Exclusive Imidazole Ligation to the $Cu^{III}_2O_2$ and $Cu^{III}Cu^{II}_2O_2$ Cores

Supporting Information

William Keown,[a] Tao A. G. Large,[a] Linus Chiang,[a,b] Erik Wasinger,[c] T. Daniel P. Stack[a]*

* Corresponding Author

[a] Department of Chemistry, Stanford University, Stanford, CA 94305, USA

[b] Current Address: Department of Chemistry, University of the Fraser Valley, Abbotsford, BC, Canada

[c] Department of Chemistry and Biochemistry, California State University, Chico, CA 95929, USA

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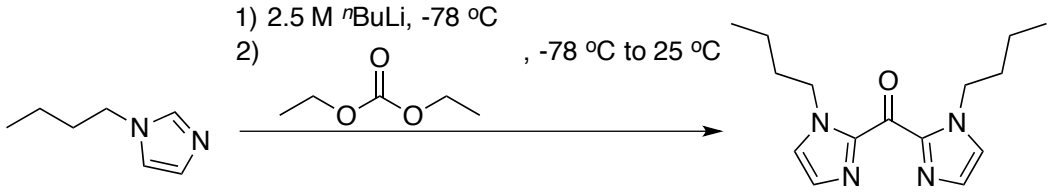
General Information:

All chemicals were obtained from commercial sources unless mentioned otherwise. THF was of HPLC grade and further purified by a Pure-Solv 400 solvent purification system (Innovative Technology) before storage over 3 Å molecular sieves. 2-MeTHF (unstabilized, Aldrich) was stored over dried 3 Å molecular sieves under a N_2 atmosphere with no further purification. Preparation and manipulation of air-sensitive materials were carried out in a N_2 drybox (MBraun, <1 ppm O_2). Low-temperature UV-Vis spectra were collected on a Varian Cary 50 Scan spectrophotometer with fiber-optic leads to a custom-designed quartz immersion probe (Hellma) of 0.1 or 1 cm optical path length in a custom-designed sample cell (ChemGlass). Reactions at -125 °C were maintained by a $N_{2(l)}$–pentane bath and reactions at -145 °C by a 3:2 pentane–2-methylbutane bath cooled by $N_{2(l)}$.

Preparation of Materials:

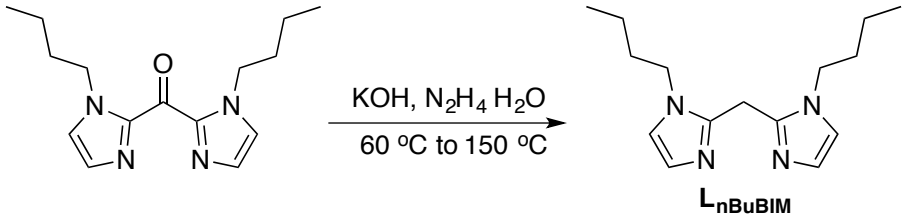
$[Cu(MeCN)_4]SbF_6$ was synthesized from Cu_2O (Aldrich) and hexafluoroantimonic acid (Aldrich) by a modified literature method.[1] Tetramethylpropylenediamine (TMPD) was obtained from Aldrich unless mentioned otherwise. Nα,Nα,Nτ-trimethylhistamine (**L_{Me3His}**) and Nτ-n-butylhistamine (**L_{nBuHis}**) were prepared according to literature procedures.[2] Ligands were stirred over CaH_2 under N_2 before vacuum distillation. 5,6-isopropylidene-L-ascorbic acid (H_2Asc, Aldrich) was dried in a vacuum oven and stored under N_2 before use.

Synthesis of bis(1-*n*-butylimidazol-2-yl)methane (L_{nBuBIM}):



Scheme S1: Synthesis of bis(1-*n*-butylimidazol-2yl)ketone intermediate.

Modified from a literature procedure:[3] To a solution of *n*-butylimidazole (5 mL, 38 mmol) in THF (50 mL) was added 2.5 M nBuLi (15.2 mL, 38 mmol) dropwise at -78 °C. The solution mixture was stirred at this temperature for 30 min, and diethylcarbonate (2.3 mL, 19 mmol) was added dropwise. The solution mixture was allowed to warm to RT overnight, where it was quenched with a saturated $NaHCO_3$ solution (50 mL) and the organic product was extracted using CH_2Cl_2 (3 x 100 mL). The organic layer was dried over Na_2SO_4, then purified by column chromatography using 9:1 $CHCl_3$–MeOH as eluent to yield bis(1-*n*-butylimidazol-2yl)ketone as a pale yellow oil. Yield: 1.6 g, 15%. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.17 (d, 4H, Ar-*H*), 4.33 (t, 4H, N-C*H*$_2$-CH$_2$), 1.80 (quintet, 4H, CH$_2$-C*H*$_2$-CH$_2$), 1.36 (sextet, 4H, CH$_2$-C*H*$_2$-CH$_3$), 0.94 (t, 6H, CH$_2$-C*H*$_3$). ^{13}C NMR (100 MHz, CD_2Cl_2): δ 175.58, 143.56, 130.05, 125.79, 48.57, 33.84, 20.34, 13.94.



Scheme S2: Synthesis of the bis(1-*n*-butylimidazol-2yl)methane (**L$_{nBuBIM}$**) ligand.

To a solution of bis(1-*n*-butylimidazol-2yl)ketone (3.2 g, 12 mmol) in N_2H_4•H_2O (40 mL, 50-60%) was added finely grounded KOH (3.2 g, 57 mmol) at room temperature. The solution mixture was stirred at 60 °C for 1 h, after which it was heated to 150 °C for 3 h. The solution mixture was cooled to room temperature, and the organic product was extracted using CH_2Cl_2 (5 x 75 mL). The organic layer was washed with H_2O (3 x 30 mL) and dried over Na_2SO_4. The crude mixture was purified by column chromatography using 20:1 $CHCl_3$–MeOH as eluent to yield bis(1-*n*-butylimidazol-2yl)methane (**L$_{nBuBIM}$**) as a pale orange oil. Yield: 0.85 g, 28%. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 6.85 (d, 4H, Ar-*H*), 4.19 (s, 2H, Ar-C*H*$_2$-Ar), 3.91 (t, 4H, N-C*H*$_2$-CH$_2$), 1.45 (quintet, 4H, CH$_2$-C*H*$_2$-CH$_2$), 1.25 (sextet, 4H, CH$_2$-C*H*$_2$-CH$_3$), 0.87 (t, 6H, CH$_2$-C*H*$_3$). ^{13}C NMR (100 MHz, CD_2Cl_2): δ 143.82, 127.61, 120.37, 46.38, 33.44, 27.70, 20.28, 13.99.

General Method of Formation for O_{nBuBIM} from O_{TMPD} at -125 °C:

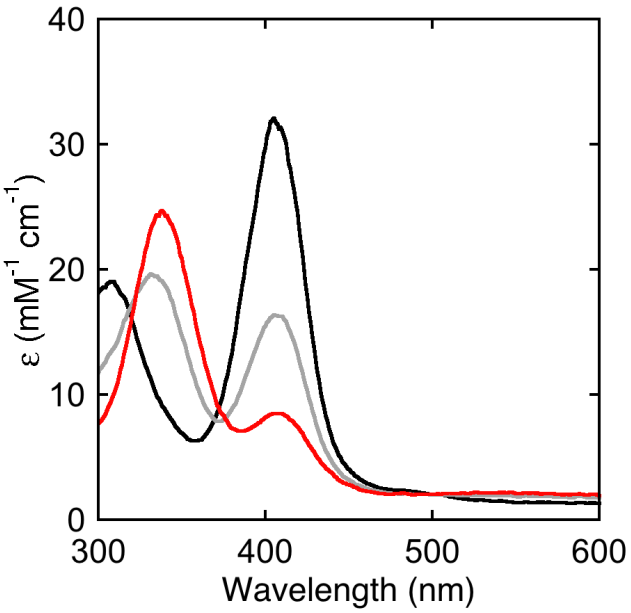


Figure S1. Optical spectra of the ligand exchange reaction of $\mathbf{O_{TMPD}}$ (blue) with 4 equiv 1-methylimidazole at -145 °C resulting in a mixture of $^{S}\mathbf{P_{1MeImd}}$ and $\mathbf{O_{TMPD}}$ (red). [Cu] = 0.9 mM, 0.1 cm path, 4:1 2-MeTHF–THF.

The aforementioned optical immersion probe and reaction vessel were charged with 5 mL 2-MeTHF under N_2, sealed with a septum, and equilibrated in a $N_{2(l)}$–pentane frozen slurry (*ca.* -125 °C). The solution was saturated with 1 atm of O_2 by sparging through a fine needle for 10 min. A 10 mM solution of $[Cu(MeCN)_4]SbF_6$ and TMPD in 500 μL of THF was injected slowly into the solution leading to the formation of $\mathbf{O_{TMPD}}$ after 10 min of stirring. The solution was sparged with N_2 through a fine needle to remove excess O_2 from the reaction vessel. 250 μL of a 20 mM solution of $\mathbf{L_{nBuBIM}}$ in THF was added to affect the maximum core capture of $\mathbf{O_{TMPD}}$ to yield $\mathbf{O_{nBuBIM}}$. All spectra presented as extinction coefficient versus wavelength have been corrected for their respective formation yields.

General Method of Formation for O_{nBuBIM} at -145 °C:

The aforementioned optical immersion probe and reaction vessel were charged with 5 mL of 4:1 2-MeTHF–THF under N_2, sealed with a septum, and equilibrated in a 3:2 pentane–2-methylbutane frozen slurry cooled by $N_2(l)$ (*ca.* -145 °C). The solution was saturated with 1 atm of O_2 by sparging through a fine needle for 10 min. 60 μL of 20 mM solutions of $[Cu(MeCN)_4]SbF_6$ in THF and $\mathbf{L_{nBuBIM}}$ in 4:1 2-MeTHF–THF were drawn up into separate syringes and injected simultaneously into the oxygenated solution. All spectra presented as extinction coefficient versus wavelength have been corrected for their respective formation yields.

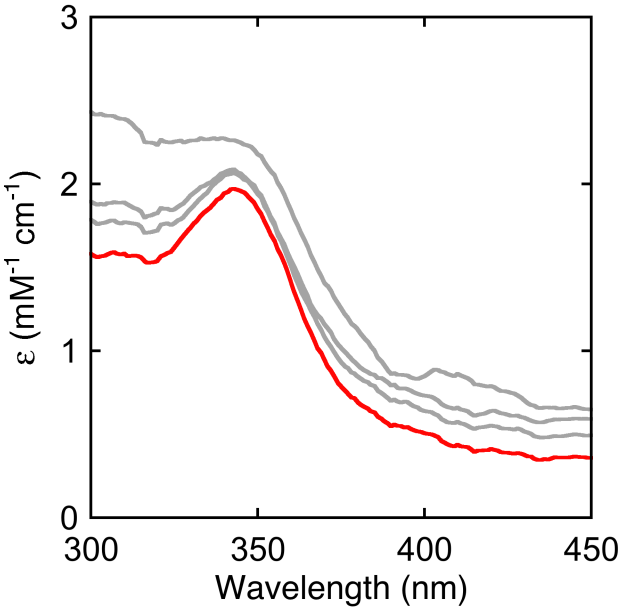


Figure S2. Optical spectra of the direct oxygenation reaction of Cu(I)- $\mathbf{L}_{\mathbf{nBuBIM}}$ at -145 °C. [Cu] = 0.1 mM, 1 cm path, 4:1 2-MeTHF–THF. Initial $\mathbf{O}_{\mathbf{nBuBIM}}$ formation is shown in red and subsequent $\mathbf{T}_{\mathbf{nBuBIM}}$ formation in grey.

General Method of Formation for $\mathbf{T}_{\mathbf{nBuBIM}}$ at -125°C:

The aforementioned optical immersion probe and reaction vessel were charged with 5 mL of 2-MeTHF under N_2, sealed with a septum, and equilibrated in a $N_{2(l)}$–pentane frozen slurry (*ca.* -125° C) or an acetone/pentane frozen slurry (*ca*. -95 °C). The solution was sparged with N_2 through a fine needle for 15 min. 60 mM solutions of $[Cu(MeCN)_4]SbF_6$ and $\mathbf{L}_{\mathbf{nBuBIM}}$ in THF were drawn up into separate 250 μL syringes and injected simultaneously into the N_2 sparged solution. The solution was then sparged with O_2 to immediately effect $\mathbf{T}_{\mathbf{nBuBIM}}$ formation. All spectra presented as extinction coefficient versus wavelength have been corrected for their respective formation yields assessed by cobaltocene titrations.

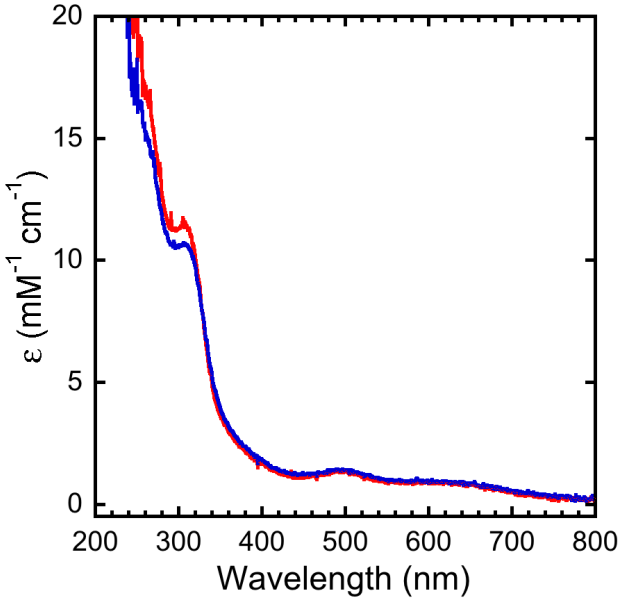


Figure S3. Optical spectra of the direct oxygenation reaction of Cu(I)-$\mathbf{L_{nBuBIM}}$ at -125 °C (red) and -95 °C (blue). [Cu] = 2.9 mM, 0.1 cm path, 2-MeTHF.

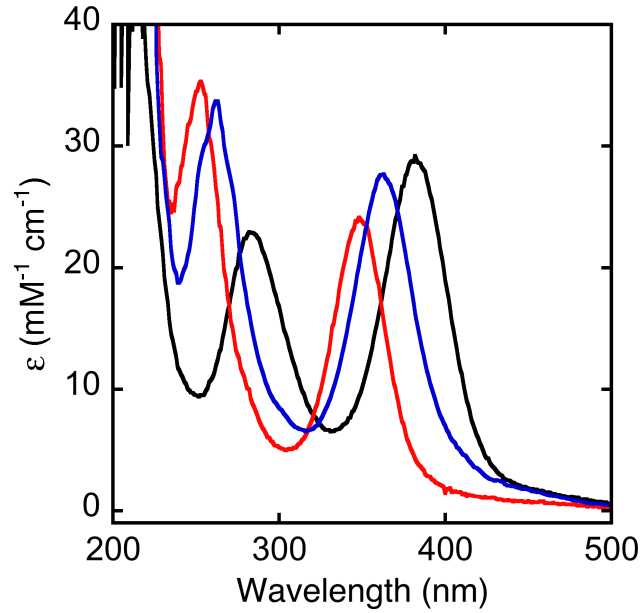


Figure S4. Optical spectra of imidazole containing **O** species (λ_{max}, nm (ε, mM^{-1} cm^{-1})): $\mathbf{O_{Me3His}}$ (black, 380 (30.2), 280 (24.5)), $\mathbf{O_{nBuHis}}$ (blue, 363 (27.8), 262 (34.2)), and $\mathbf{O_{nBuBIM}}$ (red, 349 (24.1), 251 (35.1)). [Cu] = 0.9 mM, 0.1 cm path, 2-MeTHF, -125 °C.

The blue-shifting of the intense LMCT optical transitions in $\mathbf{O_{nBuBIM}}$ relative to other **O** species is suggestive of stronger imidazole σ-interactions relative to primary, secondary, and tertiary amines, and pyridine.[4] To a first approximation, the

stronger σ-interactions increase the energy of the antibonding acceptor orbital (Table 1, Figure S4), leading to higher-energy absorption. Systematic variation of these 2 LMCT bands is consistent across a wide range of nitrogen chelates.

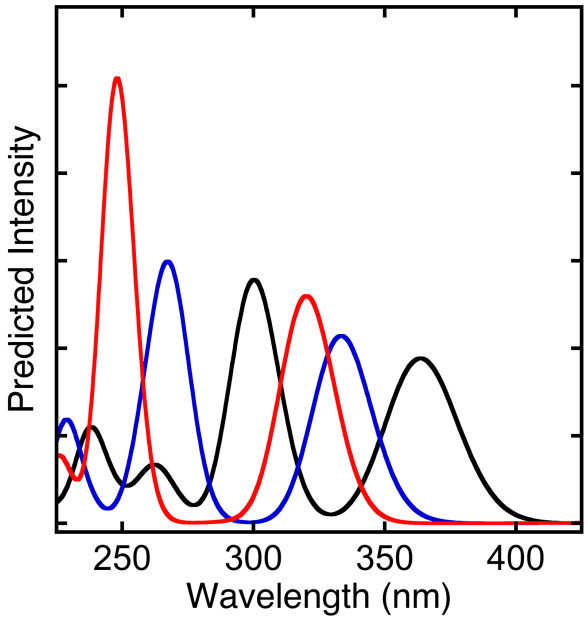
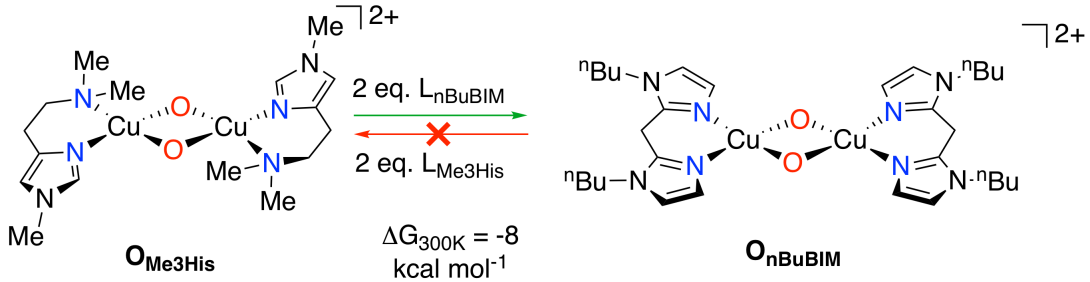


Figure S5. Time dependant DFT predicted optical spectrum of $\mathbf{O_{Me3His}}$ (black), $\mathbf{O_{nBuHis}}$ (blue), and $\mathbf{O_{nBuBIM}}$ (red).

Ligand competition experiment between $\mathbf{O_{Me3His}}$, $\mathbf{O_{nBuHis}}$ and $\mathbf{O_{nBuBIM}}$ at -125 °C:

$\mathbf{O_{Me3His}}$, $\mathbf{O_{nBuHis}}$ and $\mathbf{O_{nBuBIM}}$ are formed independently at -125 °C by the core capture method described above. To the equilibrated mixture, 250 μL of a 20 mM solution of the competing ligand (2 equiv of $\mathbf{L_{Me3His}}$, $\mathbf{L_{nBuHis}}$ or $\mathbf{L_{nBuBIM}}$) dissolved in THF was added slowly. By observing the shift in optical spectrum and appearance/disappearance of characteristic absorption maxima, it was determined that $\mathbf{L_{nBuBIM}}$ will capture the $Cu(III)_2O_2$ core from $\mathbf{L_{Me3His}}$, whereas the reverse reaction does not occur (2 equiv of $\mathbf{L_{Me3His}}$ + $\mathbf{O_{nBuBIM}}$). This establishes $\mathbf{O_{nBuBIM}}$ as the more thermodynamically stable species.



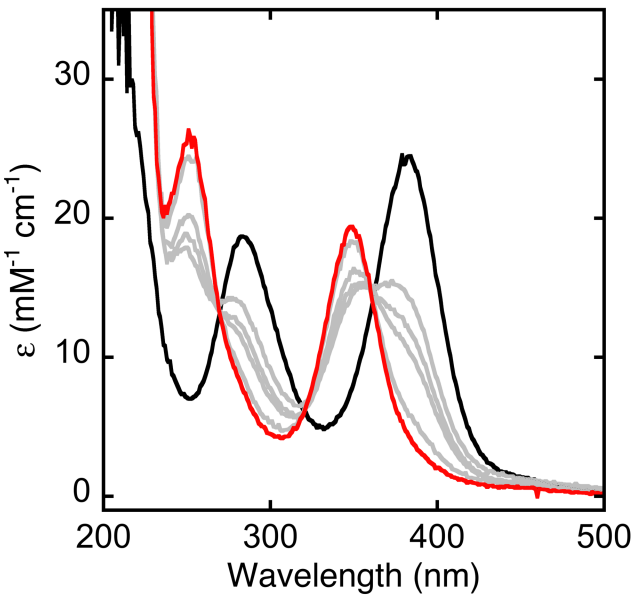


Figure S6. $Cu(III)_2O_2$ core transfer from $\mathbf{O_{Me3His}}$ (black) to $\mathbf{O_{nBuBIM}}$ (red) by the addition of 2 equiv of $\mathbf{L_{nBuBIM}}$ to $\mathbf{O_{Me3His}}$. Reaction time: 20 min, intermediate spectrum = grey. [Cu] = 0.9 mM, 0.1 cm path, 2-MeTHF, -125 °C.

Thermodynamic evaluation of ligand affinity between $\mathbf{O_{Me3His}}$, $\mathbf{O_{nBuHis}}$ and $\mathbf{O_{nBuBIM}}$:

Ligands ($\mathbf{L_{Me3His}}$, $\mathbf{L_{nBuHis}}$ and $\mathbf{L_{nBuBIM}}$) and complexes ($\mathbf{O_{Me3His}}$, $\mathbf{O_{nBuHis}}$ and $\mathbf{O_{nBuBIM}}$) were optimized at a CAM-B3LYP/6-31g* level of theory with SMD solvation in THF. Frequency calculations at the same level of theory provided zero-point corrections to the energies acquired from single point calculations performed at the CAM-B3LYP/def2TZVP level of theory with DKH2 relativistic corrections and SMD solvation in THF. A Hess' law relation based on the appropriate ligand exchange reaction holds for the energies of the **O** complexes and exchanging ligands.

Reaction of $\mathbf{O_{nBuBIM}}$ with H_2Asc at -125 °C:

$\mathbf{O_{nBuBIM}}$ is formed at -125 °C by the core-capture method described above. $\mathbf{O_{nBuBIM}}$ was titrated with 0.2 equiv increments of H_2Asc in THF, a $2H^+/2e^-$ reductant, allowing each spectrum to stabilize before the addition of more titrant. The resultant titration spectra are shown below, where lower bound estimate of formation yield of $\mathbf{O_{nBuBIM}}$ is *ca.* 80%, assessed at 349 nm.

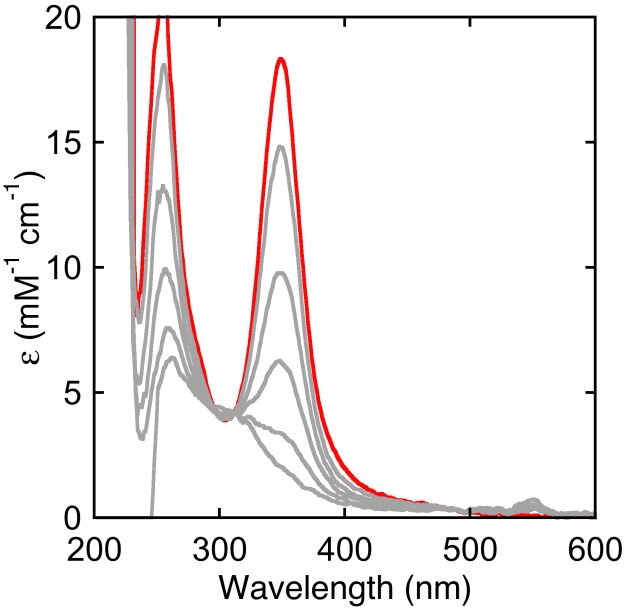


Figure S7. Spectral titration of $\mathbf{O}_{\mathbf{nBuBIM}}$ with incremental addition of 5,6-isopropylidene-L-ascorbic acid, 0.2 equiv per spectrum. [Cu] = 0.9 mM, 0.1 cm path, 2-MeTHF, -125 °C.

Reaction of $\mathbf{T}_{\mathbf{nBuBIM}}$ with cobaltocene at -125 °C:

$\mathbf{T}_{\mathbf{nBuBIM}}$ is formed at -125 °C by the direct oxygenation as described above. $\mathbf{T}_{\mathbf{nBuBIM}}$ was titrated with 0.2 equiv. increments of cobaltocene dissolved in THF, a $1e^-$ reductant, allowing each spectrum to stabilize before the addition of more titrant. The resultant titration spectra are shown below, where lower bound estimate of formation yield of $\mathbf{T}_{\mathbf{nBuBIM}}$ is *ca.* 80%, assessed at 310 nm.

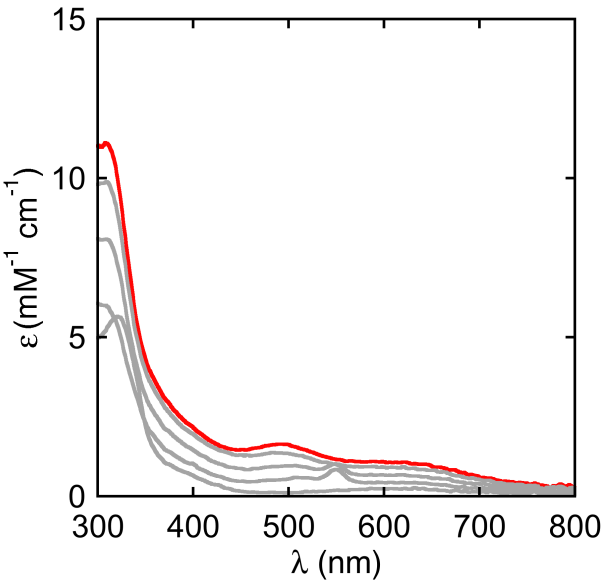


Figure S8. Spectral titration of $\mathbf{T_{nBuBIM}}$ with incremental addition of cobaltocene, 0.2 eq. per spectrum. [Cu] = 0.9 mM, 0.1 cm path, 2-MeTHF, -125 °C.

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, and subsequently frozen in $N_{2(l)}$, then stored in $N_{2(l)}$ 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 500 mA. A Si(220) monochromator 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 7 scans of the sample. Photoreduction was monitored 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.[6]

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.[6] For the complex, 6 fits over varying energy ranges and with varying background features were performed and averaged using the program EDG_FIT.[7] The reported area values (FWHM*Amplitude*100) are the average for each of the fits to the complex.

Theoretical EXAFS signals were calculated using structural models based on appropriate model complexes as input parameters to FeFF (version 7)[8] and fitted to the data using SIXPack.[9] The structural parameters R (Å), the bond distance, and the bond variance, σ^2 (Å^2) were varied for each contribution to the fit. The σ^2 is related to the Debye-Waller factor, which is a measure of thermal vibration and static disorder of the absorbers and scatterers. Coordination numbers were systematically varied during the course of the analysis, but were not allowed to vary within a given fit. The photoionization onset (E_0) was also varied for each fit, but was restrained to be a common value for all contributions within a given fit. Although EXAFS data were collected to k = 15 Å^{-1} for all samples, the EXAFS data were fitted to k = 14 Å^{-1} for $\mathbf{O_{BIM}}$ in accordance with the noise level of the data.

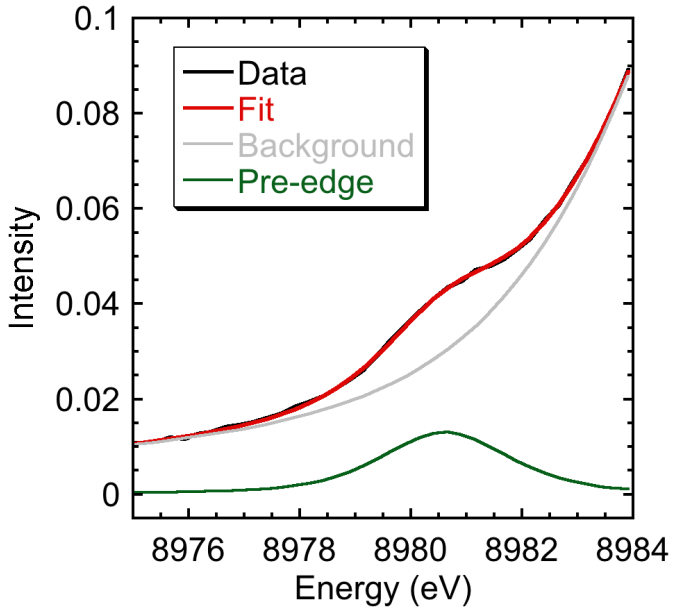
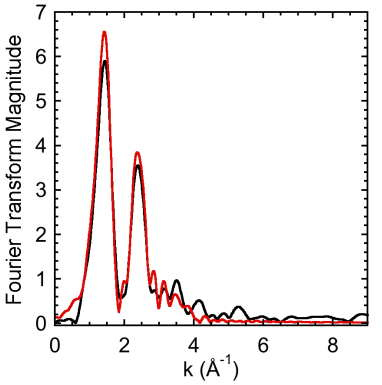
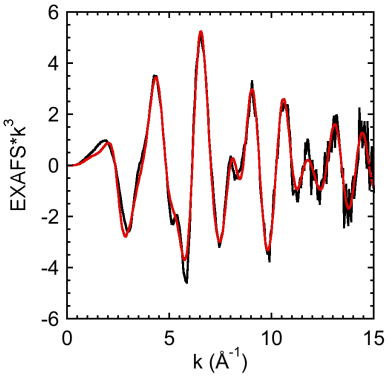


Figure S9. Data (black) and fit (red, overlaid on data) of the pre-edge energy (green) for **O$_{nBuBIM}$** indicating a Cu(III) center absorbing at 8980.7 ± 0.1 eV.





Vector	CN	Fit R (Å)	DW
Cu-N/O	2	1.84	0.00386
Cu-N/O	2	1.94	0.00514
Cu-Cu	1	2.78	0.00271
Cu-C (SS)	5	2.92	0.00726
Cu-N-C (MS)	12	3.08	0.00144
Cu-NC (MS)	16	4.16	0.00732
E0	-5.9		
R (Error)	0.0414		

Figure S10. Fourier Transform of EXAFS fit (left), EXAFS data fit (middle), and metrical parameters from fit of **O$_{nBuBIM}$** (right). Data: black; fit: red.

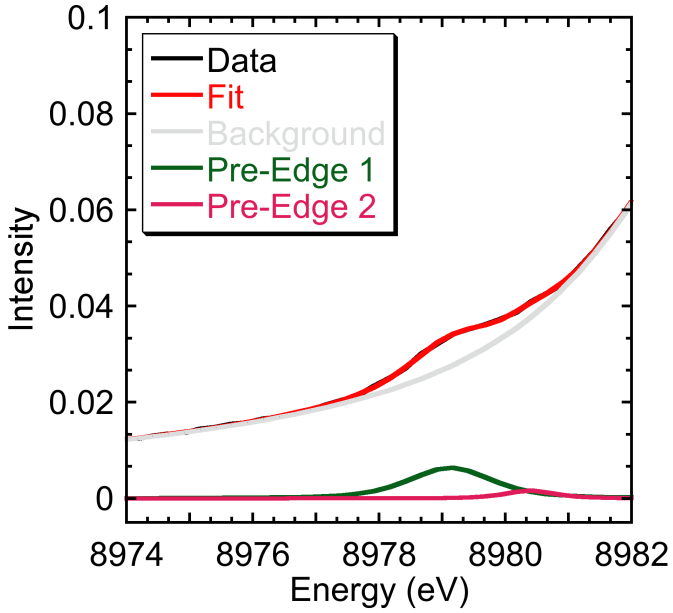
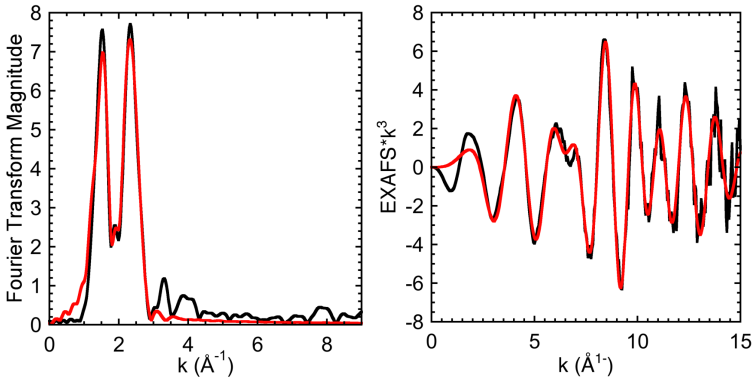


Figure S11. Data (black) and fit (red, overlaid on data) of the pre-edge energy (green) for $\mathbf{T_{nBuBIM}}$ indicating a Cu(II) center absorbing at 8979.1 ± 0.1 eV and a Cu(III) center absorbing at 8980.4 ± 0.1 eV.



Vector	Fit CN	Fit R (Å)	Fit DW
Cu-N/O	4	1.97	0.00434
Cu-Cu	2	2.67	0.00409
Cu-C	4	2.94	0.00777
Cu-N/C	8	3.16	0.00168
E0	-2.3		
R (Error)	0.0503		

Figure S12. Fourier Transform of EXAFS fit (left), EXAFS data fit (middle), and metrical parameters from fit of $\mathbf{T_{nBuBIM}}$ (right). Data: black; fit: red.

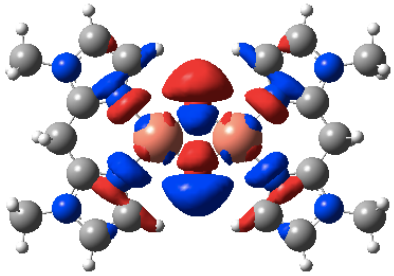
Computational Details:

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.

Time-dependent DFT Predicted Absorption Spectra of O_{nMeBIM}:

The Natural Transition Orbitals (NTO) for the 2 major ligand-to-metal charge transfer bands (LMCT) for **O_{nMeBIM}** are summarized below.



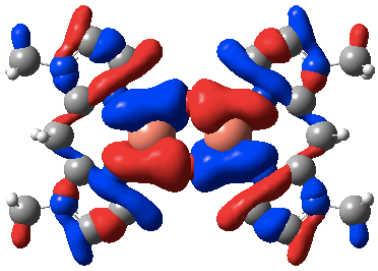
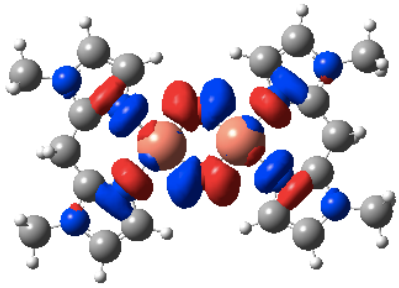


Figure S13. NTO analysis of **O_{nMeBIM}** Higher Energy LMCT (Top: Acceptor, Bottom: Donor)



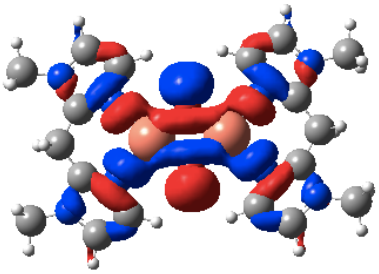


Figure S14. NTO analysis of **O_{nMeBIM}** Lower Energy LMCT (Top: Acceptor, Bottom: Donor)

Table S1: XYZ Coordinates for DFT optimized **O_{nMeBIM}** (CAM-B3LYP/6-31g*/SMD=THF)

Cu	-0.00001200	1.35432700	-0.03553100
Cu	0.00001200	-1.35432700	-0.03553100
O	-1.12934200	-0.00001200	-0.05963900
O	1.12934200	0.00001200	-0.05963900
N	1.36873700	2.64396600	0.06568200
N	-1.36873700	2.64810700	-0.07812500
C	1.25014500	3.96646900	0.09569300
C	2.70970500	2.34404500	0.15323200

C	-1.24944200	3.97082400	-0.06061700
C	-2.70910200	2.35214100	-0.18384000
H	3.05308900	1.32263400	0.15301300
H	-3.05277800	1.33158000	-0.22349700
C	0.00038500	4.77667500	0.04126600
H	-0.05082000	5.41310700	0.93414500
H	0.05245600	5.46697800	-0.81055300
N	1.36873700	-2.64810700	-0.07812500
N	-1.36873700	-2.64396600	0.06568200
C	1.24944200	-3.97082400	-0.06061700
C	2.70910200	-2.35214100	-0.18384000
C	-1.25014500	-3.96646900	0.09569300
C	-2.70970500	-2.34404500	0.15323200
H	3.05277800	-1.33158000	-0.22349700
H	-3.05308900	-1.32263400	0.15301300
C	-0.00038500	-4.77667500	0.04126600
H	-0.05245600	-5.46697800	-0.81055300
H	0.05082000	-5.41310700	0.93414500
C	-3.39888700	3.51905600	-0.22874600
H	-4.45389200	3.72954200	-0.30968300
C	3.40033200	3.50845600	0.23448900
H	4.45589600	3.71589300	0.31623800
C	-3.40033200	-3.50845600	0.23448900
H	-4.45589600	-3.71589300	0.31623800
C	3.39888700	-3.51905600	-0.22874600
H	4.45389200	-3.72954200	-0.30968300
N	-2.46776000	4.53061500	-0.15126700
N	2.46908900	4.52233700	0.19788100
N	2.46776000	-4.53061500	-0.15126700
N	-2.46908900	-4.52233700	0.19788100
C	-2.75645300	5.95801000	-0.17293800

H	-2.21843000	6.43702700	-0.99350700
H	-3.82723300	6.08684700	-0.32431300
H	-2.46842300	6.41792500	0.77490100
C	2.75722500	5.94809700	0.26900300
H	3.83151800	6.07295800	0.39784900
H	2.44500200	6.44414500	-0.65249100
H	2.23964400	6.39380600	1.12096700
C	2.75645300	-5.95801000	-0.17293800
H	3.82723300	-6.08684700	-0.32431300
H	2.46842300	-6.41792500	0.77490100
H	2.21843000	-6.43702700	-0.99350700
C	-2.75722500	-5.94809700	0.26900300
H	-2.23964400	-6.39380600	1.12096700
H	-3.83151800	-6.07295800	0.39784900
H	-2.44500200	-6.44414500	-0.65249100

Table S5: XYZ Coordinates for DFT optimized $\mathbf{T_{nMeBIM}}$

(CAM-B3LYP/6-31g*/SMD=THF)

Cu	-0.97026800	0.64574600	-0.62898100
Cu	0.00000000	0.00000000	1.76681800
Cu	0.97026800	-0.64574600	-0.62898100
O	0.67445800	0.94160000	0.40314100
O	-0.67445800	-0.94160000	0.40314100
N	-0.76967400	-1.13414500	3.04593800
N	0.76967400	1.13414500	3.04593800
N	1.37501600	2.05372900	4.92768200
N	-1.37501600	-2.05372900	4.92768200
N	0.95977200	-2.35276900	-1.53729500
N	1.51643800	-4.05512900	-2.79601700
N	2.73424900	-0.17873600	-1.32115300
N	4.57213000	-0.17373900	-2.51113800
N	-2.73424900	0.17873600	-1.32115300

N	-4.57213000	0.17373900	-2.51113800
N	-0.95977200	2.35276900	-1.53729500
N	-1.51643800	4.05512900	-2.79601700
C	0.69978000	1.03678200	4.37069100
C	1.51298700	2.25653800	2.74812200
C	1.89270400	2.83186000	3.91588300
C	-0.69978000	-1.03678200	4.37069100
C	-1.51298700	-2.25653800	2.74812200
C	-1.89270400	-2.83186000	3.91588300
C	0.00000000	-3.32916600	-1.39266700
C	1.86456400	-2.81830400	-2.38806300
C	0.33610000	-4.39020900	-2.17153900
C	3.44394500	0.95908400	-1.01410200
C	3.43879700	-0.84595900	-2.22431800
C	4.58738700	0.97234500	-1.74839800
C	-3.44394500	-0.95908400	-1.01410200
C	-3.43879700	0.84595900	-2.22431800
C	-4.58738700	-0.97234500	-1.74839800
C	0.00000000	3.32916600	-1.39266700
C	-1.86456400	2.81830400	-2.38806300
C	-0.33610000	4.39020900	-2.17153900
C	-3.10253800	2.14391600	-2.88417400
C	0.00000000	0.00000000	5.17811000
C	3.10253800	-2.14391600	-2.88417400
H	1.70054500	2.54744500	1.72844700
H	2.47605300	3.71471500	4.12630100
H	-1.70054500	-2.54744500	1.72844700
H	-2.47605300	-3.71471500	4.12630100
H	-0.84607800	-3.18635200	-0.73984800
H	-0.14264900	-5.34188300	-2.34277100
H	3.07311200	1.66954400	-0.29200100

H	5.40441000	1.67525600	-1.80266200
H	-3.07311200	-1.66954400	-0.29200100
H	-5.40441000	-1.67525600	-1.80266200
H	0.84607800	3.18635200	-0.73984800
H	0.14264900	5.34188300	-2.34277100
H	-3.94953400	2.83179300	-2.76656700
H	-3.01102100	1.98015600	-3.96640000
H	-0.72262800	0.49139200	5.84244500
H	0.72262800	-0.49139200	5.84244500
H	3.01102100	-1.98015600	-3.96640000
H	3.94953400	-2.83179300	-2.76656700
C	-5.59787100	0.58896100	-3.45692100
H	-6.01164200	1.55614800	-3.16286500
H	-5.17925800	0.66130100	-4.46319900
H	-6.39278900	-0.15608000	-3.45349500
C	5.59787100	-0.58896100	-3.45692100
H	6.01164200	-1.55614800	-3.16286500
H	5.17925800	-0.66130100	-4.46319900
H	6.39278900	0.15608000	-3.45349500
C	-1.54680300	-2.28615700	6.35692800
H	-0.57329300	-2.33792200	6.84788100
H	-2.14234600	-1.48562700	6.80068200
H	-2.06477500	-3.23533400	6.48735500
C	1.54680300	2.28615700	6.35692800
H	0.57329300	2.33792200	6.84788100
H	2.14234600	1.48562700	6.80068200
H	2.06477500	3.23533400	6.48735500
C	2.25538500	-4.88889300	-3.73331300
H	2.35313400	-4.38233700	-4.69571200
H	3.24682500	-5.11749500	-3.33664000
H	1.70514300	-5.81843600	-3.87370400

C	-2.25538500	4.88889300	-3.73331300
H	-2.35313400	4.38233700	-4.69571200
H	-3.24682500	5.11749500	-3.33664000
H	-1.70514300	5.81843600	-3.87370400

Table S6: XYZ Coordinates for DFT optimized $\mathbf{O_{TMPD}}$ (CAM-B3LYP/6-31g*/SMD=THF)

Cu	1.379533025783	-0.010692711049	0.109254955735
Cu	-1.379529432669	-0.010693025380	-0.109289460735
O	0.000000080756	-1.122791119346	-0.000003734397
O	0.000001985477	1.093831457389	-0.000021495035
N	2.624738502412	1.521400037798	0.071160628336
N	2.645149608196	-1.518858558418	-0.009453117512
N	-2.645148385797	-1.518849398361	0.009457248852
N	-2.624739327929	1.521390708404	-0.071157382363
C	4.049890355442	-1.264695438355	0.412434717093
C	2.105965081788	2.603696199346	0.942149038962
C	2.150172228288	-2.654334976222	0.805743717834
C	-2.150175170513	-2.654353851974	-0.805705564158
C	-4.022412416128	1.248893497809	-0.506400814566
C	-2.589834741041	-1.901701372205	1.442982717203
C	4.022410066581	1.248894852502	0.506405089260
C	2.589832888921	-1.901776742915	-1.442963254065
C	-2.599394385524	1.993463965198	1.334611363049
C	-4.049887709556	-1.264693871990	-0.412435333584
C	-2.105974760439	2.603719049218	-0.942111684343
C	2.599399904842	1.993540198466	-1.334586624015
C	4.657487075421	0.019739917891	-0.109842712332
C	-4.657491573427	0.019736731080	0.109839300726
H	4.053880399221	-1.243483343489	1.505778927688
H	4.644256899066	-2.129074218737	0.095170239153
H	-2.822147806072	-3.509017272188	-0.675668081094

H	-1.146157251206	-2.923640015267	-0.489319882870
H	-4.612707808983	2.142944620137	-0.276252290697
H	-4.644252057095	-2.129074234612	-0.095171243002
H	-2.777760226020	3.465835549408	-0.879444508428
H	-2.066205002964	2.251587622119	-1.974231358225
H	-1.108672936009	2.889190182105	-0.618971833878
H	4.612708729751	2.142946408756	0.276266168899
H	4.000998376656	1.137282277363	1.594216081142
H	1.555408325497	-2.119406886692	-1.707675833996
H	2.955947458625	-1.088163874233	-2.069302234832
H	3.207414563688	-2.790025796992	-1.610957427652
H	-2.996110214846	1.227144139907	2.000095778021
H	-3.206399088500	2.899636441833	1.429544362534
H	-1.568947424923	2.212387460407	1.613035686470
H	-1.555419554638	-2.119377766070	1.707694439867
H	-2.955889423760	-1.088018742092	2.069271595471
H	-3.207470217255	-2.789901837230	1.611035666502
H	2.133494129037	-2.364821098799	1.857795951966
H	2.822139265152	-3.509006699227	0.675730693341
H	1.146151816556	-2.923624563292	0.489368464513
H	1.108660420968	2.889167554487	0.619017766460
H	2.777741974698	3.465821399209	0.879508353659
H	2.066199107930	2.251531582253	1.974257478412
H	3.206288358170	2.899798862194	-1.429438257212
H	1.568938201364	2.212342580888	-1.613050164759
H	-2.133492837845	-2.364873138086	-1.857766730801
H	2.996255018897	1.227320350626	-2.000098196361
H	5.711078823639	0.019258631590	0.185889474081
H	4.652008191566	0.059888237788	-1.202421060098
H	-4.001003959476	1.137290908243	-1.594212948413
H	-4.053875477873	-1.243483348781	-1.505779594451

H	-4.652022780981	0.059882033714	1.202418022621
H	-5.711080675759	0.019251100235	-0.185902411935

Table S7: XYZ Coordinates for DFT optimized $\mathbf{O_{TMPD}}$

(CAM-B3LYP/TZVP/SMD=THF)

Cu	1.410029545356	-0.000586462134	0.074973150095
Cu	-1.410041573554	-0.000586169668	-0.075042389758
O	0.000006472091	-1.121922231537	-0.000347216274
O	-0.000009520870	1.119594507998	-0.000049459425
N	2.686380460987	1.541163795810	0.031794247566
N	2.689146681927	-1.541353728094	0.011146077007
N	-2.689117402552	-1.541382351289	-0.011104844789
N	-2.686420958919	1.541136506142	-0.031775682971
C	4.068853817595	-1.262433078785	0.487445571594
C	2.146749552437	2.643260091012	0.858790346261
C	2.158288547226	-2.653003434071	0.830767825390
C	-2.158353456102	-2.653044455889	-0.830755971820
C	-4.058047976661	1.250413617550	-0.523240782245
C	-2.699464986606	-1.957054572957	1.410381755122
C	4.057992169633	1.250478420591	0.523336676035
C	2.699763738891	-1.957082391803	-1.410312258280
C	-2.720952639919	1.977086009968	1.382568285707
C	-4.068906153221	-1.262501855947	-0.487208962176
C	-2.146816794984	2.643201156547	-0.858844025997
C	2.720936071381	1.977050089420	-1.382577175884
C	4.694849372937	0.004261293803	-0.045631775631
C	-4.694858120236	0.004231483547	0.045857306936
H	4.025467033355	-1.210601864571	1.575551588237
H	4.679456237660	-2.129511017480	0.223121623638
H	-2.839120085516	-3.504324978502	-0.761247190779
H	-1.177081758722	-2.939051444200	-0.469388691601
H	-4.670242436942	2.127147600939	-0.297162021114

H	-4.679473748133	-2.129568221536	-0.222758500650
H	-2.833338178916	3.491413980673	-0.814040549702
H	-2.051110852810	2.310783834762	-1.890171733269
H	-1.173515062002	2.939785487073	-0.484750820269
H	4.670190021939	2.127202693578	0.297229713992
H	3.996727858373	1.162072906642	1.608442835766
H	1.685948696246	-2.201793750741	-1.716145272886
H	3.076068314261	-1.152039833770	-2.036716645349
H	3.337521839934	-2.835604729569	-1.529836085605
H	-3.135164591788	1.192281791944	2.010430899952
H	-3.339745622485	2.872690643120	1.473417889262
H	-1.709468009032	2.202642191143	1.710327382235
H	-1.685642789485	-2.202086195234	1.715928717696
H	-3.075286650731	-1.151862712866	2.036873646935
H	-3.337488094303	-2.835347771700	1.530142585045
H	2.082441614961	-2.335371090657	1.868332023651
H	2.839178252675	-3.504206728563	0.761534274706
H	1.177150572926	-2.939173313711	0.469166572114
H	1.173446729349	2.939803796605	0.484671085435
H	2.833255209221	3.491484170738	0.813938000451
H	2.051051002867	2.310896618301	1.890134214605
H	3.339963828707	2.872479485538	-1.473524222131
H	1.709486323855	2.202852263912	-1.710269950633
H	-2.082830914758	-2.335503924720	-1.868371944779
H	3.134864987528	1.192099485104	-2.010439144533
H	5.737540647461	0.003303776437	0.275688389939
H	4.717683480614	0.019547952297	-1.135406407660
H	-3.996836344993	1.161928467723	-1.608342472017
H	-4.025678487275	-1.210721792002	-1.575321909453
H	-4.717585487579	0.019590130208	1.135631572562
H	-5.737580706175	0.003266369609	-0.275367558793

Table S8: XYZ Coordinates for DFT optimized $\mathbf{O_{PD}}$

(CAM-B3LYP/6-31g*/SMD=THF)

Cu	1.306270150496	0.021301288689	0.252894458982
Cu	-1.306476677777	0.021017914347	-0.254463866288
O	0.001167998257	-1.135209844785	-0.007300442831
O	-0.001820907141	1.178519194524	0.008741269760
C	3.773917164976	-1.320843262187	-0.350152033930
C	-3.772562238484	1.224413537885	0.499575499630
C	3.770732036774	1.223354590789	-0.502726064093
C	-3.769442992844	-1.320108362046	0.356800990507
C	4.547878018111	-0.030846170715	-0.135608885087
C	-4.547416739630	-0.033123023125	0.139119747790
H	4.405020804411	-2.186285948055	-0.132735851315
H	3.432356565920	-1.400333108565	-1.385463223712
H	-3.396217106973	1.172529162528	1.524717317424
H	-3.422241142490	-1.392832857733	1.390784174629
H	3.393732471809	1.164911201518	-1.527340808688
H	4.414554259913	2.103224504776	-0.428205121852
H	4.885653470803	0.034182391128	0.906908334587
H	5.448749753107	-0.067804893402	-0.754122698099
H	-4.417782299095	2.102770132057	0.419301878834
H	-4.399574327368	-2.188335186795	0.147895343741
H	-5.446627911253	-0.069826490571	0.760051430207
H	-4.887932943963	0.026682631479	-0.902799770988
N	2.569015634338	-1.382608725430	0.514558797213
H	2.051100597355	-2.245401921558	0.333893207603
H	2.851737522289	-1.420177460266	1.497889715732
N	-2.568895865660	-1.384016987692	-0.513944175348
H	-2.855945375407	-1.424840352866	-1.495813314326
H	-2.049449284001	-2.245753930237	-0.332691959993
N	-2.601490313569	1.411532657342	-0.393164734863

H	-2.102851964021	2.271287513734	-0.153870363509
H	-2.918088337795	1.523806952705	-1.360125695079
N	2.599854499815	1.413543493692	0.389810938305
H	2.100363418237	2.271788088914	0.146732974252
H	2.916635206597	1.530440956322	1.356099317993

Table S9: XYZ Coordinates for DFT optimized $\mathbf{O}_{\mathbf{Me3His}}$

(CAM-B3LYP/6-31g*/SMD=THF)

C	1.075946193799	-3.107703120469	-1.188548679575
C	-1.079145990793	3.105233953155	1.217039606945
C	-1.489974468258	2.961747018576	-1.161676007860
C	1.496631771547	-2.961658021553	1.188678708999
C	3.189739986712	1.524507297574	-0.230647701492
C	-3.193351742871	-1.526066766932	0.194154950612
C	3.296311196421	-2.611448042190	-0.434185028572
C	-3.296335025271	2.608644847639	0.453730430605
C	-4.169456120061	0.379218909835	-0.231356980460
C	4.171661571914	-0.373416309760	0.214387251650
C	-4.255630940405	1.850224029373	-0.451156544413
C	4.258888846349	-1.840707925592	0.456855299282
C	5.124998279624	3.083901496933	-0.235414998638
C	-5.128854362193	-3.084524153296	0.152541345004
C	-5.131239570251	-0.585127416485	-0.218114237205
C	5.133095257135	0.590378965812	0.171937938702
Cu	1.242470508896	-0.550402384716	-0.068115135183
Cu	-1.242860755920	0.548127811737	0.093808087275
H	0.012120480953	-2.971389775631	-1.006232467716
H	-0.014575510822	2.967429662116	1.040012182611
H	-0.412742303991	2.876982407868	-1.297199058287
H	0.420187070064	-2.875507887327	1.329708954262
H	1.328042178349	-4.172841748216	-1.172569120699
H	-1.329726824576	4.170707248444	1.199427282375

H	1.332474085097	-2.689159403347	-2.163593908582
H	-1.341101541592	2.687401280865	2.190961435072
H	-1.790216127685	4.013140612296	-1.212830314465
H	1.796019825803	-4.013304995904	1.239320735023
H	-1.989591933228	2.403360476930	-1.954024615388
H	2.000974455608	-2.403051151685	1.977877849576
H	2.437704479943	2.267893773293	-0.439734761318
H	-2.444097358672	-2.272095768419	0.403896444949
H	3.453131052400	-2.329538467713	-1.477679094026
H	-3.458901571107	2.315283841325	1.493257494244
H	-3.486321322095	3.684440135973	0.372082442405
H	3.488180226377	-3.685990037807	-0.341579728283
H	-4.083212443179	2.100117308501	-1.503357587410
H	4.088064119748	-2.074274812517	1.513151974902
H	4.358910228659	3.821787837041	-0.472621086970
H	-4.366055819634	-3.825265261566	0.391286231974
H	-5.268264753686	2.190409466201	-0.219465181638
H	5.270902569776	-2.184656627305	0.228266497718
H	-5.601016526049	-3.340362479065	-0.797409139757
H	5.610524782133	3.351702820730	0.704474847880
H	5.866033181788	3.057683131670	-1.036115840241
H	-5.880923752179	-3.067918546031	0.943144453042
H	-6.197827026986	-0.532374486701	-0.374394677984
H	6.201549524060	0.540295576291	0.315762360279
N	-1.847249333780	2.400841196535	0.163186517154
N	1.848324341404	-2.402389092788	-0.138404745242
N	2.959900989176	0.230839099597	-0.043546349372
N	-2.960862996299	-0.229592384552	0.031100646108
N	4.492269409979	1.778443178360	-0.106514935946
N	-4.494142903676	-1.777672378838	0.049327510891
O	-0.458573019614	-1.032972051362	-0.040769839957

O	0.459034013926	1.029539855613	0.078980739274

Table S10: XYZ Coordinates for DFT optimized $\mathbf{O}_{\mathbf{Me3His}}$ (CAM-B3LYP/TZVP/SMD=THF)

O	-0.458573019614	-1.032972051362	-0.040769839957
O	0.459034013926	1.029539855613	0.078980739274
Cu	1.242470508896	-0.550402384716	-0.068115135183
Cu	-1.242860755920	0.548127811737	0.093808087275
C	-4.169456120061	0.379218909835	-0.231356980460
C	-3.193351742871	-1.526066766932	0.194154950612
C	-5.131239570251	-0.585127416485	-0.218114237205
N	-4.494142903676	-1.777672378838	0.049327510891
H	-2.444097358672	-2.272095768419	0.403896444949
H	-6.197827026986	-0.532374486701	-0.374394677984
C	-5.128854362193	-3.084524153296	0.152541345004
C	4.171661571914	-0.373416309760	0.214387251650
C	3.189739986712	1.524507297574	-0.230647701492
C	5.133095257135	0.590378965812	0.171937938702
N	4.492269409979	1.778443178360	-0.106514935946
H	2.437704479943	2.267893773293	-0.439734761318
H	6.201549524060	0.540295576291	0.315762360279
C	5.124998279624	3.083901496933	-0.235414998638
N	-2.960862996299	-0.229592384552	0.031100646108
N	2.959900989176	0.230839099597	-0.043546349372
C	-4.255630940405	1.850224029373	-0.451156544413
H	-4.083212443179	2.100117308501	-1.503357587410
H	-5.268264753686	2.190409466201	-0.219465181638
C	4.258888846349	-1.840707925592	0.456855299282
H	4.088064119748	-2.074274812517	1.513151974902
H	5.270902569776	-2.184656627305	0.228266497718
C	-3.296335025271	2.608644847639	0.453730430605
H	-3.486321322095	3.684440135973	0.372082442405

H	-3.458901571107	2.315283841325	1.493257494244
C	3.296311196421	-2.611448042190	-0.434185028572
H	3.488180226377	-3.685990037807	-0.341579728283
H	3.453131052400	-2.329538467713	-1.477679094026
N	1.848324341404	-2.402389092788	-0.138404745242
C	1.075946193799	-3.107703120469	-1.188548679575
C	1.496631771547	-2.961658021553	1.188678708999
N	-1.847249333780	2.400841196535	0.163186517154
C	-1.489974468258	2.961747018576	-1.161676007860
C	-1.079145990793	3.105233953155	1.217039606945
H	-1.790216127685	4.013140612296	-1.212830314465
H	-1.989591933228	2.403360476930	-1.954024615388
H	-0.412742303991	2.876982407868	-1.297199058287
H	-1.341101541592	2.687401280865	2.190961435072
H	-1.329726824576	4.170707248444	1.199427282375
H	-0.014575510822	2.967429662116	1.040012182611
H	0.012120480953	-2.971389775631	-1.006232467716
H	1.328042178349	-4.172841748216	-1.172569120699
H	1.332474085097	-2.689159403347	-2.163593908582
H	2.000974455608	-2.403051151685	1.977877849576
H	1.796019825803	-4.013304995904	1.239320735023
H	0.420187070064	-2.875507887327	1.329708954262
H	5.610524782133	3.351702820730	0.704474847880
H	4.358910228659	3.821787837041	-0.472621086970
H	5.866033181788	3.057683131670	-1.036115840241
H	-4.366055819634	-3.825265261566	0.391286231974
H	-5.601016526049	-3.340362479065	-0.797409139757
H	-5.880923752179	-3.067918546031	0.943144453042

Table S11: XYZ Coordinates for DFT optimized ^{Me3His}**L**

(CAM-B3LYP/6-31g*/SMD=THF)

C	-0.663887680954	-0.868228253527	0.047770998098

C	-2.800690315860	-0.702564618701	-0.049227964138
C	-0.955624049736	0.470735442305	0.050436696483
N	-2.326620531667	0.564278014387	-0.009697229657
H	-3.861621852504	-0.909053513155	-0.098885578576
H	-0.319695585771	1.340734842954	0.077460037438
C	-3.104629966164	1.786819804859	-0.027516894059
N	-1.835603831494	-1.593553646528	-0.016758559745
C	0.661273799549	-1.570238215137	0.091718671814
H	0.930337269198	-1.927158711849	-0.910325708082
H	0.543738948263	-2.476309110916	0.696904496944
C	1.813993805952	-0.765138098499	0.687559259191
H	2.699834495176	-1.425731778332	0.757351430503
H	1.549644643760	-0.480455307888	1.711961846588
N	2.145473817314	0.461483207447	-0.031224551787
C	3.125887400932	1.232893697904	0.711968171782
C	2.613728933545	0.209035818538	-1.382363345958
H	3.325957460514	2.177049726099	0.195721571800
H	4.088540088188	0.701649406719	0.833793454290
H	2.740596512835	1.464426877441	1.709867479615
H	1.832115230747	-0.263888873801	-1.982004320531
H	3.509850387618	-0.439053926684	-1.411235725426
H	2.870291485951	1.158402665818	-1.862002027049
H	-2.916638439869	2.372926770692	0.875596744526
H	-4.164448071628	1.531618708993	-0.068859865848
H	-2.851560300842	2.389495743018	-0.903655011318

Table S12: XYZ Coordinates for DFT optimized $\mathbf{O}_{\mathbf{nBuHis}}$ (CAM-B3LYP/6-31g*/SMD=THF)

Cu	0.919812553656	0.944260837032	0.123145088566
Cu	-0.916206337982	-1.002645741638	-0.014782814194
O	-0.820261234168	0.732542782740	0.319463196013
O	0.834039495233	-0.808830360866	-0.106202721393

N	0.715846051160	2.827820014237	0.356027268339
N	-0.728902355759	-2.857551481153	-0.439101309211
N	-2.787445830553	-1.060960080463	0.162799945794
N	2.773574048001	1.010392848346	-0.162952727721
N	-4.818467555452	-0.419655409956	0.626550275934
N	4.795929252542	0.339334568560	-0.621821728319
C	-1.772984990626	-3.815129941073	-0.007203713365
C	1.650440021823	3.716544486409	-0.372546243473
C	-3.122694911875	-3.438569556149	-0.597093176818
C	3.076024265550	3.501349404475	0.107792409416
C	-4.895506882721	-1.730851276849	0.208518211260
C	-3.536583652889	-0.051568690830	0.588437954394
C	-3.627098853490	-2.129724371147	-0.084223143359
C	4.849970718246	1.707934585776	-0.470437033986
C	3.532481524085	-0.044507937069	-0.432932700545
C	3.587666568196	2.126811165945	-0.180317840279
H	-0.246912296909	3.007639885533	0.062591362813
H	0.747837596891	3.041093034589	1.357179728516
H	-0.609806235912	-2.919488958739	-1.454333107943
H	0.174847198888	-3.119171242554	-0.039770484459
H	-1.801698855062	-3.804466491143	1.084633547862
H	-1.486205170752	-4.817355759429	-0.336123394785
H	1.551721002832	3.498287389351	-1.438276469114
H	1.352645976323	4.754427836737	-0.203545884404
H	-3.845288279368	-4.222687531878	-0.359100241665
H	-3.039120002659	-3.411812033395	-1.691765814297
H	3.726646532239	4.236124838775	-0.372726206588
H	3.120365965938	3.704676253437	1.186029769603
C	-5.953507338558	0.421041812966	1.015707978314
H	-5.835309999741	-2.258688958004	0.157459812203
H	-3.166189690600	0.922189585926	0.868746826025

C	5.939277022571	-0.530372879201	-0.909777422284
H	5.772193076117	2.257307847824	-0.581394409952
H	3.177740565417	-1.061296991717	-0.500513207994
H	-5.542238432194	1.311813271172	1.495191774527
H	-6.528101339829	-0.127776132635	1.766025368398
H	6.459185745270	-0.111454580288	-1.775139091122
H	5.537455463994	-1.503889886764	-1.198295134196
C	6.881048832268	-0.657144719750	0.282566728431
H	7.212574278786	0.341806393932	0.591253071308
H	6.333034449667	-1.087030524822	1.129588141293
C	8.097109964096	-1.520837760555	-0.045659163621
H	8.639219946157	-1.076316406174	-0.889710117642
H	7.762203498557	-2.511223831547	-0.379287134536
C	9.038528653842	-1.672875939527	1.144199009778
H	9.409407368912	-0.698923842463	1.482767413351
H	9.906659951521	-2.287794307738	0.886859212473
H	8.532787804219	-2.148910013643	1.991710906941
C	-6.829235027984	0.795712063157	-0.174254110302
H	-6.218489439026	1.319754697043	-0.919315926137
H	-7.202369943001	-0.117672834772	-0.652672976542
C	-8.007341665373	1.671735012298	0.247104980385
H	-7.629313289955	2.592583245128	0.708650310061
H	-8.585909575809	1.152209773739	1.021329390758
C	-8.920233417241	2.022696978934	-0.922603635341
H	-8.376100337793	2.568422257350	-1.701650442379
H	-9.755428302116	2.651139941823	-0.597819033319
H	-9.340751653281	1.120829046676	-1.381353903390

Table S13: XYZ Coordinates for DFT optimized $\mathbf{O_{nBuHis}}$ (CAM-B3LYP/TZVP/SMD=THF)

Cu	0.941618819275	0.951032733646	0.077733132036
Cu	-0.947530824091	-1.013845576171	-0.004307724288

O	-0.826179218687	0.756545472447	0.293008184818
O	0.827271916705	-0.829456460766	-0.154706828631
N	0.756964797759	2.863504851752	0.320194134732
N	-0.778476126461	-2.907177465769	-0.384254719434
N	-2.842313019082	-1.058537422534	0.181508514928
N	2.827250878857	1.004625118403	-0.171738737350
N	-4.867024131140	-0.409134055748	0.622943875048
N	4.846927298409	0.338049010850	-0.611392899687
C	-1.856262375249	-3.833916885584	0.021667543560
C	1.746240416838	3.748157120092	-0.331492411042
C	-3.183121112272	-3.427688931892	-0.590361952764
C	3.142529394422	3.478800168764	0.193985928236
C	-4.947180296292	-1.716687727150	0.201768650687
C	-3.586882428116	-0.046948850077	0.598869180198
C	-3.681381634585	-2.121104333716	-0.076882321979
C	4.905969218853	1.698554512287	-0.417061507107
C	3.581847031805	-0.044337914549	-0.459160660320
C	3.644375203450	2.114760435629	-0.137901215666
H	-0.181702223420	3.062430544453	-0.021433840859
H	0.740137687499	3.038003491666	1.325373405392
H	-0.623792728209	-2.973367406112	-1.390684419433
H	0.101208684513	-3.172117152683	0.055159300698
H	-1.907500953324	-3.829982214909	1.109462251442
H	-1.590765051976	-4.839488194004	-0.306108920723
H	1.687896348837	3.579286517921	-1.405769880498
H	1.471485392306	4.784389458696	-0.131874706955
H	-3.921626494461	-4.199645505183	-0.378752610521
H	-3.076162322592	-3.387782032852	-1.678899383772
H	3.825150414236	4.219408226008	-0.220895981029
H	3.147484683888	3.625506120052	1.278605681507
C	-5.998830096449	0.434631002190	1.008426912682

H	-5.885507590995	-2.239675562690	0.137480909788
H	-3.218131756856	0.923129700988	0.885208761677
C	5.988011280090	-0.528175417925	-0.909614123490
H	5.829303150493	2.246595983470	-0.489587494664
H	3.227366296029	-1.055448964424	-0.565704400969
H	-5.587236116525	1.320074732835	1.490460729195
H	-6.579065814693	-0.110187147956	1.752889311501
H	6.511089827186	-0.100337927121	-1.764896400574
H	5.586046314489	-1.493752460146	-1.212486259319
C	6.925922689133	-0.678159018758	0.278080114285
H	7.263833452437	0.310412938040	0.600541300801
H	6.377357221386	-1.116745264446	1.116067261439
C	8.133869788067	-1.542474493671	-0.059839270375
H	8.676210755981	-1.091764343042	-0.895992356001
H	7.793720922677	-2.523444496541	-0.404632372751
C	9.074349982034	-1.715898829768	1.123376214710
H	9.450472949077	-0.751766361949	1.473124248829
H	9.936032620414	-2.330381346463	0.857833890207
H	8.568893194737	-2.199206513408	1.962571335317
C	-6.866900697502	0.818425322636	-0.179203215274
H	-6.253335652376	1.340118510259	-0.918856282814
H	-7.244598707589	-0.087675835200	-0.659807084372
C	-8.037483810845	1.699143804027	0.238922051266
H	-7.655677745171	2.613288261225	0.702647064510
H	-8.619903655101	1.182844318603	1.007575482429
C	-8.943723963954	2.060032055574	-0.928389113888
H	-8.395969460280	2.603120020618	-1.702022850840
H	-9.772675086945	2.691429049686	-0.604751900348
H	-9.368731316090	1.165608911084	-1.389557436024

Table S14: XYZ Coordinates for DFT optimized for ^{nBuHis}**L** (CAM-B3LYP/6-31g*/SMD=THF)

N	3.396653614473	-0.237744554074	-1.738667131028
N	1.871997131759	1.073452596539	1.545784016085
N	-0.129015921196	0.173245961369	1.237441479592
C	4.091231206365	-0.015951542568	-0.470633627441
C	3.380859212442	-0.731409349215	0.680956828628
C	0.794794944436	-0.745174436916	0.793570027353
C	0.575386389396	1.244281073167	1.674467585904
C	2.024803297389	-0.178426258277	0.990331238932
H	3.498897822885	-1.214900985456	-2.008037903205
H	3.854054934086	0.298504726312	-2.472835093528
H	4.094194861271	1.060477945618	-0.268487809252
H	5.143640116365	-0.342592982697	-0.488287926139
H	4.014449885690	-0.655515957781	1.572853516128
H	3.296808077626	-1.799171863265	0.443848665588
C	-1.578499548588	0.035900274608	1.204959845821
H	0.496582559229	-1.701010924244	0.388577244159
H	0.082981662590	2.115808377900	2.085247178750
H	-1.990295775249	0.790232354780	1.880825550409
H	-1.837831753153	-0.945756775713	1.613464726141
C	-2.161232962626	0.202065696721	-0.195405773295
H	-1.879958351889	1.188223440717	-0.584327771322
H	-1.711650235829	-0.541108397037	-0.865202854041
C	-3.680827922125	0.052707954540	-0.205630341896
H	-4.123047558599	0.792016570780	0.474622835713
H	-3.951355396974	-0.933341885605	0.193527982091
C	-4.278074520935	0.220789187121	-1.598719961671
H	-4.051215557191	1.211127901750	-2.009272429873
H	-5.367105090242	0.108797040228	-1.581150246112
H	-3.877225118407	-0.525525191304	-2.293819850490

Table S15: XYZ Coordinates for DFT optimized $\mathbf{O_{nBuBIM}}$ (CAM-B3LYP/6-31g*/SMD=THF)

Cu	1.334499637865	-0.017845076603	-0.075724932576
O	0.035407711062	-1.185946519445	0.169486898882
O	-0.035348761938	0.955506651772	-0.610247903086
N	2.563278776594	1.381740276837	-0.327294951494
N	2.664121960526	-1.208875535055	0.517366988785
C	3.888182262040	1.297747053037	-0.366961129940
C	2.220230951452	2.707178871569	-0.463372003891
C	3.978567697807	-1.091541792276	0.361269194578
C	2.418970738908	-2.415570664216	1.130893430963
H	1.188398313871	3.018352787073	-0.459559536108
H	1.413759493245	-2.727085692640	1.363701858779
C	4.697477970760	0.044220965592	-0.289887222528
H	5.003562000575	-0.253572708585	-1.301599277904
H	5.619501638464	0.244834921817	0.261024519064
Cu	-1.341093767979	-0.190152184355	-0.307422357605
N	-2.673730813197	1.008386441209	-0.863544791810
N	-2.593243139691	-1.537233845395	0.063940740352
C	-3.968523406378	0.964653707369	-0.569339594387
C	-2.444566717689	2.152150303277	-1.592778269624
C	-3.893077886776	-1.378604542036	0.284437532850
C	-2.300217393598	-2.872657230871	0.217957064165
H	-1.457256261676	2.399073575321	-1.948281344016
H	-1.295014784107	-3.241423184769	0.092519062925
C	-4.656095413447	-0.094700426102	0.229577194521
H	-4.835976166581	0.271647358348	1.249141120992
H	-5.641315116768	-0.288747404454	-0.202561395188
C	3.609719509770	-3.029140794735	1.342095336390
H	3.860725262268	-3.973846447545	1.798906482184
C	3.363658870661	3.425113722757	-0.593454093947
H	3.538885663706	4.482082050200	-0.721259941470
C	-3.447922620433	-3.520212074245	0.540748070430

H	-3.653527164519	-4.559400539613	0.745483160488
C	-3.625534436325	2.804108334951	-1.732227867856
H	-3.884652904064	3.722914293013	-2.235178138512
N	4.586159861570	-2.185559191952	0.855082761401
N	4.407719232459	2.526480148057	-0.535375784032
N	-4.579024801222	2.047176441431	-1.084380463571
N	-4.442854619986	-2.566770097312	0.586877987609
C	6.019897805313	-2.495829479163	0.835107316630
H	6.572499466383	-1.589384328095	1.093610234857
H	6.189049987969	-3.219176283873	1.635233458555
C	5.827628357546	2.888992740796	-0.605788569083
H	5.887459514047	3.791616152897	-1.217128529883
H	6.355167127663	2.097418959830	-1.142619114180
C	-5.982672146644	2.440600328132	-0.924527120410
H	-6.225325350206	3.076335300038	-1.778200121977
H	-6.604122461355	1.545381692712	-0.999257875064
C	-5.855348988112	-2.834543210672	0.876033204596
H	-5.878810377161	-3.653446052237	1.598611405869
H	-6.265215945297	-1.952684415897	1.369996252339
C	-6.638318315916	-3.201245902634	-0.382255815501
H	-6.560609172012	-2.382961182382	-1.109143443341
H	-6.164580780926	-4.076722063549	-0.839961755504
C	-8.112090018352	-3.500544991617	-0.099008469928
H	-8.554317696457	-3.920677531557	-1.008884031830
H	-8.183277582337	-4.283961505913	0.666011882938
C	-8.925672829768	-2.283047884516	0.332801747859
H	-9.978987998226	-2.547516624882	0.468820609814
H	-8.573383475023	-1.863138218142	1.281031779088
H	-8.880476703984	-1.490750305547	-0.423694604243
C	6.434663197165	3.125806648490	0.772847765919
H	6.331551165951	2.216232345586	1.377854666181

H	5.865757004203	3.912192270269	1.282856704902
C	7.906477420188	3.522810519551	0.683303621371
H	8.463892794654	2.736440778381	0.158644496566
H	8.000810666100	4.428817178508	0.071867269355
C	8.528657893612	3.763653952935	2.054179435023
H	8.478347852201	2.863222080619	2.676685934525
H	9.581810022572	4.048354016419	1.966933110209
H	8.009893781215	4.566774560514	2.589166951154
C	6.478631102648	-3.055904619989	-0.507171203447
H	6.291606488949	-2.316210859251	-1.295513893466
H	5.876443843766	-3.939507551093	-0.749659188888
C	7.960545148957	-3.424845244701	-0.490483870583
H	8.553453073815	-2.540757031638	-0.224030125653
H	8.140167102685	-4.166682691728	0.297573145767
C	8.438202722873	-3.974948591376	-1.829826713948
H	8.301278278904	-3.241367097277	-2.632342964112
H	9.501051018744	-4.233685871605	-1.794814344246
H	7.884592079619	-4.878490215893	-2.107917163593
C	-6.230055612356	3.175116507934	0.388691198273
H	-5.934352446550	2.529975781570	1.225590237493
H	-5.585759765031	4.061443066504	0.427828121192
C	-7.692706867424	3.585990891523	0.543132246593
H	-8.327486891431	2.691458508982	0.506779349840
H	-7.986389158388	4.208195913477	-0.311422486972
C	-7.951730591276	4.345023756147	1.839884605232
H	-9.005688815878	4.626051366846	1.929164102966
H	-7.694225288506	3.737422823917	2.714725017940
H	-7.357008594029	5.263999929350	1.886658282360

Table S16: XYZ Coordinates for DFT optimized $\mathbf{O_{nBuBIM}}$ (CAM-B3LYP/TZVP/SMD=THF)

Cu	1.372979414767	-0.017845056971	-0.047551224083

O	0.041838614773	-1.179442090160	0.253828549890
O	-0.038165474216	0.987771046564	-0.506897852726
N	2.625898781652	1.377565661340	-0.382303737789
N	2.730033262609	-1.237089538700	0.498609639568
C	3.946196732017	1.282028939453	-0.407506867053
C	2.292079224933	2.690222694988	-0.613555615188
C	4.040758598358	-1.098674762374	0.365158578797
C	2.490003481518	-2.459497965932	1.077736040455
H	1.266301893357	3.011397228926	-0.638259067814
H	1.489879047024	-2.791957277928	1.290645108599
C	4.764067207057	0.048895306146	-0.246894830357
H	5.145738914639	-0.253511928879	-1.227222802099
H	5.639578939265	0.281154596824	0.360472105003
Cu	-1.372681731420	-0.155392968796	-0.157692086601
N	-2.730975573756	1.084468248778	-0.650173180451
N	-2.639257167061	-1.522865964501	0.242101383390
C	-4.036057769045	0.975945285354	-0.451990158857
C	-2.495097108489	2.289691074649	-1.266324981359
C	-3.954805011130	-1.400152436882	0.329631949921
C	-2.322088319380	-2.841134313892	0.464253109873
H	-1.500277791931	2.596494923054	-1.535284864569
H	-1.303211146389	-3.183966224149	0.443022972711
C	-4.751839075373	-0.148282891433	0.211278099536
H	-5.064473752811	0.167752371353	1.212179765172
H	-5.668854927482	-0.360504361000	-0.339425417174
C	3.681152278599	-3.059671165774	1.294214186616
H	3.933656486323	-4.009913059957	1.731473112987
C	3.437133432706	3.388372790412	-0.781722300545
H	3.616044780820	4.430622159633	-0.981070043821
C	-3.472242408999	-3.514997842495	0.688477487483
H	-3.662395274934	-4.553003681471	0.899188946181

C	-3.682826219571	2.910470360910	-1.437936229336
H	-3.936434312120	3.857010242468	-1.882651781170
N	4.651878950616	-2.193535061967	0.844586166337
N	4.472346306126	2.491273755531	-0.652791094187
N	-4.647126161393	2.073943039574	-0.923455409560
N	-4.493635253397	-2.597180694382	0.604740729417
C	6.087436957033	-2.486566105124	0.843832750286
H	6.624813925224	-1.577694258505	1.111306444597
H	6.253829956806	-3.208277762843	1.641729219917
C	5.894181863798	2.835442330375	-0.725171704065
H	5.976567928790	3.680032666628	-1.407205215466
H	6.423188994833	1.999581655904	-1.180898952057
C	-6.071626412066	2.403494332305	-0.845273456403
H	-6.308445542739	2.987112858190	-1.733577058067
H	-6.638182052785	1.475823703481	-0.903475339780
C	-5.918802627194	-2.910076166223	0.735767911447
H	-5.995739966139	-3.747280792051	1.427764083402
H	-6.405381970093	-2.057326314297	1.204496186188
C	-6.551591304447	-3.258983692307	-0.604763711583
H	-6.405813831613	-2.427283223837	-1.300451926464
H	-6.020636854202	-4.116803739238	-1.023133720995
C	-8.038986250776	-3.582523606033	-0.492889611246
H	-8.375180204463	-3.967720475215	-1.457709867087
H	-8.179150952629	-4.395112691444	0.226101835903
C	-8.909609179342	-2.395319666288	-0.101700713482
H	-9.965826143941	-2.668697676472	-0.109943970390
H	-8.680379719865	-2.027488705016	0.900157943735
H	-8.779790897353	-1.566116983036	-0.802108841923
C	6.477262544551	3.180227502502	0.636729168878
H	6.336489659332	2.335374900733	1.317013691396
H	5.922803048137	4.022258706024	1.058648338077

C	7.957282348124	3.528814680579	0.548012382312
H	8.503203729031	2.684368661534	0.116955445635
H	8.089740589371	4.366175085593	-0.142959367656
C	8.555366314013	3.885485040516	1.900514845776
H	8.464998192925	3.055618700252	2.605276581788
H	9.615183535751	4.129350747817	1.811923072033
H	8.051926485646	4.749503107254	2.339840500194
C	6.570615542602	-3.037877335820	-0.489151221393
H	6.391241296725	-2.300109658410	-1.276076796545
H	5.981797363800	-3.923521388085	-0.741525079012
C	8.050685459257	-3.396359254555	-0.453075553701
H	8.633305491250	-2.510684086670	-0.183397097584
H	8.224099529315	-4.132820038888	0.336690908237
C	8.547903751182	-3.947010812943	-1.781145765741
H	8.416987267733	-3.219348187089	-2.585485269519
H	9.608557496251	-4.198357874157	-1.732703762211
H	8.005099118199	-4.852397112167	-2.061393893120
C	-6.417103509852	3.175976976534	0.418962601629
H	-6.143674153604	2.580712006429	1.294528914761
H	-5.815951692014	4.088221899225	0.454042755227
C	-7.896942387738	3.531368405119	0.481083998988
H	-8.492074444404	2.614068908735	0.445234561960
H	-8.166822023270	4.109992932225	-0.406918328332
C	-8.254053711043	4.321842804560	1.731051475171
H	-9.317094098241	4.566823202483	1.752418999965
H	-8.026038501589	3.755000228083	2.636703304934
H	-7.696089368141	5.259757928426	1.776861435933

Table S17: XYZ Coordinates for DFT optimized for ^{nBuBIM}**L** (CAM-B3LYP/6-31g*/SMD=THF)

N	-0.0806362305	-1.7270561026	1.5058175947
N	1.7938535807	-2.1202646142	-1.8189458145

C	-0.6929350382	-1.2691131367	0.4336835025
C	-1.0787413872	-2.0507284694	2.3932095298
C	1.4002140860	-1.1915266402	-0.9706734209
C	3.1552350239	-2.2065693581	-1.6662544615
H	-0.8583403445	-2.4659182455	3.3674677189
H	3.7487304995	-2.9033917320	-2.2429504393
C	-0.0220773022	-0.7515363180	-0.8081285925
H	-0.5571305501	-1.1091400936	-1.6917627504
H	-0.0855884057	0.3438305380	-0.8315563735
C	3.5796482476	-1.3190179712	-0.7200196189
H	4.5556132342	-1.0890456210	-0.3188413805
C	-2.2990684546	-1.7814638753	1.8475363489
H	-3.3077551616	-1.9013007427	2.2141716502
N	2.4506871125	-0.6724363535	-0.2765940455
N	-2.0472508385	-1.2812025657	0.5898487937
C	2.4277180699	0.4089767885	0.7015889747
H	1.4784518039	0.3548187228	1.2371689576
H	3.2167886522	0.2048804482	1.4305111852
C	-3.0600968941	-0.7970909931	-0.3412125518
H	-3.9716215961	-1.3705498405	-0.1538484508
H	-2.7349617440	-1.0320998244	-1.3579823263
C	-3.3327856404	0.6978451676	-0.1975466590
H	-2.4015059119	1.2536596435	-0.3633846022
H	-3.6448527277	0.9056569416	0.8333731712
C	-4.4031840303	1.1828441863	-1.1726288172
H	-4.0864747889	0.9608738157	-2.1998098971
H	-5.3282771640	0.6160116272	-1.0066298957
C	-4.6881350508	2.6751165061	-1.0393012542
H	-3.7875136325	3.2692940858	-1.2312228420
H	-5.4563653011	2.9981879127	-1.7492798202
H	-5.0401266957	2.9236971558	-0.0318060947

C	2.6307543900	1.7826869732	0.0687121175
H	1.8409458595	1.9596978343	-0.6723301847
H	3.5814125032	1.7885922522	-0.4786987608
C	2.6240153500	2.9012514483	1.1078666975
H	1.6774045852	2.8753520182	1.6627445879
H	3.4165287433	2.7169483719	1.8444710952
C	2.8150324152	4.2822172055	0.4893519552
H	2.0163575947	4.5106307161	-0.2254046100
H	2.8099565898	5.0647863801	1.2550895597
H	3.7681858424	4.3478959766	-0.0474776796

Table S18: XYZ Coordinates for DFT optimized $\mathbf{O_{NH3}}$

(CAM-B3LYP/DEF2TZVP/SMD=THF)

Cu	-1.38390300	0.00000000	0.00000000
Cu	1.38390300	0.00000000	0.00000000
O	0.00000000	1.15531700	0.00000000
O	0.00000000	-1.15531700	0.00000000
N	2.69615000	1.40933700	0.08132500
N	3.80226800	3.25063800	-0.27254300
N	2.69615000	-1.40933700	-0.08132500
N	3.80226800	-3.25063800	0.27254300
N	-2.69615000	-1.40933700	0.08132500
N	-3.80226800	-3.25063800	-0.27254300
N	-2.69615000	1.40933700	-0.08132500
N	-3.80226800	3.25063800	0.27254300
C	2.82044000	2.45118700	-0.73772000
C	3.62065100	1.54493800	1.09338600
C	4.31277300	2.69489200	0.88024800
C	2.82044000	-2.45118700	0.73772000
C	3.62065100	-1.54493800	-1.09338600
C	4.31277300	-2.69489200	-0.88024800
C	-3.62065100	-1.54493800	1.09338600

C	-2.82044000	-2.45118700	-0.73772000
C	-4.31277300	-2.69489200	0.88024800
C	-3.62065100	1.54493800	-1.09338600
C	-2.82044000	2.45118700	0.73772000
C	-4.31277300	2.69489200	-0.88024800
C	2.04716700	2.70803700	-1.97537600
C	2.04716700	-2.70803700	1.97537600
C	-2.04716700	-2.70803700	-1.97537600
C	-2.04716700	2.70803700	1.97537600
H	-5.10966900	3.16286100	-1.43074000
H	3.71554600	0.81795300	1.87978300
H	5.10966900	3.16286100	1.43074000
H	3.71554600	-0.81795300	-1.87978300
H	5.10966900	-3.16286100	-1.43074000
H	-3.71554600	-0.81795300	1.87978300
H	-5.10966900	-3.16286100	1.43074000
H	-3.71554600	0.81795300	-1.87978300
H	1.22285100	2.00219100	-2.04346200
H	1.64014100	3.72044000	-1.97547200
H	2.68456700	2.60646300	-2.85735700
H	1.22285100	-2.00219100	2.04346200
H	1.64014100	-3.72044000	1.97547200
H	2.68456700	-2.60646300	2.85735700
H	-1.22285100	-2.00219100	-2.04346200
H	-1.64014100	-3.72044000	-1.97547200
H	-2.68456700	-2.60646300	-2.85735700
H	-1.22285100	2.00219100	2.04346200
H	-1.64014100	3.72044000	1.97547200
H	-2.68456700	2.60646300	2.85735700
C	-4.23290600	4.50228300	0.88236700
H	-5.09870100	4.87252900	0.33979800

H	-4.50652600	4.33736500	1.92345500
H	-3.43283600	5.24030900	0.83113400
C	-4.23290600	-4.50228300	-0.88236700
H	-5.09870100	-4.87252900	-0.33979800
H	-4.50652600	-4.33736500	-1.92345500
H	-3.43283600	-5.24030900	-0.83113400
C	4.23290600	-4.50228300	0.88236700
H	5.09870100	-4.87252900	0.33979800
H	4.50652600	-4.33736500	1.92345500
H	3.43283600	-5.24030900	0.83113400
C	4.23290600	4.50228300	-0.88236700
H	5.09870100	4.87252900	-0.33979800
H	4.50652600	4.33736500	-1.92345500
H	3.43283600	5.24030900	-0.83113400

Table S19: XYZ Coordinates for DFT optimized $\mathbf{O_{NH3}}$

(CAM-B3LYP/6-31g*/SMD=THF)

Cu	0.00000000	1.33780600	0.00005600
Cu	0.00000000	-1.33780600	0.00005600
O	0.00000000	0.00000000	-1.14283000
O	0.00000000	0.00000000	1.14306200
N	-0.08893100	2.62143100	1.41487900
N	0.08786700	2.62127600	-1.41512400
N	-0.08786700	-2.62127600	-1.41512400
N	0.08893100	-2.62143100	1.41487900
H	0.06829300	-2.13575700	-2.30065900
H	-0.07245100	-2.13735000	2.30024800
H	0.07245100	2.13735000	2.30024800
H	-0.06829300	2.13575700	-2.30065900
H	1.01272700	-3.05699700	1.47155800
H	0.60185400	-3.37256600	-1.34800500
H	-0.60185400	3.37256600	-1.34800500

H	-1.01272700	3.05699700	1.47155800
H	0.59637700	3.37654100	1.34527400
H	1.00943600	3.06184300	-1.46926200
H	-1.00943600	-3.06184300	-1.46926200
H	-0.59637700	-3.37654100	1.34527400

Table S20: XYZ Coordinates for DFT optimized $\mathbf{O_{MeNH2}}$

(CAM-B3LYP/DEF2TZVP/SMD=THF)

Cu	-0.03856300	1.56348200	-0.19682200
Cu	-0.09799700	-1.15325000	-0.33791100
O	-0.23733700	0.27001900	-1.43949000
O	0.10688800	0.13863500	0.90582600
N	0.11307200	2.80834700	1.30982100
N	-0.23319600	2.95597400	-1.55589300
N	-0.27262500	-2.40219200	-1.83213600
N	0.07409400	-2.55607900	1.01066800
H	0.58090000	-2.13782700	1.78964900
H	0.94772900	2.53038500	1.82466300
H	-0.14132300	2.48001500	-2.45266300
H	0.64866900	-3.32447700	0.66518700
H	-0.82287500	-3.21739600	-1.56398300
H	0.26486800	3.76889400	1.00642900
H	0.52848000	3.63085400	-1.49912600
H	-0.80372900	-1.91125600	-2.55030400
C	-1.06849300	2.72904200	2.19668100
H	-0.93653300	3.37742500	3.06360200
H	-1.95068200	3.03931200	1.64106600
H	-1.18701500	1.69842500	2.52089100
C	-1.54093000	3.64289000	-1.47374300
H	-1.61428300	4.16074300	-0.51957000
H	-1.64769200	4.36368200	-2.28498800
H	-2.33296800	2.90010500	-1.54007100

C	1.04176100	-2.81960000	-2.36668500
H	1.59260200	-1.93433800	-2.67585000
H	1.59450600	-3.33345200	-1.58259900
H	0.91328500	-3.48666500	-3.21964600
C	-1.24198700	-3.05606200	1.46716900
H	-1.77723100	-3.48341400	0.62087900
H	-1.11595500	-3.81765900	2.23767700
H	-1.81258100	-2.22251400	1.87039000

Table S21: XYZ Coordinates for DFT optimized $\mathbf{O_{MeNH2}}$ (CAM-B3LYP/6-31g*/SMD=THF)

Cu	-1.30561300	-0.03298500	-0.27836900
Cu	1.30422900	-0.03262500	0.27743000
O	-0.00206300	1.12349500	0.00557100
O	0.00014600	-1.18480700	-0.00396400
N	-2.51684800	-1.46636600	-0.62095200
N	-2.57351700	1.38090800	-0.46610000
N	2.56856100	1.38471000	0.46557500
N	2.51581500	-1.46701500	0.61661700
C	-2.95677600	1.93329600	0.85266700
C	3.55575200	-1.70854500	-0.40756300
C	-3.54306500	-1.71524700	0.41522800
C	2.95694600	1.93169600	-0.85392900
H	-2.05216100	2.25691000	1.36742600
H	-3.63374400	2.78115400	0.72978100
H	4.12175500	-2.61071000	-0.16582300
H	3.63086700	2.78206800	-0.73164700
H	-4.10919300	-2.61830100	0.17718000
H	-3.05010700	-1.84154600	1.38012800
H	3.07542700	-1.83279300	-1.37906600
H	2.05400300	2.25073500	-1.37451500
H	-3.45152900	1.15687000	1.43785600

H	-4.22532500	-0.86628300	0.46293900
H	3.45663500	1.15438500	-1.43360800
H	4.23595100	-0.85723200	-0.44381600
H	2.10435400	2.11528600	1.00915000
H	1.90879000	-2.28679000	0.68477100
H	-1.91034400	-2.28521600	-0.70284400
H	-2.11498100	2.11005600	-1.01632800
H	2.95475900	-1.36197000	1.53441200
H	3.40125700	1.11869700	0.99439500
H	-3.40861600	1.10957800	-0.98827700
H	-2.96755700	-1.35456300	-1.53213700

Table S22: XYZ Coordinates for DFT optimized $\mathbf{O_{Me2NH}}$

(CAM-B3LYP/6-31g*/SMD=THF)

Cu	-1.34832600	-0.00016500	-0.00028900
Cu	1.34802600	-0.00016400	0.00018200
O	-0.00012700	1.14460100	-0.00288200
O	-0.00012600	-1.14497200	0.00283400
N	-2.53140100	-1.52739100	-0.05439200
N	-2.53118200	1.52728600	0.05409100
N	2.53119500	1.52653900	-0.05535800
N	2.53142900	-1.52662900	0.05560600
C	-2.97529000	1.82603600	1.43283800
C	3.63621800	-1.60135900	-0.91974800
C	3.63734500	1.60154300	0.91843200
C	-3.63709500	-1.60122600	0.92003100
C	-3.63857900	1.60143200	-0.91837900
C	2.97941900	-1.82063400	1.43398900
C	2.97706700	1.82114800	-1.43433600
C	-2.97807500	-1.82547100	-1.43240900
H	-2.10887200	1.82626200	2.09633100
H	-3.45502100	2.80843600	1.46334300

H	4.08502800	-2.59848800	-0.89062400
H	3.45779000	2.80297800	-1.46716100
H	-4.08388200	-2.59932800	0.89359800
H	-3.25345000	-1.40558000	1.92249900
H	-3.25677500	1.40553200	-1.92149900
H	-4.40216000	0.86624000	-0.66449900
H	-4.08489800	2.59972600	-0.89125900
H	3.69220500	-1.06244600	1.75783700
H	3.46067600	-2.80221900	1.46639500
H	2.11483000	-1.81977700	2.09985000
H	3.25340700	1.40980600	1.92154000
H	4.39982800	0.86387600	0.66876600
H	4.08573600	2.59884800	0.88878900
H	-3.45840400	-2.80760100	-1.46236800
H	-2.11279900	-1.82598700	-2.09739600
H	-3.69118700	-1.06911100	-1.75941300
H	3.25079000	-1.40987700	-1.92233700
H	2.11153000	1.82004000	-2.09896200
H	-3.68826100	1.07019400	1.76134200
H	-4.40083800	-0.86570700	0.66755000
H	3.68977300	1.06342800	-1.75944300
H	4.39878600	-0.86338200	-0.67122900
H	1.85023000	2.24652000	0.19798100
H	1.85036200	-2.24690800	-0.19662200
H	-1.85004500	-2.24684100	0.19941200
H	-1.85001700	2.24643400	-0.20107500

Table S23: XYZ Coordinates for DFT optimized $\mathbf{O_{Me2NH}}$ (CAM-B3LYP/DEF2TZVP/SMD=THF)

Cu	1.37776400	-0.00086400	-0.00060900
Cu	-1.37726200	-0.00047100	0.00045900
O	0.00007300	-1.18178200	0.00772300

O	0.00034400	1.18023700	-0.00754200
N	2.59385200	1.55743500	-0.02773800
N	2.59567700	-1.55766400	0.02699100
N	-2.59561400	-1.55863600	-0.03177000
N	-2.59405500	1.55889300	0.03229000
C	3.05034300	-1.87169800	1.39797200
C	-3.68361400	1.57861000	-0.96119700
C	-3.68771100	-1.57627100	0.95911200
C	3.68183800	1.56966500	0.96745200
C	3.68648400	-1.56707800	-0.96507800
C	-3.05086500	1.86067900	1.40567500
C	-3.05000200	-1.86075200	-1.40595900
C	3.05161800	1.87225000	-1.39745600
H	2.18929200	-1.89289900	2.06294100
H	3.54544300	-2.84518400	1.41206500
H	-4.14031000	2.57038200	-0.98987300
H	-3.54839200	-2.83244300	-1.42809800
H	4.13505600	2.56255700	1.00856500
H	3.27664800	1.31689400	1.94501900
H	3.28354100	-1.31490200	-1.94379600
H	4.44493500	-0.84353000	-0.68036600
H	4.14221300	-2.55889300	-1.00525300
H	-3.75051800	1.09708900	1.73383300
H	-3.54754600	2.83321100	1.42749400
H	-2.19007700	1.87850900	2.07125300
H	-3.28542700	-1.33564900	1.94081300
H	-4.44320200	-0.84685600	0.68047000
H	-4.14576300	-2.56740400	0.98726900
H	3.54435900	2.84697500	-1.41034500
H	2.19216100	1.89124300	-2.06491800
H	3.75517700	1.11370800	-1.72946800

H	-3.27925300	1.33809100	-1.94212600
H	-2.18768200	-1.88054500	-2.06983400
H	3.75117000	-1.11145500	1.73194000
H	4.44283700	0.84783300	0.68527300
H	-3.74764100	-1.09618300	-1.73616000
H	-4.44094000	0.85004400	-0.68501500
H	-1.91721500	-2.27380700	0.23224000
H	-1.91392800	2.27332500	-0.22963600
H	1.91274800	2.26795000	0.24210200
H	1.91684900	-2.26962900	-0.24500100

Table S24: XYZ Coordinates for DFT optimized $\mathbf{O_{Me3N}}$

(CAM-B3LYP/DEF2TZVP/SMD=THF)

Cu	0.00000000	1.45397600	0.00063700
Cu	0.00000000	-1.45397600	0.00063700
O	0.00000000	0.00000000	-1.09199100
O	0.00000000	0.00000000	1.09317200
N	-0.24361700	2.63199500	1.67409900
N	0.08817700	2.65227300	-1.67216700
N	-0.08817700	-2.65227300	-1.67216700
N	0.24361700	-2.63199500	1.67409900
C	0.37796100	4.09480200	-1.51924700
C	0.90824200	2.32223400	2.55465100
C	1.15054600	2.07604600	-2.53677200
C	-1.15054600	-2.07604600	-2.53677200
C	0.33817400	-4.09905000	1.52569500
C	1.24051100	-2.48337300	-2.30818700
C	-0.33817400	4.09905000	1.52569500
C	-1.24051100	2.48337300	-2.30818700
C	1.51013300	-2.14900700	2.28098500
C	-0.37796100	-4.09480200	-1.51924700
C	-0.90824200	-2.32223400	2.55465100

C	-1.51013300	2.14900700	2.28098500
H	1.29501300	4.22703700	-0.95082500
H	0.50836200	4.53792900	-2.51023100
H	-1.16673300	-2.60607200	-3.49242800
H	-0.96052400	-1.02204200	-2.70488600
H	0.50153300	-4.54629600	2.51016300
H	-0.50836200	-4.53792900	-2.51023100
H	-0.79413600	-2.84040000	3.51050300
H	-1.82388200	-2.65684800	2.07007500
H	-0.95972600	-1.25193000	2.72550700
H	-0.50153300	4.54629600	2.51016300
H	0.58407300	4.49429700	1.11311700
H	-1.42714600	1.42740600	-2.48250700
H	-2.00556000	2.88317500	-1.64437400
H	-1.26970600	3.02272500	-3.25890300
H	2.33086100	-2.35334100	1.59490900
H	1.68853800	-2.67226100	3.22424800
H	1.44845700	-1.08137800	2.45965100
H	1.42714600	-1.42740600	-2.48250700
H	2.00556000	-2.88317500	-1.64437400
H	1.26970600	-3.02272500	-3.25890300
H	2.11266500	2.19467800	-2.04125900
H	1.16673300	2.60607200	-3.49242800
H	0.96052400	1.02204200	-2.70488600
H	0.95972600	1.25193000	2.72550700
H	0.79413600	2.84040000	3.51050300
H	1.82388200	2.65684800	2.07007500
H	-1.68853800	2.67226100	3.22424800
H	-1.44845700	1.08137800	2.45965100
H	-2.11266500	-2.19467800	-2.04125900
H	-2.33086100	2.35334100	1.59490900

H	-0.58407300	-4.49429700	1.11311700
H	-1.29501300	-4.22703700	-0.95082500
H	-0.44636500	4.59783600	-1.02895900
H	-1.17910200	4.35157100	0.88670600
H	0.44636500	-4.59783600	-1.02895900
H	1.17910200	-4.35157100	0.88670600

Table S25: XYZ Coordinates for DFT optimized $\mathbf{O_{Me3N}}$

(CAM-B3LYP/6-31g*/SMD=THF)

Cu	0.00000000	1.41330300	0.00284300
Cu	0.00000000	-1.41330300	0.00284300
O	0.00000000	0.00000000	-1.07400300
O	0.00000000	0.00000000	1.07896400
N	-0.24383300	2.57098900	1.63061600
N	0.07671600	2.59339800	-1.62981700
N	-0.07671600	-2.59339800	-1.62981700
N	0.24383300	-2.57098900	1.63061600
C	0.35964400	4.04086600	-1.50627000
C	0.89064000	2.27893800	2.53815600
C	1.13247700	2.04036700	-2.51587800
C	-1.13247700	-2.04036700	-2.51587800
C	0.34496500	-4.04004100	1.50698400
C	1.24769200	-2.42901000	-2.27241900
C	-0.34496500	4.04004100	1.50698400
C	-1.24769200	2.42901000	-2.27241900
C	1.51156500	-2.09697500	2.23938400
C	-0.35964400	-4.04086600	-1.50627000
C	-0.89064000	-2.27893800	2.53815600
C	-1.51156500	2.09697500	2.23938400
H	1.28996200	4.19256000	-0.95826500
H	0.46852900	4.46477300	-2.51011900
H	-1.11573400	-2.57520800	-3.47079300

H	-0.96172500	-0.98134600	-2.68450400
H	0.50714500	-4.46675600	2.50259300
H	-0.46852900	-4.46477300	-2.51011900
H	-0.74125200	-2.79663500	3.49135400
H	-1.81623400	-2.63366700	2.08004700
H	-0.95683700	-1.20746500	2.71237400
H	-0.50714500	4.46675600	2.50259300
H	0.57603300	4.44952400	1.09740900
H	-1.44935400	1.37046600	-2.42950100
H	-2.01666700	2.85665700	-1.62566000
H	-1.25981400	2.95121600	-3.23505700
H	2.33811200	-2.32039500	1.56087400
H	1.67830000	-2.61602100	3.18918300
H	1.46064200	-1.02488100	2.40912900
H	1.44935400	-1.37046600	-2.42950100
H	2.01666700	-2.85665700	-1.62566000
H	1.25981400	-2.95121600	-3.23505700
H	2.10630800	2.18309700	-2.04269500
H	1.11573400	2.57520800	-3.47079300
H	0.96172500	0.98134600	-2.68450400
H	0.95683700	1.20746500	2.71237400
H	0.74125200	2.79663500	3.49135400
H	1.81623400	2.63366700	2.08004700
H	-1.67830000	2.61602100	3.18918300
H	-1.46064200	1.02488100	2.40912900
H	-2.10630800	-2.18309700	-2.04269500
H	-2.33811200	2.32039500	1.56087400
H	-0.57603300	-4.44952400	1.09740900
H	-1.28996200	-4.19256000	-0.95826500
H	-0.45984400	4.55195400	-1.00990300
H	-1.19297100	4.30221400	0.87590800

H	0.45984400	-4.55195400	-1.00990300
H	1.19297100	-4.30221400	0.87590800

Table S26: XYZ Coordinates for DFT optimized $\mathbf{O_{Himd}}$

(CAM-B3LYP/DEF2TZVP/SMD=THF)

Cu	-1.38961600	0.00000000	0.00000000
Cu	1.38961600	0.00000000	0.00000000
O	0.00000000	1.15117700	0.00000000
O	0.00000000	-1.15117700	0.00000000
N	2.67289500	1.43532600	0.09304300
N	3.50363300	3.42391400	-0.15005200
N	2.67289500	-1.43532600	-0.09304300
N	3.50363300	-3.42391400	0.15005200
N	-2.67289500	-1.43532600	0.09304300
N	-3.50363300	-3.42391400	-0.15005200
N	-2.67289500	1.43532600	-0.09304300
N	-3.50363300	3.42391400	0.15005200
C	2.46649300	2.62995700	-0.44028800
C	3.88371000	1.47156900	0.75196900
C	4.41079200	2.71796800	0.60333800
C	2.46649300	-2.62995700	0.44028800
C	3.88371000	-1.47156900	-0.75196900
C	4.41079200	-2.71796800	-0.60333800
C	-3.88371000	-1.47156900	0.75196900
C	-2.46649300	-2.62995700	-0.44028800
C	-4.41079200	-2.71796800	0.60333800
C	-3.88371000	1.47156900	-0.75196900
C	-2.46649300	2.62995700	0.44028800
C	-4.41079200	2.71796800	-0.60333800
H	-5.32617900	3.15482700	-0.96050200
H	4.27447600	0.61630200	1.27233000
H	5.32617900	3.15482700	0.96050200

H	4.27447600	-0.61630200	-1.27233000
H	5.32617900	-3.15482700	-0.96050200
H	-4.27447600	-0.61630200	1.27233000
H	-5.32617900	-3.15482700	0.96050200
H	-4.27447600	0.61630200	-1.27233000
H	-1.59642900	2.91717600	1.00259700
H	1.59642900	2.91717600	-1.00259700
H	1.59642900	-2.91717600	1.00259700
H	-1.59642900	-2.91717600	-1.00259700
H	-3.59932300	4.38743600	0.43890300
H	3.59932300	4.38743600	-0.43890300
H	3.59932300	-4.38743600	0.43890300
H	-3.59932300	-4.38743600	-0.43890300

Table S27: XYZ Coordinates for DFT optimized $\mathbf{O_{Himd}}$ (CAM-B3LYP/6-31g*/SMD=THF)

Cu	-0.000389	1.352797	-0.043463
Cu	0.000389	-1.352797	-0.043463
O	-1.132389	-0.000892	-0.079766
O	1.132389	0.000892	-0.079766
N	-1.407345	-2.605858	0.095226
N	-3.396155	-3.442806	-0.138952
N	1.407345	-2.617963	-0.091358
N	3.386052	-3.448066	0.234790
N	1.407345	2.605858	0.095226
N	3.396155	3.442806	-0.138952
N	-1.407345	2.617963	-0.091358
N	-3.386052	3.448066	0.234790
C	-2.600664	-2.413960	-0.445024
C	-1.448501	-3.805772	0.775323
C	-2.692786	-4.335469	0.634067
C	2.577611	-2.416013	0.493181

C	1.477434	-3.826818	-0.752787
C	2.715326	-4.352843	-0.552913
C	1.448501	3.805772	0.775323
C	2.600664	2.413960	-0.445024
C	2.692786	4.335469	0.634067
C	-1.477434	3.826818	-0.752787
C	-2.577611	2.416013	0.493181
C	-2.715326	4.352843	-0.552913
H	-3.172695	5.267909	-0.894089
H	-0.593119	-4.191338	1.306865
H	-3.134565	-5.245635	1.007255
H	0.643621	-4.221976	-1.311206
H	3.172695	-5.267909	-0.894089
H	0.593119	4.191338	1.306865
H	3.134565	5.245635	1.007255
H	-0.643621	4.221976	-1.311206
H	-2.848239	1.543850	1.066231
H	-2.893557	-1.551332	-1.021975
H	2.848239	-1.543850	1.066231
H	2.893557	1.551332	-1.021975
H	-4.338316	3.541625	0.569088
H	-4.361184	-3.542263	-0.432633
H	4.338316	-3.541625	0.569088
H	4.361184	3.542263	-0.432633

Table S28: XYZ Coordinates for DFT optimized $\mathbf{O_{1Meimd}}$

(CAM-B3LYP/DEF2TZVP/SMD=THF)

Cu	-1.38674500	0.00000000	0.00000000
Cu	1.38674500	0.00000000	0.00000000
O	0.00000000	1.15487000	0.00000000
O	0.00000000	-1.15487000	0.00000000
N	2.67299400	1.42875600	0.03581100

N	3.50953600	3.40268300	-0.36039800
N	2.67299400	-1.42875600	-0.03581100
N	3.50953600	-3.40268300	0.36039800
N	-2.67299400	-1.42875600	0.03581100
N	-3.50953600	-3.40268300	-0.36039800
N	-2.67299400	1.42875600	-0.03581100
N	-3.50953600	3.40268300	0.36039800
C	2.47200400	2.58612400	-0.57919900
C	3.88592800	1.50668800	0.68140600
C	4.41375100	2.73887000	0.43886800
C	2.47200400	-2.58612400	0.57919900
C	3.88592800	-1.50668800	-0.68140600
C	4.41375100	-2.73887000	-0.43886800
C	-3.88592800	-1.50668800	0.68140600
C	-2.47200400	-2.58612400	-0.57919900
C	-4.41375100	-2.73887000	0.43886800
C	-3.88592800	1.50668800	-0.68140600
C	-2.47200400	2.58612400	0.57919900
C	-4.41375100	2.73887000	-0.43886800
H	-5.33307100	3.19798200	-0.75787500
H	4.27908200	0.68911500	1.25814700
H	5.33307100	3.19798200	0.75787500
H	4.27908200	-0.68911500	-1.25814700
H	5.33307100	-3.19798200	-0.75787500
H	-4.27908200	-0.68911500	1.25814700
H	-5.33307100	-3.19798200	0.75787500
H	-4.27908200	0.68911500	-1.25814700
C	-3.65819800	4.75914300	0.87300400
H	-4.58631400	4.83689100	1.43680100
H	-2.81790800	4.98221700	1.52574900
H	-3.67372300	5.46647200	0.04472500

C	-3.65819800	-4.75914300	-0.87300400
H	-4.58631400	-4.83689100	-1.43680100
H	-2.81790800	-4.98221700	-1.52574900
H	-3.67372300	-5.46647200	-0.04472500
C	3.65819800	-4.75914300	0.87300400
H	4.58631400	-4.83689100	1.43680100
H	2.81790800	-4.98221700	1.52574900
H	3.67372300	-5.46647200	0.04472500
C	3.65819800	4.75914300	-0.87300400
H	4.58631400	4.83689100	-1.43680100
H	2.81790800	4.98221700	-1.52574900
H	3.67372300	5.46647200	-0.04472500
H	-1.60044400	2.84281400	1.15465800
H	1.60044400	2.84281400	-1.15465800
H	1.60044400	-2.84281400	1.15465800
H	-1.60044400	-2.84281400	-1.15465800

Table S29: XYZ Coordinates for DFT optimized **O_{1Meimd}**

(CAM-B3LYP/6-31g*/SMD=THF)

Cu	-1.352755	0.000000	0.000000
Cu	1.352755	-0.000000	0.000000
O	0.000000	1.133461	0.000000
O	-0.000000	-1.133461	0.000000
N	2.617548	1.402195	0.055284
N	3.461223	3.377549	-0.329887
N	2.617548	-1.402195	-0.055284
N	3.461223	-3.377549	0.329887
N	-2.617548	-1.402195	0.055284
N	-3.461223	-3.377549	-0.329887
N	-2.617548	1.402195	-0.055284
N	-3.461223	3.377549	0.329887
C	2.429030	2.560828	-0.560110

C	3.824510	1.482961	0.713796
C	4.355379	2.712892	0.479106
C	2.429030	-2.560828	0.560110
C	3.824510	-1.482961	-0.713796
C	4.355379	-2.712892	-0.479106
C	-3.824510	-1.482961	0.713796
C	-2.429030	-2.560828	-0.560110
C	-4.355379	-2.712892	0.479106
C	-3.824510	1.482961	-0.713796
C	-2.429030	2.560828	0.560110
C	-4.355379	2.712892	-0.479106
H	-5.273459	3.174118	-0.809048
H	4.216076	0.663888	1.296231
H	5.273459	3.174118	0.809048
H	4.216076	-0.663888	-1.296231
H	5.273459	-3.174118	-0.809048
H	-4.216076	-0.663888	1.296231
H	-5.273459	-3.174118	0.809048
H	-4.216076	0.663888	-1.296231
C	-3.613871	4.733783	0.839032
H	-4.547309	4.811418	1.398479
H	-2.776108	4.957615	1.498799
H	-3.623607	5.441158	0.007854
C	-3.613871	-4.733783	-0.839032
H	-4.547309	-4.811418	-1.398479
H	-2.776108	-4.957615	-1.498799
H	-3.623607	-5.441158	-0.007854
C	3.613871	-4.733783	0.839032
H	4.547309	-4.811418	1.398479
H	2.776108	-4.957615	1.498799
H	3.623607	-5.441158	0.007854

C	3.613871	4.733783	-0.839032
H	4.547309	4.811418	-1.398479
H	2.776108	4.957615	-1.498799
H	3.623607	5.441158	-0.007854
H	-1.561219	2.824874	1.143903
H	1.561219	2.824874	-1.143903
H	1.561219	-2.824874	1.143903
H	-1.561219	-2.824874	-1.143903

Table S30: XYZ Coordinates for DFT optimized $\mathbf{O_{2Meimd}}$

(CAM-B3LYP/DEF2TZVP/SMD=THF)

Cu	-1.38759500	0.00000000	0.00000000
Cu	1.38759500	0.00000000	0.00000000
O	0.00000000	1.15197100	0.00000000
O	0.00000000	-1.15197100	0.00000000
N	2.70609100	1.40639900	-0.08346800
N	3.80353600	3.17750100	-0.67021300
N	2.70609100	-1.40639900	0.08346800
N	3.80353600	-3.17750100	0.67021300
N	-2.70609100	-1.40639900	-0.08346800
N	-3.80353600	-3.17750100	-0.67021300
N	-2.70609100	1.40639900	0.08346800
N	-3.80353600	3.17750100	0.67021300
C	2.76263500	2.38590200	-0.98216900
C	3.73702200	1.58504800	0.81738900
C	4.42971300	2.69666900	0.45693200
C	2.76263500	-2.38590200	0.98216900
C	3.73702200	-1.58504800	-0.81738900
C	4.42971300	-2.69666900	-0.45693200
C	-3.73702200	-1.58504800	0.81738900
C	-2.76263500	-2.38590200	-0.98216900
C	-4.42971300	-2.69666900	0.45693200

C	-3.73702200	1.58504800	-0.81738900
C	-2.76263500	2.38590200	0.98216900
C	-4.42971300	2.69666900	-0.45693200
C	1.87539800	2.57407600	-2.15518900
C	1.87539800	-2.57407600	2.15518900
C	-1.87539800	-2.57407600	-2.15518900
C	-1.87539800	2.57407600	2.15518900
H	-5.28661100	3.17981300	-0.89114300
H	3.89437200	0.90956000	1.63857300
H	5.28661100	3.17981300	0.89114300
H	3.89437200	-0.90956000	-1.63857300
H	5.28661100	-3.17981300	-0.89114300
H	-3.89437200	-0.90956000	1.63857300
H	-5.28661100	-3.17981300	0.89114300
H	-3.89437200	0.90956000	-1.63857300
H	0.87981900	2.20272200	-1.91937400
H	1.81485000	3.62886500	-2.42251500
H	2.25911900	2.02490900	-3.01885100
H	0.87981900	-2.20272200	1.91937400
H	1.81485000	-3.62886500	2.42251500
H	2.25911900	-2.02490900	3.01885100
H	-0.87981900	-2.20272200	-1.91937400
H	-1.81485000	-3.62886500	-2.42251500
H	-2.25911900	-2.02490900	-3.01885100
H	-0.87981900	2.20272200	1.91937400
H	-1.81485000	3.62886500	2.42251500
H	-2.25911900	2.02490900	3.01885100
H	-4.07848900	3.99589800	1.19469600
H	4.07848900	3.99589800	-1.19469600
H	4.07848900	-3.99589800	1.19469600
H	-4.07848900	-3.99589800	-1.19469600

Table S31: XYZ Coordinates for DFT optimized $\mathbf{O_{2Meimd}}$

(CAM-B3LYP/6-31g*/SMD=THF)

Cu	1.356846	-0.000000	-0.000000
Cu	-1.356846	0.000000	-0.000000
O	0.000000	1.130828	0.000000
O	-0.000000	-1.130828	0.000000
N	-2.652489	1.381354	0.058344
N	-3.740757	3.176350	0.596264
N	-2.652489	-1.381354	-0.058344
N	-3.740757	-3.176350	-0.596264
N	2.652489	-1.381354	0.058344
N	3.740757	-3.176350	0.596264
N	2.652489	1.381354	-0.058344
N	3.740757	3.176350	-0.596264
C	-2.717984	2.376449	0.938124
C	-3.663279	1.564182	-0.865625
C	-4.349332	2.687638	-0.536205
C	-2.717984	-2.376449	-0.938124
C	-3.663279	-1.564182	0.865625
C	-4.349332	-2.687638	0.536205
C	3.663279	-1.564182	-0.865625
C	2.717984	-2.376449	0.938124
C	4.349332	-2.687638	-0.536205
C	3.663279	1.564182	0.865625
C	2.717984	2.376449	-0.938124
C	4.349332	2.687638	0.536205
C	-1.855461	2.576156	2.131075
C	-1.855461	-2.576156	-2.131075
C	1.855461	-2.576156	2.131075
C	1.855461	2.576156	-2.131075
H	5.191886	3.179580	0.995285

H	-3.815567	0.881920	-1.687049
H	-5.191886	3.179580	-0.995285
H	-3.815567	-0.881920	1.687049
H	-5.191886	-3.179580	0.995285
H	3.815567	-0.881920	-1.687049
H	5.191886	-3.179580	-0.995285
H	3.815567	0.881920	1.687049
H	-0.854068	2.198571	1.921942
H	-1.793396	3.637236	2.383737
H	-2.261430	2.043822	2.997943
H	-0.854068	-2.198571	-1.921942
H	-1.793396	-3.637236	-2.383737
H	-2.261430	-2.043822	-2.997943
H	0.854068	-2.198571	1.921942
H	1.793396	-3.637236	2.383737
H	2.261430	-2.043822	2.997943
H	0.854068	2.198571	-1.921942
H	1.793396	3.637236	-2.383737
H	2.261430	2.043822	-2.997943
H	4.016871	4.007065	-1.106729
H	-4.016871	4.007065	1.106729
H	-4.016871	-4.007065	-1.106729
H	4.016871	-4.007065	1.106729

Table S32: XYZ Coordinates for DFT optimized **$O_{15Meimd}$**

(CAM-B3LYP/DEF2TZVP/SMD=THF)

Cu	-1.38485500	0.00000000	0.00000000
Cu	1.38485500	0.00000000	0.00000000
O	0.00000000	1.15785700	0.00000000
O	0.00000000	-1.15785700	0.00000000
N	2.67205800	1.42559900	0.03581600
N	3.52903200	3.38707100	-0.37212500

N	2.67205800	-1.42559900	-0.03581600
N	3.52903200	-3.38707100	0.37212500
N	-2.67205800	-1.42559900	0.03581600
N	-3.52903200	-3.38707100	-0.37212500
N	-2.67205800	1.42559900	-0.03581600
N	-3.52903200	3.38707100	0.37212500
C	2.48246500	2.57711800	-0.58771700
C	3.88550300	1.49934100	0.68347700
C	4.43635700	2.72471900	0.43888200
C	2.48246500	-2.57711800	0.58771700
C	3.88550300	-1.49934100	-0.68347700
C	4.43635700	-2.72471900	-0.43888200
C	-3.88550300	-1.49934100	0.68347700
C	-2.48246500	-2.57711800	-0.58771700
C	-4.43635700	-2.72471900	0.43888200
C	-3.88550300	1.49934100	-0.68347700
C	-2.48246500	2.57711800	0.58771700
C	-4.43635700	2.72471900	-0.43888200
H	4.27212400	0.68316600	1.26675000
H	4.27212400	-0.68316600	-1.26675000
H	-4.27212400	-0.68316600	1.26675000
H	-4.27212400	0.68316600	-1.26675000
C	-3.68385800	4.73772100	0.89332000
H	-4.61179500	4.81104000	1.45860100
H	-2.84412900	4.95958700	1.54699600
H	-3.70433200	5.45364900	0.07217700
C	-3.68385800	-4.73772100	-0.89332000
H	-4.61179500	-4.81104000	-1.45860100
H	-2.84412900	-4.95958700	-1.54699600
H	-3.70433200	-5.45364900	-0.07217700
C	3.68385800	-4.73772100	0.89332000

H	4.61179500	-4.81104000	1.45860100
H	2.84412900	-4.95958700	1.54699600
H	3.70433200	-5.45364900	0.07217700
C	3.68385800	4.73772100	-0.89332000
H	4.61179500	4.81104000	-1.45860100
H	2.84412900	4.95958700	-1.54699600
H	3.70433200	5.45364900	-0.07217700
H	-1.61388100	2.83853600	1.16554000
H	1.61388100	2.83853600	-1.16554000
H	1.61388100	-2.83853600	1.16554000
H	-1.61388100	-2.83853600	-1.16554000
C	-5.71478700	3.33425500	-0.88210200
H	-6.35758000	3.57462700	-0.03152200
H	-5.54397100	4.25885600	-1.43879300
H	-6.24879000	2.63916500	-1.52830400
C	-5.71478700	-3.33425500	0.88210200
H	-6.35758000	-3.57462700	0.03152200
H	-5.54397100	-4.25885600	1.43879300
H	-6.24879000	-2.63916500	1.52830400
C	5.71478700	-3.33425500	-0.88210200
H	6.35758000	-3.57462700	-0.03152200
H	5.54397100	-4.25885600	-1.43879300
H	6.24879000	-2.63916500	-1.52830400
C	5.71478700	3.33425500	0.88210200
H	6.35758000	3.57462700	0.03152200
H	5.54397100	4.25885600	1.43879300
H	6.24879000	2.63916500	1.52830400

Table S32: XYZ Coordinates for DFT optimized $\mathbf{O_{15Meimd}}$

(CAM-B3LYP/6-31g*/SMD=THF)

Cu	-1.352339	0.000000	0.000000
Cu	1.352339	-0.000000	0.000000

O	0.000000	1.134121	0.000000
O	-0.000000	-1.134121	0.000000
N	2.617715	1.399453	0.049990
N	3.471126	3.367592	-0.343388
N	2.617715	-1.399453	-0.049990
N	3.471126	-3.367592	0.343388
N	-2.617715	-1.399453	0.049990
N	-3.471126	-3.367592	-0.343388
N	-2.617715	1.399453	-0.049990
N	-3.471126	3.367592	0.343388
C	2.438154	2.549792	-0.577583
C	3.818106	1.486789	0.721083
C	4.365342	2.713399	0.487325
C	2.438154	-2.549792	0.577583
C	3.818106	-1.486789	-0.721083
C	4.365342	-2.713399	-0.487325
C	-3.818106	-1.486789	0.721083
C	-2.438154	-2.549792	-0.577583
C	-4.365342	-2.713399	0.487325
C	-3.818106	1.486789	-0.721083
C	-2.438154	2.549792	0.577583
C	-4.365342	2.713399	-0.487325
H	4.203223	0.672746	1.315221
H	4.203223	-0.672746	-1.315221
H	-4.203223	-0.672746	1.315221
H	-4.203223	0.672746	-1.315221
C	-3.625282	4.715714	0.869084
H	-4.556313	4.789218	1.433954
H	-2.785282	4.932091	1.528526
H	-3.638731	5.437111	0.049535
C	-3.625282	-4.715714	-0.869084

H	-4.556313	-4.789218	-1.433954
H	-2.785282	-4.932091	-1.528526
H	-3.638731	-5.437111	-0.049535
C	3.625282	-4.715714	0.869084
H	4.556313	-4.789218	1.433954
H	2.785282	-4.932091	1.528526
H	3.638731	-5.437111	0.049535
C	3.625282	4.715714	-0.869084
H	4.556313	4.789218	-1.433954
H	2.785282	4.932091	-1.528526
H	3.638731	5.437111	-0.049535
H	-1.576712	2.811911	1.171686
H	1.576712	2.811911	-1.171686
H	1.576712	-2.811911	1.171686
H	-1.576712	-2.811911	-1.171686
C	-5.631333	3.335495	-0.958162
H	-6.291299	3.586640	-0.121083
H	-5.441994	4.255148	-1.521431
H	-6.161261	2.639921	-1.611886
C	-5.631333	-3.335495	0.958162
H	-6.291299	-3.586640	0.121083
H	-5.441994	-4.255148	1.521431
H	-6.161261	-2.639921	1.611886
C	5.631333	-3.335495	-0.958162
H	6.291299	-3.586640	-0.121083
H	5.441994	-4.255148	-1.521431
H	6.161261	-2.639921	-1.611886
C	5.631333	3.335495	0.958162
H	6.291299	3.586640	0.121083
H	5.441994	4.255148	1.521431
H	6.161261	2.639921	1.611886

Table S33: XYZ Coordinates for DFT optimized $\mathbf{O_{12Meimd}}$

(CAM-B3LYP/DEF2TZVP/SMD=THF)

Cu	-1.38390300	0.00000000	0.00000000
Cu	1.38390300	0.00000000	0.00000000
O	0.00000000	1.15531700	0.00000000
O	0.00000000	-1.15531700	0.00000000
N	2.69615000	1.40933700	0.08132500
N	3.80226800	3.25063800	-0.27254300
N	2.69615000	-1.40933700	-0.08132500
N	3.80226800	-3.25063800	0.27254300
N	-2.69615000	-1.40933700	0.08132500
N	-3.80226800	-3.25063800	-0.27254300
N	-2.69615000	1.40933700	-0.08132500
N	-3.80226800	3.25063800	0.27254300
C	2.82044000	2.45118700	-0.73772000
C	3.62065100	1.54493800	1.09338600
C	4.31277300	2.69489200	0.88024800
C	2.82044000	-2.45118700	0.73772000
C	3.62065100	-1.54493800	-1.09338600
C	4.31277300	-2.69489200	-0.88024800
C	-3.62065100	-1.54493800	1.09338600
C	-2.82044000	-2.45118700	-0.73772000
C	-4.31277300	-2.69489200	0.88024800
C	-3.62065100	1.54493800	-1.09338600
C	-2.82044000	2.45118700	0.73772000
C	-4.31277300	2.69489200	-0.88024800
C	2.04716700	2.70803700	-1.97537600
C	2.04716700	-2.70803700	1.97537600
C	-2.04716700	-2.70803700	-1.97537600
C	-2.04716700	2.70803700	1.97537600
H	-5.10966900	3.16286100	-1.43074000

H	3.71554600	0.81795300	1.87978300
H	5.10966900	3.16286100	1.43074000
H	3.71554600	-0.81795300	-1.87978300
H	5.10966900	-3.16286100	-1.43074000
H	-3.71554600	-0.81795300	1.87978300
H	-5.10966900	-3.16286100	1.43074000
H	-3.71554600	0.81795300	-1.87978300
H	1.22285100	2.00219100	-2.04346200
H	1.64014100	3.72044000	-1.97547200
H	2.68456700	2.60646300	-2.85735700
H	1.22285100	-2.00219100	2.04346200
H	1.64014100	-3.72044000	1.97547200
H	2.68456700	-2.60646300	2.85735700
H	-1.22285100	-2.00219100	-2.04346200
H	-1.64014100	-3.72044000	-1.97547200
H	-2.68456700	-2.60646300	-2.85735700
H	-1.22285100	2.00219100	2.04346200
H	-1.64014100	3.72044000	1.97547200
H	-2.68456700	2.60646300	2.85735700
C	-4.23290600	4.50228300	0.88236700
H	-5.09870100	4.87252900	0.33979800
H	-4.50652600	4.33736500	1.92345500
H	-3.43283600	5.24030900	0.83113400
C	-4.23290600	-4.50228300	-0.88236700
H	-5.09870100	-4.87252900	-0.33979800
H	-4.50652600	-4.33736500	-1.92345500
H	-3.43283600	-5.24030900	-0.83113400
C	4.23290600	-4.50228300	0.88236700
H	5.09870100	-4.87252900	0.33979800
H	4.50652600	-4.33736500	1.92345500
H	3.43283600	-5.24030900	0.83113400

C	4.23290600	4.50228300	-0.88236700
H	5.09870100	4.87252900	-0.33979800
H	4.50652600	4.33736500	-1.92345500
H	3.43283600	5.24030900	-0.83113400

Table S33: XYZ Coordinates for DFT optimized **$O_{12Meimd}$**

(CAM-B3LYP/6-31g*/SMD=THF)

Cu	-1.357222	0.000000	0.000000
Cu	1.357222	-0.000000	0.000000
O	0.000000	1.129880	0.000000
O	-0.000000	-1.129880	0.000000
N	2.646665	1.384683	0.098963
N	3.727548	3.258460	-0.164584
N	2.646665	-1.384683	-0.098963
N	3.727548	-3.258460	0.164584
N	-2.646665	-1.384683	0.098963
N	-3.727548	-3.258460	-0.164584
N	-2.646665	1.384683	-0.098963
N	-3.727548	3.258460	0.164584
C	2.732713	2.486741	-0.641974
C	3.611845	1.461152	1.080714
C	4.287860	2.626875	0.923211
C	2.732713	-2.486741	0.641974
C	3.611845	-1.461152	-1.080714
C	4.287860	-2.626875	-0.923211
C	-3.611845	-1.461152	1.080714
C	-2.732713	-2.486741	-0.641974
C	-4.287860	-2.626875	0.923211
C	-3.611845	1.461152	-1.080714
C	-2.732713	2.486741	0.641974
C	-4.287860	2.626875	-0.923211
C	1.908684	2.833915	-1.827376

C	1.908684	-2.833915	1.827376
C	-1.908684	-2.833915	-1.827376
C	-1.908684	2.833915	1.827376
H	-5.105638	3.065349	-1.473583
H	3.747646	0.680531	1.812712
H	5.105638	3.065349	1.473583
H	3.747646	-0.680531	-1.812712
H	5.105638	-3.065349	-1.473583
H	-3.747646	-0.680531	1.812712
H	-5.105638	-3.065349	1.473583
H	-3.747646	0.680531	-1.812712
H	1.108994	2.103437	-1.941041
H	1.457266	3.823750	-1.711524
H	2.519647	2.849233	-2.736079
H	1.108994	-2.103437	1.941041
H	1.457266	-3.823750	1.711524
H	2.519647	-2.849233	2.736079
H	-1.108994	-2.103437	-1.941041
H	-1.457266	-3.823750	-1.711524
H	-2.519647	-2.849233	-2.736079
H	-1.108994	2.103437	1.941041
H	-1.457266	3.823750	1.711524
H	-2.519647	2.849233	2.736079
C	-4.133928	4.547379	0.707336
H	-5.016854	4.886373	0.166234
H	-4.378786	4.449089	1.766589
H	-3.332963	5.279378	0.584337
C	-4.133928	-4.547379	-0.707336
H	-5.016854	-4.886373	-0.166234
H	-4.378786	-4.449089	-1.766589
H	-3.332963	-5.279378	-0.584337

C	4.133928	-4.547379	0.707336
H	5.016854	-4.886373	0.166234
H	4.378786	-4.449089	1.766589
H	3.332963	-5.279378	0.584337
C	4.133928	4.547379	-0.707336
H	5.016854	4.886373	-0.166234
H	4.378786	4.449089	-1.766589
H	3.332963	5.279378	-0.584337

Table S34: XYZ Coordinates for DFT optimized $\mathbf{O_{EtNH2}}$

(CAM-B3LYP/6-31g*/SMD=THF)

Cu	0.003516563924	1.338558528688	0.055355088926
Cu	-0.003516563924	-1.338558528688	0.055355088926
O	0.000000000000	0.000000000000	-1.096111802110
O	0.000000000000	0.000000000000	1.205509677468
N	-0.068527686534	2.613676829747	1.478853418177
N	0.131880883459	2.600013381625	-1.372146914450
N	-0.131880883459	-2.600013381625	-1.372146914450
N	0.068527686534	-2.613676829747	1.478853418177
C	1.506806385012	2.589937061621	-1.938899781712
C	-1.145200542439	-3.442759504282	1.697507129146
C	1.145200542439	3.442759504282	1.697507129146
C	-1.506806385012	-2.589937061621	-1.938899781712
H	1.724284185762	1.554865890510	-2.206731331858
H	1.989069527888	2.755925102348	1.796023117941
H	-1.989069527888	-2.755925102348	1.796023117941
H	-1.724284185762	-1.554865890510	-2.206731331858
H	2.187037438099	2.883910277808	-1.135864062118
H	1.303885734653	4.046028218942	0.800854844228
H	-2.187037438099	-2.883910277808	-1.135864062118
H	-1.303885734653	-4.046028218942	0.800854844228
H	0.534065385353	-2.312520286806	-2.093125994499

H	0.245904058536	-2.051150446653	2.314814463179
H	-0.245904058536	2.051150446653	2.314814463179
H	-0.534065385353	2.312520286806	-2.093125994499
H	0.883216013366	-3.223906631607	1.370362094577
H	0.124563121966	-3.553495139259	-1.105382494049
H	-0.124563121966	3.553495139259	-1.105382494049
H	-0.883216013366	3.223906631607	1.370362094577
C	1.642002651204	3.512608006979	-3.134407393135
H	1.430439934567	4.551878188477	-2.862536355019
H	2.663662710460	3.466578009638	-3.522331527054
H	0.960495551191	3.218601169401	-3.939267312350
C	1.011793393728	4.325561933201	2.924296279351
H	1.919584081974	4.921956628785	3.052355489143
H	0.164819751676	5.012835434920	2.826329867157
H	0.869380272549	3.725982894148	3.828998936855
C	-1.642002651204	-3.512608006979	-3.134407393135
H	-1.430439934567	-4.551878188477	-2.862536355019
H	-2.663662710460	-3.466578009638	-3.522331527055
H	-0.960495551191	-3.218601169401	-3.939267312350
C	-1.011793393728	-4.325561933201	2.924296279351
H	-1.919584081974	-4.921956628785	3.052355489143
H	-0.164819751676	-5.012835434920	2.826329867157
H	-0.869380272549	-3.725982894148	3.828998936854

Table S35: XYZ Coordinates for DFT optimized $\mathbf{O_{nPrNH2}}$

(CAM-B3LYP/6-31g*/SMD=THF)

Cu	0.000000000000	0.000000000000	-1.337816698217
Cu	0.000000000000	0.000000000000	1.361147464677
O	0.000000000000	1.127873220768	0.011320593196
O	0.000000000000	-1.127873220768	0.011320593196
N	0.068217328952	-1.385167940029	-2.670715924099
N	-0.068217328952	1.385167940029	-2.670715924099

N	0.105237009964	1.390783733914	2.689783881841
N	-0.105237009964	-1.390783733914	2.689783881841
C	0.350345840177	2.747718911123	-2.255573838244
C	-0.630421124542	-2.708770147690	2.251930657743
C	-0.350345840177	-2.747718911123	-2.255573838244
C	0.630421124542	2.708770147690	2.251930657743
H	1.384217725671	2.678378872335	-1.909489853167
H	0.264352946654	-3.030320218499	-1.400592371818
H	-1.651860128465	-2.550376848372	1.897819587798
H	0.031855386618	3.029998895699	1.399050435230
H	-0.264352946654	3.030320218499	-1.400592371818
H	-1.384217725671	-2.678378872335	-1.909489853167
H	1.651860128465	2.550376848372	1.897819587798
H	-0.031855386618	-3.029998895699	1.399050435230
H	-0.831429010979	1.526597343768	3.081477252096
H	-0.677028123628	-1.064316071805	3.473546129209
H	1.029027611682	-1.428363265461	-3.023547880811
H	0.499799009861	1.109327678034	-3.476254030301
H	0.831429010979	-1.526597343768	3.081477252096
H	0.677028123628	1.064316071805	3.473546129209
H	-1.029027611682	1.428363265461	-3.023547880811
H	-0.499799009861	-1.109327678034	-3.476254030301
C	0.222877926730	3.754366661048	-3.388863364849
H	-0.818186606213	3.779638633322	-3.734998777907
H	0.833216548124	3.425859978209	-4.239439962481
C	-0.222877926730	-3.754366661048	-3.388863364849
H	-0.833216548124	-3.425859978209	-4.239439962481
H	0.818186606213	-3.779638633322	-3.734998777907
C	0.594393033262	3.738146235280	3.371535038886
H	1.196648623582	3.382342344730	4.216528885384
H	-0.435992098228	3.839986413040	3.735316834596

C	-0.594393033262	-3.738146235280	3.371535038886
H	0.435992098228	-3.839986413040	3.735316834596
H	-1.196648623582	-3.382342344730	4.216528885384
C	1.114013437007	5.092674029190	2.902706896186
H	0.507004431651	5.488518946453	2.081357542087
H	2.148519455977	5.020559360571	2.549564879387
C	0.657705740831	5.148426158435	-2.950660929699
H	0.043318766017	5.514116288965	-2.120855321970
H	1.702427912358	5.153061661761	-2.621124114734
C	-0.657705740831	-5.148426158435	-2.950660929699
H	-0.043318766017	-5.514116288965	-2.120855321970
H	-1.702427912358	-5.153061661761	-2.621124114734
C	-1.114013437007	-5.092674029190	2.902706896186
H	-2.148519455977	-5.020559360571	2.549564879387
H	-0.507004431651	-5.488518946453	2.081357542087
H	0.565617419555	5.862811591510	-3.773884991524
H	1.090818440190	5.823033205520	3.716742435345
H	-1.090818440190	-5.823033205520	3.716742435345
H	-0.565617419555	-5.862811591510	-3.773884991524

Table S36: XYZ Coordinates for DFT optimized $\mathbf{O_{iPrNH2}}$

(CAM-B3LYP/6-31g*/SMD=THF)

Cu	1.294978846414	-0.088803835298	-0.034925297462
Cu	-1.364760405161	-0.132553087141	0.172860767898
O	-0.049436914411	1.046079690691	0.120778201018
O	-0.007610062393	-1.272201370130	0.140922505475
N	2.631219564914	-1.452726323924	0.014528257526
N	2.516617857436	1.356267134148	-0.280869483158
N	-2.692197511909	1.243126436890	0.253585717890
N	-2.602087369135	-1.585699579107	0.027192065494
H	-3.240918322373	-1.617700474760	0.825863930740
H	2.305427032040	-2.233378491055	-0.558693708504

H	3.301965129066	1.298797035431	0.370974387691
H	-2.016342022814	-2.422919470728	0.095700025830
H	3.524016023169	-1.159687796632	-0.389855812865
H	1.990194717020	2.193500680444	-0.016054287214
H	-3.627632333881	0.856418531318	0.410003357239
C	2.846322280453	-1.941388209767	1.411960155130
H	1.868234903569	-2.296264703060	1.746631907363
C	3.030987488577	1.537112771306	-1.667985683065
H	3.570932685281	0.615444391102	-1.911578616305
C	-2.427767661132	2.306552890989	1.265604388240
H	-1.450767404894	2.718714371834	1.005940344666
C	-3.388639597375	-1.637586918778	-1.242548561725
H	-4.005274352516	-0.732659467167	-1.255399340871
C	3.989916634876	2.718971035489	-1.719417273691
H	4.364210620378	2.861966948120	-2.736671168646
H	3.480293841476	3.639653045449	-1.413673559239
H	4.849616129289	2.563158894877	-1.060170570078
C	3.834672763334	-3.095476288021	1.413605146060
H	3.940438940253	-3.503659971771	2.422405616996
H	3.495890769932	-3.903514272660	0.757805204144
H	4.823992291256	-2.765093338105	1.076430788686
C	-2.342691381205	1.662854355298	2.635871272151
H	-1.546414625534	0.910314860183	2.661594977149
H	-2.120994154505	2.414520934450	3.396415361486
H	-3.289975965189	1.181062344928	2.905492716898
C	-4.291289619002	-2.861349514374	-1.242653566132
H	-4.881726394292	-2.891226074376	-2.162442181873
H	-3.700176235581	-3.782396818453	-1.189703230523
H	-4.983955681535	-2.842998633642	-0.395502513743
C	1.856800233039	1.721164042533	-2.611361974224
H	1.138457208155	0.902634562637	-2.525241974830

H	1.335771560228	2.656247382295	-2.387177694294
H	2.205848589791	1.764401169615	-3.644270602115
C	3.281887704676	-0.779330313686	2.285614110020
H	3.390973326207	-1.107110284212	3.320574049727
H	4.239073828039	-0.364258106374	1.954329477320
H	2.517626233579	0.012492251140	2.247534695312
C	-2.449395489714	-1.608402464524	-2.435432942145
H	-1.861602555374	-0.686252853342	-2.463949622348
H	-1.762962582686	-2.458496653502	-2.417647514111
H	-3.031147886834	-1.659763742028	-3.356886138609
H	-2.727486094571	1.670369639700	-0.674533981519
C	-3.492105434291	3.388138288896	1.183146981964
H	-3.268067850147	4.184023150058	1.896185002077
H	-3.534614887095	3.831198754707	0.184974545168
H	-4.479918783363	2.986454661608	1.427393614836

Table S37: XYZ Coordinates for DFT optimized $\mathbf{O_{tBuNH2}}$ (CAM-B3LYP/6-31g*/SMD=THF)

Cu	1.327231113733	0.080797085008	-0.404097439682
Cu	-1.372230300927	-0.098114760532	-0.383914352125
O	-0.092036201952	1.111428054812	-0.227417965239
O	0.050071392068	-1.144378792443	-0.364697101345
N	2.790201118693	-1.139806653735	-0.773382716451
N	2.411365086560	1.658005043945	-0.633364803064
N	-2.865943760713	1.126461571841	-0.553636752857
N	-2.487521137691	-1.645924563286	-0.647197664633
H	-1.854191794792	-2.288766713193	-1.130688597049
H	2.813172542564	-1.245270295546	-1.792329973671
H	1.738532490411	2.318135153960	-1.031978880994
H	-3.239967312433	-1.446883991505	-1.312759429437
H	3.653159206439	-0.642957251242	-0.543277309941
H	3.112961602016	1.503491707373	-1.363170575445

H	-3.636877582629	0.700762876141	-0.034680864417
C	2.900876891420	-2.518235990489	-0.159756255018
C	3.080288280245	2.333490373690	0.534757085915
C	-2.849565487977	2.588172479010	-0.171976297700
C	-3.080718924657	-2.381406607913	0.529300850845
C	3.745217889956	3.604430224817	0.009369180005
H	4.235188798378	4.136738670202	0.829352699699
H	4.505364191053	3.372025326373	-0.744351509735
H	3.007242976167	4.278531195234	-0.438032099252
C	4.353193797155	-2.968468743899	-0.316284061801
H	4.480279778463	-3.972966907398	0.097077373175
H	4.645267897415	-2.998911647238	-1.371543540038
H	5.038700155699	-2.297915679120	0.214287056708
C	-2.312404905640	2.705410117916	1.249831887753
H	-1.284352889958	2.342520756296	1.307944768815
H	-2.333906449854	3.751505192541	1.568110541751
H	-2.931709348561	2.133689379552	1.950613592019
C	-3.761598739784	-3.636808096370	-0.013699511453
H	-4.193306914743	-4.212302439743	0.809864553052
H	-4.569737466039	-3.381840277692	-0.707715391520
H	-3.044539756253	-4.279219802952	-0.535352076893
C	4.117937956500	1.380721520751	1.113474060279
H	3.645477045650	0.485446032648	1.529596135492
H	4.850898021928	1.080860964166	0.355301656317
H	4.664384032484	1.874546209821	1.921132986850
C	2.521932573755	-2.418577576117	1.312803255894
H	2.629754303292	-3.395880116343	1.791652944350
H	3.174060688276	-1.715952874636	1.842502386673
H	1.483986849310	-2.094529445892	1.423107794934
C	-4.099418860325	-1.477589075691	1.214617912118
H	-3.618038990422	-0.613583735665	1.685102959939

H	-4.865921410505	-1.130765396538	0.510817370412
H	-4.609964639002	-2.034468801111	2.004517995534
C	2.015746601431	2.675430779104	1.570014648350
H	2.485186074465	3.169094809974	2.425057599750
H	1.264816540559	3.355008955884	1.156365010766
H	1.503397291576	1.778878521866	1.928656135180
C	1.972388678516	-3.464135514707	-0.914286334900
H	0.935880363415	-3.130975535045	-0.842160492097
H	2.251998295383	-3.523077182530	-1.972830927785
H	2.053391087985	-4.469845367012	-0.492390175384
C	-1.956285657306	-2.751688591013	1.488464043044
H	-1.220074538779	-3.402977753279	1.008422330007
H	-1.437604890319	-1.862424014122	1.856021980626
H	-2.373316901297	-3.284715817800	2.347138256075
C	-1.986361549791	3.340244117999	-1.178502541318
H	-0.960995611161	2.968175473890	-1.164812753390
H	-2.389517984336	3.232609230350	-2.192461451371
H	-1.981164458092	4.406325215646	-0.935046258424
C	-4.293806107031	3.085879614257	-0.238330124753
H	-4.333006178782	4.149910562979	0.011731605397
H	-4.713585691064	2.960745561293	-1.242190965744
H	-4.931271498992	2.549843157771	0.473989254005
H	-3.150596801510	1.070842523043	-1.537042489625

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