052	-3.42623290
C	2.36645200	-4.02190300	-1.73014100
H	2.83244400	-3.69451700	-2.66575100
H	2.64078700	-5.07375900	-1.62017800
C	0.46493603	4.68215252	-1.52009190
H	0.96537003	5.53093052	-1.99120890
H	-0.47633197	5.07604652	-1.12375290
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C	-2.12866600	-1.17610100	3.49818000
H	-2.11305500	-2.20223100	3.11944400
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C	-3.48089500	-0.54795900	3.23788900
H	-4.21170900	-1.05474700	3.87225800
H	-3.47965900	0.49673400	3.56690000
C	2.23058503	4.81936652	0.34593710
H	2.55991603	5.84561952	0.34969210
C	3.98996400	-3.57592100	0.20968500
H	4.64931000	-4.42876900	0.22432900
C	-5.19077400	-0.81284300	1.33627900
H	-6.14154500	-0.94322000	1.82770200
C	-6.18260700	-0.89453700	-0.97390200
H	-5.77905500	-1.01847000	-1.97689600
H	-6.80231500	-1.75527400	-0.72665800
H	-6.79083000	0.00918700	-0.93860500
C	3.77113903	4.13268052	2.21405410
H	4.70559303	4.39142052	1.71718810
H	3.47598903	4.94899552	2.87179810
H	3.91229503	3.22832952	2.80165910
C	5.13144100	-2.44104100	2.14474900
H	6.13035800	-2.52810800	1.71867600
H	5.03381500	-1.47596200	2.63800200
H	4.98007800	-3.23645900	2.87405900
N	4.13706600	-2.53270000	1.09377800
N	-5.08272200	-0.79426300	-0.03424200
N	2.73406803	3.89218352	1.22796110
C	-1.94857497	2.91135952	-1.69600290

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H	-1.85130897	3.44854952	-0.75283990
C	-0.79599697	1.63957452	-3.38346390
H	-1.44319197	0.79874452	-3.14472090
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H	0.61618800	-2.86359300	-4.27414400
H	0.31316800	-1.19569800	-3.71961300
H	1.88475300	-1.94601000	-3.42157200
C	-1.15824900	-2.74879900	-2.25782700
H	-1.43630800	-3.52981100	-2.97640900
H	-1.55666000	-3.00736100	-1.27447100
H	-1.59047500	-1.80036800	-2.57519400
C	0.23398500	-1.25620700	3.17292300
H	1.10784200	-0.73209700	2.78654200
H	0.34962600	-1.39966700	4.25480000
H	0.16058800	-2.23269800	2.68991200
C	-0.82373700	0.88091600	3.43984900
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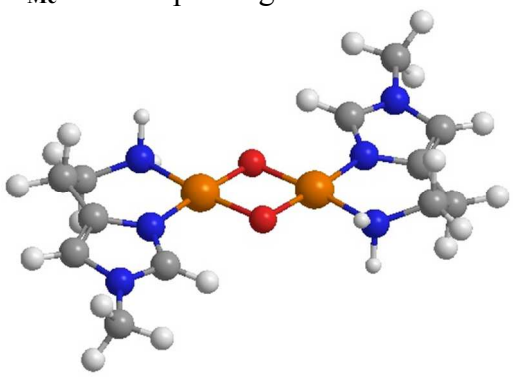
O_{Me} M06/tzvp – singlet



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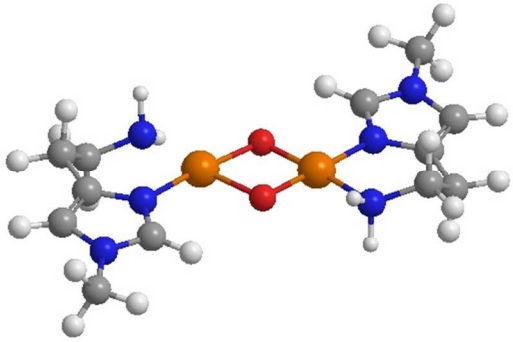
O	1.07866700	0.49511600	-0.06505000
Cu	-0.56929200	1.23783300	0.03807300
Cu	0.56929200	-1.23783300	-0.03807300
C	0.61158100	-4.18345500	0.13062300
C	-1.38555400	-3.35427300	-0.16215800
C	-0.25917700	-5.22298400	0.05096300
N	-1.51179100	-4.68080100	-0.12769900
H	-2.20705700	-2.67005300	-0.30492300
H	-0.10351400	-6.28788200	0.11036500

C	-0.61158100	4.18345500	-0.13062300
C	1.38555400	3.35427300	0.16215800
C	0.25917700	5.22298400	-0.05096300
N	1.51179100	4.68080100	0.12769900
H	2.20705700	2.67005300	0.30492300
H	0.10351400	6.28788200	-0.11036500
N	-0.11477500	-3.02146400	-0.00484500
N	0.11477500	3.02146400	0.00484500
C	2.07925800	-4.17233400	0.33366200
H	2.31580000	-3.95159000	1.38181600
H	2.47761700	-5.16614100	0.12509300
C	-2.07925800	4.17233400	-0.33366200
H	-2.31580000	3.95159000	-1.38181600
H	-2.47761700	5.16614100	-0.12509300
C	2.77086000	-3.15750100	-0.54835200
H	3.85414400	-3.28437800	-0.48401100
H	2.47813700	-3.27927600	-1.59260200
C	-2.77086000	3.15750100	0.54835200
H	-3.85414400	3.28437800	0.48401100
H	-2.47813700	3.27927600	1.59260200
N	-2.43565600	1.78487700	0.13511800
H	-2.86417900	1.10258400	0.75749400
H	-2.80238400	1.60527900	-0.80029200
N	2.43565600	-1.78487700	-0.13511800
H	2.80238400	-1.60527900	0.80029200
H	2.86417900	-1.10258400	-0.75749400
C	-2.74742900	-5.42748100	-0.27925100
H	-3.57336100	-4.72426500	-0.35906100
H	-2.70584000	-6.04034900	-1.17877300
H	-2.89958600	-6.06851600	0.58766600
C	2.74742900	5.42748100	0.27925100
H	2.70584000	6.04034900	1.17877300
H	3.57336100	4.72426500	0.35906100
H	2.89958600	6.06851600	-0.58766600

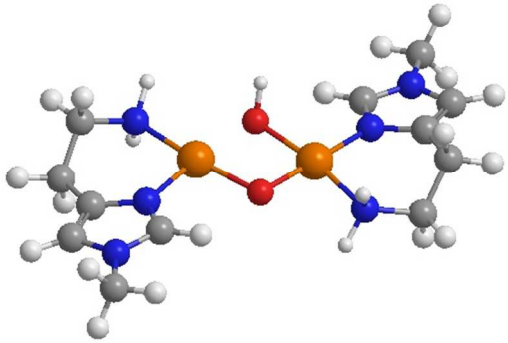
O_{Me} electron reduced M06/tzvp – doublet



Cu	-1.26709000	0.61741300	0.00766900

Cu	1.28698100	-0.57505700	0.01853900
O	0.59777100	1.09257700	-0.04383600
O	-0.42746900	-1.12693300	0.04229300
N	4.82662400	1.43635000	0.05076700
N	-4.84857800	-1.44578300	-0.02888900
N	3.12423300	0.07658300	-0.03046200
N	-3.14289500	-0.07900700	0.06525900
N	-1.89114600	2.57481900	-0.07022300
N	1.85285500	-2.47152700	0.10768700
C	4.27060200	-0.67390700	-0.17722500
C	3.49568800	1.33645500	0.10797700
C	5.33525900	0.16976800	-0.12347700
C	-4.29480600	0.66656800	0.18340800
C	-3.51426100	-1.33874100	-0.06397700
C	-5.36045400	-0.17784400	0.12233900
C	4.23700400	-2.14438400	-0.36555300
C	-4.27330500	2.14096400	0.35856500
C	3.21850600	-2.81976100	0.52560300
C	-3.26404900	2.84179300	-0.52792100
H	2.83386900	2.17585800	0.24924200
H	6.39511400	-0.01345400	-0.19672200
H	-2.85445000	-2.18453700	-0.18413000
H	-6.42205900	0.00409000	0.17180600
H	4.00673100	-2.38943700	-1.41014400
H	5.22874000	-2.55195000	-0.16205100
H	-4.05322600	2.39552500	1.40351600
H	-5.27152300	2.53268300	0.15182200
H	3.34746700	-3.90433200	0.48275700
H	3.34672300	-2.50899900	1.56469700
H	-3.46274400	3.91753500	-0.52810300
H	-3.35419400	2.49051800	-1.55887800
H	-1.22359100	3.05437200	-0.66728700
H	-1.77108500	2.96895300	0.86059400
H	1.67312900	-2.84389000	-0.82367000
H	1.16170500	-2.89211600	0.72309400
C	-5.61969300	-2.66647900	-0.16211900
H	-6.28013500	-2.78683200	0.69579400
H	-6.21689500	-2.63886300	-1.07338300
H	-4.93477600	-3.51074500	-0.20780900
C	5.60357300	2.65406700	0.18684800
H	4.92220000	3.50037900	0.24207400
H	6.20620700	2.61681600	1.09393400
H	6.25813100	2.77454600	-0.67524200

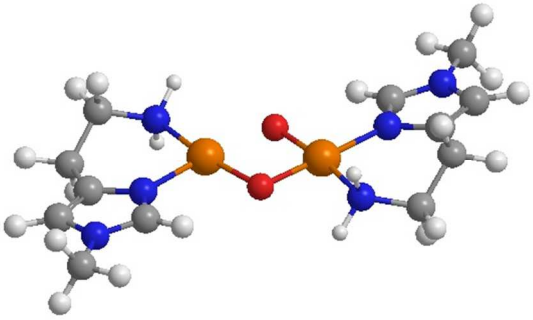
O_{Me} H-atom reduced M06/tzvp – doublet



O	-0.43428600	0.96905600	0.01012500
O	0.57829500	-1.22265900	-0.26524300
Cu	1.32601300	0.48734400	-0.02607500
Cu	-1.35852600	-0.68097700	-0.10848500
C	-4.31401300	-0.57456300	0.27921300
C	-3.44781600	1.38064000	-0.11914900
C	-5.32775400	0.33080800	0.27042800
N	-4.76314100	1.55878300	0.02062300
H	-2.74822800	2.17436100	-0.33159600
H	-6.38935800	0.21293100	0.41780700
C	4.26536500	0.75269400	-0.22628400
C	3.64126500	-1.29381100	0.18591400
C	5.38634200	-0.00742100	-0.11771800
N	4.97398500	-1.29319900	0.13955900
H	3.04256200	-2.16606900	0.39809200
H	6.43046700	0.24914100	-0.20027400
N	-3.13876900	0.10211100	0.03102500
N	3.17681900	-0.07137400	-0.03569000
C	-4.35293500	-2.04107500	0.51189500
H	-4.07492600	-2.27235000	1.54891700
H	-5.38031200	-2.39218300	0.39813400
C	4.10986400	2.20911800	-0.46956100
H	3.79886200	2.40179800	-1.50449500
H	5.07748700	2.69983900	-0.35216000
C	-3.46006300	-2.82071700	-0.43205500
H	-3.68551000	-3.88787500	-0.36697300
H	-3.62367400	-2.50781800	-1.46561900
C	3.11559400	2.83835300	0.48738300
H	3.15598700	3.92848600	0.41834300
H	3.34179700	2.56046100	1.51865000
N	1.73434400	2.39402900	0.19026500
H	1.07588300	2.69104700	0.90875500
H	1.39905800	2.81173600	-0.67795200
N	-2.02573800	-2.59518200	-0.11322700
H	-1.83018600	-2.97024100	0.81482900
H	-1.44732900	-3.14202500	-0.74630600

C	-5.48681200	2.81801100	-0.07788700
H	-4.78095500	3.61863300	-0.28873000
H	-6.21748100	2.76448700	-0.88385300
H	-5.99478200	3.02805700	0.86262000
C	5.85229600	-2.43883800	0.34086000
H	6.52592300	-2.24448000	1.17415500
H	5.24881900	-3.31524600	0.56722900
H	6.43119600	-2.62490100	-0.56278600
H	0.84499600	-1.55894800	-1.12973000

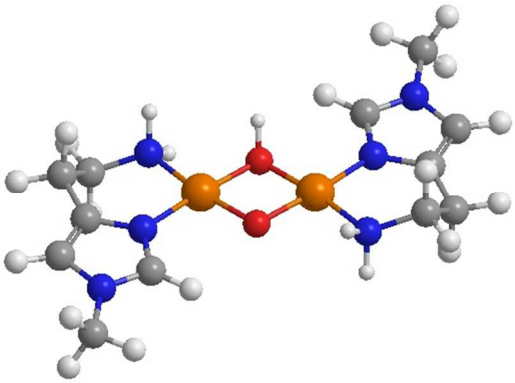
O_{Me} H-atom reduced minus H-atom M06/tzvp – singlet



O	-0.41632200	1.03131700	0.11110100
O	0.64105100	-1.23438100	0.13314600
Cu	1.30209200	0.51570900	0.06899700
Cu	-1.29859000	-0.66482200	0.09713600
C	-4.30733900	-0.58010100	0.23738700
C	-3.44128900	1.39462000	-0.00785000
C	-5.33407800	0.30976000	0.17399800
N	-4.76851700	1.55415600	0.02350200
H	-2.74985100	2.21411700	-0.12911200
H	-6.40273000	0.17490200	0.21976800
C	4.25311600	0.76427200	-0.21172100
C	3.59763900	-1.28100600	0.14880700
C	5.36149000	-0.01956400	-0.16596600
N	4.92795700	-1.30610700	0.05683900
H	2.99426700	-2.15458600	0.33733900
H	6.40789600	0.21665400	-0.27246700
N	-3.12491200	0.11829600	0.12187900
N	3.15522100	-0.04345100	-0.01191900
C	-4.35335700	-2.05305100	0.41450600
H	-4.18462100	-2.31402000	1.46726800
H	-5.35841400	-2.40296100	0.17001000
C	4.12528900	2.22507200	-0.42588900
H	3.86424000	2.44001700	-1.46953700
H	5.08983700	2.69984600	-0.24031100
C	-3.34334400	-2.79568000	-0.43302100
H	-3.57266100	-3.86446400	-0.42515000
H	-3.38669000	-2.45540100	-1.47026100

C	3.08069200	2.84022600	0.47575700
H	3.11566900	3.92988200	0.40100100
H	3.24713200	2.56913400	1.51969900
N	1.72819400	2.40003500	0.09644600
H	1.01965700	2.78863400	0.71498200
H	1.50447300	2.71700200	-0.84748600
N	-1.97484500	-2.57108000	0.06593000
H	-1.90255600	-2.94059100	1.01241700
H	-1.31176100	-3.10047700	-0.49460500
C	-5.49095900	2.80374500	-0.11682000
H	-4.77446000	3.62134300	-0.15998500
H	-6.08302200	2.79504300	-1.03168700
H	-6.15143200	2.94916600	0.73700900
C	5.77533100	-2.47747500	0.18359400
H	6.42815500	-2.37366800	1.04929500
H	5.14445600	-3.35458300	0.30898700
H	6.38156400	-2.59354700	-0.71353900

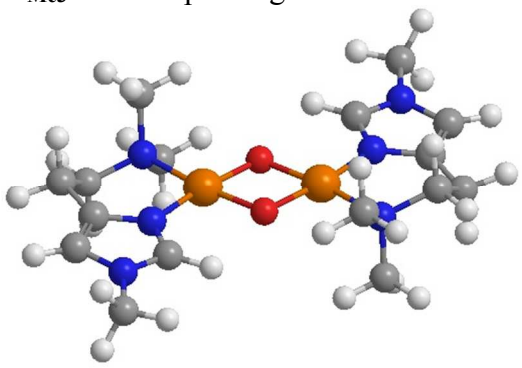
O_{Me} with H-atom – doublet



O	-1.07866700	-0.49511600	0.06505000
O	1.07866700	0.49511600	-0.06505000
Cu	-0.56929200	1.23783300	0.03807300
Cu	0.56929200	-1.23783300	-0.03807300
C	0.61158100	-4.18345500	0.13062300
C	-1.38555400	-3.35427300	-0.16215800
C	-0.25917700	-5.22298400	0.05096300
N	-1.51179100	-4.68080100	-0.12769900
H	-2.20705700	-2.67005300	-0.30492300
H	-0.10351400	-6.28788200	0.11036500
C	-0.61158100	4.18345500	-0.13062300
C	1.38555400	3.35427300	0.16215800
C	0.25917700	5.22298400	-0.05096300
N	1.51179100	4.68080100	0.12769900
H	2.20705700	2.67005300	0.30492300
H	0.10351400	6.28788200	-0.11036500
N	-0.11477500	-3.02146400	-0.00484500

N	0.11477500	3.02146400	0.00484500
C	2.07925800	-4.17233400	0.33366200
H	2.31580000	-3.95159000	1.38181600
H	2.47761700	-5.16614100	0.12509300
C	-2.07925800	4.17233400	-0.33366200
H	-2.31580000	3.95159000	-1.38181600
H	-2.47761700	5.16614100	-0.12509300
C	2.77086000	-3.15750100	-0.54835200
H	3.85414400	-3.28437800	-0.48401100
H	2.47813700	-3.27927600	-1.59260200
C	-2.77086000	3.15750100	0.54835200
H	-3.85414400	3.28437800	0.48401100
H	-2.47813700	3.27927600	1.59260200
N	-2.43565600	1.78487700	0.13511800
H	-2.86417900	1.10258400	0.75749400
H	-2.80238400	1.60527900	-0.80029200
N	2.43565600	-1.78487700	-0.13511800
H	2.80238400	-1.60527900	0.80029200
H	2.86417900	-1.10258400	-0.75749400
C	-2.74742900	-5.42748100	-0.27925100
H	-3.57336100	-4.72426500	-0.35906100
H	-2.70584000	-6.04034900	-1.17877300
H	-2.89958600	-6.06851600	0.58766600
C	2.74742900	5.42748100	0.27925100
H	2.70584000	6.04034900	1.17877300
H	3.57336100	4.72426500	0.35906100
H	2.89958600	6.06851600	-0.58766600
H	-1.53760686	-0.65081272	-0.77195053

O_{Me3} M06/tzvp – singlet

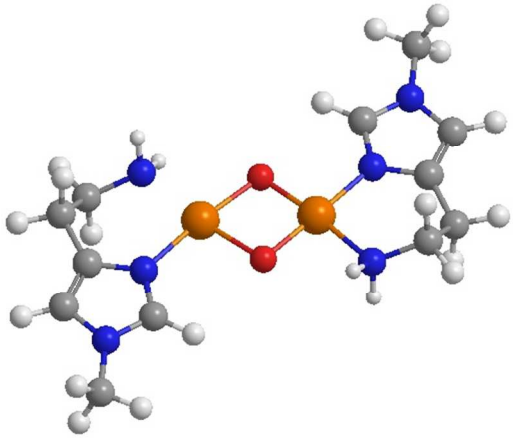


O	-1.06046700	-0.46768700	0.05757300
O	1.06046700	0.46768700	-0.05757300
Cu	-0.56485200	1.26735800	0.03691100
Cu	0.56485200	-1.26735800	-0.03691100
C	0.38192200	-4.23633800	0.13217100
C	-1.53958800	-3.22706100	-0.05844700
C	-0.58453400	-5.19139400	0.12555100

N	-1.78819500	-4.53503200	0.01156300
H	-2.30236200	-2.47037500	-0.16064000
H	-0.52717400	-6.26553800	0.19284200
C	-0.38192200	4.23633800	-0.13217100
C	1.53958800	3.22706100	0.05844700
C	0.58453400	5.19139400	-0.12555100
N	1.78819500	4.53503200	-0.01156300
H	2.30236200	2.47037500	0.16064000
H	0.52717400	6.26553800	-0.19284200
N	-0.23489300	-3.01308300	0.01384700
N	0.23489300	3.01308300	-0.01384700
C	1.85205000	-4.36299200	0.24358300
H	2.16548900	-4.32711000	1.29189600
H	2.15351800	-5.34538600	-0.12518700
C	-1.85205000	4.36299200	-0.24358300
H	-2.16548900	4.32711000	-1.29189600
H	-2.15351800	5.34538600	0.12518700
C	2.58851900	-3.32164000	-0.56344100
H	3.66068600	-3.54915600	-0.55548800
H	2.25307600	-3.33396900	-1.60342300
C	-2.58851900	3.32164000	0.56344100
H	-3.66068600	3.54915600	0.55548800
H	-2.25307600	3.33396900	1.60342300
N	-2.44638000	1.92322300	0.07753400
N	2.44638000	-1.92322300	-0.07753400
C	-3.09102600	-5.16697700	-0.08428300
H	-3.24289000	-5.82896000	0.76682500
H	-3.85719900	-4.39500100	-0.08251300
H	-3.15828200	-5.74294700	-1.00657900
C	3.09102600	5.16697700	0.08428300
H	3.85719900	4.39500100	0.08251300
H	3.24289000	5.82896000	-0.76682500
H	3.15828200	5.74294700	1.00657900
C	-3.23476200	1.06061100	0.97739400
H	-3.18341300	0.02792900	0.63800600
H	-2.83785600	1.13275000	1.99015400
H	-4.27784800	1.39341500	0.96831600
C	2.95246200	-1.78227200	1.30099500
H	3.97341900	-2.17484200	1.35898300
H	2.95383200	-0.72735100	1.57156700
H	2.31493100	-2.32240000	1.99983900
C	3.23476200	-1.06061100	-0.97739400
H	2.83785600	-1.13275000	-1.99015400
H	3.18341300	-0.02792900	-0.63800600
H	4.27784800	-1.39341500	-0.96831600
C	-2.95246200	1.78227200	-1.30099500

H	-2.95383200	0.72735100	-1.57156700
H	-3.97341900	2.17484200	-1.35898300
H	-2.31493100	2.32240000	-1.99983900

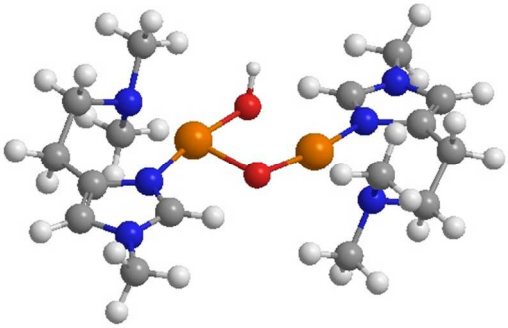
O_{Me3} electron reduced M06/tzvp – doublet



Cu	-1.26709000	0.61741300	0.00766900
Cu	1.28698100	-0.57505700	0.01853900
O	0.59777100	1.09257700	-0.04383600
O	-0.42746900	-1.12693300	0.04229300
N	4.82662400	1.43635000	0.05076700
N	-4.84857800	-1.44578300	-0.02888900
N	3.12423300	0.07658300	-0.03046200
N	-3.14289500	-0.07900700	0.06525900
N	-1.89114600	2.57481900	-0.07022300
N	1.85285500	-2.47152700	0.10768700
C	4.27060200	-0.67390700	-0.17722500
C	3.49568800	1.33645500	0.10797700
C	5.33525900	0.16976800	-0.12347700
C	-4.29480600	0.66656800	0.18340800
C	-3.51426100	-1.33874100	-0.06397700
C	-5.36045400	-0.17784400	0.12233900
C	4.23700400	-2.14438400	-0.36555300
C	-4.27330500	2.14096400	0.35856500
C	3.21850600	-2.81976100	0.52560300
C	-3.26404900	2.84179300	-0.52792100
H	2.83386900	2.17585800	0.24924200
H	6.39511400	-0.01345400	-0.19672200
H	-2.85445000	-2.18453700	-0.18413000
H	-6.42205900	0.00409000	0.17180600
H	4.00673100	-2.38943700	-1.41014400
H	5.22874000	-2.55195000	-0.16205100
H	-4.05322600	2.39552500	1.40351600
H	-5.27152300	2.53268300	0.15182200
H	3.34746700	-3.90433200	0.48275700
H	3.34672300	-2.50899900	1.56469700

H	-3.46274400	3.91753500	-0.52810300
H	-3.35419400	2.49051800	-1.55887800
H	-1.22359100	3.05437200	-0.66728700
H	-1.77108500	2.96895300	0.86059400
H	1.67312900	-2.84389000	-0.82367000
H	1.16170500	-2.89211600	0.72309400
C	-5.61969300	-2.66647900	-0.16211900
H	-6.28013500	-2.78683200	0.69579400
H	-6.21689500	-2.63886300	-1.07338300
H	-4.93477600	-3.51074500	-0.20780900
C	5.60357300	2.65406700	0.18684800
H	4.92220000	3.50037900	0.24207400
H	6.20620700	2.61681600	1.09393400
H	6.25813100	2.77454600	-0.67524200

O_{Me3} H-atom reduced M06/tzvp – doublet



O	-0.42446200	0.96904000	-0.09799900
O	0.36580600	-1.27181800	-0.34390300
Cu	1.38854900	0.47238600	-0.05833000
Cu	-1.40088900	-0.61894000	-0.17695000
C	-4.31824300	-0.14318200	0.24174500
C	-3.13955800	1.66538400	-0.05564700
C	-5.16855800	0.91605000	0.28112600
N	-4.40749000	2.04539100	0.09505100
H	-2.30928800	2.33253300	-0.22762100
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H	2.04233700	4.09833300	-1.19026400
H	2.27450600	2.53766900	-2.01029400
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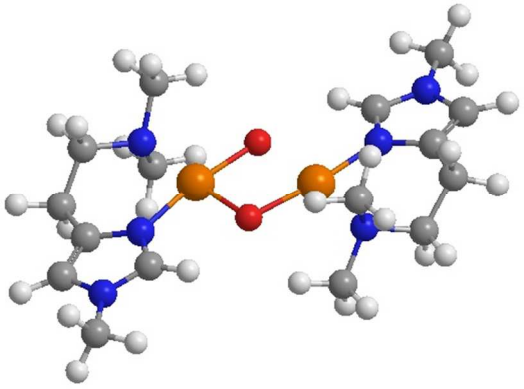
O_{Me3} H-atom reduced minus H-atom M06/tzvp - singlet



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H	6.40452600	-0.53741400	0.10543700
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C	-4.56234800	-1.61998700	0.44974400
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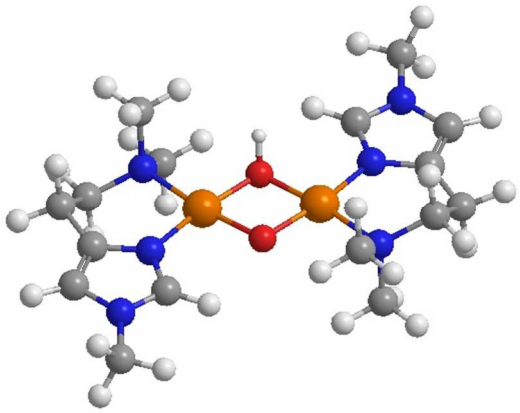
O_{Me3} with H-atom - doublet



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C	0.38322812	-4.23576158	0.13553564
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H	-1.40483161	-0.61966288	-0.82952750

Full Bibliography of Gaussian 09:
Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.;
Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009..

X-ray Absorption Spectroscopy (XAS):

The samples were loaded into Lucite XAS cells with 37 μm Kapton windows by direct immersion of the cell into the solution at -125°C, frozen in liquid nitrogen (LN_2), and stored under LN_2 until use. Cu K-edge X-ray absorption data were collected on wiggler beam line 7-3 at the Stanford Synchrotron Radiation Lightsource under ring conditions of 3.0 GeV and 450-500 mA. A Si (220) monochrometer was used for energy selection and detuned 50% to minimize harmonic components of the X-ray beam. During data collection, samples were maintained at 10–15 K using an Oxford Instruments CF1208 continuous flow liquid helium cryostat. Data were measured in fluorescence mode, monitoring the Cu Kα fluorescence signal with a 30-element Ge solid-state array detector. Internal energy calibration was performed by simultaneous measurement of the transmission signal through a Cu reference foil. The first inflection point of the copper reference data was aligned to 8980.3 eV. Data represent averages of 6 scans of the sample. The data were monitored for photoreduction and only scans with main edge shifts of less than 0.5 eV were included in the final data averages. Data reduction was performed according to established methods.[9]

The intensities and energies of the 1s→3d pre-edge features were quantified using pseudo-Voigt line-shapes to model the rising edge background and absorption features of the Cu complexes according to established methods.[11] For $\mathbf{T_{Me3}}$, 7 fits over varying energy ranges and with varying background features were performed and averaged using the program EDG_FIT.[10] The reported area values (FWHM*Amplitude*100) are the average for each of the fits to a given complex.

Theoretical EXAFS signals were calculated using structural models based on appropriate model complexes as input parameters to FeFF (version 7)[11] and fit to the data using SIXPACK.[12] EXAFS data were fit to k = 14 $Å^{-1}$ for $\mathbf{T_{Me3}}$ in accord with the noise level of the data. The structural parameters that were varied during the refinements include the bond distance (R) and the Debye-Waller factor (σ^2). The σ^2 is a measure of thermal vibration and static disorder of the absorbers and scatterers. The ΔE_0 (eV) value representing the ionization threshold value was also varied for each fit, but was restrained to be a common value for all contributions within a given fit. Coordination numbers were systematically varied during the course of the analysis, but were not allowed to vary within a given fit.

It should be noted that the Cu-N-C multiple scattering waves (~3.20 Å, Table S1) for $\mathbf{T_{Me3}}$

was found to have an abnormally low Debye-Waller factor if the coordination number was fixed at 10 in the fits, as anticipated expected from the model. However, it was found that artificially expanding the coordination number up to 14 did not impact the overall fit. In such cases, the fit error changed insignificantly (<0.005); none of the distances varied by more than 0.02 Å (the resolution of the experiment); the Debye-Waller values for the other waves varied by less than 10%; and the visual quality of the fit was unchanged. Alternatively, completely removing the wave increased the fit error by 50-100%. Therefore, the Cu-N-C multiple scattering wave is a necessary component of the fit, but the fit is effectively invariant to differences in the contribution's coordination number. Most importantly, in no case did this effect vary the Cu-O or Cu-N distances by more than 0.01 Å.

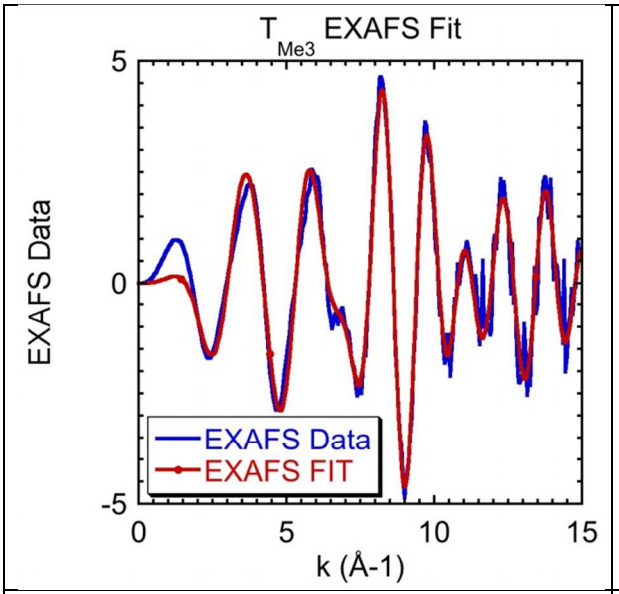

Figure S18: EXAFS (blue) and Fit (red) of $\mathbf{T_{Me3}}$.

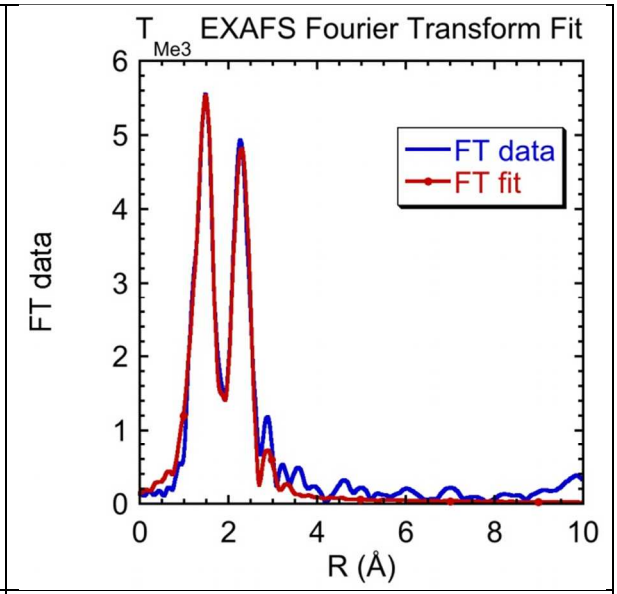

Figure S19: Fourier Transform of EXAFS (blue) and Fit (red) of $\mathbf{T_{Me3}}$.

Table S3. $\mathbf{T_{Me3}}$ EXAFS Fit table.

$\mathbf{T_{Me3}}$		E_0	R (error)
k=1-15 (1/Å)		-11.1	0.0564
	CN	R (Å)	DW (Å^2)
Cu-O/N	1	1.92	0.00097
Cu-O/N	3	2.03	0.00404
Cu-Cu	2	2.67	0.00497
Cu-C(SS)	5	2.88	0.00452
Cu-NC(MS)	10	3.20	0.00121

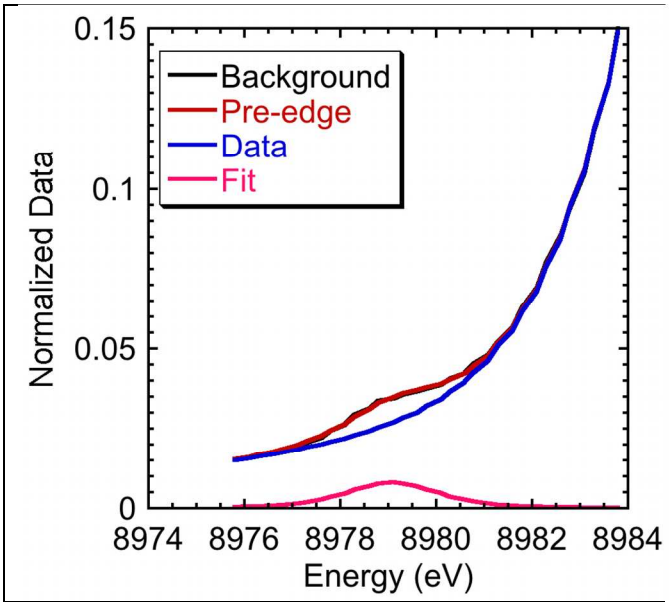

Figure S20. Fits to pre-edge data for $\mathbf{T_{Me3}}$ indicating a Cu(II) center absorbing at 8979.1 ± 0.1 eV.

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