Supporting Information

for

Substrate and Lewis Acid Coordination Promote O-O Bond Cleavage of an Unreactive $L_2Cu^{II}_2(O_2^{2-})$ Species to Form $L_2Cu^{III}_2(O)_2$ Cores with Enhanced Oxidative Reactivity.

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1. UV-Vis experiments.

1.1 Reaction of $[(MeAN)_2Cu_2(O_2^{2-})]^{2+}$ towards external substrates.

3 mL of a $[(MeAN)Cu^{I}](BAr^{F})$ solution (0.2 mM) in acetone were placed in a 10 mm path quartz cell equipped with a stir bar and it was capped with a rubber septum. After cooling down the cell to -90 ºC, dioxygen was added to generate the corresponding $[(MeAN)_2Cu^{II}_2(O_2^{2-})]^{2+}$ ($^{S}\mathbf{P}^{MeAN}$) (λ_{max}: 365 nm; ε = 22 mM^{-1} cm^{-1}). After complete formation, 100 μL of an acetone solution containing excess of the corresponding substrate were added. No spectral change was observed with substituted phenols, PPh_3, DHA, thioanisole, Me_2Fc, or Fc within 30 minutes after substrate addition. On the other hand, addition of Me_8Fc or $Me_{10}Fc$ (10 equiv.) led to decay of the $^{S}\mathbf{P}^{MeAN}$ UV-Vis features with concomitant formation of 1 equiv. of the corresponding Me_nFc^{+} (**Figure S1**). NOTE: the formation of only one equiv. suggests a disproportion reaction.

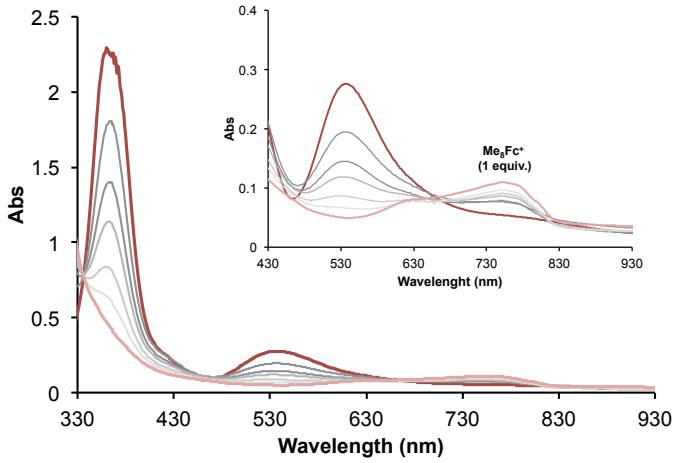


Figure S1. UV-vis spectra for the 1e⁻ reduction of $^{S}\mathbf{P}^{MeAN}$ (**brown spectrum**) by $Me_{10}Fc$ (10 equiv). The decay of $^{S}\mathbf{P}^{MeAN}$ features concluded 1 minute after the addition of the reductant with concomitant formation of 1 equiv. of $Me_{10}Fc^{+}$ (**pink spectrum**).

1.2 Reaction of $[(MeAN)_2Cu_2(O_2^{2-})]^{2+}$ with substituted sodium phenolates (4-NO_2, 4-CN, 4-Cl, 4-Me, 4-MeO and 2,6-F_2)

2.9 mL of a $[(MeAN)Cu^{I}](BAr^{F})$ solution (0.1 mM) in acetone were placed in a 10 mm path quartz cell equipped with a stir bar and it was capped with a rubber septum. After cooling down the cell to -90 ºC, dioxygen was added to generate the corresponding $[(MeAN)_2Cu^{II}_2(O_2^{2-})]^{2+}$ (0.05 mM. After complete formation, 100 μL of an acetone solution containing the corresponding 4-substituted sodium phenolate were added (0.2 mM). Initial formation of a putative $[(MeAN)_2Cu^{III}_2(O^{2-})_2(R\text{-}PhO^{-})]^{+}$ was observed followed by its decay (**Figures S3-S7**). Kinetic analysis was performed by fitting the exponential decay of $[(MeAN)_2Cu^{III}_2(O^{2-})_2(R\text{-}PhO^{-})]^{+}$ at 400 nm. Pseudo-first-order rate constants k_{obs} obtained for each substrate are summarized in **Table S1** and plotted in **Figure S2** (Hammett plot). Note: the reaction rates (k_{obs}) were plotted against σ^{+}. When k_{obs} was plotted against σ, a poor linear correlation was observed, confirming the proposed mechanism in which during the rate determining step, electrophilic attack of the Cu_2O_2 to the arene leads to formation of a carbocation intermediate. This analysis has also been previously carried out in the reactivity of other Cu_2O_2 species towards phenolates (see references S1-S4).[1-4]

Table S1. Summary of kinetic experiments for the reactivity of $^{S}P^{MeAN}$ towards substituted sodium phenolates.

R-PhO$^-$	σ_p^+	[R-PhO$^-$]$_0$ (mM)	k_{obs} (s^{-1})
4-MeO	-0.778	0.2	0.29 ± 0.02
4-Me	-0.31	0.2	0.082 ± 0.003
4-Cl	0.114	0.2	0.039 ± 0.004
4-CN	0.659	0.2	0.0061 ± 0.0001
2,6-F_2	-	0.2	0.00194 ± 0.0004

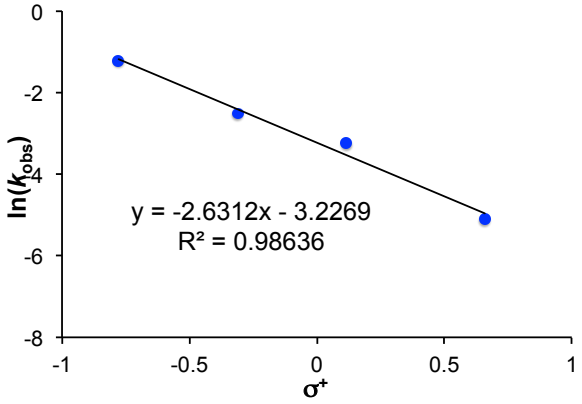


Figure S2. Hammett plot (ln (k_{obs}) vs. σ+) for the reaction of $^{S}P^{MeAN}$ (0.05 mM) towards 4-substituted phenolates (see Table S1).[1-4]

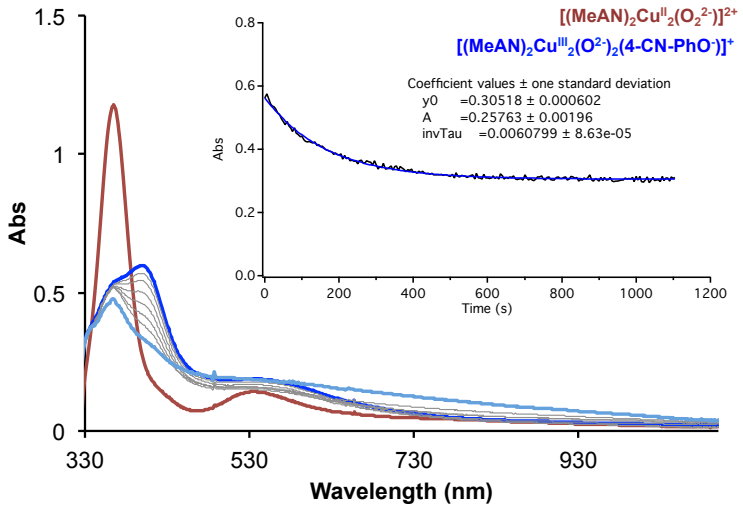


Figure S3. UV-vis spectra for the reaction of $^{S}P^{MeAN}$ (0.05 mM) (**brown spectrum**) towards 4-CN-phenolate (0.2 mM) to form the [(MeAN)$_2$Cu$^{III}_2$(O^{2-})$_2$(4-CN-PhO$^-$)]$^+$ (**blue spectrum**). Inset: kinetic traces (400 nm) for the decay of [(MeAN)$_2$Cu$^{III}_2$(O^{2-})$_2$(4-CN-PhO$^-$)]$^+$.

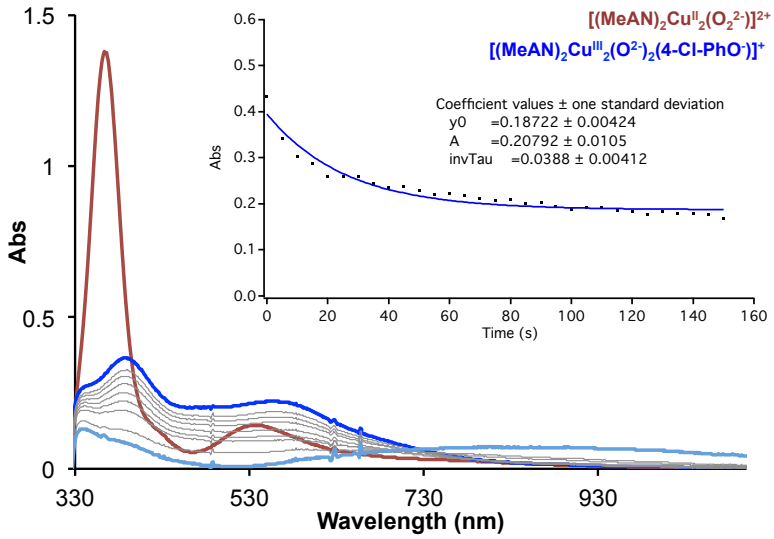


Figure S4. UV-vis spectra for the reaction of $^{S}P^{MeAN}$ (0.05 mM) (**brown spectrum**) towards 4-Cl-phenolate (0.2 mM) to form the $[(MeAN)_2Cu^{III}_2(O^{2-})_2(4\text{-Cl-PhO}^-)]^+$ (**blue spectrum**). Inset: kinetic traces (400 nm) for the decay of $[(MeAN)_2Cu^{III}_2(O^{2-})_2(4\text{-Cl-PhO}^-)]^+$.

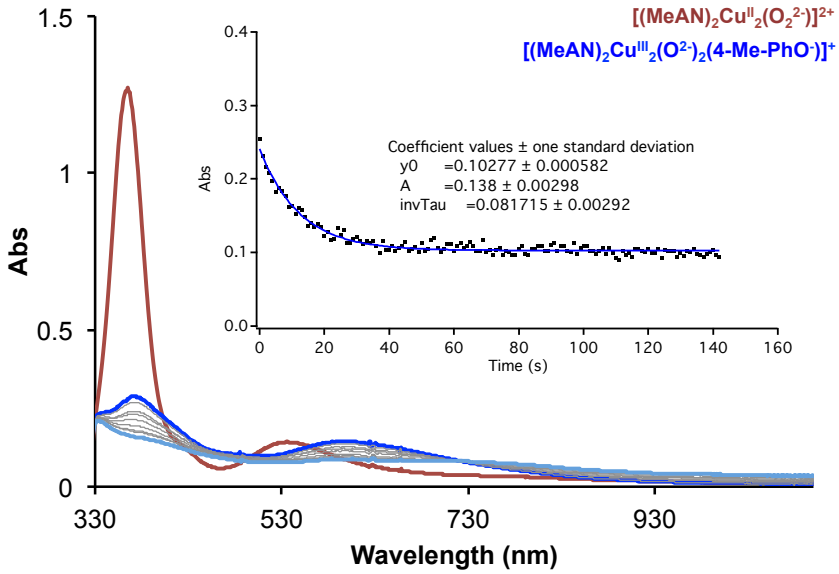


Figure S5. UV-vis spectra for the reaction of $^{S}P^{MeAN}$ (0.05 mM) (**brown spectrum**) towards 4-Me-phenolate (0.2 mM) to form the $[(MeAN)_2Cu^{III}_2(O^{2-})_2(4\text{-Me-PhO}^-)]^+$ (**blue spectrum**). Inset: kinetic traces (400 nm) for the decay of $[(MeAN)_2Cu^{III}_2(O^{2-})_2(4\text{-Me-PhO}^-)]^+$.

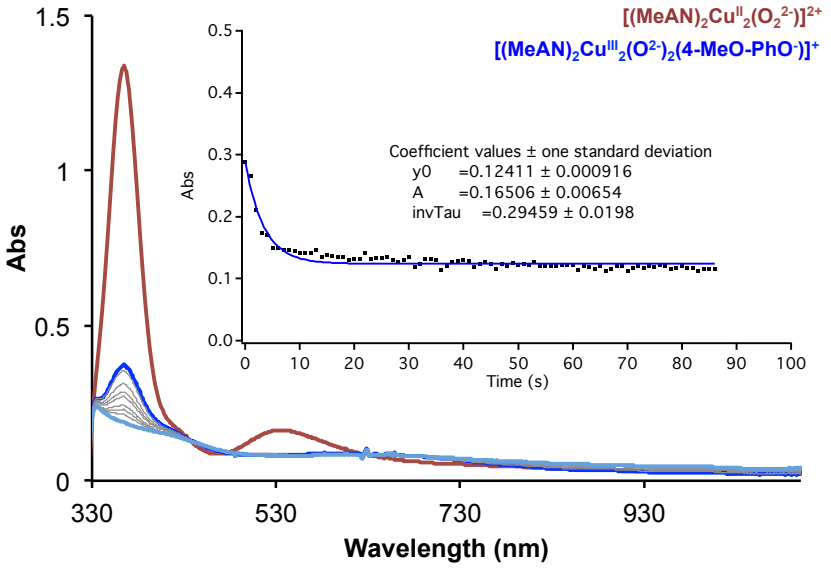


Figure S6. UV-vis spectra for the reaction of $^{S}P^{MeAN}$ (0.05 mM) (**brown spectrum**) towards 4-MeO-phenolate (0.2 mM) to form the $[(MeAN)_2Cu^{III}{}_2(O^{2-})_2(4\text{-MeO-PhO}^-)]^+$ (**blue spectrum**). Inset: kinetic traces (400 nm) for the decay of $[(MeAN)_2Cu^{III}{}_2(O^{2-})_2(4\text{-MeO-PhO}^-)]^+$.

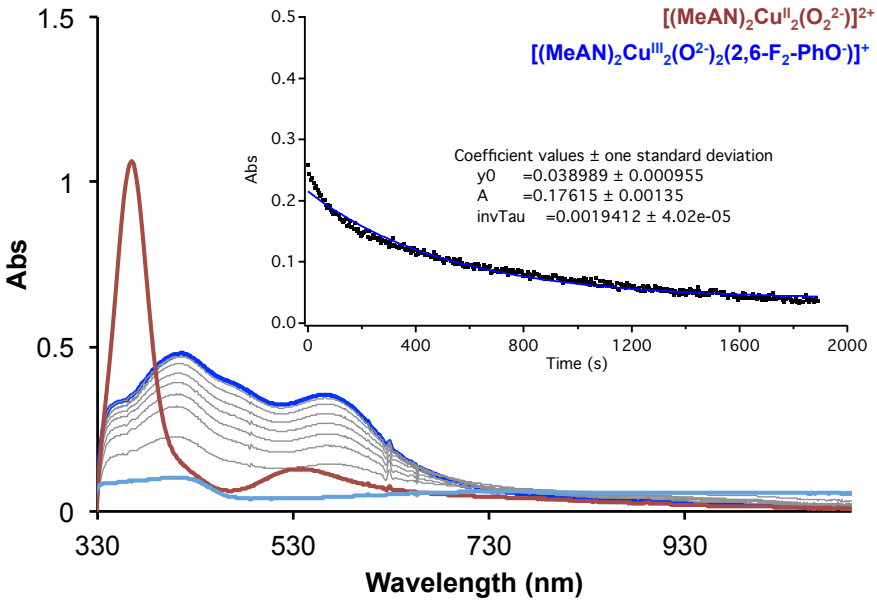


Figure S7. UV-vis spectra for the reaction of $^{S}P^{MeAN}$ (0.05 mM) (**brown spectrum**) towards 2,6-F_2-phenolate (0.2 mM) to form the $[(MeAN)_2Cu^{III}{}_2(O^{2-})_2(2,6\text{-}F_2\text{-PhO}^-)]^+$ (**blue spectrum**). Inset: kinetic traces (400 nm) for the decay of $[(MeAN)_2Cu^{III}{}_2(O^{2-})_2(2,6\text{-}F_2\text{-PhO}^-)]^+$. Note: slight deviation of the kinetic trace observed (400 nm) from the calculated exponential decay fit is attributed to the slow accumulation of the $[(MeAN)_2Cu^{III}{}_2(O^{2-})_2(2,6\text{-}F_2\text{-PhO}^-)]^+$ during the first 50 seconds of reaction coupled with its decay (i.e., formation of $[(MeAN)_2Cu^{III}{}_2(O^{2-})_2(2,6\text{-}F_2\text{-PhO}^-)]^+$ and its decay have similar reaction rates).

1.3 Generation of Lewis acid adducts of $[(MeAN)_2Cu_2(O_2^{2-})]^{2+}$ (O^{MeAN}-LA)

3 mL of a $[(MeAN)Cu^{I}](BAr^{F})$ solution (0.2 mM) in acetone were placed in a 10 mm path quartz cell equipped with a stir bar and capped with a rubber septum. After cooling the cell to -90 ºC, O_2 was added to generate the corresponding $^{S}P^{MeAN}$ (λ_{max}: 365 nm; ε = 22 mM^{-1} cm^{-1}). After complete formation, 100 μL of an acetone solution containing the corresponding equivalents of Lewis acids (0.2 mM $DMF{\cdot}CF_3SO_3H$, 0.1 mM $Sc(CF_3SO_3)_3$, or 0.1 mM $B(C_6F_5)_3$) were added to generate the corresponding (**O^{MeAN}-LA**) species (**Figure S8**). NOTE: addition of $(NBu_4^{+})(CF_3SO_3^{-})$ didn't lead to the isomerization of the $^{S}P^{MeAN}$ to the **O** species.

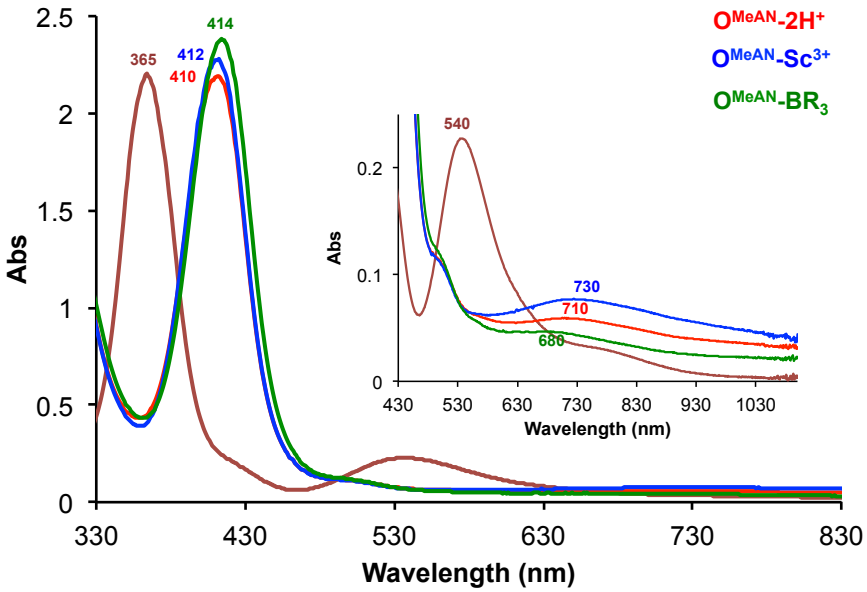


Figure S8. UV-vis spectra of $^{S}P^{MeAN}$ (brown) and the different **O^{MeAN}-LA** species **O^{MeAN}-2H^{+}** (red), **O^{MeAN}-Sc^{3+}** (blue), and **O^{MeAN}-2BR$_3$** (green).

1.4 Lewis Acid titration and reversibility experiments

1.4.1 **O^{MeAN}-$2H^+$**: After formation of **$^{S}P^{MeAN}$** (0.1 mM, -90 ºC), consecutive additions of sub-stoichiometric and stoichiometric amounts of DMF·CF_3SO_3H (0.05 – 0.2 mM) were added, observing full formation of **O^{MeAN}-$2H^+$** (λ_{max}: 410 nm; ε = 21 mM^{-1} cm^{-1}). NOTE: addition of excess amounts of DMF·CF_3SO_3H (up to 1 mM) led to the slow decomposition of **O^{MeAN}-$2H^+$**.

Formation of **O^{MeAN}-$2H^+$** could be reversed by addition of proton sponge (1,8-bis(dimethylamino)naphthalene) in excess (0.6 mM) leading to full regeneration of **$^{S}P^{MeAN}$** (**Figure S9**). **O^{MeAN}-$2H^+$** could be formed again by re-addition of DMF·CF_3SO_3H (0.6 mM were required in order to full formation, due to the presence of proton sponge excess in solution).

Note: addition of excess equivalents of Na(CF_3SO_3) did not lead to any spectral change associated with O-O bond cleavage.

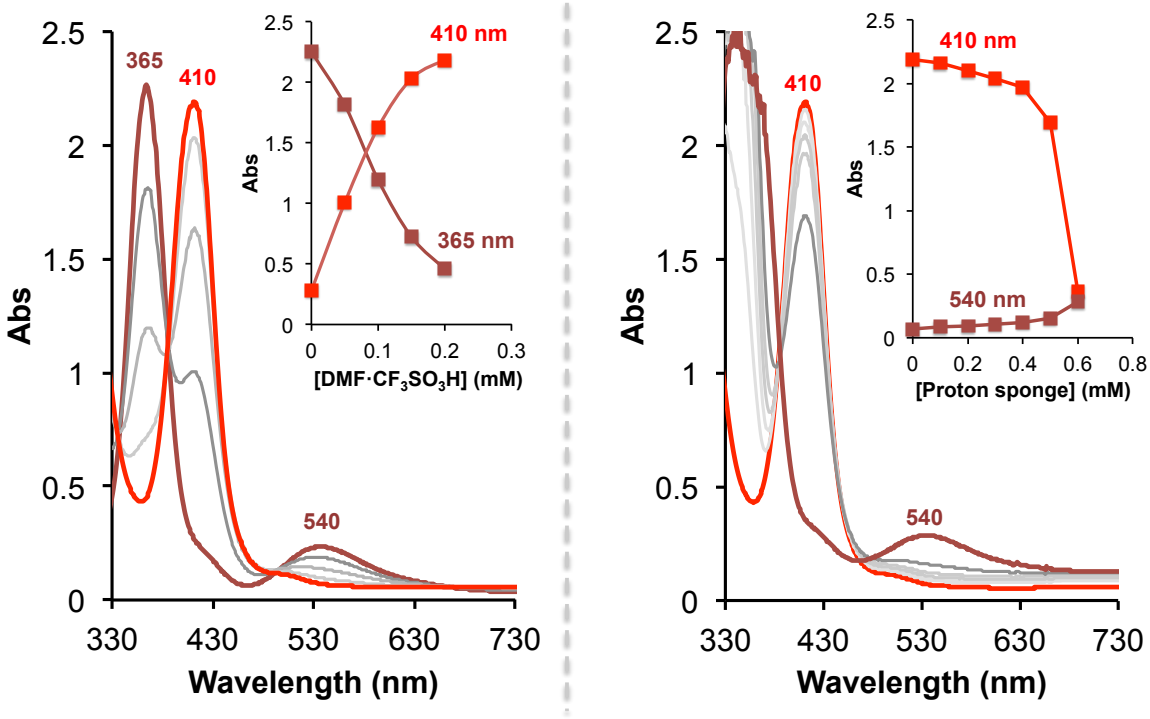


Figure S9. Titration (left) and reversibility experiments (right) of the **$^{S}P^{MeAN}$/O^{MeAN}-$2H^+$** equilibrium (see above for experimental details).

1.4.2 **O^{MeAN}-Sc^{3+}**: After formation of **$^{S}P^{MeAN}$** (0.1 mM, -90 ºC), consecutive additions of sub-stoichiometric and stoichiometric amounts of $Sc(CF_3SO_3)_3$ (0.025 – 0.15 mM) were added, observing full formation of **O^{MeAN}-Sc^{3+}** (λ_{max}: 412 nm; ε = 23 mM^{-1} cm^{-1}).

Formation of **O^{MeAN}-Sc^{3+}** could be reversed by addition of 1,10-phenantroline in excess (0.8 mM), leading only to partial formation (75%) of **$^{S}P^{MeAN}$** (**Figure S10**) due to the ability of 1,10-phenantroline to trap Cu(I) (430 and 455 nm bands, see Figure S10). **O^{MeAN}-Sc^{3+}** could be partially formed again by re-addition of $Sc(CF_3SO_3)_3$ (0.2 mM were required in order to full formation, due to the presence of excess 1,10-phenanthroline in solution).

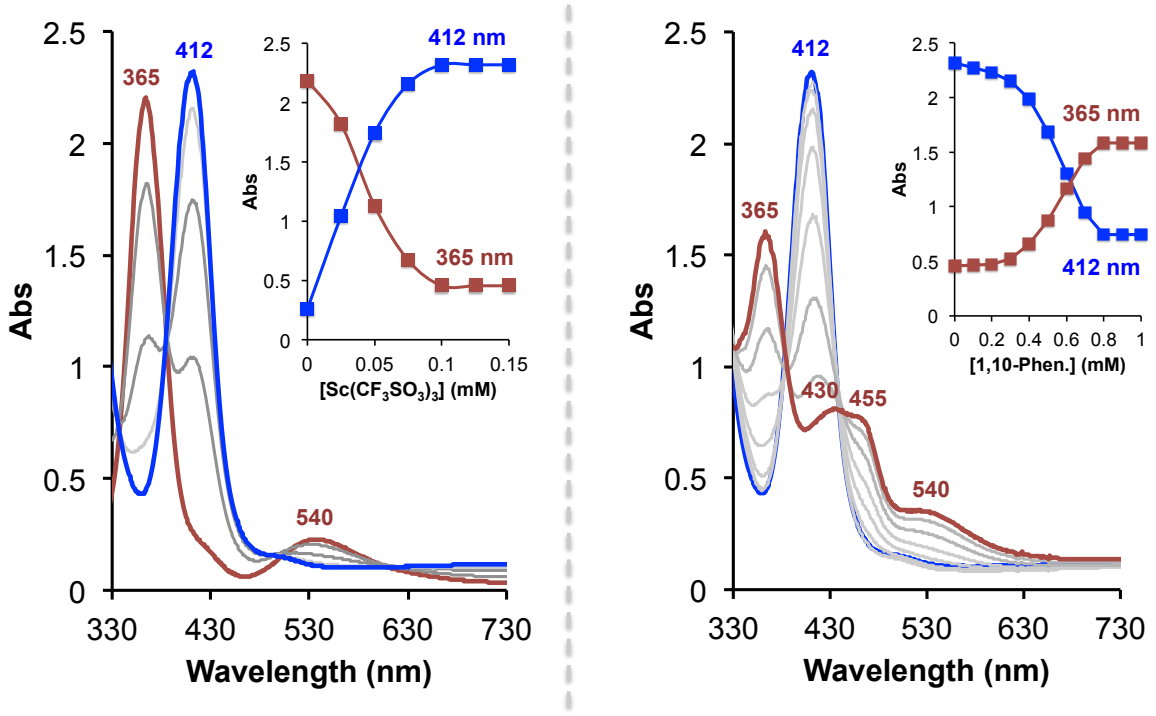


Figure S10. Titration (left) and reversibility experiments (right) of the **$^{S}P^{MeAN}$/O^{MeAN}-Sc^{3+}** equilibrium (see above for experimental details).

1.4.3 **O^{MeAN}-2BR_3**: After formation of **$^{S}P^{MeAN}$** (0.1 mM, -90 ºC), consecutive additions of sub-stoichiometric and stoichiometric amounts of $B(C_6F_5)_3$ (0.05 – 0.30 mM) were added, observing full formation of **O^{MeAN}-2BR_3** (λ_{max}: 414 nm,; ε = 24 mM^{-1} cm^{-1}).

Formation of **O^{MeAN}-2BR_3** could be reversed by addition of TASF (tris(dimethylamino)sulfonium difluorotrimethylsilicate) in excess (0.6 mM), leading only to partial formation (60%) of **$^{S}P^{MeAN}$** (**Figure S11**). However, **O^{MeAN}-2BR_3** could be partially formed again by re-addition of $B(C_6F_5)_3$.

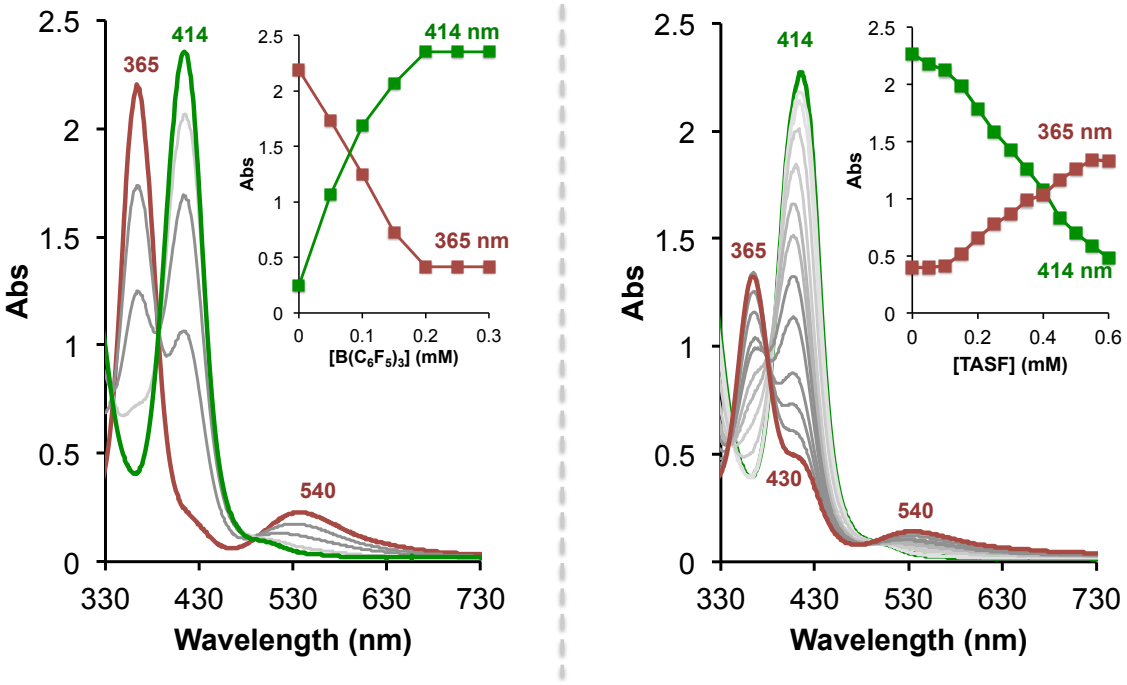


Figure S11. Titration (left) and reversibility experiments (right) of the **$^{S}P^{MeAN}$/O^{MeAN}-2BR_3** equilibrium (see above for experimental details).

1.5 Reactivity of O^{MeAN}-LA towards external substrates

After generation of the corresponding (**O^{MeAN}-LA**) as described above (Section 2.3), 100 μL of an acetone solution containing excess of the corresponding substrate (PPh_3, DHA, thioanisole, and Fc (e^-)) were added. No spectral change was observed, not even 30 minutes after substrate addition. On the other hand, addition of $Me_{10}Fc$, Me_8Fc or Me_2Fc (**$^SP^{MeAN}$** was not able to be reduced by Me_2Fc) led to decay of the UV-vis features of the (**O^{MeAN}-LA**) cores (**Figure S12**). NOTE: the formation of only one equiv. of Me_2Fe^+ and regeneration of 0.5 equiv. of **$^SP^{MeAN}$** suggests a disproportion reaction after electron transfer.

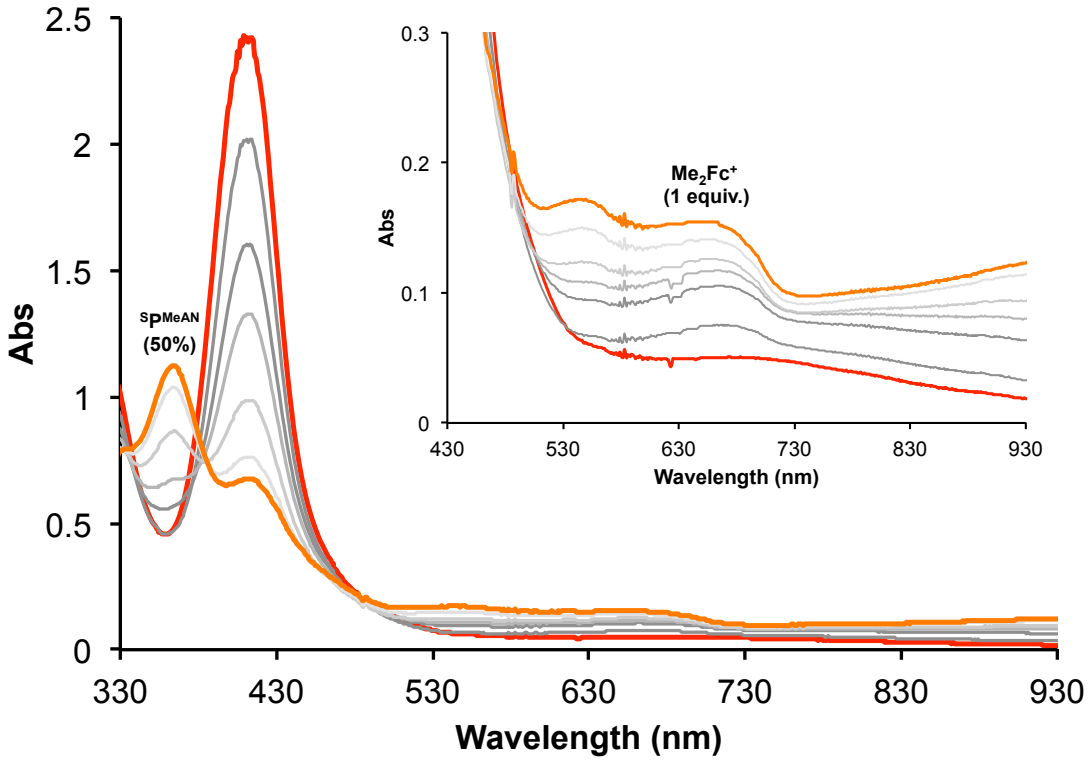


Figure S12. UV-vis for the $1e^-$ reduction of **O^{MeAN}-$2H^+$** by Me_2Fc (10 equiv.). The decay of **O^{MeAN}-$2H^+$** features concluded 1 minute after the addition of the reductant with concomitant formation of 1 equiv. of Me_2Fc^+ (**orange spectrum**) and 50% of **$^SP^{MeAN}$**. Note: similar results were obtained in the reduction of **O^{MeAN}-$2BR_3$** and **O^{MeAN}-Sc^{3+}** with Me_2Fc.

1.5.1 Reaction of **O^{MeAN}-LA** towards C-H bonds (BNAH, BNAD and BzImH): Kinetic studies

After generation of the corresponding (**O^{MeAN}-LA**) as described above (Section 1.3), 100 μL of an acetone solution containing various amounts of the corresponding substrate (BNAH, BNAD or BzImH) were added, causing the decay of the **O^{MeAN}-LA** spectral features. The absorbance changes (λ = 400 nm) were fitted to single exponential decays. In all the cases (BNAH, BNAD and BzImH), a linear correlation between the reaction rate (k_{obs}) and the substrate concentration was found, from which we obtained the second-order rate constant (slope). NOTE: regeneration of 0.2-0.3 equiv. of **^{S}P^{MeAN}** suggests a secondary disproportion reaction after hydride transfer.

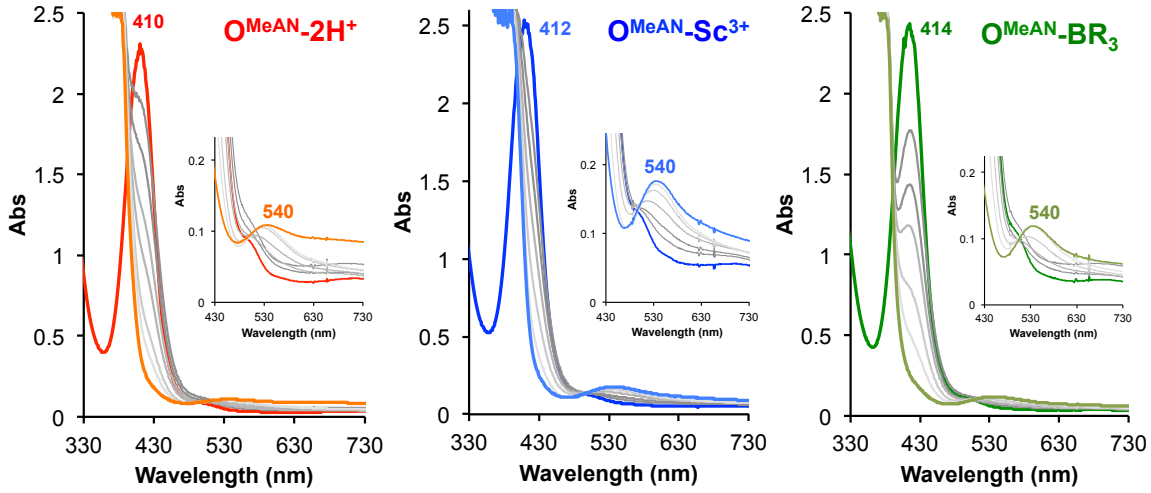


Figure S13. UV-vis spectral changes (decay) of the reaction between **O^{MeAN}-LA** and BNAH.

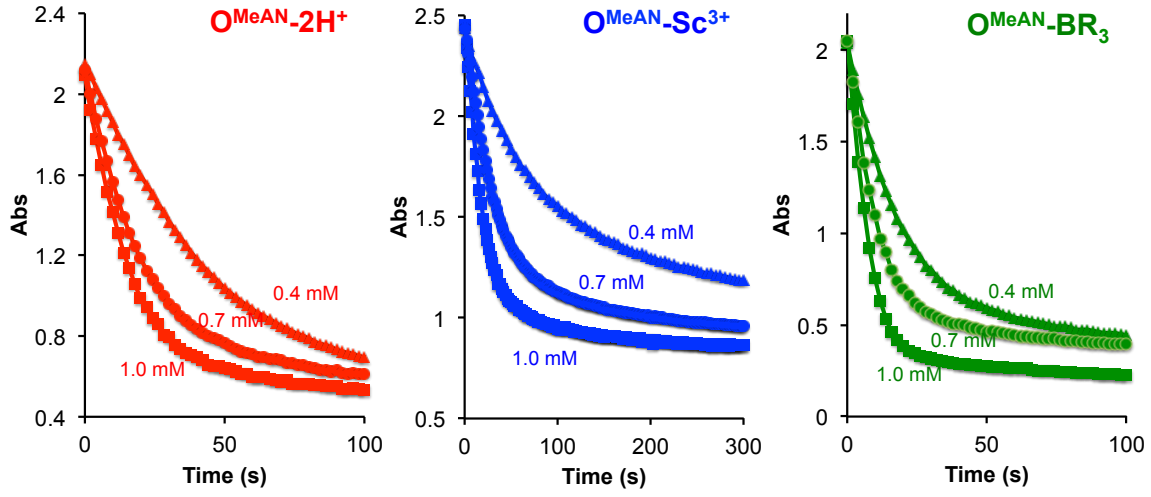


Figure S14. Decay (400 nm) of the UV-vis features of **O^{MeAN}-LA** upon addition of different amounts of BNAH (4, 7 and 10 equiv.)

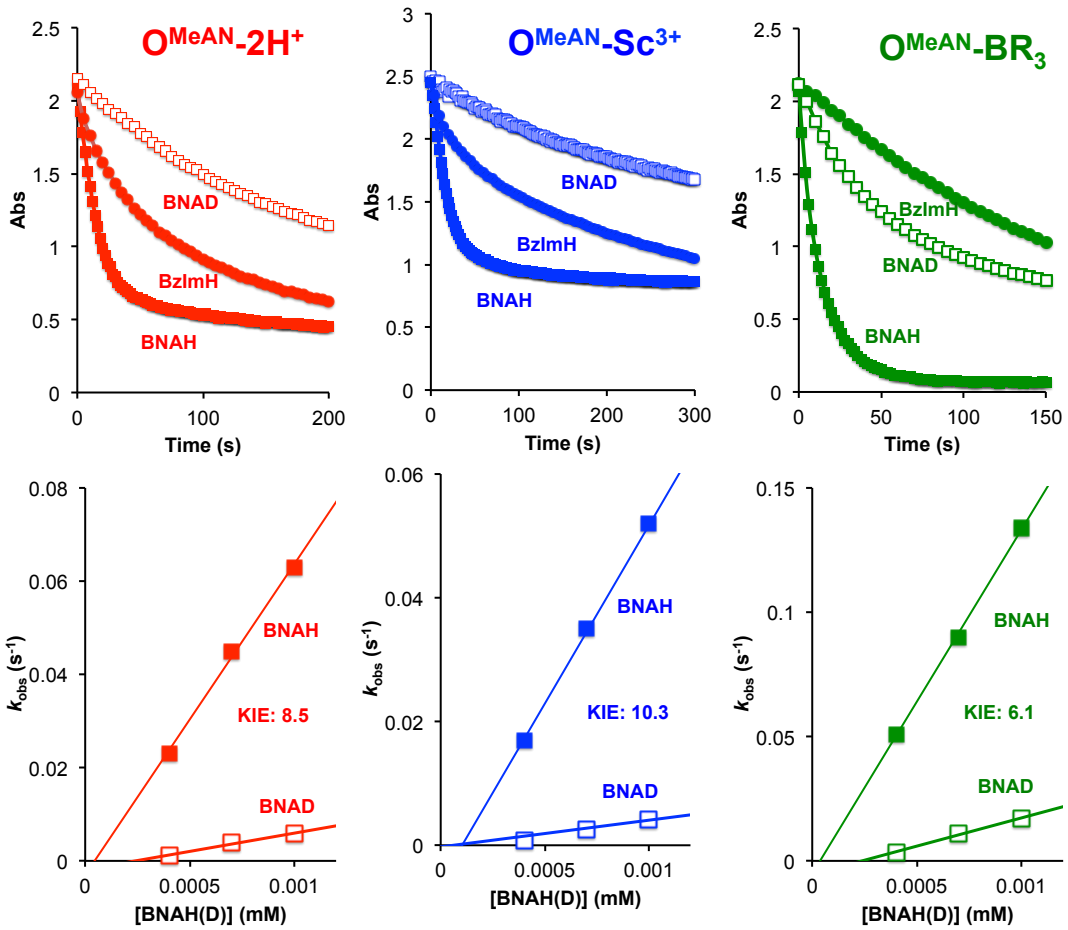


Figure S15. Top: decay (400 nm) of the UV-vis features of **O^{MeAN}-LA** upon addition of BNAH, BNAD or BzIMH (10 equiv.). Bottom: kinetic isotope effect (KIE) calculated from plotting the different reaction rates (pseudo-first-order fitting and linear correlation (k_{obs} vs. [BNAH(D)]) obtained from the decay of the UV-vis features of **O^{MeAN}-LA** upon addition of different amounts of BNAH or BNAD (4, 7 and 10 equiv.).

1.5.2 Reaction of **O^{MeAN}-LA** towards O-H bonds (substituted phenols): Kinetic studies

After generation of the corresponding (**O^{MeAN}-LA**) as described above (Section 21.3), 100 μL of an acetone solution containing various amounts of the corresponding substrate (substituted phenols) were added, causing the decay of the **O^{MeAN}-LA** spectral features. The absorbance changes (λ = 400 nm) were fitted to single exponential decays. In all the cases, a linear correlation between the reaction rate (k_{obs}) and the substrate concentration was found, from which we obtained the second-order rate constant (slope).

The deuterated 4-MeO-C_6H_4OD was prepared by the reaction of the 4-MeO-phenolate (110 mg, 0.75 mmols) with acetic acid-*d* (1.5 mL, 25 mmols). The resulting product was dried under vacuum to eliminate the excess of acetic acid-*d,* and the resulting white solid was dissolved in MeTHF. The resulting solution was filtered and the organic solvent was evaporated under vacuum, leading to the isolation of the 4-MeO-C_6H_4OD as a white powder (44 mg, 47%). The purity of the product was confirmed by ^{1}H-NMR (95% deuterated).

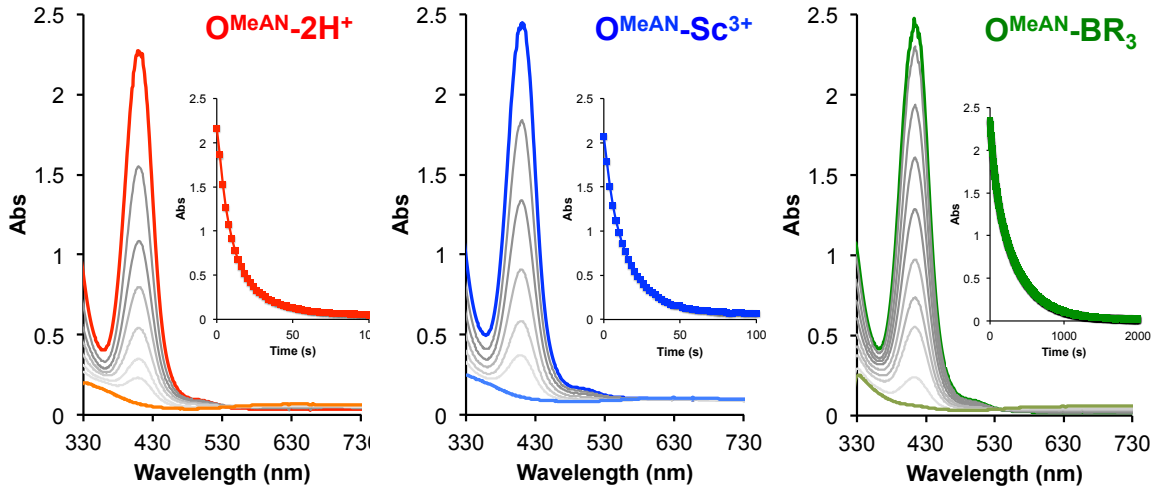


Figure S16. Decay (400 nm) of the UV-vis features of **O^{MeAN}-LA** upon addition of 4-MeO-Phenol (11 equiv.).

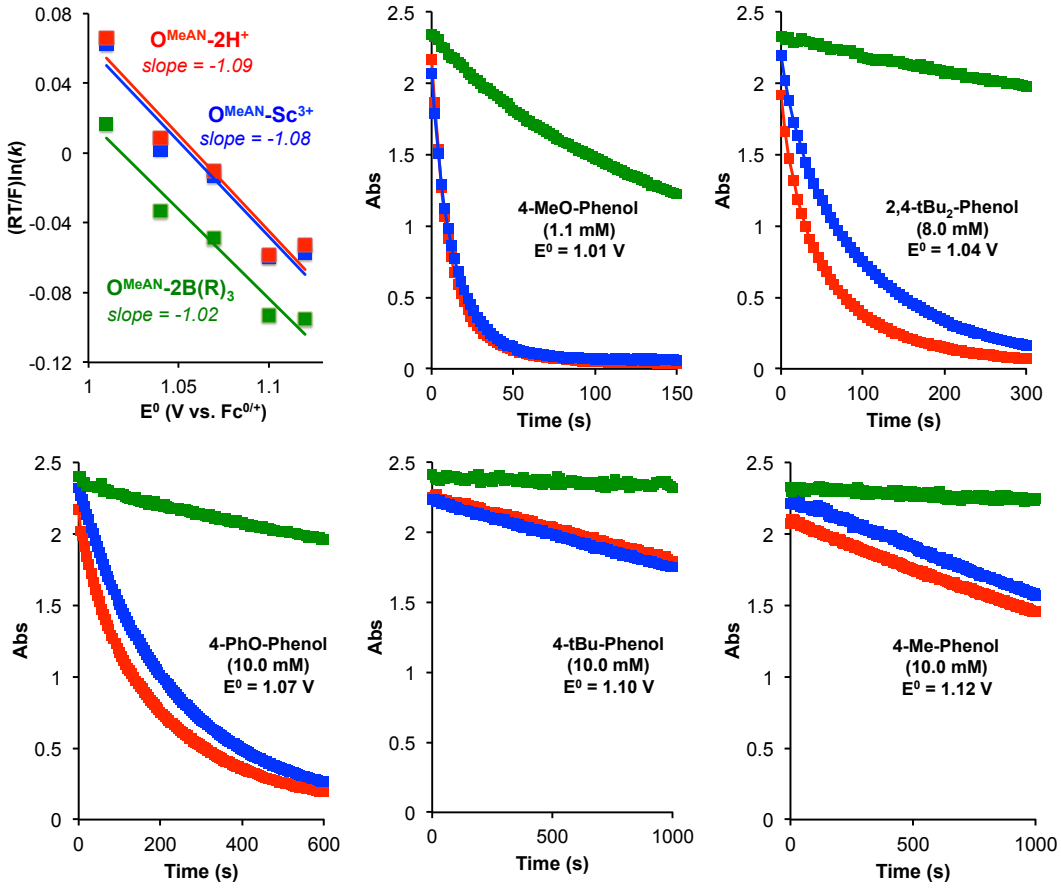


Figure S17. Decay (400 nm) of the UV-vis features of **O^{MeAN}-LA** upon addition of different substituted phenols. Top left: correlation of rate with phenol reduction potential.

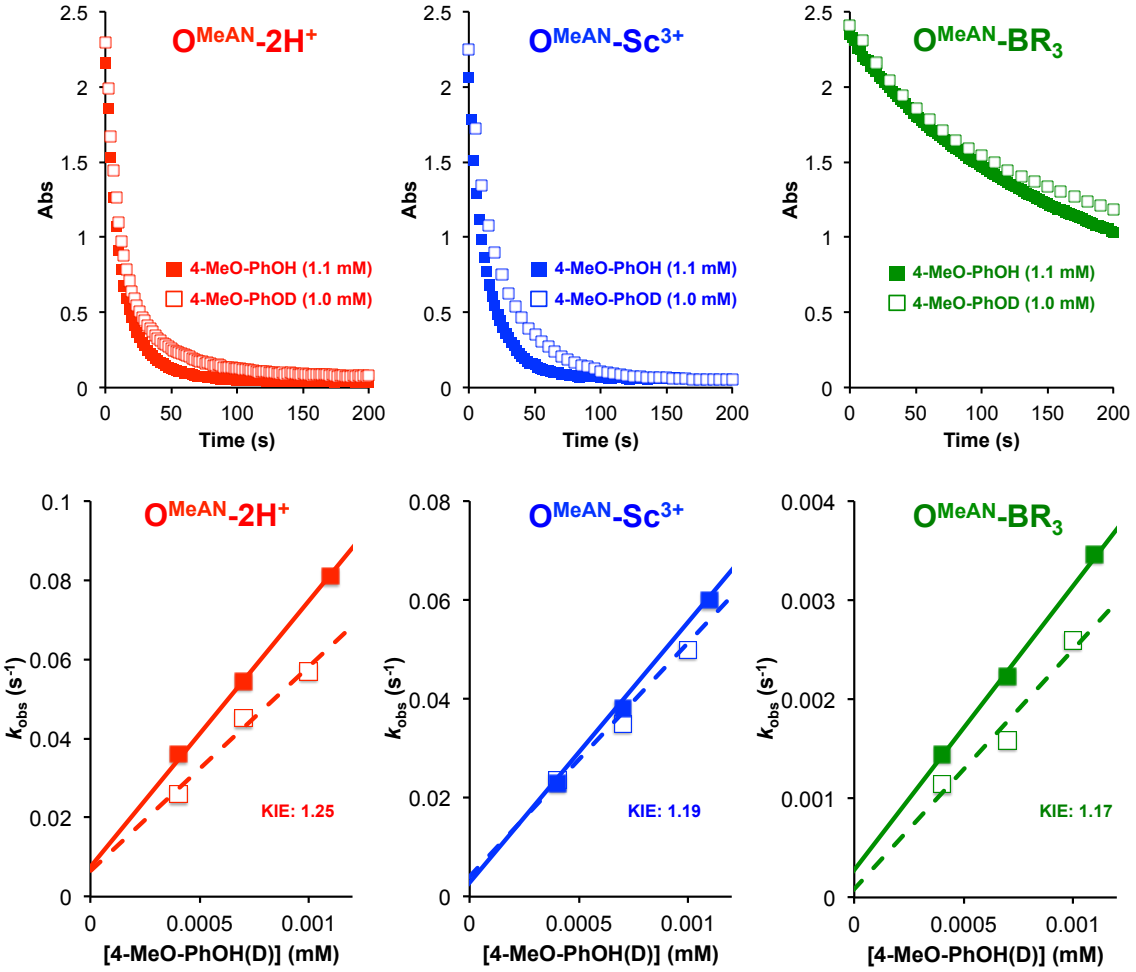


Figure S18. Kinetic isotope effect (KIE) calculated from plotting the different reaction rates (obtained by fitting the pseudo-first order exponential decays, see top) and linear correlation (k_{obs} vs. [4-MeO-PhOH(D)]) obtained from the reaction of **O^{MeAN}-LA** upon with different amounts of 4-MeO-PhOH or 4-MeO-PhOD.

2. Product analysis.

2.1 Reaction of $[(MeAN)_2Cu_2(O_2^{2-})]^{2+}$ with substituted sodium phenolates: catechol quantification.

10 mL of a $[(MeAN)Cu^{I}](BAr^{F})$ solution (0.32 mM) in acetone prepared in the glovebox were placed in a 100 mL Schlenk flask equipped with a stir bar and capped with a rubber septum. After cooling the flask to -90 ºC (5 minutes at -90 ºC), dioxygen was added to generate the corresponding $[(MeAN)_2Cu^{II}_2(O_2^{2-})]^{2+}$ (0.166 mM). After complete formation, 250 μL of an acetone solution containing the corresponding 4-substituted sodium phenolate were added (1 mM) and the reaction mixture was stirred for 30 minutes at -90 ºC. After that, the reaction crude was quenched by addition of 3 mL of an aqueous HCl solution (0.5 M). After warming up, the reaction organic solvents (acetone) were evaporated under vacuum and the resulting aqueous solution was extracted with CH_2Cl_2 (3 x 10 mL). The organic fractions were dried over $MgSO_4$ and the solvents were removed under vacuum. The resulting solid product was dissolved in 0.7 mL of acetone-d_6 containing 10 μL of an 0.32 mM acetophenone solution as internal standard. The catechol formation was quantified by ^{1}H-NMR (**Table S2**).

Table S2. Catechol quantification from the reaction of $[(MeAN)_2Cu_2(O_2^{2-})]^{2+}$ with substituted sodium phenolates

R-PhO$^-$Na$^+$	σ_p^+	[R-Catechol] (ppm)	Yield (%)
4-Me	-0.31	6.49 (2H)	29
4-Cl	0.114	6.72 (2H)	35
4-CN	0.659	7.15 (2H)	41
2,6-F_2	-	6.65 (3H)	30

2.2 Reaction of O^{MeAN}-LA with BNAH: quantification of oxidation products.

10 mL of a $[(MeAN)Cu^{I}](BAr^{F})$ solution (0.32 mM) in acetone prepared in the glovebox were placed in a 100 mL Schlenk flask equipped with a stir bar and capped with a rubber septum. After cooling the flask to -90 ºC (5 minutes at -90 ºC), dioxygen was added to generate the corresponding $[(MeAN)_2Cu^{II}_2(O_2^{2-})]^{2+}$ (0.166 mM). After complete formation, 250 μL of an acetone solution containing the corresponding equiv. of Lewis acid (0.32 mM DMF·TfOH, 0.166 mM $Sc(CF_3SO_3)$, or 0.32 mM $B(C_6F_5)_3$) were added. After 1 minute (to make sure the corresponding **O^{MeAN}-LA** complex is formed), 250 μL of an acetone solution containing 10 equiv. of BNAH were added (1.66 mM). After 30 minutes, the reaction crude was quenched by addition of 3 mL of an aqueous HCl solution (0.1 M, 1.1 equiv). The solution was then allowed to warm up to room temp under vacuum and all solvent was removed, yielding a green solid. The ^{1}H-NMR of the resulting green residue was taken in DMSO-D_6 and BNA^+ integration was compared to 1,2-dichloroethane as an internal standard.

Table S3. BNA^+ quantification in the oxidation of BNAH by **O^{MeAN}-LA**. NOTE: Control experiments (without copper) showed that BNAH was oxidized to the corresponding BNA^+ by the Lewis acids. The amount of product derived from that oxidation was subtracted from the values obtained from the quantity obtained in the **O^{MeAN}-LA** oxidations.

O^{MeAN}-LA	μmols BNA^+ (control[a])	Yield (%)
O^{MeAN}-2H+	2.8 (1.2)	99
O^{MeAN}-Sc^{3+}	2.4 (0.8)	99
O^{MeAN}-2BR_3	1.9 (0.7)	75

[a]μmols of BNA^+ obtained in the control reaction without Cu complex.

2.3 Reaction of $\mathbf{O^{MeAN}}$**-LA** *with 2,4-tBu$_2$-phenol: quantification of oxidation products.*

10 mL of a [(MeAN)Cu^{I}](BAr^{F}) solution (0.32 mM) in acetone prepared in the glovebox were placed in a 100 mL Schlenk flask equipped with a stir bar and capped with a rubber septum. After cooling down the flask to -90 ºC (5 minutes at -90 ºC), dioxygen was added to generate the corresponding $[(MeAN)_2Cu^{II}_2(O_2^{2-})]^{2+}$ (0.166 mM). After complete formation, 250 μL of an acetone solution containing the corresponding equiv. of Lewis acid (0.32mM DMF·TfOH, 0.166 mM $Sc(CF_3SO_3)$, or 0.32 mM $B(C_6F_5)_3$) were added. After 1 minute (to make sure the corresponding $\mathbf{O^{MeAN}}$**-LA** complex is formed), 250 μL of an acetone solution containing 50 equiv. of 2,4-tBu_2-phenol were added (8.3 mM). After 2 hours, the reaction crude was quenched by addition of 3 mL of an aqueous HCl solution (0.5 M). After warming up, the reaction organic solvents (acetone) were evaporated under vacuum and the resulting aqueous solution was extracted with CH_2Cl_2 (3 x 10 mL). The organic fractions were dried over $MgSO_4$ and the solvents were removed under vacuum. The resulting solid product was solved with 0.7 mL of acetone-d_6 and the C-C coupling product was quantified using 1,2-dichloroethane as an internal standard.

Table S4. C-C coupled product quantification in the oxidation of 2,4-tBu_2-Phenol by $\mathbf{O^{MeAN}}$**-LA**. Note: the final yield of C-C coupled product was calculated based on a stoichiometry where 1 equiv. of $\mathbf{O^{MeAN}}$**-LA** leads to 0.5 equiv. of coupling product.[5]

$\mathbf{O^{MeAN}}$**-LA**	Yield (%)
$\mathbf{O^{MeAN}}$**-2H+**	67
$\mathbf{O^{MeAN}}$**-Sc^{3+}**	57
$\mathbf{O^{MeAN}}$**-2BR_3**	66

3. rRaman experiments.

Generation of $[(MeAN)_2Cu_2(O_2^{2-})]^{2+}$ ($^{S}\mathbf{P}^{MeAN}$): 0.57 μL of a $[(MeAN)Cu^{I}]^{+}$ (1.0 mM) solution in acetone were placed in a 5 mm rubber septum capped NMR tube. After cooling the NMR tub to -90 ºC (acetone/$N_{2(liq)}$ bath), dioxygen was bubbled through the solution mixture to generate the $[(MeAN)_2Cu_2(O_2^{2-})]^{2+}$ complex (1 mM).

$[(MeAN)_2Cu^{III}_2(O^{2-})_2(2,6\text{-}F_2\text{-}PhO^{-})]^{+}$($\mathbf{O}^{MeAN}$-$\mathbf{F_2PhO}^{-}$): 0.57 μL of a $[(MeAN)Cu^{I}]^{+}$ (1.0 mM) solution in acetone were placed in a 5 mm rubber septum capped NMR tube. After cooling the NMR tube to -90 ºC (acetone/$N_{2(liq)}$ bath), dioxygen was bubbled through the solution mixture to generate the form the $[(MeAN)_2Cu_2(O_2^{2-})]^{2+}$ complex (0.5 mM). To generate the $[(MeAN)_2Cu^{III}_2(O^{2-})_2(2,6\text{-}F_2\text{-}PhO^{-})]^{+}$, 50 μL of an acetone solution containing sodium 2,6-F_2-phenolate (3 mM) was added. Two samples were generated, depending on the time they were frozen (10/300 seconds after addition of phenolate).

$[(MeAN)_2Cu^{III}_2(O^{2-})_2(DMF{\cdot}CF_3SO_3H)_2]^{2+}$ ($\mathbf{O}^{MeAN}$-$\mathbf{2H}^{+}$): 0.57 μL of a $[(MeAN)Cu^{I}]^{+}$ (1.0 mM) solution in acetone were placed in a 5 mm rubber septum capped NMR tube. After cooling the NMR tube to -90 ºC (acetone/$N_{2(liq)}$ bath), dioxygen was bubbled through the solution mixture to generate the form the $[(MeAN)_2Cu_2(O_2^{2-})]^{2+}$ complex (0.5 mM). To generate the $\mathbf{O}^{MeAN}$-$\mathbf{2H}^{+}$, 50 μL of an acetone solution containing 2 equiv. of $DMF{\cdot}CF_3SO_3H$ (1 mM) were added.

$[(MeAN)_2Cu^{III}_2(O^{2-})_2(Sc(CF_3SO_3)_3)]^{2+}$ ($\mathbf{O}^{MeAN}$-$\mathbf{Sc}^{3+}$): 0.57 μL of a $[(MeAN)Cu^{I}]^{+}$ (1.0 mM) solution in acetone were placed in a 5 mm rubber septum capped NMR tube. After cooling the NMR tube to -90 ºC (acetone/$N_{2(liq)}$ bath), dioxygen was bubbled through the solution mixture to generate the form the $[(MeAN)_2Cu_2(O_2^{2-})]^{2+}$ complex (0.5 mM). To generate the $\mathbf{O}^{MeAN}$-$\mathbf{Sc}^{3+}$, 50 μL of an acetone solution containing 1 equiv. of $Sc(CF_3SO_3)_3$ (0.5 mM) were added.

$[(MeAN)_2Cu^{III}_2(O^{2-})_2(B(C_6F_5)_3)_2]^{2+}$ ($\mathbf{O}^{MeAN}$-$\mathbf{2BR_3}$) 0.57 μL of a $[(MeAN)Cu^{I}]^{+}$ (1.0 mM) solution in acetone were placed in a 5 mm rubber septum capped NMR tube. After cooling the NMR tube to -90 ºC (acetone/$N_{2(liq)}$ bath), dioxygen was bubbled through the solution mixture to generate the form the $[(MeAN)_2Cu_2(O_2^{2-})]^{2+}$ complex (0.5 mM). To generate the $\mathbf{O}^{MeAN}$-$\mathbf{2BR_3}$, 50 μL of an acetone solution containing 2 equiv. of $B(C_6F_5)_3$ (0.5 mM) were added.

4. DFT calculations.

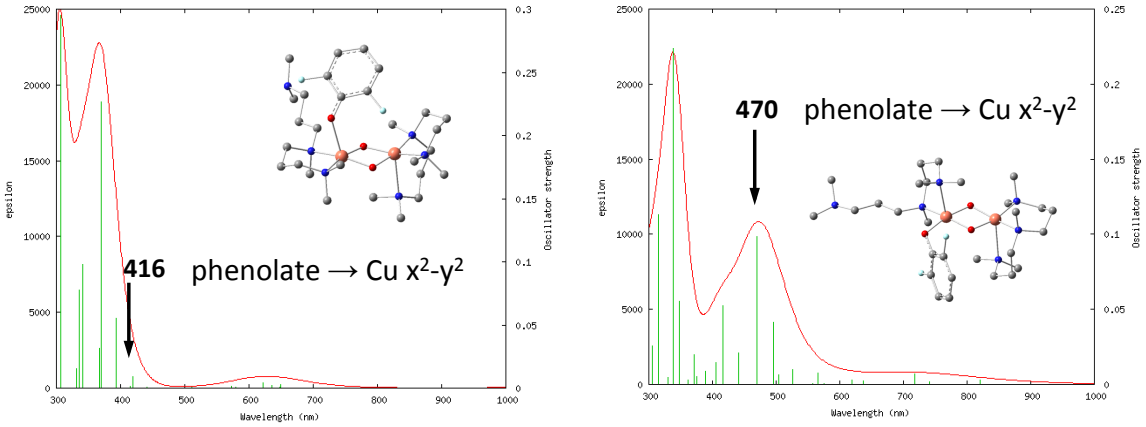


Figure S19. TD-DFT calculated absorption spectra of $[(MeAN)_2Cu^{III}_2(O^{2-})_2(2,6\text{-}F_2\text{-}PhO^-)]^+$ with phenolate occupying an axial (left) or equatorial (right) position. The phenolate → Cu LMCT is indicated (416 nm and weak for axial phenolate, 470 nm and intense for equatorial phenolate).

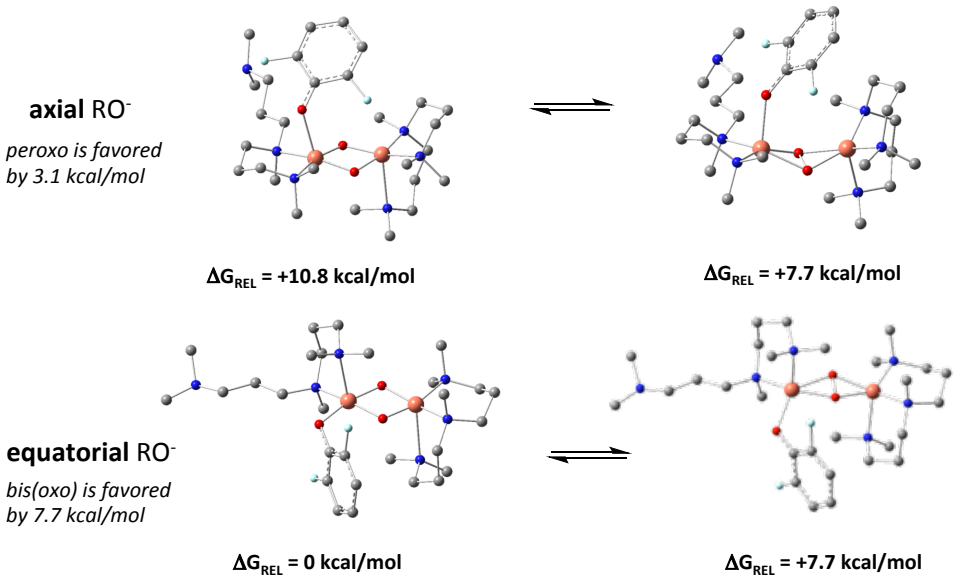


Figure S20. Relative energies (ΔG, 298 K) of $^{S}\mathbf{P}^{MeAN}$ and $\mathbf{O}^{MeAN}$ isomers with axial (top) or equatorial (bottom) phenolate coordination. The relative energies include a correction of -12 kcal/mol as determined by previous calibration of the B3LYP functional to bis(μ-oxo)/peroxo equilibria.[2]

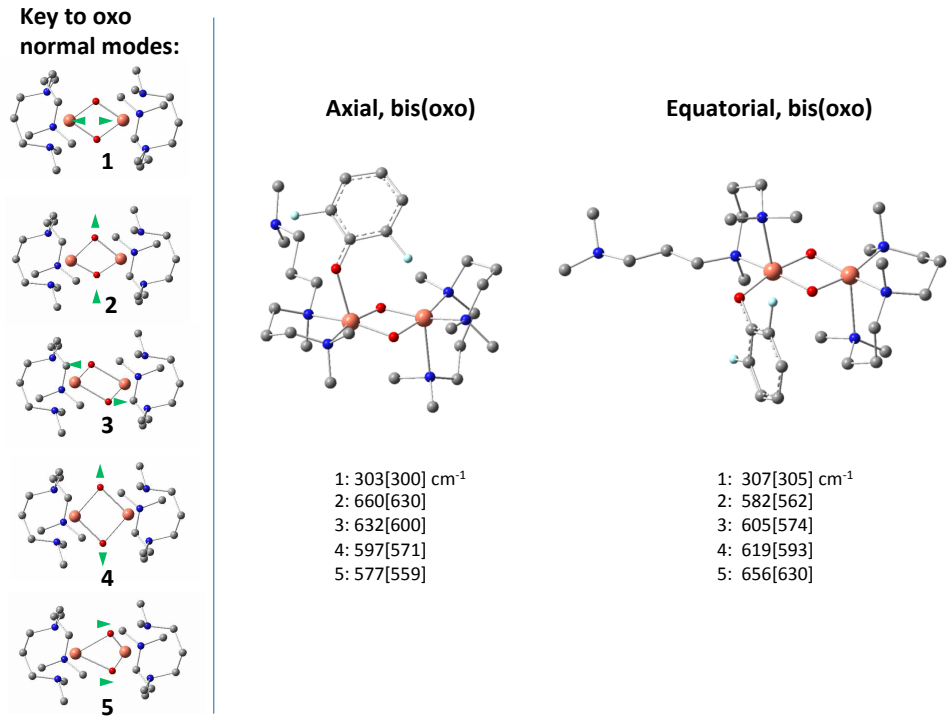


Figure S21. Calculated normal modes and $^{16}O_2/^{18}O_2$ isotope effects for 2,6-F_2-PhO$^-$-coordinated $\mathbf{O}^{\mathbf{MeAN}}$.

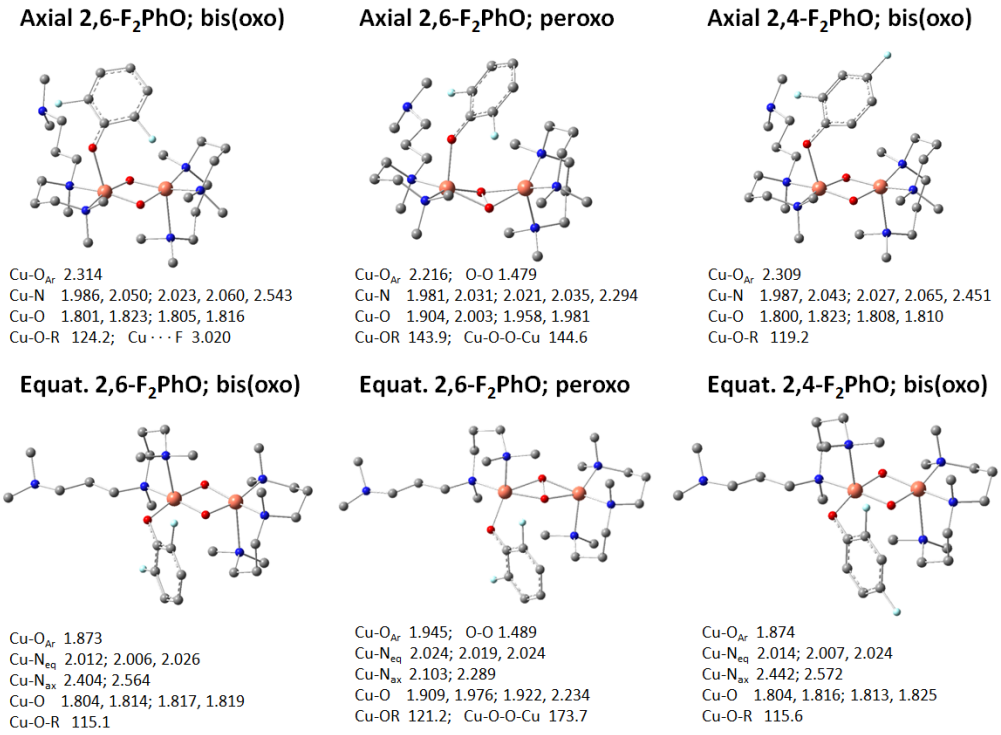


Figure S22. DFT-calculated structures and relevant bond metrics (Å; °) for 2,6-F_2-PhO$^-$- and 2,4-F_2-PhO$^-$-coordinated $^{\mathbf{S}}\mathbf{P}^{\mathbf{MeAN}}$ and $\mathbf{O}^{\mathbf{MeAN}}$.

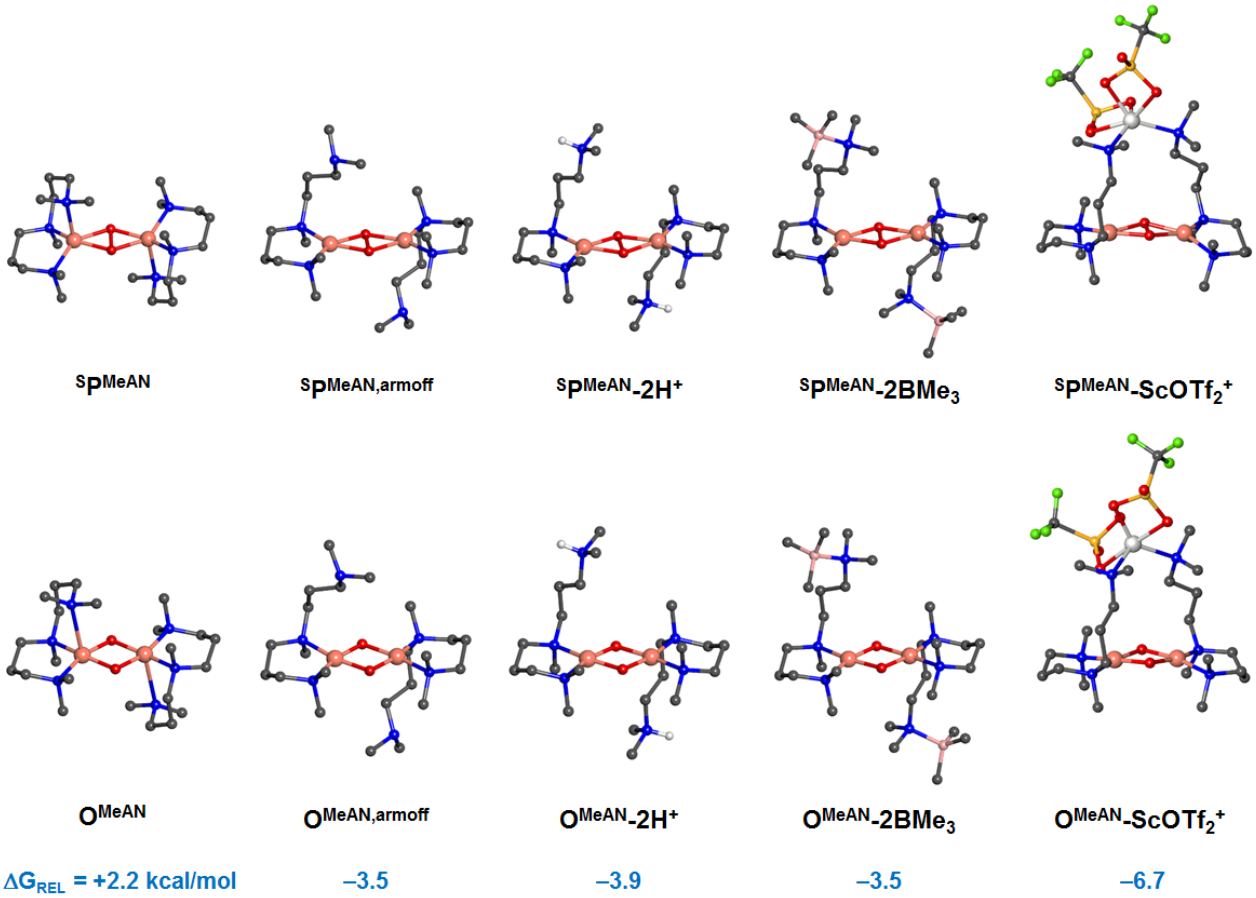


Figure S23. DFT-optimized structures and relative energies of $^{S}\mathbf{P}^{\mathbf{MeAN}}$ and $\mathbf{O}^{\mathbf{MeAN}}$ and their Lewis acid adducts $\mathbf{O}^{\mathbf{MeAN}}$**-LA** and $^{S}\mathbf{P}^{\mathbf{MeAN}}$**-LA**. The relative energy of the bis(μ-oxo) isomer relative to peroxo is given for each complex, which includes an energy correction of -12 kcal/mol as determined by previous calibration of the B3LYP functional to bis(μ-oxo)/peroxo equilibria.[6]

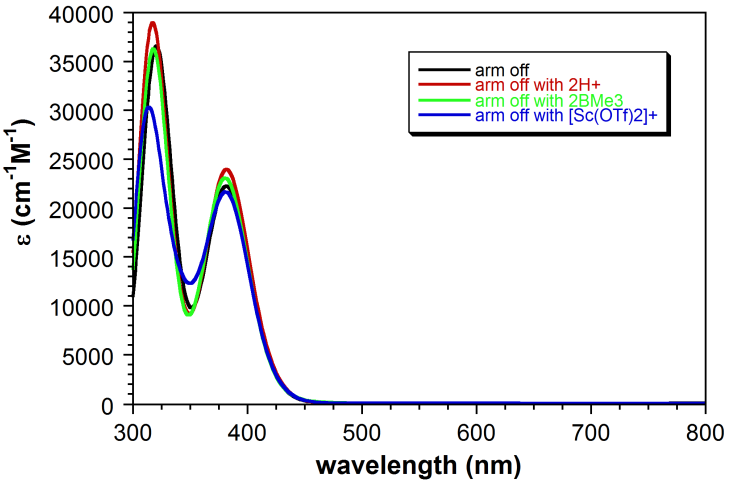
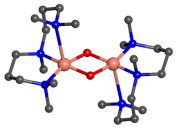
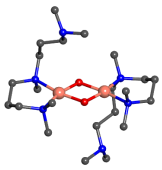
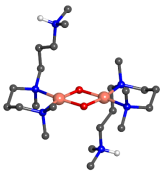
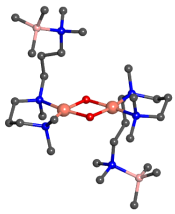
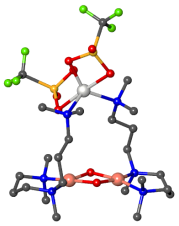
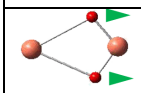
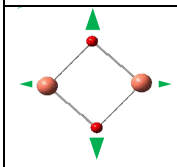
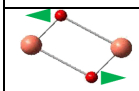
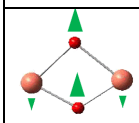


Figure S24. Time-dependent DFT-calculated absorption spectra of $\mathbf{O^{MeAN}}$ with the axial N uncoordinated (black), $\mathbf{O^{MeAN}\text{-}2H^{+}}$ (red), $\mathbf{O^{MeAN}\text{-}2BMe_3}$ (green), and $\mathbf{O^{MeAN}\text{-}ScOTf_2^{+}}$ (blue). Calculated $\pi^*_\sigma \rightarrow d_{xy}$ and $\sigma^* \rightarrow d_{xy}$ LMCTs are at 321/382, 317/382, 318/381, and 312/382 nm, respectively.

Table S5. DFT-calculated normal modes in $Cu^{III}_2(\mu\text{-}O)_2$ models. Calculated frequencies (cm^{-1}, scaled by 0.966 according to reference 7) are given for $^{16}O_2$ and ($^{18}O_2$) isotopologues.

					
Normal Mode:	**O^{MeAN}**	**O^{MeAN}_{armoff}**	**O^{MeAN}-2H$^+$**	**O^{MeAN}-2BMe_3**	**O^{MeAN}-ScOTf_2^+**
	645 (*616*)	659 (*630*)	665 (*636*)	664 (*635*)	659 (*629*)
	611 (*581*)	623 (*593*)	625 (*596*)	625 (*596*)	627 (*597*)
	604 (*579*)	618 (*593*)	618 (*592*)	620 (*594*)	618 (*592*)
	577 (*557*)	593 (*574*)	592 (*573*)	592 (*572*)	593 (*572*)

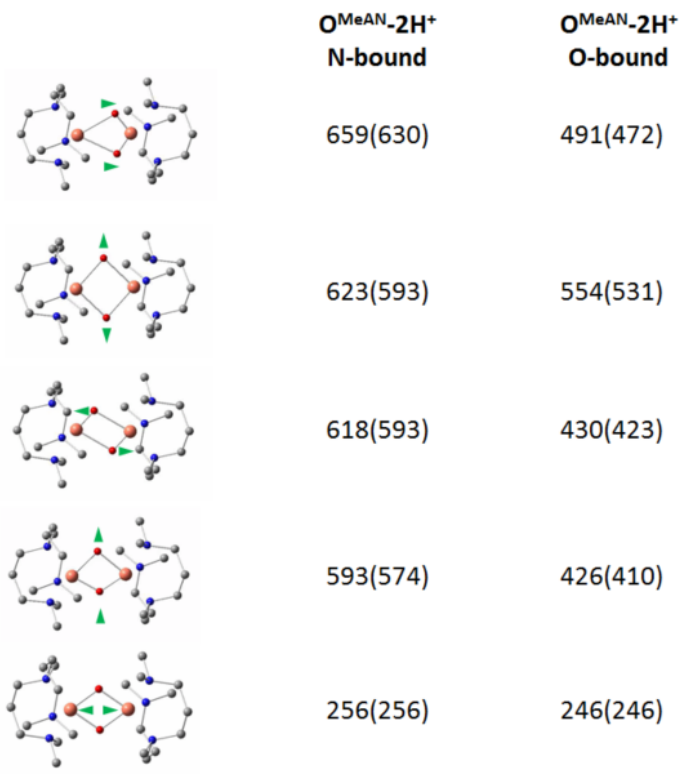


Figure S25. Comparison of DFT-calculated normal mode frequencies for N-bound vs. O-bound $\mathbf{O^{MeAN}}$**-2H**$^{+}$. The significantly weaker Cu-O bonding in the O-bound isomer results in very low frequency modes inconsistent with the observed resonance Raman data for $\mathbf{O^{MeAN}}$.

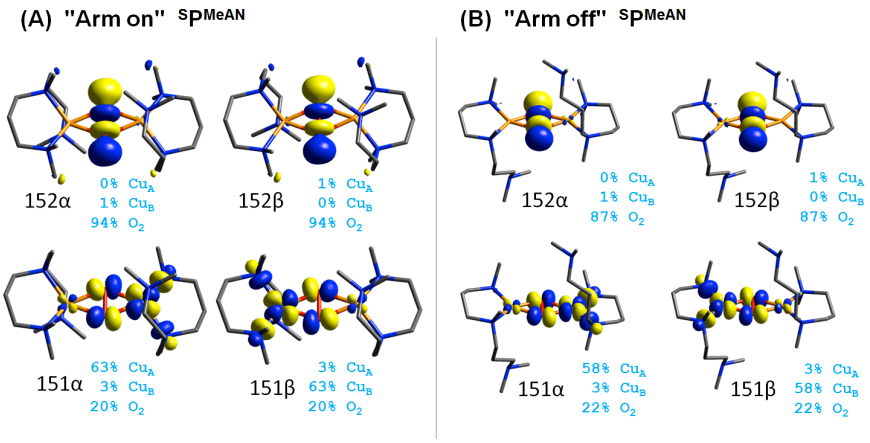


Figure S26. Comparison of LUMO (Cu dx^2-y^2 + O_2 π^*_σ) and LUMO+1 (O_2 σ^*) in the "arm on" and "arm off" isomers of $\mathbf{^{S}P^{MeAN}}$. Note the "arm off" isomer shows more unoccupied O_2 π^*_σ character (MO 151), which implies slightly higher Cu-O covalency, and less unoccupied O_2 σ^* character (MO 152), which implies stronger Cu → O_2 σ^* backbonding and thus a weaker O–O bond.

xyz coordinates for DFT structures:

$^{S}P^{MeAN}$

Cu	-1.8267	-0.0161	0.8021
Cu	1.8268	0.0164	0.6845
O	-0.0100	0.0041	-0.0007
O	0.0101	-0.0026	1.4873
N	2.2486	-2.2900	0.9876
N	3.0171	0.6624	2.2000
N	2.8757	0.6246	-0.9481
N	-2.2489	2.2904	0.4978
N	-3.0171	-0.6628	-0.7129
N	-2.8752	-0.6234	2.4352
C	-3.5363	2.8912	0.9366
H	-3.6215	2.8294	2.0240
H	-4.3855	2.3687	0.4947
H	-3.5952	3.9528	0.6492
C	-1.1490	3.0196	1.1844
H	-1.1706	4.0933	0.9411
H	-0.1906	2.6028	0.8772
H	-1.2503	2.9057	2.2664
C	-2.0792	2.4762	-0.9762
H	-2.1799	3.5479	-1.2166
H	-1.0532	2.1812	-1.2178
C	-3.0498	1.6740	-1.8535
H	-4.0909	1.8792	-1.5840
H	-2.9410	2.0592	-2.8757
C	-2.7804	0.1669	-1.9538
H	-3.4032	-0.2575	-2.7547
H	-1.7339	0.0076	-2.2335
C	-2.5584	-2.0527	-1.0386
H	-2.7219	-2.7213	-0.1941
H	-3.1086	-2.4416	-1.9046
H	-1.4924	-2.0311	-1.2694
C	-4.4816	-0.6816	-0.3757
H	-4.8316	0.3524	-0.3553
H	-5.0121	-1.1889	-1.1942
C	-4.8379	-1.3517	0.9590
H	-4.5246	-2.4005	0.9755
H	-5.9335	-1.3790	1.0083
C	-4.3623	-0.6109	2.2156
H	-4.8419	-1.0472	3.1032
H	-4.6703	0.4378	2.1612
C	-2.4103	-1.9965	2.8056
H	-2.6191	-2.7068	2.0061
H	-2.9157	-2.3340	3.7189
H	-1.3341	-1.9694	2.9788
C	-2.5420	0.2902	3.5720
H	-3.0417	-0.0447	4.4894
H	-1.4623	0.2896	3.7302
H	-2.8711	1.3035	3.3419
C	3.5361	-2.8907	0.5486
H	4.3852	-2.3685	0.9910
H	3.6215	-2.8282	-0.5387
H	3.5948	-3.9525	0.8353
C	1.1488	-3.0188	0.3004
H	0.1904	-2.6020	0.6075
H	1.2503	-2.9044	-0.7816
H	1.1702	-4.0926	0.5432
C	2.0787	-2.4767	2.4614
H	2.1793	-3.5486	2.7011
H	1.0526	-2.1820	2.7030
C	3.0490	-1.6751	3.3395
H	2.9397	-2.0608	4.3614
H	4.0902	-1.8804	3.0702
C	2.7799	-0.1679	3.4404
H	3.4027	0.2558	4.2417
H	1.7334	-0.0086	3.7199
C	2.5583	2.0521	2.5265
H	3.1081	2.4404	3.3930
H	1.4921	2.0305	2.7567
H	2.7223	2.7212	1.6825
C	4.4816	0.6813	1.8632
H	5.0120	1.1883	2.6821
H	4.8317	-0.3526	1.8425
C	4.8382	1.3520	0.5289
H	4.5250	2.4008	0.5128
H	5.9337	1.3792	0.4797
C	4.3627	0.6118	-0.7282
H	4.8425	1.0485	-1.6155
H	4.6705	-0.4369	-0.6742
C	2.4109	1.9979	-1.3179
H	2.9165	2.3359	-2.2309
H	2.6194	2.7077	-0.5179
H	1.3347	1.9710	-1.4915
C	2.5426	-0.2884	-2.0854
H	2.8720	-1.3018	-1.8559
H	3.0423	0.0471	-3.0027
H	1.4629	-0.2879	-2.2436

O^{MeAN}

Cu	-1.4349	-0.1291	0.8006
Cu	1.4350	0.1295	0.6859
O	-0.0429	-0.0054	-0.3630
O	0.0430	0.0054	1.8495
N	2.2943	-2.5061	0.9598
N	2.7220	0.5823	2.1708
N	2.5949	0.5346	-0.9128
N	-2.2942	2.5061	0.5261
N	-2.7222	-0.5827	-0.6838
N	-2.5947	-0.5333	2.3996
C	-3.6132	3.0922	0.8641
H	-3.8017	2.9854	1.9361
H	-4.4174	2.5872	0.3252
H	-3.6566	4.1660	0.6134
C	-1.2524	3.2452	1.2780
H	-1.2084	4.3073	0.9832
H	-0.2797	2.7875	1.0953
H	-1.4608	3.1971	2.3499
C	-2.0183	2.6621	-0.9285
H	-2.1734	3.7158	-1.2231
H	-0.9592	2.4366	-1.0813
C	-2.8492	1.7616	-1.8521
H	-3.9215	1.8908	-1.6723
H	-2.6910	2.1287	-2.8752
C	-2.4553	0.2791	-1.9055
H	-2.9919	-0.1977	-2.7371
H	-1.3837	0.1935	-2.1006
C	-2.3264	-1.9849	-1.0600
H	-2.4868	-2.6658	-0.2240
H	-2.9296	-2.3251	-1.9089
H	-1.2725	-1.9907	-1.3366
C	-4.1891	-0.5529	-0.3586
H	-4.4971	0.4908	-0.3091
H	-4.7198	-1.0156	-1.2011
C	-4.5779	-1.2370	0.9510
H	-4.2827	-2.2909	0.9717
H	-5.6734	-1.2407	0.9952
C	-4.0818	-0.4821	2.1818
H	-4.5582	-0.8786	3.0877
H	-4.3571	0.5722	2.0986
C	-2.1834	-1.9035	2.8526
H	-2.3793	-2.6439	2.0769
H	-2.7422	-2.1775	3.7541
H	-1.1177	-1.8897	3.0743
C	-2.2550	0.4360	3.4916
H	-2.7653	0.1395	4.4149
H	-1.1768	0.4373	3.6446
H	-2.5824	1.4333	3.2023
C	3.6131	-3.0924	0.6215
H	4.4175	-2.5876	1.1603
H	3.8015	-2.9855	-0.4505
H	3.6564	-4.1662	0.8720
C	1.2522	-3.2445	0.2077
H	0.2797	-2.7866	0.3910
H	1.4603	-3.1958	-0.8642
H	1.2080	-4.3068	0.5019
C	2.0184	-2.6626	2.4143
H	2.1735	-3.7165	2.7084
H	0.9593	-2.4373	2.5672
C	2.8493	-1.7624	3.3381
H	2.6915	-2.1299	4.3611
H	3.9216	-1.8914	3.1580
C	2.4551	-0.2801	3.3920
H	2.9915	0.1965	4.2239
H	1.3835	-0.1948	3.5871
C	2.3258	1.9842	2.5477
H	2.9287	2.3241	3.3969
H	1.2719	1.9898	2.8239
H	2.4863	2.6656	1.7121
C	4.1889	0.5530	1.8458
H	4.7194	1.0153	2.6886
H	4.4972	-0.4906	1.7958
C	4.5778	1.2379	0.5366
H	4.2823	2.2917	0.5164
H	5.6733	1.2418	0.4925
C	4.0821	0.4836	-0.6947
H	4.5585	0.8806	-1.6003
H	4.3575	-0.5707	-0.6121
C	2.1835	1.9048	-1.3654
H	2.7426	2.1792	-2.2667
H	2.3790	2.6450	-0.5895
H	1.1179	1.8909	-1.5875
C	2.2556	-0.4344	-2.0052
H	2.5833	-1.4317	-1.7163
H	2.7659	-0.1374	-2.9283
H	1.1774	-0.4359	-2.1583

$^{S}P^{MeAN}$ with axial N uncoordinated

Cu	-1.7382	-0.4633	0.5213
Cu	1.7673	0.1749	0.4815
O	0.0157	-0.2012	-0.2647
O	0.0280	-0.1728	1.2390
N	-2.2881	3.8269	-0.1556
N	-2.9364	-0.6832	-1.0532
N	-2.8430	-0.7897	2.1402
C	-2.6659	4.8719	-1.1240
H	-2.9324	5.7840	-0.5813
H	-3.5383	4.5610	-1.7045
H	-1.8466	5.1142	-1.8271
C	-1.1939	4.3069	0.7059
H	-0.2734	4.5440	0.1389
H	-0.9520	3.5441	1.4536
H	-1.5131	5.2134	1.2296
C	-1.9059	2.5661	-0.8171
H	-1.0926	2.7226	-1.5551
H	-1.4902	1.9174	-0.0385
C	-3.0944	1.8714	-1.5060
H	-3.9438	1.8627	-0.8135
H	-3.4142	2.4673	-2.3679
C	-2.7903	0.4598	-2.0426
H	-3.4573	0.2294	-2.8835
H	-1.7635	0.4170	-2.4195
C	-2.4127	-1.9272	-1.7185
H	-2.5538	-2.7859	-1.0609
H	-2.9503	-2.1055	-2.6568
H	-1.3480	-1.8100	-1.9269
C	-4.3931	-0.8879	-0.7177
H	-4.8584	0.0950	-0.6213
H	-4.8641	-1.3909	-1.5720
C	-4.6450	-1.6802	0.5713
H	-4.1335	-2.6497	0.5526
H	-5.7156	-1.9149	0.5982
C	-4.3163	-0.9007	1.8505
H	-4.7971	-1.3667	2.7201
H	-4.7065	0.1185	1.7644
C	-2.3320	-2.0639	2.7466
H	-2.4985	-2.9003	2.0655
H	-2.8506	-2.2628	3.6916
H	-1.2611	-1.9671	2.9344
C	-2.6117	0.3320	3.1076
H	-3.1761	0.1555	4.0307
H	-1.5479	0.3944	3.3417
H	-2.9387	1.2730	2.6605
H	5.6400	1.8759	0.4467
C	4.5901	1.5603	0.4446
C	4.3871	0.6860	-0.7993
H	4.0061	2.4863	0.3845
C	4.3304	0.8240	1.7647
N	2.9454	0.3671	-1.1128
H	4.9176	-0.2575	-0.6556
H	4.8198	1.1732	-1.6823
N	2.8703	0.6221	2.0736
H	4.7819	1.3674	2.6045
H	4.7954	-0.1657	1.7257
C	2.8728	-0.8528	-2.0149
C	2.3468	1.5244	-1.8654
C	2.2839	1.8806	2.6432
C	2.7186	-0.4829	3.0761
C	3.2498	-2.1970	-1.3638
H	3.5339	-0.6495	-2.8674
H	1.8490	-0.8970	-2.3995
H	2.4532	2.4404	-1.2820
H	2.8606	1.6528	-2.8249
H	1.2868	1.3357	-2.0438
H	2.4064	2.7038	1.9372
H	2.7873	2.1368	3.5826
H	1.2197	1.7288	2.8313
H	3.2824	-0.2468	3.9860
H	1.6631	-0.6006	3.3262
H	3.0946	-1.4158	2.6506
C	2.0839	-2.9054	-0.6501
H	4.0746	-2.0781	-0.6518
H	3.6335	-2.8383	-2.1648
N	2.5304	-4.0141	0.2130
H	1.3438	-3.2447	-1.4035
H	1.5551	-2.1984	-0.0025
C	3.1118	-5.1245	-0.5623
C	1.4125	-4.5021	1.0389
H	3.4195	-5.9188	0.1247
H	3.9984	-4.7890	-1.1064
H	2.3969	-5.5538	-1.2896
H	0.5852	-4.9228	0.4365
H	1.0156	-3.6793	1.6428
H	1.7728	-5.2839	1.7149

O^{MeAN} with axial N uncoordinated

Cu	-1.3783	-0.3677	0.4027
Cu	1.4350	0.1266	0.4058
O	0.0342	-0.1482	-0.7166
O	0.0219	-0.0905	1.5149
N	-2.1195	3.9086	0.0565
N	-2.6231	-0.5757	-1.1458
N	-2.5847	-0.6841	1.9583
C	-2.7740	4.9643	-0.7373
H	-3.0566	5.7881	-0.0748
H	-3.6851	4.5838	-1.2060
H	-2.1156	5.3680	-1.5298
C	-0.9690	4.4668	0.7876
H	-0.1883	4.8706	0.1154
H	-0.5180	3.6892	1.4125
H	-1.3094	5.2777	1.4392
C	-1.6929	2.7683	-0.7757
H	-1.0175	3.0915	-1.5936
H	-1.1040	2.1062	-0.1332
C	-2.8837	1.9956	-1.3738
H	-3.6346	1.8572	-0.5866
H	-3.3663	2.6074	-2.1432
C	-2.5084	0.6543	-2.0361
H	-3.1605	0.4603	-2.8964
H	-1.4782	0.6791	-2.3972
C	-2.0701	-1.7524	-1.9076
H	-2.2311	-2.6666	-1.3344
H	-2.5870	-1.8374	-2.8690
H	-1.0041	-1.6046	-2.0704
C	-4.0820	-0.8470	-0.8619
H	-4.5973	0.1103	-0.7689
H	-4.4925	-1.3543	-1.7423
C	-4.3342	-1.6684	0.4001
H	-3.7756	-2.6113	0.3895
H	-5.3939	-1.9470	0.4080
C	-4.0503	-0.8617	1.6647
H	-4.5024	-1.3379	2.5428
H	-4.4887	0.1359	1.5687
C	-2.0454	-1.9302	2.6059
H	-2.1733	-2.7852	1.9398
H	-2.5863	-2.1180	3.5394
H	-0.9864	-1.7870	2.8149
C	-2.4267	0.4678	2.9087
H	-3.0183	0.2772	3.8106
H	-1.3749	0.5721	3.1694
H	-2.7795	1.3831	2.4292
H	5.4347	1.7250	0.3815
C	4.3794	1.4300	0.3771
C	4.1498	0.5543	-0.8527
H	3.8069	2.3634	0.3260
C	4.0970	0.6695	1.6703
N	2.6968	0.2506	-1.1358
H	4.6782	-0.3904	-0.7160
H	4.5606	1.0311	-1.7496
N	2.6305	0.4891	1.9607
H	4.5383	1.1838	2.5321
H	4.5468	-0.3259	1.6156
C	2.5977	-1.0319	-1.9519
C	2.1441	1.3765	-1.9716
C	2.0840	1.7470	2.5779
C	2.4724	-0.6437	2.9346
C	2.9864	-2.3295	-1.2173
H	3.2505	-0.8832	-2.8208
H	1.5684	-1.0888	-2.3122
H	2.2867	2.3230	-1.4473
H	2.6757	1.4128	-2.9280
H	1.0824	1.2085	-2.1420
H	2.2221	2.5872	1.8952
H	2.6144	1.9530	3.5135
H	1.0223	1.6095	2.7764
H	3.0605	-0.4321	3.8340
H	1.4201	-0.7435	3.1951
H	2.8289	-1.5691	2.4770
C	1.8327	-3.0274	-0.4711
H	3.8019	-2.1558	-0.5055
H	3.3914	-3.0080	-1.9759
N	2.3100	-4.0649	0.4626
H	1.1150	-3.4403	-1.2086
H	1.2728	-2.2999	0.1256
C	2.9529	-5.1921	-0.2372
C	1.1977	-4.5552	1.2947
H	3.2764	-5.9333	0.5000
H	3.8376	-4.8521	-0.7813
H	2.2719	-5.6903	-0.9529
H	0.3985	-5.0385	0.7015
H	0.7588	-3.7207	1.8507
H	1.5767	-5.2869	2.0149

O^{MeAN}-$2H^+$

Cu	-1.3502	-0.3729	0.7801
Cu	1.4545	0.1698	0.7529
O	0.0498	-0.1457	-0.3539
O	0.0558	-0.0636	1.8666
N	-2.3901	3.9505	-1.0042
N	-2.6095	-0.7545	-0.7371
N	-2.5441	-0.6708	2.3538
C	-1.5802	4.5144	-2.1499
H	-1.8249	5.5706	-2.2551
H	-1.8291	3.9894	-3.0697
H	-0.5225	4.3917	-1.9163
C	-2.1304	4.7248	0.2707
H	-1.0947	4.5634	0.5696
H	-2.8092	4.3666	1.0436
H	-2.3070	5.7821	0.0781
C	-2.1700	2.4556	-0.7861
H	-1.0913	2.3047	-0.7064
H	-2.6310	2.2448	0.1802
C	-2.7878	1.6014	-1.8994
H	-3.8796	1.6724	-1.8654
H	-2.4900	1.9935	-2.8781
C	-2.3172	0.1360	-1.9352
H	-2.7903	-0.3425	-2.8010
H	-1.2351	0.1013	-2.0753
C	-2.1894	-2.1467	-1.1411
H	-2.3137	-2.8424	-0.3116
H	-2.8020	-2.4867	-1.9820
H	-1.1431	-2.1226	-1.4417
C	-4.0869	-0.7505	-0.4404
H	-4.4203	0.2877	-0.3970
H	-4.5904	-1.2251	-1.2914
C	-4.4758	-1.4418	0.8646
H	-4.1428	-2.4841	0.8964
H	-5.5705	-1.4866	0.8892
C	-4.0289	-0.6603	2.0970
H	-4.5141	-1.0563	2.9972
H	-4.3255	0.3878	1.9952
C	-2.1153	-2.0028	2.9040
H	-2.3617	-2.8013	2.2034
H	-2.6329	-2.1919	3.8500
H	-1.0387	-1.9839	3.0726
C	-2.2538	0.3863	3.3823
H	-2.8308	0.1732	4.2885
H	-1.1898	0.3853	3.6095
H	-2.5425	1.3632	2.9913
H	-3.3814	4.0836	-1.2351
H	5.6550	1.3479	0.7582
C	4.5612	1.2809	0.7451
C	4.1771	0.4634	-0.4862
H	4.2071	2.3149	0.6843
C	4.1355	0.6037	2.0440
N	2.7009	0.4411	-0.7901
H	4.5043	-0.5667	-0.3341
H	4.6864	0.8479	-1.3783
N	2.6500	0.5941	2.2974
H	4.6062	1.0923	2.9055
H	4.4648	-0.4393	2.0350
C	2.4240	-0.5426	-1.9168
C	2.2799	1.7956	-1.3049
C	2.1923	1.9509	2.7594
C	2.3820	-0.4000	3.3924
C	2.8627	-2.0079	-1.7398
H	2.9367	-0.1470	-2.8018
H	1.3489	-0.4984	-2.0997
H	2.4025	2.5526	-0.5307
H	2.8956	2.0694	-2.1673
H	1.2336	1.7517	-1.6045
H	2.4256	2.7071	2.0086
H	2.7037	2.2095	3.6922
H	1.1160	1.9216	2.9271
H	2.9598	-0.1198	4.2793
H	1.3192	-0.4023	3.6253
H	2.6860	-1.3950	3.0617
C	2.0804	-2.7869	-0.6771
H	3.9390	-2.0844	-1.5530
H	2.6919	-2.4559	-2.7245
N	2.4932	-4.2530	-0.5919
H	1.0078	-2.7803	-0.8778
H	2.2438	-2.3849	0.3240
C	2.2468	-5.0227	-1.8712
C	1.8164	-4.9310	0.5800
H	3.5025	-4.2790	-0.4102
H	2.5238	-6.0624	-1.7026
H	2.8567	-4.6092	-2.6711
H	1.1877	-4.9503	-2.1192
H	0.7433	-4.9523	0.3916
H	2.0331	-4.3678	1.4868
H	2.2030	-5.9455	0.6666

O^{MeAN}-$2H^+$ (O-protonated)

Cu	-1.4305	-0.4204	0.9383
Cu	1.5476	0.4809	0.7337
O	-0.0950	0.2699	-0.3261
O	0.2057	-0.1985	1.9881
N	2.1336	-3.9251	1.3602
N	2.9878	0.6407	2.2349
N	2.6328	1.1636	-0.8821
N	-2.4410	3.9292	-0.3568
N	-2.8068	-0.8206	-0.5679
N	-2.5505	-0.9387	2.5936
C	-3.1404	5.0525	-0.9612
H	-4.2036	5.0018	-0.6819
H	-3.0526	5.0127	-2.0456
H	-2.7345	5.9895	-0.5715
C	-2.0673	4.0034	1.0486
H	-1.1996	4.6714	1.1422
H	-1.8014	3.0142	1.4218
H	-2.8863	4.4333	1.6320
C	-2.1665	2.7133	-1.1102
H	-2.0557	2.9725	-2.1648
H	-1.2367	2.2771	-0.7304
C	-3.3110	1.6659	-0.9321
H	-3.5274	1.5531	0.1352
H	-4.2223	2.0475	-1.3996
C	-2.9091	0.3112	-1.5653
H	-3.6456	0.0189	-2.3231
H	-1.9486	0.3944	-2.0749
C	-2.2083	-2.0120	-1.2684
H	-2.1981	-2.8713	-0.5967
H	-2.7973	-2.2651	-2.1568
H	-1.1849	-1.7970	-1.5729
C	-4.2183	-1.1836	-0.1626
H	-4.7755	-0.2541	-0.0206
H	-4.6773	-1.7094	-1.0095
C	-4.3289	-2.0163	1.1117
H	-3.7269	-2.9302	1.0583
H	-5.3692	-2.3543	1.1864
C	-4.0180	-1.2025	2.3649
H	-4.4063	-1.7045	3.2601
H	-4.5184	-0.2314	2.2959
C	-1.9318	-2.1713	3.1861
H	-1.9954	-2.9982	2.4768
H	-2.4577	-2.4488	4.1067
H	-0.8853	-1.9801	3.4142
C	-2.4654	0.1781	3.5936
H	-3.1128	-0.0366	4.4512
H	-1.4463	0.2897	3.9606
H	-2.7861	1.1112	3.1270
C	2.9936	-5.0760	1.5893
H	3.3139	-5.1099	2.6292
H	3.8728	-5.0017	0.9343
H	2.4546	-5.9905	1.3225
C	1.3714	-3.8478	0.1216
H	1.0107	-2.8313	-0.0351
H	1.9865	-4.1831	-0.7178
H	0.5088	-4.5256	0.2006
C	2.0508	-2.8481	2.3381
H	1.9987	-3.2945	3.3359
H	1.1461	-2.2694	2.1392
C	3.2923	-1.9023	2.2554
H	4.1719	-2.4329	2.6287
H	3.4958	-1.6603	1.2074
C	3.0500	-0.6144	3.0787
H	3.8542	-0.4791	3.8119
H	2.1184	-0.6835	3.6414
C	2.5117	1.7687	3.1096
H	3.1488	1.8539	3.9968
H	1.4841	1.5966	3.4273
H	2.5519	2.7080	2.5572
C	4.4029	0.9576	1.8072
H	4.9378	1.3249	2.6922
H	4.8811	0.0211	1.5075
C	4.5150	1.9552	0.6578
H	3.9643	2.8798	0.8633
H	5.5683	2.2506	0.5854
C	4.1175	1.3454	-0.6830
H	4.4857	1.9618	-1.5130
H	4.5820	0.3594	-0.7824
C	2.0263	2.4827	-1.2616
H	2.4829	2.8558	-2.1855
H	2.1899	3.2112	-0.4664
H	0.9555	2.3543	-1.4126
C	2.4748	0.2071	-2.0296
H	2.7240	-0.8041	-1.7005
H	3.1436	0.4954	-2.8483
H	1.4554	0.2310	-2.4113
H	0.1844	0.0531	2.9167
H	-0.0462	-0.0314	-1.2390

$^{S}P^{MeAN}$-2H^{+}

Cu	-1.6671	-0.5332	0.7900
Cu	1.7930	0.2844	0.7509
O	0.0711	-0.1977	-0.0027
O	0.0802	-0.1561	1.4974
N	-2.5652	3.7880	-1.0215
N	-2.8614	-0.9166	-0.7680
N	-2.7924	-0.8054	2.4140
C	-1.7241	4.3275	-2.1566
H	-1.9280	5.3928	-2.2572
H	-1.9849	3.8183	-3.0820
H	-0.6739	4.1630	-1.9145
C	-2.3079	4.5616	0.2542
H	-1.2812	4.3773	0.5700
H	-3.0076	4.2237	1.0175
H	-2.4559	5.6218	0.0540
C	-2.3834	2.2887	-0.7946
H	-1.3074	2.1198	-0.6989
H	-2.8654	2.0910	0.1647
C	-3.0041	1.4470	-1.9157
H	-4.0952	1.5287	-1.8847
H	-2.6987	1.8425	-2.8906
C	-2.5580	-0.0264	-1.9593
H	-3.0358	-0.4842	-2.8346
H	-1.4758	-0.0782	-2.1094
C	-2.4456	-2.3067	-1.1777
H	-2.6099	-3.0131	-0.3643
H	-3.0270	-2.6297	-2.0482
H	-1.3860	-2.3009	-1.4380
C	-4.3343	-0.9111	-0.4473
H	-4.6683	0.1281	-0.4185
H	-4.8614	-1.4053	-1.2736
C	-4.6966	-1.5763	0.8874
H	-4.3390	-2.6105	0.9353
H	-5.7901	-1.6491	0.9143
C	-4.2717	-0.7791	2.1265
H	-4.7929	-1.1557	3.0157
H	-4.5525	0.2713	2.0005
C	-2.3991	-2.1230	3.0173
H	-2.6562	-2.9416	2.3440
H	-2.9231	-2.2692	3.9687
H	-1.3218	-2.1295	3.1934
C	-2.4732	0.2782	3.4031
H	-3.0484	0.1249	4.3232
H	-1.4080	0.2548	3.6362
H	-2.7300	1.2512	2.9808
H	-3.5489	3.9437	-1.2695
H	5.8627	1.5696	0.7864
C	4.7726	1.4544	0.7678
C	4.4378	0.6564	-0.4992
H	4.3762	2.4744	0.7222
C	4.3764	0.7556	2.0731
N	2.9685	0.5936	-0.8327
H	4.7941	-0.3679	-0.3682
H	4.9602	1.0825	-1.3655
N	2.8951	0.7311	2.3483
H	4.8691	1.2375	2.9272
H	4.7112	-0.2860	2.0436
C	2.7218	-0.3940	-1.9581
C	2.5164	1.9329	-1.3546
C	2.4259	2.0702	2.8390
C	2.6209	-0.2863	3.4171
C	3.1365	-1.8628	-1.7529
H	3.2645	-0.0187	-2.8351
H	1.6533	-0.3421	-2.1865
H	2.6566	2.7051	-0.5987
H	3.0946	2.2026	-2.2453
H	1.4584	1.8788	-1.6176
H	2.6404	2.8438	2.1001
H	2.9344	2.3237	3.7760
H	1.3488	2.0293	3.0127
H	3.1841	-0.0354	4.3231
H	1.5548	-0.2951	3.6462
H	2.9252	-1.2758	3.0699
C	2.3231	-2.6168	-0.6961
H	4.2068	-1.9451	-1.5372
H	2.9860	-2.3225	-2.7351
N	2.6557	-4.1051	-0.6391
H	1.2485	-2.5440	-0.8787
H	2.5296	-2.2457	0.3091
C	2.3296	-4.8487	-1.9159
C	1.9808	-4.7570	0.5487
H	3.6673	-4.1869	-0.4891
H	2.5571	-5.9029	-1.7631
H	2.9368	-4.4611	-2.7309
H	1.2690	-4.7192	-2.1310
H	0.9021	-4.7115	0.4002
H	2.2643	-4.2196	1.4529
H	2.3083	-5.7939	0.6103

O^{MeAN}-2BMe_3

Cu	-1.3872	-0.4370	0.5621
Cu	1.3815	0.2602	0.6262
O	0.0342	-0.1323	-0.5248
O	-0.0480	-0.0110	1.6934
N	-2.4226	3.9115	-1.0259
N	-2.5570	-0.8864	-0.9937
N	-2.5920	-0.8488	2.1051
C	-2.2840	4.5182	-2.3888
H	-2.4936	5.5859	-2.3182
H	-2.9978	4.0707	-3.0768
H	-1.2655	4.3721	-2.7663
C	-1.3932	4.5576	-0.1414
H	-0.3865	4.3157	-0.5003
H	-1.5145	4.1937	0.8797
H	-1.5283	5.6368	-0.1548
C	-2.0479	2.4432	-1.0705
H	-1.0088	2.3860	-1.4162
H	-2.0645	2.1072	-0.0329
C	-2.9163	1.5403	-1.9546
H	-3.9468	1.5356	-1.6005
H	-2.9523	1.9500	-2.9700
C	-2.3719	0.1103	-2.1345
H	-2.8701	-0.3421	-3.0012
H	-1.2993	0.1383	-2.3377
C	-1.9812	-2.1945	-1.4759
H	-2.0871	-2.9637	-0.7103
H	-2.5126	-2.5186	-2.3766
H	-0.9260	-2.0522	-1.7041
C	-4.0277	-1.0713	-0.7228
H	-4.4829	-0.0829	-0.6509
H	-4.4569	-1.5719	-1.5994
C	-4.3517	-1.8474	0.5520
H	-3.8660	-2.8287	0.5747
H	-5.4282	-2.0530	0.5401
C	-4.0573	-1.0350	1.8097
H	-4.5076	-1.5076	2.6911
H	-4.4942	-0.0371	1.7087
C	-2.0189	-2.1122	2.6860
H	-2.1405	-2.9403	1.9865
H	-2.5419	-2.3556	3.6168
H	-0.9596	-1.9578	2.8888
C	-2.4638	0.2497	3.1224
H	-3.0281	-0.0251	4.0200
H	-1.4133	0.3874	3.3707
H	-2.8682	1.1753	2.7095
H	5.5306	1.6126	0.7633
C	4.4411	1.5086	0.7042
C	4.1407	0.6243	-0.5046
H	4.0571	2.5263	0.5796
C	3.9782	0.8794	2.0152
N	2.6837	0.5292	-0.8703
H	4.5003	-0.3843	-0.2949
H	4.6741	0.9903	-1.3907
N	2.4839	0.8252	2.2010
H	4.3906	1.4285	2.8704
H	4.3452	-0.1499	2.0745
C	2.4918	-0.5231	-1.9561
C	2.2335	1.8385	-1.4658
C	1.9465	2.1882	2.5397
C	2.2027	-0.0972	3.3537
C	3.0267	-1.9423	-1.6971
H	2.9886	-0.1293	-2.8518
H	1.4172	-0.5557	-2.1484
H	2.3026	2.6401	-0.7303
H	2.8672	2.0900	-2.3226
H	1.2001	1.7381	-1.7945
H	2.1630	2.8939	1.7369
H	2.4133	2.5476	3.4628
H	0.8679	2.1153	2.6783
H	2.7079	0.2823	4.2482
H	1.1289	-0.1438	3.5229
H	2.5788	-1.0950	3.1213
C	2.3562	-2.6693	-0.5258
H	4.1109	-1.9404	-1.5787
H	2.8297	-2.4771	-2.6328
N	2.5927	-4.1631	-0.4238
H	1.2706	-2.5180	-0.5793
H	2.7039	-2.2590	0.4249
C	1.9958	-4.8567	-1.6095
C	1.8242	-4.6064	0.7891
H	2.1252	-5.9322	-1.4869
H	2.5017	-4.5498	-2.5222
H	0.9270	-4.6251	-1.6846
H	0.7864	-4.2613	0.7217
H	2.2892	-4.1903	1.6834
H	1.8379	-5.6923	0.8513
B	-4.0725	4.2478	-0.3447
C	-4.0570	5.7987	0.1642
H	-3.7512	6.5257	-0.6050
H	-5.0906	6.0633	0.4372
H	-3.4432	5.9832	1.0578
C	-5.1798	4.0630	-1.5285
H	-5.0902	4.8088	-2.3325
H	-5.2273	3.0746	-2.0048
H	-6.1671	4.2279	-1.0681
C	-4.2716	3.2109	0.8975
H	-4.3603	2.1532	0.6036
H	-3.4841	3.2802	1.6651
H	-5.2144	3.4684	1.4038
B	4.3347	-4.6377	-0.2139
C	4.9890	-3.5444	0.8029
H	5.9953	-3.9005	1.0731
H	5.1288	-2.5410	0.3723
H	4.4445	-3.4244	1.7532
C	5.0470	-4.6658	-1.6809
H	5.0326	-3.7244	-2.2463
H	6.1093	-4.9064	-1.5147
H	4.6568	-5.4527	-2.3438
C	4.3279	-6.1363	0.4337
H	5.3670	-6.5010	0.4221
H	3.9945	-6.1831	1.4806
H	3.7412	-6.8751	-0.1353

$^{S}P^{MeAN}$-2BMe_3

Cu	-1.6359	-0.6574	0.5507
Cu	1.7590	0.4153	0.4706
O	0.0620	-0.1831	-0.2698
O	0.0738	-0.1077	1.2279
N	-2.5617	3.6231	-0.8957
N	-2.8325	-1.1361	-0.9722
N	-2.6566	-1.0470	2.2225
C	-2.2799	4.1972	-2.2506
H	-2.3770	5.2817	-2.1963
H	-2.9960	3.8226	-2.9784
H	-1.2630	3.9385	-2.5668
C	-1.5161	4.1589	0.0412
H	-0.5256	3.7982	-0.2590
H	-1.7341	3.8245	1.0562
H	-1.5256	5.2462	0.0128
C	-2.3519	2.1220	-0.9165
H	-1.3097	1.9480	-1.2142
H	-2.4584	1.8013	0.1223
C	-3.2770	1.3050	-1.8264
H	-4.2951	1.3014	-1.4345
H	-3.3379	1.7740	-2.8138
C	-2.7789	-0.1246	-2.1056
H	-3.3751	-0.5452	-2.9266
H	-1.7371	-0.0936	-2.4385
C	-2.2376	-2.4089	-1.5155
H	-2.2970	-3.2067	-0.7747
H	-2.7842	-2.7219	-2.4122
H	-1.1916	-2.2369	-1.7755
C	-4.2647	-1.3920	-0.5755
H	-4.7699	-0.4271	-0.5053
H	-4.7402	-1.9539	-1.3898
C	-4.4393	-2.1358	0.7548
H	-3.8802	-3.0783	0.7658
H	-5.4953	-2.4234	0.8205
C	-4.1260	-1.2836	1.9904
H	-4.5390	-1.7509	2.8934
H	-4.5985	-0.3024	1.8819
C	-2.0254	-2.2575	2.8490
H	-2.1783	-3.1371	2.2236
H	-2.4713	-2.4408	3.8334
H	-0.9542	-2.0824	2.9642
C	-2.4905	0.1086	3.1652
H	-3.0024	-0.1046	4.1108
H	-1.4290	0.2692	3.3580
H	-2.9196	1.0103	2.7238
H	5.5453	2.3403	0.4836
C	4.5001	2.0096	0.4690
C	4.3395	1.1063	-0.7615
H	3.9072	2.9268	0.3779
C	4.2344	1.3035	1.8035
N	2.9128	0.7663	-1.1130
H	4.8713	0.1702	-0.5805
H	4.7946	1.5802	-1.6410
N	2.7803	1.0198	2.0780
H	4.6250	1.9024	2.6362
H	4.7589	0.3432	1.8153
C	2.8811	-0.3554	-2.1387
C	2.2724	1.9574	-1.7770
C	2.0934	2.2575	2.5805
C	2.6788	-0.0373	3.1389
C	3.3980	-1.7431	-1.7162
H	3.4778	-0.0062	-2.9918
H	1.8429	-0.4334	-2.4757
H	2.3083	2.8262	-1.1203
H	2.8024	2.1954	-2.7062
H	1.2310	1.7266	-2.0064
H	2.1865	3.0677	1.8557
H	2.5450	2.5744	3.5275
H	1.0361	2.0395	2.7393
H	3.1833	0.3004	4.0517
H	1.6277	-0.2301	3.3588
H	3.1513	-0.9570	2.7885
C	2.4162	-2.5438	-0.8508
H	4.3701	-1.6726	-1.2263
H	3.5749	-2.2735	-2.6573
N	2.7048	-4.0240	-0.6910
H	1.4081	-2.4586	-1.2769
H	2.3761	-2.1428	0.1639
C	2.5946	-4.7114	-2.0180
C	1.6000	-4.5565	0.1774
H	2.7458	-5.7808	-1.8698
H	3.3588	-4.3462	-2.7003
H	1.6021	-4.5407	-2.4499
H	0.6269	-4.2880	-0.2487
H	1.6906	-4.1338	1.1785
H	1.6768	-5.6398	0.2382
B	-4.1982	4.1495	-0.3073
C	-4.0385	5.7036	0.1659
H	-3.6178	6.3722	-0.6021
H	-5.0492	6.0854	0.3792
H	-3.4530	5.8460	1.0859
C	-5.2551	4.0440	-1.5446
H	-5.0464	4.7484	-2.3638
H	-5.3796	3.0487	-1.9914
H	-6.2423	4.3254	-1.1446
C	-4.5709	3.1740	0.9439
H	-4.7837	2.1303	0.6659
H	-3.8141	3.1607	1.7448
H	-5.4927	3.5599	1.4061
B	4.2988	-4.4021	0.0912
C	4.4958	-3.3058	1.2813
H	5.3850	-3.5964	1.8615
H	4.6813	-2.2786	0.9315
H	3.6617	-3.2700	2.0006
C	5.4661	-4.3394	-1.0463
H	5.5805	-3.3829	-1.5733
H	6.4229	-4.5214	-0.5313
H	5.3773	-5.1262	-1.8105
C	4.1753	-5.9183	0.6834
H	5.1794	-6.2196	1.0208
H	3.5124	-6.0182	1.5552
H	3.8655	-6.6725	-0.0576

O^{MeAN}-Sc(OTf)$_2$

Cu	-1.3534	-0.2854	0.4712
Cu	1.4108	0.3264	0.7356
O	0.0806	0.2574	-0.4972
O	-0.0837	0.0363	1.7155
N	-2.7156	4.0621	-0.8311
N	-2.4250	-0.6246	-1.1872
N	-2.6032	-0.9954	1.8589
C	-4.2157	4.1298	-0.7658
H	-4.5173	5.1609	-0.5754
H	-4.5703	3.4905	0.0430
H	-4.6594	3.8035	-1.7112
C	-2.2424	4.8303	-2.0306
H	-2.6435	4.4017	-2.9532
H	-1.1523	4.8203	-2.0726
H	-2.5965	5.8595	-1.9693
C	-2.2477	2.6205	-0.8915
H	-1.1542	2.6324	-0.8888
H	-2.5864	2.1624	0.0441
C	-2.7436	1.8134	-2.1069
H	-3.8354	1.7577	-2.1167
H	-2.4599	2.3292	-3.0308
C	-2.1233	0.4142	-2.2573
H	-2.4778	-0.0128	-3.2038
H	-1.0350	0.4884	-2.3044
C	-1.8418	-1.9241	-1.6834
H	-2.0038	-2.7203	-0.9576
H	-2.3203	-2.2066	-2.6266
H	-0.7720	-1.7928	-1.8423
C	-3.9161	-0.7678	-1.0328
H	-4.3328	0.2286	-0.8766
H	-4.3061	-1.1465	-1.9857
C	-4.3588	-1.6628	0.1217
H	-3.9632	-2.6795	0.0358
H	-5.4473	-1.7667	0.0457
C	-4.0611	-1.0434	1.4839
H	-4.5803	-1.5950	2.2770
H	-4.4236	-0.0106	1.5018
C	-2.0916	-2.3714	2.1789
H	-2.1700	-3.0261	1.3112
H	-2.6793	-2.7980	2.9986
H	-1.0474	-2.2972	2.4814
C	-2.4849	-0.1477	3.0933
H	-3.1098	-0.5766	3.8840
H	-1.4453	-0.1236	3.4136
H	-2.8182	0.8638	2.8665
H	5.7198	0.1672	1.1439
C	4.6373	0.0324	1.0402
C	3.9829	0.6481	2.2758
H	4.4783	-1.0503	0.9893
C	4.2095	0.7277	-0.2498
N	2.5081	0.3553	2.4124
H	4.1164	1.7311	2.2438
H	4.4683	0.2857	3.1895
N	2.8032	0.4140	-0.6902
H	4.8762	0.4536	-1.0760
H	4.2746	1.8116	-0.1201
C	1.8947	1.3242	3.4159
C	2.3490	-1.0306	2.9867
C	2.7619	-0.9392	-1.3473
C	2.3884	1.4457	-1.6986
C	1.8225	2.8024	2.9728
H	2.5019	1.2377	4.3243
H	0.8985	0.9408	3.6436
H	2.8511	-1.7604	2.3515
H	2.7978	-1.0634	3.9847
H	1.2886	-1.2677	3.0496
H	3.0945	-1.7098	-0.6518
H	3.4224	-0.9386	-2.2206
H	1.7395	-1.1460	-1.6597
H	3.0792	1.4227	-2.5483
H	1.3767	1.2292	-2.0373
H	2.4199	2.4337	-1.2379
C	0.4156	3.2144	2.4818
H	2.5720	3.0056	2.2036
H	2.1011	3.4184	3.8327
N	0.3261	4.5853	1.8477
H	-0.2701	3.1972	3.3336
H	0.0481	2.4939	1.7476
C	0.7297	5.6592	2.8181
C	1.2134	4.6516	0.6383
H	0.5828	6.6333	2.3504
H	1.7854	5.5595	3.0885
H	0.1122	5.5890	3.7144
H	1.0049	3.7957	-0.0087
H	2.2699	4.6384	0.9221
H	1.0190	5.5781	0.0959
Sc	-1.8571	5.0414	1.1062
O	-2.4185	8.4855	-1.3641
S	-2.0880	7.8172	0.0643
O	-0.7687	6.7400	0.1592
O	-3.2204	6.7374	0.7320
C	-1.7992	9.2547	1.4551
F	-3.0217	9.6195	1.9085
F	-1.0468	8.6986	2.4380
F	-1.1571	10.2758	0.8427
O	-2.6912	3.0792	4.8055
S	-3.1670	3.9225	3.5176
O	-2.8494	3.2456	1.9812
O	-2.4158	5.4118	3.1959
C	-5.1578	4.3216	3.6162
F	-5.2880	5.5488	4.1695
F	-5.6174	4.2935	2.3409
F	-5.7150	3.3545	4.3786

$^{S}P^{MeAN}$-Sc(OTf)$_2$

Cu	-1.6086	-0.3698	0.3338
Cu	1.8165	0.2887	0.7600
O	0.1585	0.1424	-0.1931
O	-0.0173	0.1284	1.2684
N	-2.8153	4.0079	-0.8233
N	-2.5573	-0.6532	-1.3956
N	-2.8366	-1.0382	1.7488
C	-4.3185	4.0433	-0.7648
H	-4.6438	5.0566	-0.5302
H	-4.6658	3.3710	0.0189
H	-4.7468	3.7492	-1.7276
C	-2.3667	4.8341	-1.9953
H	-2.8342	4.4840	-2.9203
H	-1.2820	4.7830	-2.1047
H	-2.6645	5.8725	-1.8455
C	-2.3236	2.5768	-0.9391
H	-1.2276	2.6004	-0.9127
H	-2.6793	2.0740	-0.0341
C	-2.7935	1.8288	-2.2031
H	-3.8851	1.7959	-2.2437
H	-2.4746	2.3855	-3.0908
C	-2.2110	0.4200	-2.4103
H	-2.5577	0.0603	-3.3886
H	-1.1190	0.4686	-2.4475
C	-1.9743	-1.9384	-1.9174
H	-2.1769	-2.7571	-1.2265
H	-2.4125	-2.1822	-2.8920
H	-0.8943	-1.8259	-2.0266
C	-4.0498	-0.7961	-1.2538
H	-4.4696	0.2015	-1.1086
H	-4.4430	-1.1872	-2.2016
C	-4.5018	-1.6840	-0.0867
H	-4.0777	-2.6911	-0.1550
H	-5.5842	-1.8189	-0.1988
C	-4.2737	-1.0707	1.3006
H	-4.8485	-1.6233	2.0557
H	-4.6309	-0.0358	1.3039
C	-2.3605	-2.4145	2.1064
H	-2.4253	-3.0797	1.2444
H	-2.9731	-2.8243	2.9182
H	-1.3209	-2.3587	2.4350
C	-2.7289	-0.1685	2.9638
H	-3.3550	-0.5695	3.7698
H	-1.6906	-0.1378	3.2981
H	-3.0646	0.8402	2.7258
H	5.9817	-0.0372	1.4376
C	4.8996	-0.1209	1.2823
C	4.2248	0.7047	2.3863
H	4.6728	-1.1882	1.3859
C	4.6114	0.3764	-0.1398
N	2.7391	0.4784	2.5155
H	4.3867	1.7674	2.1864
H	4.6815	0.4828	3.3595
N	3.2179	0.0867	-0.6363
H	5.3202	-0.0691	-0.8494
H	4.7492	1.4616	-0.1780
C	2.1099	1.6124	3.2926
C	2.4901	-0.7978	3.2682
C	3.1224	-1.3314	-1.1177
C	2.9036	1.0050	-1.7770
C	2.0594	2.9535	2.5174
H	2.6681	1.7255	4.2299
H	1.1004	1.2834	3.5567
H	2.9818	-1.6307	2.7637
H	2.8849	-0.7159	4.2874
H	1.4168	-0.9918	3.3090
H	3.3739	-2.0239	-0.3127
H	3.8139	-1.4893	-1.9536
H	2.1022	-1.5299	-1.4508
H	3.6471	0.8868	-2.5741
H	1.9153	0.7658	-2.1726
H	2.9164	2.0385	-1.4241
C	0.5984	3.3957	2.2862
H	2.5742	2.8510	1.5571
H	2.6036	3.7179	3.0786
N	0.3963	4.7021	1.5519
H	0.0967	3.5043	3.2509
H	0.0780	2.6081	1.7251
C	0.8444	5.8589	2.3987
C	1.1535	4.7263	0.2546
H	0.6425	6.7869	1.8639
H	1.9177	5.7958	2.6050
H	0.2922	5.8513	3.3401
H	0.9195	3.8304	-0.3262
H	2.2329	4.7688	0.4299
H	0.8616	5.6150	-0.3100
Sc	-1.9130	4.9210	1.1503
O	-3.3690	8.5019	-0.6275
S	-2.7145	7.7209	0.6188
O	-1.2643	6.8617	0.3425
O	-3.5492	6.3829	1.2694
C	-2.3863	8.9956	2.1671
F	-3.4433	8.8710	3.0038
F	-1.2296	8.6080	2.7574
F	-2.2976	10.2362	1.6381
O	-3.1241	2.7539	4.6559
S	-3.2557	3.9769	3.6146
O	-3.4868	3.6021	1.9683
O	-1.8877	4.9578	3.3722
C	-4.8031	5.1899	4.1716
F	-4.3032	6.4396	4.3080
F	-5.7362	5.1189	3.1939
F	-5.2611	4.6968	5.3457

O^{MeAN}-2,6-F_2PhO$^-$ (axial)

Cu	0.1414	1.5823	-0.0012
Cu	-1.9607	-0.3691	-0.1008
O	-0.2307	-0.0846	-0.5730
O	-1.6497	1.3710	0.2622
N	5.5696	-1.8582	-1.8493
N	1.9422	1.6000	-0.9805
N	0.0556	3.4619	0.6334
C	5.2968	-2.3108	-3.2242
H	6.2366	-2.6049	-3.7025
H	4.8589	-1.5014	-3.8143
H	4.6065	-3.1763	-3.2554
C	6.2484	-2.9254	-1.0935
H	5.6318	-3.8399	-0.9967
H	6.4918	-2.5678	-0.0876
H	7.1815	-3.1956	-1.5988
C	4.3369	-1.4452	-1.1515
H	3.5660	-2.2432	-1.1952
H	4.5863	-1.3022	-0.0927
C	3.7493	-0.1234	-1.6780
H	4.5148	0.6525	-1.5696
H	3.5087	-0.2000	-2.7436
C	2.4857	0.2014	-0.8650
H	1.6714	-0.4723	-1.1430
H	2.6822	0.0613	0.1919
C	1.6369	1.9158	-2.4059
H	1.0903	2.8560	-2.4811
H	2.5562	1.9992	-2.9947
H	1.0191	1.1147	-2.8092
C	2.9359	2.5610	-0.3997
H	3.2302	2.1396	0.5638
H	3.8120	2.5885	-1.0581
C	2.4096	3.9817	-0.2011
H	2.0297	4.4082	-1.1360
H	3.2657	4.6063	0.0811
C	1.3876	4.0847	0.9280
H	1.2086	5.1368	1.1880
H	1.7730	3.5655	1.8078
C	-0.7079	4.2392	-0.3883
H	-0.1516	4.2839	-1.3247
H	-0.8884	5.2599	-0.0320
H	-1.6583	3.7330	-0.5618
C	-0.7261	3.4342	1.9130
H	-0.8074	4.4512	2.3135
H	-1.7128	3.0234	1.7110
H	-0.2023	2.7807	2.6097
H	4.0850	-2.2951	3.0988
C	3.0654	-1.9313	3.0407
C	1.9792	-2.7233	3.4438
C	2.8310	-0.6530	2.5590
C	0.6806	-2.2029	3.3295
H	2.1394	-3.7218	3.8317
C	1.5488	-0.0479	2.4032
F	3.9401	0.1027	2.1122
C	0.5106	-0.9209	2.8304
H	-0.1876	-2.7771	3.6337
O	1.3566	1.1408	1.9175
F	-0.8117	-0.4313	2.6917
H	-1.8802	-4.1975	0.3975
C	-2.0313	-3.1427	0.6616
N	-1.8651	-2.3272	-0.6018
C	-3.3645	-2.9809	1.3914
H	-1.2130	-2.8454	1.3243
C	-0.4835	-2.6332	-1.1056
C	-2.8673	-2.8021	-1.6329
C	-3.5551	-1.6107	2.0363
H	-3.3657	-3.7162	2.2052
H	-4.2124	-3.2510	0.7550
H	-0.4188	-3.6971	-1.3617
H	0.2380	-2.3863	-0.3295
H	-0.2561	-2.0241	-1.9753
H	-2.6864	-3.8789	-1.7553
H	-3.8637	-2.6960	-1.2079
C	-2.8430	-2.1310	-3.0154
N	-3.6540	-0.4585	1.0697
H	-4.4679	-1.6112	2.6471
H	-2.7102	-1.3973	2.6901
H	-1.8210	-2.0377	-3.3933
H	-3.3427	-2.8291	-3.6987
C	-3.5915	-0.7939	-3.1159
C	-4.9324	-0.5460	0.3057
C	-3.7039	0.7981	1.8873
N	-2.9565	0.2988	-2.3439
H	-3.6874	-0.5127	-4.1802
H	-4.6085	-0.9279	-2.7294
H	-4.9236	-1.3897	-0.3775
H	-5.0614	0.3683	-0.2647
H	-5.7751	-0.6574	0.9983
H	-2.7882	0.8814	2.4676
H	-3.7685	1.6545	1.2183
H	-4.5785	0.7679	2.5485
C	-1.6986	0.7330	-2.9896
C	-3.8429	1.4838	-2.2754
H	-1.8757	1.1146	-4.0084
H	-0.9816	-0.0851	-3.0254
H	-1.2597	1.5155	-2.3732
H	-4.8537	1.1912	-1.9864
H	-3.9108	2.0019	-3.2461
H	-3.4407	2.1711	-1.5260

O^{MeAN}-2,6-F_2PhO^- (equatorial)

Cu	0.6141	-0.1903	0.2319
Cu	-2.1301	-0.7921	-0.1100
O	-0.4825	-1.4856	-0.4231
O	-1.0420	0.4684	0.5843
N	-2.5840	0.7347	-2.1194
N	-3.7380	0.0217	0.8164
N	-2.9584	-2.4951	-0.7702
N	1.1784	-1.2789	2.2999
N	2.2439	-0.9325	-0.6851
N	7.2490	-0.1648	-1.0905
C	2.1591	-0.5625	3.1426
H	1.8706	0.4894	3.1831
H	3.1587	-0.6255	2.7091
H	2.1996	-0.9814	4.1627
C	-0.1354	-1.2476	2.9727
H	-0.1239	-1.7861	3.9351
H	-0.8762	-1.6992	2.3114
H	-0.4139	-0.2052	3.1341
C	1.5799	-2.6802	2.0381
H	1.8602	-3.1851	2.9801
H	0.6980	-3.1946	1.6401
C	2.7167	-2.8163	1.0159
H	3.6153	-2.2900	1.3548
H	2.9946	-3.8774	0.9756
C	2.3423	-2.4104	-0.4167
H	3.0724	-2.8287	-1.1210
H	1.3601	-2.8214	-0.6693
C	1.9342	-0.7348	-2.1367
H	1.8437	0.3353	-2.3317
H	2.7232	-1.1557	-2.7683
H	0.9880	-1.2285	-2.3567
C	3.4835	-0.1697	-0.3157
H	3.3077	0.8577	-0.6380
H	3.5320	-0.1372	0.7721
C	4.7997	-0.7079	-0.8966
H	4.7699	-0.7292	-1.9916
H	4.9742	-1.7326	-0.5537
C	5.9643	0.1964	-0.4590
H	6.0458	0.1865	0.6478
H	5.7361	1.2295	-0.7511
C	7.7509	-1.4644	-0.6105
H	7.0557	-2.2655	-0.8748
H	7.9012	-1.4813	0.4865
H	8.7103	-1.6809	-1.0911
C	8.2513	0.8858	-0.8391
H	8.4691	1.0209	0.2379
H	9.1867	0.6278	-1.3463
H	7.8942	1.8404	-1.2394
C	-3.6526	0.5510	-3.1245
H	-4.6372	0.5913	-2.6539
H	-3.5463	-0.4240	-3.6077
H	-3.6143	1.3265	-3.9087
C	-1.2652	0.6393	-2.7851
H	-0.4907	0.7661	-2.0307
H	-1.1467	-0.3467	-3.2390
H	-1.1382	1.4097	-3.5637
C	-2.6785	2.0813	-1.4917
H	-2.7364	2.8537	-2.2794
H	-1.7508	2.2333	-0.9394
C	-3.8419	2.2565	-0.5126
H	-3.8888	3.3245	-0.2625
H	-4.8051	2.0269	-0.9800
C	-3.6647	1.5346	0.8270
H	-4.4333	1.8799	1.5329
H	-2.6819	1.7793	1.2347
C	-3.5426	-0.4156	2.2380
H	-4.3575	-0.0401	2.8675
H	-2.5932	-0.0153	2.5872
H	-3.5186	-1.5024	2.3086
C	-5.0883	-0.4103	0.3294
H	-5.8379	-0.0173	1.0296
H	-5.2565	0.0666	-0.6359
C	-5.2630	-1.9190	0.1612
H	-5.0737	-2.4595	1.0936
H	-6.3188	-2.0967	-0.0737
C	-4.4422	-2.4835	-0.9961
H	-4.7529	-3.5128	-1.2182
H	-4.6206	-1.8819	-1.8915
C	-2.5800	-3.5204	0.2550
H	-2.9099	-4.5145	-0.0665
H	-3.0423	-3.2877	1.2138
H	-1.4961	-3.5015	0.3661
C	-2.2944	-2.8599	-2.0627
H	-2.5646	-2.1263	-2.8202
H	-2.6268	-3.8542	-2.3816
H	-1.2161	-2.8423	-1.9144
O	1.4680	1.3843	0.7790
C	0.7414	2.4887	0.6596
C	0.7226	3.2507	-0.5270
C	-0.0685	2.9946	1.6962
C	-0.0128	4.4134	-0.6933
F	1.4666	2.7479	-1.6054
C	-0.8309	4.1493	1.5823
F	-0.1029	2.2768	2.8946
C	-0.7997	4.8665	0.3774
H	0.0192	4.9404	-1.6385
H	-1.4353	4.4748	2.4199
H	-1.3879	5.7697	0.2707

$^{S}P^{MeAN}$-2,6-F_2PhO$^-$ (axial)

Cu	0.8072	1.6606	-0.7711
Cu	-1.9823	-0.3854	-0.6580
O	-0.1388	0.0703	-1.2209
O	-1.0688	1.2167	-1.3164
N	5.0996	-3.2509	0.1838
N	2.7314	1.0881	-1.0811
N	0.9513	3.6355	-0.7200
C	5.7230	-3.6139	-1.1001
H	6.6391	-4.1827	-0.9108
H	5.9950	-2.7157	-1.6606
H	5.0571	-4.2313	-1.7344
C	4.8392	-4.4628	0.9793
H	4.1324	-5.1568	0.4839
H	4.4200	-4.1830	1.9515
H	5.7788	-4.9985	1.1500
C	3.8505	-2.4884	-0.0068
H	3.1432	-3.0399	-0.6622
H	3.3677	-2.3946	0.9734
C	4.0760	-1.0727	-0.5680
H	4.8047	-0.5631	0.0721
H	4.4989	-1.1220	-1.5776
C	2.7328	-0.3290	-0.5768
H	2.0138	-0.8731	-1.1966
H	2.3325	-0.2839	0.4347
C	3.0498	1.1312	-2.5338
H	2.9455	2.1472	-2.9130
H	4.0715	0.7881	-2.7336
H	2.3403	0.4903	-3.0626
C	3.6556	1.9417	-0.2690
H	3.4413	1.7018	0.7759
H	4.6933	1.6594	-0.4900
C	3.4893	3.4544	-0.4849
H	3.6531	3.7247	-1.5338
H	4.2994	3.9421	0.0714
C	2.1748	4.0446	0.0445
H	2.2296	5.1428	0.0468
H	2.0140	3.6982	1.0686
C	0.9270	4.2134	-2.0932
H	1.8022	3.8951	-2.6577
H	0.9090	5.3099	-2.0510
H	0.0324	3.8542	-2.6064
C	-0.2663	4.0881	0.0197
H	-0.2585	5.1791	0.1390
H	-1.1498	3.7910	-0.5483
H	-0.2903	3.5979	0.9913
H	1.0033	-1.8003	4.5978
C	0.4991	-0.9208	4.2145
C	-0.6611	-0.4155	4.8210
C	1.0144	-0.2835	3.0962
C	-1.2711	0.7218	4.2711
H	-1.0809	-0.8975	5.6950
C	0.4609	0.8740	2.4704
F	2.1742	-0.8328	2.5060
C	-0.7098	1.3154	3.1505
H	-2.1731	1.1452	4.6975
O	0.9671	1.4646	1.4306
F	-1.3830	2.4276	2.5887
H	-2.0082	-2.8772	2.3097
C	-2.1202	-1.9188	1.7825
N	-1.8211	-2.1451	0.3221
C	-3.4925	-1.3120	2.0969
H	-1.3450	-1.2464	2.1553
C	-0.3806	-2.5431	0.2213
C	-2.6991	-3.2453	-0.2079
C	-3.6736	0.1379	1.6379
H	-3.5790	-1.3045	3.1900
H	-4.3095	-1.9482	1.7424
H	-0.2087	-3.4955	0.7384
H	0.2363	-1.7659	0.6726
H	-0.0924	-2.6355	-0.8231
H	-2.4791	-4.1521	0.3750
H	-3.7334	-2.9698	0.0060
C	-2.5780	-3.5693	-1.7049
N	-3.7053	0.3375	0.1484
H	-4.6040	0.5465	2.0585
H	-2.8500	0.7445	2.0109
H	-1.5496	-3.8378	-1.9649
H	-3.1662	-4.4820	-1.8627
C	-3.1294	-2.5073	-2.6703
C	-4.9615	-0.2382	-0.4097
C	-3.6887	1.8102	-0.1248
N	-2.3009	-1.2728	-2.7488
H	-3.2351	-2.9495	-3.6756
H	-4.1327	-2.2129	-2.3438
H	-4.9736	-1.3193	-0.2856
H	-5.0302	-0.0055	-1.4709
H	-5.8341	0.1885	0.1008
H	-2.7995	2.2419	0.3343
H	-3.6431	1.9724	-1.2027
H	-4.5878	2.2863	0.2855
C	-1.0154	-1.5545	-3.4395
C	-3.0032	-0.2221	-3.5277
H	-1.1951	-1.9499	-4.4518
H	-0.4249	-2.2774	-2.8772
H	-0.4365	-0.6338	-3.4936
H	-3.9898	-0.0339	-3.1024
H	-3.1337	-0.5127	-4.5815
H	-2.4167	0.6978	-3.4706

$^{S}P^{MeAN}$-2,6-F_2PhO$^-$ (equatorial)

Cu	1.0488	-0.2402	0.5185
Cu	-2.5113	-0.7575	-0.3081
O	-0.6804	-1.2976	-0.2793
O	-0.8686	-0.0832	0.5663
N	-2.5180	0.9286	-1.8527
N	-4.0448	-0.0820	0.8246
N	-3.3073	-2.4290	-1.1085
N	1.1784	-1.5511	2.1726
N	2.6180	-0.9017	-0.5585
N	7.5953	-0.0229	-1.1277
C	2.1459	-0.9474	3.1304
H	1.8111	0.0648	3.3656
H	3.1387	-0.8886	2.6857
H	2.2084	-1.5386	4.0551
C	-0.1516	-1.6314	2.8392
H	-0.0980	-2.2731	3.7304
H	-0.8735	-2.0299	2.1278
H	-0.4615	-0.6250	3.1187
C	1.5890	-2.9285	1.7660
H	1.7374	-3.5394	2.6705
H	0.7409	-3.3457	1.2128
C	2.8387	-3.0038	0.8786
H	3.7141	-2.5812	1.3830
H	3.0651	-4.0682	0.7409
C	2.6577	-2.3990	-0.5196
H	3.4498	-2.7551	-1.1901
H	1.7016	-2.7369	-0.9333
C	2.2494	-0.4580	-1.9397
H	2.1933	0.6313	-1.9501
H	2.9760	-0.8074	-2.6810
H	1.2663	-0.8665	-2.1835
C	3.8901	-0.2440	-0.1131
H	3.6981	0.8300	-0.1726
H	4.0301	-0.4801	0.9442
C	5.1614	-0.6173	-0.8904
H	5.0543	-0.3825	-1.9550
H	5.3493	-1.6932	-0.8083
C	6.3620	0.1701	-0.3392
H	6.5234	-0.0941	0.7267
H	6.1213	1.2407	-0.3674
C	8.1231	-1.3921	-0.9954
H	7.4042	-2.1192	-1.3819
H	8.3562	-1.6567	0.0544
H	9.0419	-1.4836	-1.5836
C	8.6196	0.9535	-0.7174
H	8.9171	0.8424	0.3432
H	9.5136	0.8279	-1.3370
H	8.2399	1.9703	-0.8626
C	-3.5147	0.9317	-2.9495
H	-4.5290	0.8878	-2.5484
H	-3.3628	0.0604	-3.5903
H	-3.4234	1.8361	-3.5720
C	-1.1491	0.8949	-2.4338
H	-0.4223	0.8744	-1.6232
H	-1.0317	-0.0120	-3.0313
H	-0.9594	1.7743	-3.0684
C	-2.6383	2.1733	-1.0398
H	-2.5578	3.0489	-1.7045
H	-1.7765	2.1874	-0.3730
C	-3.9072	2.2896	-0.1886
H	-3.9439	3.3230	0.1785
H	-4.8143	2.1592	-0.7875
C	-3.9171	1.4004	1.0599
H	-4.7342	1.7071	1.7301
H	-2.9729	1.5431	1.5949
C	-3.8453	-0.7489	2.1486
H	-4.5964	-0.4090	2.8733
H	-2.8471	-0.5038	2.5140
H	-3.9190	-1.8304	2.0474
C	-5.3998	-0.4078	0.2727
H	-6.1553	-0.1307	1.0227
H	-5.5572	0.2283	-0.6008
C	-5.6042	-1.8714	-0.1467
H	-5.4633	-2.5504	0.6999
H	-6.6599	-1.9707	-0.4267
C	-4.7794	-2.3234	-1.3601
H	-5.1458	-3.2963	-1.7185
H	-4.9087	-1.6009	-2.1724
C	-2.9830	-3.5571	-0.1867
H	-3.2895	-4.5154	-0.6251
H	-3.4909	-3.4279	0.7679
H	-1.9064	-3.5544	-0.0088
C	-2.5882	-2.6601	-2.3955
H	-2.7928	-1.8375	-3.0797
H	-2.9114	-3.6009	-2.8587
H	-1.5160	-2.6955	-2.1975
O	1.5388	1.6132	0.2156
C	0.7017	2.6017	0.4621
C	0.4638	3.6364	-0.4717
C	-0.0364	2.7399	1.6603
C	-0.3988	4.7011	-0.2555
F	1.1206	3.5344	-1.7053
C	-0.9247	3.7724	1.9221
F	0.1387	1.7363	2.6339
C	-1.1063	4.7718	0.9539
H	-0.5258	5.4472	-1.0306
H	-1.4560	3.7922	2.8660
H	-1.7904	5.5908	1.1387

O^{MeAN}-2,4-F_2PhO$^-$ (axial)

Cu	-0.2688	1.5821	-0.5742
Cu	1.8553	-0.0848	0.4230
O	0.0865	0.2609	0.5952
O	1.5382	1.3487	-0.6324
N	-5.6343	-1.3483	2.0613
N	-2.1413	1.8613	0.1932
N	-0.1666	3.1128	-1.8363
C	-5.8133	-0.8114	3.4210
H	-6.8300	-1.0266	3.7651
H	-5.6805	0.2737	3.4245
H	-5.1017	-1.2514	4.1470
C	-5.9286	-2.7917	2.0456
H	-5.2474	-3.3746	2.6955
H	-5.8393	-3.1753	1.0239
H	-6.9545	-2.9607	2.3891
C	-4.2737	-1.1017	1.5466
H	-3.5053	-1.5023	2.2412
H	-4.1703	-1.6539	0.6044
C	-3.9865	0.3845	1.2639
H	-4.7848	0.7687	0.6194
H	-4.0029	0.9621	2.1945
C	-2.6136	0.4861	0.5830
H	-1.8406	0.0744	1.2362
H	-2.6092	-0.0907	-0.3374
C	-1.9932	2.7232	1.4018
H	-1.4698	3.6462	1.1521
H	-2.9702	2.9806	1.8233
H	-1.4110	2.1783	2.1436
C	-3.1008	2.4530	-0.7926
H	-3.2615	1.6824	-1.5496
H	-4.0470	2.6493	-0.2746
C	-2.6137	3.7370	-1.4637
H	-2.3576	4.5069	-0.7277
H	-3.4571	4.1436	-2.0344
C	-1.4779	3.4962	-2.4548
H	-1.3054	4.3934	-3.0645
H	-1.7485	2.6690	-3.1144
C	0.4609	4.2515	-1.1013
H	-0.1918	4.5909	-0.2972
H	0.6496	5.0877	-1.7841
H	1.4017	3.9032	-0.6731
C	0.7472	2.6844	-2.9444
H	0.8431	3.4961	-3.6748
H	1.7186	2.4369	-2.5213
H	0.3164	1.7958	-3.4039
H	-2.3954	-4.0309	-2.1060
C	-1.6396	-3.2849	-2.3153
C	-0.3611	-3.6400	-2.7394
C	-1.9197	-1.9336	-2.1882
C	0.6065	-2.6825	-3.0238
F	-0.0518	-5.0038	-2.8891
C	-0.9896	-0.8750	-2.4225
F	-3.2260	-1.5849	-1.7779
C	0.2940	-1.3284	-2.8573
H	1.5825	-2.9974	-3.3759
O	-1.2899	0.3849	-2.2640
H	1.0359	-0.5651	-3.0629
H	1.7545	-3.8675	1.1300
C	1.9226	-2.9371	0.5718
N	1.6928	-1.7813	1.5208
C	3.2908	-2.9904	-0.1101
H	1.1435	-2.8611	-0.1935
C	0.2780	-1.9258	2.0047
C	2.6143	-1.9010	2.7132
C	3.5565	-1.8427	-1.0839
H	3.3024	-3.9134	-0.7022
H	4.1032	-3.0994	0.6146
H	0.1841	-2.8577	2.5742
H	-0.3914	-1.9378	1.1475
H	0.0047	-1.0794	2.6279
H	2.3872	-2.8677	3.1835
H	3.6364	-1.9642	2.3467
C	2.5286	-0.7956	3.7784
N	3.6848	-0.4849	-0.4482
H	4.4759	-2.0417	-1.6506
H	2.7317	-1.7739	-1.7941
H	1.4923	-0.6258	4.0842
H	3.0316	-1.1968	4.6672
C	3.2225	0.5321	3.4348
C	4.9028	-0.4435	0.4153
C	3.9000	0.5110	-1.5482
N	2.5736	1.2784	2.3291
H	3.2686	1.1576	4.3440
H	4.2566	0.3278	3.1378
H	4.7989	-1.0906	1.2789
H	5.0646	0.5748	0.7557
H	5.7762	-0.7666	-0.1637
H	3.0717	0.4593	-2.2505
H	3.9232	1.5130	-1.1223
H	4.8456	0.2941	-2.0590
C	1.2759	1.8406	2.7670
C	3.4144	2.4173	1.8902
H	1.4012	2.5326	3.6153
H	0.5830	1.0475	3.0425
H	0.8374	2.3691	1.9224
H	4.4363	2.0898	1.6948
H	3.4567	3.2129	2.6514
H	2.9897	2.8187	0.9664

O^{MeAN}-2,4-F_2PhO$^-$ (equatorial)

Cu	0.7178	-0.1390	0.1105
Cu	-1.9832	-0.9760	-0.0477
O	-0.2971	-1.5981	-0.3049
O	-0.9730	0.4534	0.3905
N	-2.5906	0.0875	-2.3097
N	-3.6187	-0.0980	0.7581
N	-2.7094	-2.8214	-0.3531
N	1.3537	-0.9638	2.3196
N	2.3963	-0.9095	-0.6916
N	7.3665	0.0490	-1.1366
C	2.2996	-0.1125	3.0722
H	1.9650	0.9232	2.9979
H	3.3019	-0.1819	2.6456
H	2.3589	-0.4103	4.1334
C	0.0429	-0.9381	2.9994
H	0.0852	-1.3981	4.0011
H	-0.6788	-1.4756	2.3830
H	-0.2842	0.0973	3.0839
C	1.8270	-2.3635	2.2156
H	2.1338	-2.7416	3.2078
H	0.9722	-2.9640	1.8865
C	2.9661	-2.5621	1.2083
H	3.8403	-1.9602	1.4781
H	3.2934	-3.6069	1.2866
C	2.5675	-2.3410	-0.2570
H	3.3152	-2.8004	-0.9159
H	1.6056	-2.8250	-0.4512
C	2.0919	-0.8997	-2.1561
H	1.9273	0.1314	-2.4766
H	2.9149	-1.3301	-2.7356
H	1.1857	-1.4819	-2.3226
C	3.5937	-0.0519	-0.4022
H	3.3764	0.9250	-0.8359
H	3.6261	0.1020	0.6758
C	4.9418	-0.5849	-0.9111
H	4.9287	-0.7212	-1.9982
H	5.1583	-1.5594	-0.4624
C	6.0575	0.4136	-0.5593
H	6.1229	0.5230	0.5433
H	5.7872	1.3989	-0.9601
C	7.9191	-1.1693	-0.5188
H	7.2652	-2.0250	-0.7061
H	8.0529	-1.0660	0.5756
H	8.8947	-1.3893	-0.9638
C	8.3163	1.1655	-0.9858
H	8.5116	1.4217	0.0733
H	9.2700	0.9002	-1.4537
H	7.9225	2.0558	-1.4872
C	-3.6721	-0.3378	-3.2239
H	-4.6459	-0.2534	-2.7369
H	-3.5263	-1.3820	-3.5133
H	-3.6938	0.2718	-4.1437
C	-1.2849	-0.0684	-2.9890
H	-0.5016	0.2103	-2.2861
H	-1.1320	-1.1115	-3.2740
H	-1.2097	0.5622	-3.8906
C	-2.7437	1.5229	-1.9457
H	-2.8652	2.1261	-2.8636
H	-1.8116	1.8255	-1.4655
C	-3.8943	1.8219	-0.9807
H	-4.0027	2.9141	-0.9410
H	-4.8509	1.4514	-1.3639
C	-3.6483	1.3886	0.4680
H	-4.4272	1.8171	1.1146
H	-2.6788	1.7709	0.7911
C	-3.3591	-0.2286	2.2302
H	-4.1814	0.2162	2.8023
H	-2.4292	0.2898	2.4554
H	-3.2609	-1.2760	2.5138
C	-4.9475	-0.7008	0.4153
H	-5.7041	-0.2286	1.0563
H	-5.1737	-0.4307	-0.6162
C	-5.0205	-2.2216	0.5453
H	-4.7655	-2.5577	1.5549
H	-6.0675	-2.5084	0.3940
C	-4.1960	-2.9452	-0.5170
H	-4.4417	-4.0152	-0.5286
H	-4.4407	-2.5376	-1.5016
C	-2.2340	-3.6082	0.8297
H	-2.5142	-4.6619	0.7208
H	-2.6738	-3.2192	1.7478
H	-1.1502	-3.5121	0.8831
C	-2.0576	-3.3812	-1.5797
H	-2.4016	-2.8236	-2.4487
H	-2.3261	-4.4377	-1.6930
H	-0.9796	-3.2640	-1.4820
O	1.4580	1.5651	0.3517
C	0.5972	2.5838	0.2817
C	0.3889	3.2994	-0.9197
C	-0.1537	3.0074	1.4004
C	-0.5184	4.3580	-0.9984
H	0.9467	2.9827	-1.7935
C	-1.0703	4.0479	1.3610
F	0.0266	2.3444	2.6165
C	-1.2366	4.7028	0.1439
H	-0.6803	4.8978	-1.9227
H	-1.6339	4.3314	2.2393
F	-2.1660	5.7440	0.0726

$^{S}P^{MeAN}$-2,4-F_2PhO$^-$ (axial)

Cu	0.9312	1.8239	-0.0014
Cu	-1.9594	0.0943	-0.8642
O	-0.0556	0.6053	-1.0904
O	-0.9273	1.7509	-0.7462
N	5.0978	-3.1884	-0.9970
N	2.8418	1.3612	-0.5196
N	1.1352	3.6260	0.8051
C	5.7854	-3.0131	-2.2876
H	6.6823	-3.6405	-2.3087
H	6.0993	-1.9739	-2.4155
H	5.1473	-3.2925	-3.1489
C	4.7851	-4.6113	-0.7804
H	4.1006	-5.0212	-1.5484
H	4.3162	-4.7406	0.2007
H	5.7098	-5.1975	-0.8007
C	3.8663	-2.3792	-0.9149
H	3.1811	-2.6092	-1.7586
H	3.3430	-2.6678	0.0050
C	4.1297	-0.8633	-0.8673
H	4.8634	-0.6666	-0.0774
H	4.5622	-0.5201	-1.8137
C	2.8053	-0.1408	-0.5811
H	2.0714	-0.3964	-1.3519
H	2.4030	-0.4681	0.3764
C	3.1529	1.9394	-1.8546
H	3.0742	3.0259	-1.8232
H	4.1633	1.6734	-2.1858
H	2.4219	1.5609	-2.5729
C	3.7917	1.8238	0.5401
H	3.5742	1.2150	1.4223
H	4.8207	1.6181	0.2172
C	3.6681	3.3098	0.9111
H	3.8311	3.9509	0.0379
H	4.4956	3.5336	1.5956
C	2.3746	3.6853	1.6466
H	2.4599	4.6981	2.0662
H	2.2114	2.9788	2.4647
C	1.1158	4.6804	-0.2478
H	1.9793	4.5792	-0.9037
H	1.1267	5.6802	0.2043
H	0.2095	4.5587	-0.8449
C	-0.0612	3.7927	1.6829
H	-0.0232	4.7533	2.2116
H	-0.9590	3.7522	1.0643
H	-0.0766	2.9687	2.3953
H	0.3841	-3.4925	3.3489
C	0.0680	-2.4588	3.3980
C	-1.0010	-2.0573	4.1953
C	0.7084	-1.4837	2.6485
C	-1.4144	-0.7305	4.2485
F	-1.6789	-3.0258	4.9544
C	0.3651	-0.0980	2.6310
F	1.7627	-1.9149	1.8125
C	-0.7388	0.2239	3.4805
H	-2.2509	-0.4510	4.8785
O	1.0124	0.7907	1.9257
H	-1.0515	1.2614	3.5179
H	-2.2896	-3.3792	0.8109
C	-2.3076	-2.2834	0.7223
N	-1.9525	-1.9160	-0.6951
C	-3.6411	-1.7406	1.2483
H	-1.5044	-1.8899	1.3473
C	-0.5356	-2.3484	-0.9225
C	-2.8680	-2.6297	-1.6507
C	-3.6875	-0.2173	1.4075
H	-3.7655	-2.1632	2.2527
H	-4.4921	-2.1101	0.6678
H	-0.4552	-3.4411	-0.8594
H	0.1057	-1.8929	-0.1680
H	-0.1964	-2.0117	-1.8993
H	-2.7319	-3.7102	-1.4942
H	-3.8934	-2.3912	-1.3622
C	-2.6881	-2.3124	-3.1435
N	-3.6859	0.5528	0.1168
H	-4.5804	0.0711	1.9809
H	-2.8088	0.1083	1.9704
H	-1.6659	-2.5298	-3.4678
H	-3.3228	-3.0274	-3.6818
C	-3.1191	-0.9058	-3.5905
C	-4.9561	0.3084	-0.6247
C	-3.6003	2.0119	0.4377
N	-2.2187	0.1838	-3.1217
H	-3.1919	-0.8802	-4.6910
H	-4.1208	-0.6979	-3.1995
H	-5.0156	-0.7267	-0.9537
H	-4.9980	0.9561	-1.4992
H	-5.8189	0.5280	0.0169
H	-2.6949	2.1942	1.0155
H	-3.5359	2.5784	-0.4923
H	-4.4795	2.3336	1.0093
C	-0.9157	0.1272	-3.8339
C	-2.8223	1.5119	-3.3980
H	-1.0600	0.2279	-4.9211
H	-0.4060	-0.8145	-3.6313
H	-0.2789	0.9295	-3.4634
H	-3.8111	1.5777	-2.9417
H	-2.9286	1.6958	-4.4782
H	-2.1822	2.2792	-2.9566

$^{S}P^{MeAN}$-2,4-F_2PhO$^-$ (equatorial)

Cu	1.1577	-0.1648	0.4756
Cu	-2.4025	-0.9449	-0.2714
O	-0.5527	-1.4133	-0.2349
O	-0.7634	-0.1054	0.4452
N	-2.5034	0.5001	-2.0440
N	-3.9395	-0.1464	0.7752
N	-3.1714	-2.7318	-0.8111
N	1.2872	-1.3099	2.2348
N	2.7691	-0.8885	-0.5116
N	7.6979	0.1969	-1.1596
C	2.2199	-0.5869	3.1443
H	1.8433	0.4272	3.2891
H	3.2141	-0.5261	2.7033
H	2.2950	-1.0935	4.1167
C	-0.0511	-1.3715	2.8880
H	0.0078	-1.9313	3.8323
H	-0.7485	-1.8518	2.2038
H	-0.3941	-0.3551	3.0749
C	1.7466	-2.7075	1.9723
H	1.8827	-3.2239	2.9355
H	0.9267	-3.1982	1.4378
C	3.0248	-2.8295	1.1334
H	3.8718	-2.3317	1.6174
H	3.2866	-3.8945	1.1078
C	2.8667	-2.3716	-0.3212
H	3.6929	-2.7588	-0.9306
H	1.9380	-2.7884	-0.7251
C	2.4045	-0.6106	-1.9360
H	2.3281	0.4686	-2.0691
H	3.1451	-1.0260	-2.6279
H	1.4318	-1.0640	-2.1398
C	4.0088	-0.1391	-0.1239
H	3.7610	0.9182	-0.2481
H	4.1701	-0.3039	0.9441
C	5.2915	-0.4910	-0.8928
H	5.1776	-0.2791	-1.9615
H	5.5112	-1.5591	-0.7902
C	6.4676	0.3425	-0.3565
H	6.6514	0.0848	0.7074
H	6.1863	1.4033	-0.3817
C	8.2714	-1.1554	-1.0458
H	7.5730	-1.9017	-1.4333
H	8.5227	-1.4226	-0.0008
H	9.1872	-1.2109	-1.6429
C	8.6937	1.2031	-0.7514
H	9.0069	1.0921	0.3047
H	9.5842	1.1133	-1.3822
H	8.2787	2.2079	-0.8824
C	-3.5347	0.3281	-3.0937
H	-4.5349	0.3414	-2.6571
H	-3.3945	-0.6306	-3.5981
H	-3.4739	1.1266	-3.8505
C	-1.1541	0.3937	-2.6599
H	-0.4030	0.5237	-1.8812
H	-1.0319	-0.5993	-3.0981
H	-1.0110	1.1538	-3.4438
C	-2.6161	1.8492	-1.4184
H	-2.5726	2.6196	-2.2061
H	-1.7316	1.9688	-0.7932
C	-3.8593	2.0747	-0.5504
H	-3.8885	3.1474	-0.3184
H	-4.7832	1.8691	-1.1006
C	-3.8332	1.3561	0.8037
H	-4.6433	1.7400	1.4419
H	-2.8829	1.5801	1.2969
C	-3.7248	-0.6181	2.1782
H	-4.4807	-0.1951	2.8525
H	-2.7313	-0.3048	2.5012
H	-3.7770	-1.7041	2.2292
C	-5.2903	-0.5693	0.2827
H	-6.0488	-0.1961	0.9867
H	-5.4594	-0.0717	-0.6743
C	-5.4714	-2.0823	0.0864
H	-5.3115	-2.6261	1.0226
H	-6.5272	-2.2401	-0.1650
C	-4.6482	-2.6953	-1.0550
H	-4.9968	-3.7184	-1.2580
H	-4.8023	-2.1071	-1.9652
C	-2.8104	-3.7068	0.2594
H	-3.1022	-4.7248	-0.0287
H	-3.3066	-3.4489	1.1940
H	-1.7315	-3.6580	0.4155
C	-2.4631	-3.1334	-2.0617
H	-2.6932	-2.4222	-2.8543
H	-2.7724	-4.1375	-2.3789
H	-1.3881	-3.1189	-1.8771
O	1.5475	1.6585	-0.0782
C	0.6613	2.6303	0.0864
C	0.4197	3.6016	-0.9170
C	-0.1046	2.7774	1.2682
C	-0.5484	4.5992	-0.7667
H	0.9949	3.5262	-1.8324
C	-1.0848	3.7400	1.4502
F	0.1204	1.8628	2.3148
C	-1.2947	4.6378	0.4065
H	-0.7384	5.3205	-1.5520
H	-1.6606	3.7877	2.3647
F	-2.3094	5.5962	0.5462

5. References.

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