Electronic Supporting Information for:

Encapsulation of synthetic tricopper cluster in a synthetic cryptand enables facile redox processes from Cu\textsuperscript{i}Cu\textsuperscript{i}Cu\textsuperscript{i} to Cu\textsuperscript{ii}Cu\textsuperscript{ii}Cu\textsuperscript{ii} states

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1. Materials and Methods

**General**: All reactions were carried out under a nitrogen atmosphere in an MBraun glovebox or using Schlenk techniques.

**Instrumentation**: Nuclear magnetic resonance (NMR) spectra were recorded on DXP 400 MHz (\textsuperscript{1}H: 400 MHz) and AVIII 600 MHz (\textsuperscript{1}H: 600 MHz) at ambient temperature. Chemical shift values for protons were referenced to the residual proton resonance of acetone-\textsubscript{d}\textsubscript{6} (\textdelta: 2.05 ppm) and tetrahydrofuran-\textsubscript{d}\textsubscript{8} (THF-\textsubscript{d}\textsubscript{8}, \textdelta: 1.72 ppm and 3.58 ppm). X-ray crystallographic analyses were performed under a cold nitrogen stream (Oxford Cryosystems Cryostream) at 100 K (4a, 4b, 4c, 4a-BAR\textsubscript{6}) on a Bruker D8 Venture instrument with Mo Ka ra-
diation source (λ = 0.7107 Å) and a Photon II detector. Elemental analyses were performed by Midwest Micro Lab (Indianapolis, IN, http://midwestlab.com/). ESI mass spectra were recorded on a Bruker MicrOTOF. EPR measurements were performed in 4 mm low-pressure quartz tubes on a Bruker EMXPlus X-band EPR spectrometer equipped with a Coldedge cryostat with small-volume power saturation. Solid-state IR was recorded on a Bruker Alpha II FTIR spectrometer. Cyclic voltammogram was performed using Bio-Logic SAS SP-50 with a glassy carbon working electrode, a platinum wire counter electrode and a Ag/Ag⁺ reference electrode (a commercial leakless miniature Ag/AgCl reference is used for aqueous solution and a Ag/AgNO₃ (0.01 M) reference electrode is used for organic solution).

Materials: Anhydrous acetone and anhydrous methanol were purchased from Acros and Alfa Aesar, respectively, and were used as received. Dichloromethane, acetonitrile, diethyl ether, tetrahydrofuran, and fluorenbene were dried and degassed under nitrogen using a Pure Process Technologies (PPT, Nashua, NH) solvent purification system, and stored over 4 Å molecular sieves. Acetone-d₅ (Cambridge Isotope Laboratories, Inc.) was purified by distillation, deoxygenated by three freeze-pump-thaw cycles, and dried over 4 Å molecular sieves prior to use. Tetrahydrofuran-d₅ (Cambridge Isotope Laboratories, Inc.) was deoxygenated by three freeze-pump-thaw cycles and dried over 4 Å molecular sieves prior to use. Tetraakis(acetonitrile)copper(I) hexafluorophosphate (Sigma-Aldrich), paraformaldehyde (Acros), tris(2-aminoethyl) amine (TREN, TCI), cobaltocene (Strem), tetrabutylammonium tetrafluoroborate (Sigma-Aldrich), tetra-n-butylammonium chloride (Combi-Blocks), decamethylferrocene (Sigma-Aldrich), silver hexafluorophosphate (Strem), iodine (VWR), sodium iodide (Sigma-Aldrich), triazabicyclocdecene (TBD, Sigma-Aldrich), dioxygen (Praxair), and ¹⁸O-dioxygen (Sigma-Aldrich) were purchased and used without further purification. Sodium tetrakis[3,5-trifluoromethyl]phenylborate was prepared by a published method.¹ AcOH (glacial, Fisher) and heptane (anhydrous, Alfa Aesar) were deoxygenated by three freeze-pump-thaw cycles before use.

**Synthesis and characterization of [TREN₂Cu⁴Cu⁴Cu⁴(μ₂-OH)][PF₆]₃ (4b)**

Tetrakis(acetonitrile)copper(I) hexafluorophosphate (93.3 mg, 0.251 mmol), paraformaldehyde (150 mg, 5.0 mmol), and acetonitrile (10 mL) were added to a 20 mL scintillation vial equipped with a septum under nitrogen atmosphere. Tris(2-aminoethyl) amine (TREN, 0.150 mL, 1.00 mmol) was injected with a syringe. Four other vials with the same suspension were prepared in parallel. The five vials were sealed and heated at 80 °C with vigorous stirring for two days, during which the solution turned dark brown. After the reaction, the solution was allowed to cool down and transferred back to the glovebox. The dark brown suspension from five vials was combined and filtered under a nitrogen atmosphere. The brown filtrate was dried under vacuum to afford an orange oil-like residue. Dichloromethane (10 mL) was added to the residue, and the resulting suspension was allowed to sit overnight at room temperature to yield a mixture of a blue solid and a yellow solid, which was collected by filtration and washed with additional dichloromethane (ca. 10 mL), and extracted into acetone (15 mL). The acetone solution was filtered, and all volatiles were removed under vacuum to yield a blue solid. The product was reashed with dichloromethane (ca. 10 mL) and dried under vacuum to afford 106.8 mg of 4b (18% yield). Single crystals of 4b suitable for X-ray diffraction were obtained by diffusing diethyl ether to an acetone solution of 4b at ~30 °C. Elemental analysis, Calcd for C₉₆H₇₃Cu₁₂F₁₃N₁₆O₆P₇: C, 31.52; H, 5.36; N, 16.34. found C, 31.75; H, 5.39; N, 16.06.

Infrared spectrum (ATR), νOH = 3440 cm⁻¹ (Fig. 6); UV-Vis spectrum (acetone, Fig. S1), λmax = 655 nm (800 M⁻¹cm⁻¹), 790 nm (870 M⁻¹cm⁻¹);
ESI-MS spectrum (Fig. S2), M/z = 312.2;
EPR spectrum (acetonitrile, 50 K, Fig. S16), g₁ = 2.14, g₂ = 2.25, g₃ = 2.01, A₃ = 146 MHz.

Fig. S1. (A) UV-Vis spectra of \([\text{TREN}_4\text{Cu}^0\text{Cu}^I\text{Cu}^{III}(\mu_3\text{-OH})]\)(PF₆)₃ (4b) at various concentration in acetone at room temperature; Beer’s law plots for the peak at 790 nm (B, ε = 870 M⁻¹cm⁻¹) and 655 nm (C, ε = 800 M⁻¹cm⁻¹).

Fig. S2. ESI-MS spectrum (MeCN) and simulation of \([\text{TREN}_4\text{Cu}^0\text{Cu}^I\text{Cu}^{III}(\mu_3\text{-OH})]\)(PF₆)₃.

Synthesis and characterization of \([\text{TREN}_4\text{Cu}^0\text{Cu}^I\text{Cu}^{III}(\mu_3\text{-OH})]\)(BArF)₄ (4b-BArF₄)

\[
\begin{align*}
\text{[TREN}_4\text{Cu}^0\text{Cu}^I\text{Cu}^{III}(\mu_3\text{-OH})]\text{(PF}_6\text{)}₃ & \xrightarrow{6 \text{ equiv. TBACl acetone}} \text{[TREN}_4\text{Cu}^0\text{Cu}^I\text{Cu}^{III}(\mu_3\text{-OH})]\text{Cl}_3 \downarrow + \text{TBA PF}_6 \\
\text{NaCl} \downarrow + \text{[TREN}_4\text{Cu}^0\text{Cu}^I\text{Cu}^{III}(\mu_3\text{-OH})]\text{(BArF)}₄ & \xleftarrow{4 \text{ equiv. NaBArF}} \text{dichloromethane}
\end{align*}
\]

Yield: 95.7%

To an acetone (1 mL) solution of tetra-n-butyrammonium chloride (60.8 mg, 0.219 mmol), an acetone (4 mL) solution of \([\text{TREN}_4\text{Cu}^0\text{Cu}^I\text{Cu}^{III}(\mu_3\text{-OH})]\)(PF₆)₃ (40.0 mg, 0.0292 mmol) was added dropwise with stirring. A blue precipitate was formed immediately and collected by filtration. After being washed by acetone (ca. 2 mL), the blue solid was dried under vacuum. Then, a dichloromethane (3 mL) suspension of the obtained blue solid was added to a dichloromethane (2 mL) suspension of sodium tetrakis[(3,5-trifluoromethyl)phenyl]borate (103.5 mg, 0.117 mmol). The mixture was allowed to stir at room temperature overnight. After filtration, the blue filtrate was collected and dried under vacuum. The obtained blue solid was washed with diethyl ether (ca. 3 mL, three times) and dried under vacuum to afford the desired product 4b-BArF₄ (98.3 mg, 96% yield).

Elemental analysis, Calcd for C₁₃₂H₁₀₉B₄Cu₃F₇₂N₁₆O C, 44.96; H, 3.12; N, 6.36. found C,
Synthesis and characterization of \([\text{TREN}_4\text{Cu}^1\text{Cu}^1\text{Cu}^1(\mu_3-\text{OH})](\text{PF}_6)_2\) (4a)

To an acetone (6 mL) solution of \([\text{TREN}_4\text{Cu}^1\text{Cu}^1\text{Cu}^1(\mu_3-\text{OH})](\text{PF}_6)_3\) (4b, 40.0 mg, 0.0292 mmol), an acetone (2 mL) solution of CoCp \(_2\) (6.1 mg, and 0.0321 mmol, 1.1 eq) was added under nitrogen atmosphere. The mixture was stirred at room temperature for five minutes, during which the color of the solution turns yellow. All volatiles were removed under vacuum, and the yielded yellow residue was washed by THF \((ca. 15\text{ mL})\). After dried under vacuum, the solid was dissolved in acetone \((ca. 1.5\text{ ml})\). Slow diffusion of diethyl ether to the acetone solution at \(-30^\circ\text{C}\) afford colorless crystals of 4a (6.7 mg, yield 19%) suitable for XRD (Fig. S11). \(^1\)H NMR analysis of the crystals (Fig. S3) shows a mixture of 4a (marked with blue dots) and a small amount of impurity that appears to be the protonated species \([4a+\text{H}]\) with sharp resonances at 9.20, 4.34, 3.30, 2.72, 2.45, and 2.36 ppm (marked with red dots, Fig. S3). We believe that the protonation of 4a was due to the residual water in acetone-\(d_6\), which cannot be completely removed without causing the decomposition of acetone-\(d_6\). Unfortunately, we were unable to obtain a solution of 4a in THF-\(d_8\) due to its low solubility. Other NMR solvents, e.g. acetonitrile-\(d_3\), cause rapid decomposition of 4a back to 4b. To confirm these sharp resonances (9.20, 4.34, 3.30, 2.72, 2.45, and 2.36 ppm) are from protonated 4a, we prepared the \(\text{BARF}_4\) analog 4a-\(\text{BARF}_4\), which can be dissolved and analyzed in THF-\(d_8\) \((\text{infra vide})\).

Infrared spectrum, vOH = 3516 cm\(^{-1}\) (Fig. 6).

Fig. S3. \(^1\)H NMR spectrum (600 MHz, acetone-\(d_6\)) of 4a (blue dots). The peaks marked with green dots are from residual diethyl ether. The peaks marked with red dots are from protonated 4a.
Fig. S4. UV-Vis spectrum of $[\text{TREN}_4\text{Cu}^I\text{Cu}^I\text{Cu}^I(\mu_3\text{-OH})](\text{PF}_6)_2$ (4a) in acetone at room temperature. The UV-Vis sample was generated in-situ from the treatment of $[\text{TREN}_4\text{Cu}^I\text{Cu}^I\text{Cu}^I(\mu_3\text{-OH})](\text{PF}_6)_3$ (4b) with one equivalent of Cp$_2$Co.

Fig. S5. ESI-MS spectrum (MeCN) and simulation of $[\text{TREN}_4\text{Cu}^I\text{Cu}^I\text{Cu}^I(\mu_3\text{-OH})](\text{PF}_6)_2$ (4a).

**Synthesis and characterization of $[\text{TREN}_4\text{Cu}^I\text{Cu}^I\text{Cu}^I(\mu_3\text{-OH})](\text{BAr}_4^F)_2$ (4a-BAr$^F_4$)**

$[\text{TREN}_4\text{Cu}^I\text{Cu}^I\text{Cu}^I(\mu_3\text{-OH})](\text{BAr}_4^F)_3 + \text{Cp}_2\text{Co}$ $\xrightarrow{\text{Fluorobenzene}} [\text{TREN}_4\text{Cu}^I\text{Cu}^I\text{Cu}^I(\mu_3\text{-OH})](\text{BAr}_4^F)_2$

| 1 equiv. |
| 2.4 equiv. |

Yield: 50.5%

To a suspension of 4b-BAr$^F_4$ (10.0 mg, 0.00284 mmol) in fluorobenzene (1 mL), a dichloromethane (0.2 mL) solution of Cp$_2$Co (1.3 mg, 0.0068 mmol) was added with stirring. The blue 4b-BAr$^F_4$ was gradually dissolved and the solution turned yellow. After filtration, the yellow filtrate was allowed to sit at room temperature overnight. Colorless needle-like crystals of 4a-BAr$^F_4$ suitable for single-crystal X-ray diffraction were obtained. The mother liquid was pipetted out and the crystals were washed by fluorobenzene (ca. 5 mL) for three times. The obtained white solid was dissolved in THF (1.5 mL) and treated with triazabicyclodecene (2.0 mg, 0.014 mmol). After about one minute, the resulting suspension was filtered, and the filtrate was dried under vacuum. The obtained solid was washed with fluorobenzene (ca. 8 mL, five times) and dried under vacuum to afford 4a-BAr$^F_4$ (3.8 mg, 51 % yield). (Fig. S12). $^1$H NMR (600 MHz, THF-$d_8$, Fig. S6) δ 7.79 (br, 16H), 7.58 (br, 8H), 3.98 (br, 12H), 3.28 (br,
12H), 2.92 (br, 12H), 2.44 (br, 12H), 2.19 (br, 24H), 1.35 (s, 1H); 
Elemental analysis, Calcd for C_{10}H_{9}B_{2}Cu_{3}F_{28}N_{16}O: C, 45.10; H, 3.67; N, 8.42. found C, 45.17; H, 3.84; N, 8.45.

Fig. S6. ^1^H NMR spectrum (600 MHz, THF-d$_8$) of 4a-BAr$_F^4$. The peaks marked with blue dots are from residual fluorobenzene. The peaks marked with green spots are from residual THF.

**Synthesis and characterization of [TREN$_4$Cu$^I$Cu$^{II}$Cu$^{II}$($\mu_3$-OH)] (PF$_6$)$_4$ (4c)**

To an acetone (3 mL) solution of [TREN$_4$Cu$^I$Cu$^{II}$Cu$^{II}$($\mu_3$-OH)] (PF$_6$)$_3$ (20.0 mg, 0.0140 mmol), an acetone (4 mL) solution of decamethylferrocenium hexafluorophosphate (9.4 mg, 0.020 mmol) was added under nitrogen atmosphere. The mixture was allowed to stir at room temperature for ten minutes. The solution was dried under vacuum and the yielded solid was re-dissolved in acetone (ca. 1 mL). THF (ca. 15 mL) was then added to the acetone solution with stirring. The obtained suspension was filtered and the dark blue precipitate was collected and dried under vacuum to afford 4c (10.6 mg, 50 % yield) as a dark blue powder.

Elemental analysis, Calcd for 4c•(CH$_3$C(O)CH$_3$)$_2$: C$_{42}$H$_{85}$Cu$_3$F$_{22}$N$_{16}$OP$_4$: C, 30.90; H, 5.25; N, 13.73. found C, 30.05; H, 5.26; N, 13.70.

UV-Vis spectrum (acetone, Fig. S7), $\lambda_{\text{max}}$ = 680 nm (970 M$^{-1}$cm$^{-1}$), 850 nm (1250 M$^{-1}$cm$^{-1}$); Infrared spectrum, vOH = 3372 cm$^{-1}$ (Fig. 6).
Fig. S7. UV-Vis spectrum of [TREN₄CuᴵCuᴵᴵ(µ₃-OH)](PF₆)₄ in acetonitrile at room temperature. Two maxima at 680 nm and 850 nm were observed.

In order to obtain crystals of [TREN₄CuᴵCuᴵᴵ(µ₃-OH)]²⁺ for single-crystal X-ray diffraction analysis, [TREN₄CuᴵCuᴵᴵ(µ₃-OH)](PF₆)₄ (10.0 mg, 0.00659 mmol) and tetra-n-butylammonium tetrafluoroborate (TBABF₄, 2.0 mg, 0.0060 mmol) was dissolved in acetone (ca. 1 mL). Slow diffusion of diethyl ether to the mixture of [TREN₄CuᴵCuᴵᴵ(µ₃-OH)](PF₆)₄ and TBABF₄ at −30°C afford single crystals of [TREN₄CuᴵCuᴵᴵ(µ₃-OH)](PF₆)(BF₄)₃ (Fig. S13).

Fig. S8. ¹H NMR (400 MHz, CD₃CN) spectrum of [TREN₄CuᴵCuᴵᴵ(µ₃-OH)](PF₆)₄ (4c).
The peak marked with a red dot is from residual CD$_2$HCN from the NMR solvent. The peak marked with a green dot is from residual acetone. The peak marked with a green dot is from residual water.

**Synthesis and characterization of decamethylferrocenium hexafluorophosphate**

\[
\text{Me}_{10}\text{Fc} + \text{AgPF}_6 \xrightarrow{\text{acetone, N}_2, \text{room temperature}} \text{Me}_{10}\text{Fc}^+\text{PF}_6^- + \text{Ag}
\]

Yield: 80%

To an acetone suspension (5 mL) of decamethylferrocene (154.6 mg, 0.4738 mmol), an acetone solution (2 mL) of AgPF$_6$ (100.0 mg, 0.3955 mmol) was added dropwise with stirring. The obtained mixture was allowed to stir at room temperature for three hours. After filtration, the green filtrate was collected and dried under vacuum. The green-yellow solid was then dissolved in acetone (ca. 5 mL). Diethyl ether (ca. 15 mL) was added to the acetone solution to precipitate out the product. The green solid was collected with filtration and dried under vacuum.

Block crystals of the product were obtained by diffusing diethyl ether into an acetone solution (5 mL) at room temperature overnight (149.9 mg, Yield 80.3%).

Elemental analysis, Calcd for C$_{20}$H$_{30}$F$_6$FeP: C, 50.97; H, 6.42 found C, 51.42; H, 6.38.
2. UV-Vis spectroscopy Studies Details

Determining the molar extinction coefficient of NaI3 in an acetone/heptane (2:3) mixture

\[ \text{NaI} + I_2 \rightarrow \text{NaI}_3 \]

**Fig. S9.** Solutions of NaI with various concentrations were prepared by adding a solution of I2 (0.2 mL, 1.2 mM) to NaI (2 mL, 50 mM, excess) in acetone/heptane (2:3) sequentially. The UV-Vis traces of the solutions were recorded at 0.0109 mM (trace 1), 0.0200 mM (trace 2), 0.0277 mM (trace 3), 0.0343 mM (trace 4), and 0.0400 mM (trace 5). The molar extinction coefficient of NaI3 at 364 nm was calculated as \(2.13 \times 10^4\) cm\(^{-1}\)M\(^{-1}\).

**Quantification of H\(_2\)O\(_2\) produced from the reaction of 4a and O\(_2\):**

\[
\begin{align*}
\text{A} & \quad \text{Cu}_3(\text{I,II}) \quad 1 \text{ eq CoCp}_2 \quad \text{C} & \quad \text{Cu}_3(\text{I,I}) \quad \text{excess O}_2 \quad \text{Cu}_3(\text{I,II}) \\
\text{trace 1} & \quad \text{trace 2} & \quad \text{H}_2\text{O}_2 & \quad \text{H}_2\text{O} \\
\text{B} & \quad \text{H}_2\text{O}_2 + 3 \text{ NaI} + 2 \text{ H}^+ \rightarrow 2 \text{ H}_2\text{O} + I_3^- + 3 \text{ Na}^+ \\
\text{trace 6} & \quad \text{trace 5} & \quad \text{trace 4} \\
\end{align*}
\]

**Scheme S1.** (A) H\(_2\)O\(_2\) quantification from the stoichiometric reaction between 4a and O\(_2\). (B) The reaction of H\(_2\)O\(_2\) and NaI.

In glovebox, an acetone solution of \([\text{TREN}]_4\text{Cu}^\text{II}\text{Cu}^\text{II}(\mu_\text{-OH})(\text{PF}_6)_3\) (4b, 1.4 mg, 1.0 \(\mu\)mol, 2.00 mL, 0.5 mM) was transferred to a Schlenk quartz cuvette. The cuvette was sealed and transferred to the UV-Vis spectrometer (Fig. S9, trace 1). Under nitrogen protection, an ace-
A toluene solution of Cp₂Co (0.19 mg, 1.0 μmol, 0.500 mL acetone) and acetic acid (0.30 mg, 20.5 μmol, 5 equiv., 0.500 mL acetone) were injected to the cuvette. The 790 nm and 655 nm bands of complex 4b (CuII/Cu/CuI) were bleached instantaneously (Fig. S10, trace 2, Scheme 1), indicating the formation of complex 4a (CuI/Cu/CuI). Oxygen gas (0.500 mL, 20.5 μmol, 20.5 equiv.) was injected to the cuvette (Fig. S10, trace 3). The progress of oxygen reduction reaction was monitored by taking a UV-Vis spectrum every 60 seconds. Two bands at 790 nm and 655 nm grew in over 5 minutes, indicating the reformation of complex 4b (CuII/Cu/CuI) in 96% spectroscopic yield. The solution in the Schlenk quartz cuvette was purged with N₂ for five minutes to remove the excess oxygen (Fig. S10, trace 4). The cuvette was sealed and transferred back into glovebox. The solution in cuvette was transferred to a scintillation vial. Additional acetone (0.354 mL, calculated based on absorbance increase at 790 nm after purging) was added to the scintillation vial in order to compensate the solvent loss during the N₂ purging process. To the combined acetone solution, heptane (6 ml) was added in order to precipitate all the copper complexes. The obtained suspension was then filtered, and the filtrate (2 mL) was transferred to a new Schlenk quartz cuvette (Fig. S10, trace 5). Acetone/heptane (2:3) solution of NaI (7.5 mg, 50 μmol, 0.500 mL) was injected to the solution in the cuvette (Fig. S10, trace 6). The reaction between H₂O₂ and NaI affords I₃⁻ (Scheme S1, B), the yield of which can be determined by its characteristic absorbance at λmax = 364 nm (ε = 2.1 × 10⁴ M⁻¹ cm⁻¹). The H₂O₂ quantification results from three independent trials are summarized in Table S1.

| Entry | Experiment 1 | Experiment 2 | Experiment 3 | average  |
|-------|--------------|--------------|--------------|---------|
| Absorbance / I₃⁻ | 0.817 | 0.813 | 0.847 | 0.826 |
| Amount / mmol | 9.57 × 10⁻⁵ | 9.52 × 10⁻⁵ | 9.92 × 10⁻⁵ | 9.67 × 10⁻⁵ |
| Yield of H₂O₂ | 96% | 95% | 99% | 97% |

Table S1. Yields of H₂O₂ in three independent trials.

Fig. S10. UV-Vis traces for H₂O₂ quantification. The absorbances of the spectra were normalized based on solution volume to account for dilution.
3. X-ray Crystallographic Data

The single crystal X-ray diffraction studies were carried out on a Bruker Kappa Photon II CPAD diffractometer equipped with Cu K$_\text{α}$ radiation ($\lambda = 1.54178$) for 4a, a Bruker Kappa Photon II CPAD diffractometer equipped with Mo K$_\text{α}$ radiation ($\lambda = 0.71073$ Å) for 4b, and a Nonius Kappa diffractometer equipped with a Bruker APEX-II CCD and Mo K$_\text{α}$ radiation ($\lambda = 0.71073$ Å) for 4c. Crystals were mounted on MiTeGen Micromounts with Paratone oil, and data were collected in a nitrogen gas stream at 100 K. The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SHELXT) produced a complete phasing model for refinement. All nonhydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-2014). All carbon bonded hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-2014. Due to the disorder of the Cu positions in the structure, the hydroxide hydrogen atoms were placed at idealized locations and restrained using DFIX commands to fit to the disorder model of each structure. Their thermals were fixed to that of the parent oxygen atom. Platon SQUEEZ was used to remove the electron density from the lattice due to the disordered solvent contribution. 4a and 4b both had 4 voids with 34 electrons in each. 4c had 2 large voids of 600 electrons. In all cases, the disordered solvent appeared to be a mixture of acetone and diethyl ether.

**Fig. S11**: X-ray structure (CIF: 1984893, 100 K) of 4a with thermal ellipsoids of 20% probability. Hydrogen atoms and anion PF$_6^-$ are omitted for clarity. Selected bond lengths (Å) for 4a: Ave. Cu–O = 1.885(5), Ave. Cu...Cu = 3.098, Cu–N = 2.057-2.538.
**Fig. S12**: X-ray structure (CIF: 1984894, 100 K) of 4b with thermal ellipsoids of 50% probability. Hydrogen atoms, solvent molecules, and anion PF$_6^-$ are omitted for clarity. Selected bond lengths (Å) for 4b: Ave. Cu–O = 1.913(6), Ave. Cu···Cu = 3.112, Cu–N = 2.060-2.491.

**Fig. S13**: X-ray structure (CIF: 1984895, 100 K) of 4c with thermal ellipsoids of 30% probability. Hydrogen atoms, solvent molecules, and anion BF$_4^-$/PF$_6^-$ are omitted for clarity. Selected bond lengths (Å) for 4c: Ave. Cu–O = 1.937(3), Ave. Cu···Cu = 3.181, Cu–N = 2.093-2.300.
**Fig. S14:** X-ray structure (CIF: 1987932, 100 K) of 4a-BArF$_4$ with thermal ellipsoids of 50% probability. Hydrogen atoms, solvent molecules, and anion BArF$_4^-$ are omitted for clarity. Selected bond lengths (Å) for 4a-BArF$_4$: Ave. Cu–O = 1.913(2), Ave. Cu⋯Cu = 3.129, Cu–N = 2.049-2.559.

**Table S2:** Crystal Data and Structure Refinement for 4a, 4b, 4c, and 4a-BArF$_4$.

|   | 4a        | 4b        | 4c        | 4a-BArF$_4$ |
|---|-----------|-----------|-----------|-------------|
| CCDC | 1984893   | 1984894   | 198495    | 1987932     |
| Empirical formula, FW (g/mol) | C$_{36}$H$_{73}$Cu$_3$F$_{12}$N$_{16}$ | C$_{28}$H$_{91}$Cu$_3$F$_{18}$N$_{16}$ | C$_{30}$H$_{79}$B$_3$Cu$_3$F$_{18}$N$_{16}$ | C$_{100}$H$_{97}$B$_2$Cu$_3$F$_{48}$N$_{16}$O$_2$, 2663.17 |
| Color | Colorless Block | Blue Block | Blue Block | Colorless Block |
| Temperature (K) | 100 | 100 | 100 | 100 |
| Wavelength (Å) | 1.54178 | 0.71073 | 0.71073 | 0.71073 |
| Crystal system, Space group | Cubic, Pa-3 | Monoclinic, C 1 c 1 | Monoclinic, C 1 2/c 1 | Triclinic, P-1 |
| Unit cell dimensions a (Å) | 17.4900(2) | 22.6031(11) | 35.673(3) | 12.4878(13) |
| b (Å) | 17.4900(2) | 17.2489(8) | 21.1666(16) | 15.1031(17) |
| c (Å) | 17.4900(2) | 17.6361(8) | 21.0194(17) | 15.1131(17) |
| α(°) | 90° | 90° | 90° | 77.567(3) |
| β(°) | 90° | 100.981(2) | 102.442(2) | 88.651(3) |
| γ(°) | 90° | 90° | 90° | 85.637(3) |
| Volume (Å$^3$) | 5350.19(18) | 6750.0(5) | 15498(2) | 2775.4(5) |
| Z | 4.00008 | 4 | 8 | 1 |
| Density (calc., g/cm$^3$) | 1.523 | 1.521 | 1.200 | 1.593 |
| Absorption coefficient (mm$^{-1}$) | 2.729 | 1.108 | 0.917 | 0.706 |
| F(000) | 2536 | 3196 | 5760 | 1346 |
| Theta range for data collection (°) | 6.198 to 68.078 | 2.932 to 25.393 | 1.126 to 25.437 | 3.113 to 25.380 |
| Index ranges | Reflections collected | Independent reflections, R_int | Completeness to 2θ_max (%) | Absorption correction | Refinement method | Data / restraints / parameters | Goodness-of-fit | Final R indices [I>2sigma(I)] | Largest diff. peak and hole (e \cdot Å⁻³) |
|--------------|----------------------|--------------------------------|--------------------------|----------------------|-----------------|-----------------------------|----------------|-----------------------------|--------------------------------------|
| -20<=h<=19, -20<=k<=20, -16<=l<=20 | 33351                | 1628 [R(int) = 0.0331, R(sigma) = 0.0104] | 99.4                     | Semi-empirical from equivalents | Full-matrix least-squares on F² | 1628 / 196 / 201 | 1.047                      | R1 = 0.0679, wR2 = 0.1844               | 0.359 and -0.218                      |
| -27<=h<=27, -20<=k<=20, -20<=l<=21 |                       | 12117 [R(int) = 0.0465, R(sigma) = 0.0347] | 99.2                     | Semi-empirical from equivalents | Full-matrix least-squares on F² | 12117 / 194 / 867 | 1.037                      | R1 = 0.0530, wR2 = 0.1221               | 0.479 and -0.470                      |
| -42<=h<=43, -25<=k<=25, -25<=l<=24 |                       | 14249 [R(int) = 0.0763, R(sigma) = 0.0452] | 99.9                     | Semi-empirical from equivalents | Full-matrix least-squares on F² | 14249 / 52 / 837 | 1.028                      | R1 = 0.0616, wR2 = 0.1770               | 0.732 and -0.316                      |
| -15<=h<=15, -18<=k<=18, -18<=l<=18 |                       | 10153 [R(int) = 0.0801, R(sigma) = 0.0439] | 99.8                     | Semi-empirical from equivalents | Full-matrix least-squares on F² | 10153 / 564 / 1124 | 1.128                      | R1 = 0.0791, wR2 = 0.1663               | 0.409 and -0.546                      |

4. ESI-MS details

**ESI-MS analysis of the reaction of complex 4a and ¹⁸O₂ in the presence of acetic acid**

To an acetone solution (5 mL) of complex 4b (2.2 mg, 0.0016 mmol) in a 20 mL scintillation vial equipped with a septum, CoCp₂ (0.27 mg, 0.0015 mmol) was added under nitrogen atmosphere to generate complex 4a in situ. Excess ¹⁸O₂ (0.5 mL, 0.02 mmol) and acetic acid (2.1 mg, 0.035 mmol) was inject to the vial and the obtained mixture was allowed to stir at room temperature for five minutes, during which the color of the solution changed from yellow to blue, indicating complex 4a was oxidized back to complex 4b. ESI-MS analysis of the resulting blue solution (Fig. S15) showed that less than 10% of μ₃⁻¹⁶O ligand in 4a was replaced by ¹⁸O during its aerobic oxidation to 4b.
Fig. S15. ESI-MS analysis of complex 4b from the reaction of complex 4a and \(^{18}\text{O}_2\) in the presence of acetic acid (red), and simulated mass spectrum with 90% 4b-\(^{16}\text{O}\) and 10% 4b-\(^{18}\text{O}\) (black).

5. X-band EPR details

EPR spectra were recorded on a Bruker EMXPlus X-band EPR spectrometer equipped with Coldedge cryostat with small-volume power saturation. All samples were measured in 4 mm septum-capped EPR quartz tubes (Wilmad Lab glass, 727-SQ-250MM). Complex 4b (4.1 mg, 3 µmol) was dissolved in acetonitrile (6.0 mL) to make a 0.50 mM solution of 4b, and 0.20 mL of the solution was transferred into the EPR tube under nitrogen atmosphere, frozen in liquid nitrogen, and used for EPR measurement. The spectrum was collected at 50 K with a modulation frequency of 100 kHz and a modulation amplitude of 10 G using 30 dB attenuation. A time constant of 40.96 ms and a conversion time of 50.15 ms were used. All spectra were baseline-corrected using Igor Pro (Wavemetrics, Lake Oswego, OR) software. Spectral simulations were performed using the EasySpin toolbox with MATLAB.²

Fig. S16. X-band EPR spectrum (frozen MeCN, 50K, 0.5 mM) of complex 4b; \(g_1 = 2.14, g_2 = 2.25, g_3 = 2.01\), \(A_2 = 146\) MHz.
6. Electrochemistry details

Fig. S17. Solution cyclic voltammogram of 4b (1 mM) in DMF (0.1 M TBAPF$_6$) with a scan rate of 0.100 V/s. Working electrode: glassy carbon; counter electrode: Pt wire; reference electrode: Ag/AgNO$_3$.

Fig. S18. Solution cyclic voltammogram of 4 (1 mM) and 3 (1 mM) in phosphate buffer (pH = 5.8, 0.1 M) with a scan rate of 0.100 V/s. Working electrode: glassy carbon; counter electrode: Pt wire; reference electrode: leakless Ag/AgCl electrode (eDAQ).
Fig. S19. (A) Scan rate dependant cyclic voltammetry of 3a (1 mM, pH = 5.8 phosphate buffer). (B) Plot of cathodic and anodic potentials against log ν (scan rate, V/s). The number of electrons involved in the redox process can be calculated using Laviron’s equation. The slope obtained from the plot is equal to:

\[ \frac{2.3RT}{\alpha Fn} \]

where \( \alpha \) is the electron-transfer coefficient and assumed to be 0.5 for irreversible process. \( R \) (8.314 J·K\(^{-1}\)·mol\(^{-1}\)) is the ideal gas constant. \( T \) (298K) is temperature. \( F \) (96485 C·mol\(^{-1}\)) is Faraday constant. \( n \) is the number of electrons involved. \( n_c \), the number of electrons involved in the cathodic process, was calculated to be 2.0. And \( n_a \), the number of electrons involved in the anodic process, was calculated to be 2.1. This result suggests that both the oxidation and the reduction are two-electron processes.

Scheme S2. Proposed redox behavior of 3a based on its CV at different pH. Under acidic conditions, 3a is protonated to form 3b with a \( \mu_3 \)-hydroxo ligand. The ca. 800 μV separation of the redox couple at low pH indicates a substantial barrier for electron transfer. Under basic conditions, 3b is deprotonated to afford 3a. The central \( \mu_3 \)-oxo ligand in 3a binds to the three copper centers tighter than \( \mu_3 \)-hydroxo, attenuating the redox-induced geometric change and lowering the barrier for electron transfer. Consequently, the redox of 3a is more reversible under basic conditions.

Evaluation of the electron self-exchange rate constants \( k_{el} \) and \( k_{hom} \).
The standard electrochemical electron self-exchange rate constant \( k_{el} \) (cm s\(^{-1}\)) for the 4a/4b
and 4b/4c redox couples was estimated using an electrochemical method published previously.\textsuperscript{5} Under quasi-reversible conditions, $k_{el}$ can be derived from Eq. 1:\textsuperscript{6,7}

$$
\Psi = k_{el}(D_R/D_O)^{\alpha/2}(RT/nF\pi D_R)^{1/2}V^{-1/2} \quad (1)
$$

where $\Psi$ is a kinetic parameter, $D_R$ and $D_O$ are the diffusion coefficients (cm$^2$/s) of the reduced and oxidized species, respectively, $\alpha$ is the transfer coefficient for the electrode process, $R$ is gas constant (8.314 J K$^{-1}$ mol$^{-1}$), $T$ is temperature ($T = 298.15$ K in this case), $n$ is the number of electrons transferred in each step ($n = 1$ in this case), $F$ is Faraday constant (96485.3 C mol$^{-1}$), and $v$ is the potential scan rate (V s$^{-1}$). The kinetic parameter $\Psi$ is also related to the peak-to-peak separation ($\Delta E_p$ / mV) of the anodic and cathodic waves in cyclic voltammogram by using the empirical equation (Eq. 2):\textsuperscript{6}

$$
\Psi = (-0.6288+0.0021n\Delta E_p)/(1-0.017n\Delta E_p) \quad (2)
$$

where $n$ is the number of electrons transferred in each step. Cyclic voltammograms of 4a/4b and 4b/4c (1 mM in MeCN + 0.1 M Bu$_4$NPF$_6$) were measured at different potential scan rates (0.5-5.0 V s$^{-1}$ range) in the suitable potential regions (Fig. S20A and S20C). Current interrupt (CI) measurement was performed before the cyclic voltammetry to account for uncompensated resistance ($R_u$). The values of $\Psi$ were calculated from the experimental $\Delta E_p$ values (80 mV – 140 mV) using the Eq. 2. The value of $D_O$ and $D_R$ was obtained using the Randles-Sevcik equations ($9.4(6)\times10^{-7}$ cm$^2$ s$^{-1}$ and $9.4(6)\times10^{-7}$ cm$^2$ s$^{-1}$ for 4a/4b redox couple; 1.5(1)×10$^{-6}$ cm$^2$ s$^{-1}$ and 1.4(1)×10$^{-6}$ cm$^2$ s$^{-1}$ for 4b/4c redox couple). Since $D_O = D_R$ in both redox cases and $0<\alpha<1$, $(D_O/D_R)^{\alpha/2}$ is approximated equal to 1.\textsuperscript{7} An estimate of the values of $k_{el}$ was obtained from the $\Psi$ vs $v^{-1/2}$ plot using Eq. 1 ($7.8(2)\times10^{-3}$ cm s$^{-1}$ for 4a/4b redox couple, Fig.S19B; 7.6(2)×10$^{-3}$ cm s$^{-1}$ for 4b/4c redox couple, Fig.S19D). A correlation between $k_{el}$ and the homogeneous electron self-exchange rate constant $k_{hom}$ (L mol$^{-1}$ s$^{-1}$) has been described by Weaver et al. (Eq. 3):\textsuperscript{8}

$$
k_{hom} = 4\pi N_A r^2_{el} 10^{-19} \quad (3)
$$

where $k_{el}$ is the electrochemical rate constant (cm s$^{-1}$), $N_A$ is the Avogadro constant (mol$^{-1}$), and $r$ is the internuclear distance for self-exchange (Å). The value of $r$ (11.2 Å) was estimated based on atomic coordinate of the X-ray single-crystal structure 4b using chemcraft software. The value of $k_{hom}$ was calculated as $7.4(2)\times10^{5}$ L mol$^{-1}$ s$^{-1}$ for 4a/4b redox couple and $7.2(2)\times10^{5}$ L mol$^{-1}$ s$^{-1}$ for 4b/4c redox couple.
Fig. S20. Scan rate dependent cyclic voltammograms for 4a/4b redox couple (A) and 4b/4c redox couple (C). \( \Psi \) vs \( \nu^{1/2} \) plots for 4a/4b redox couple (B) and 4b/4c redox couple (D).

7. Computational details

All computations were performed using ORCA software packages. The geometry optimization was carried out using BP86 method with a mixed basis set (def2-TZVP for the copper atoms and def2-SVP for all light atoms, C, N, O, H), followed by a frequency calculation. For both complex 3 and 4 in Cu\textsuperscript{II}Cu\textsuperscript{III} and Cu\textsuperscript{II}Cu\textsuperscript{II}Cu\textsuperscript{II} oxidation states, the structures were optimized at three spin states (singlet, triplet, broken symmetry triplet for Cu\textsuperscript{II}Cu\textsuperscript{II}Cu\textsuperscript{II}; doublet, quartet, and broken symmetry quartet for Cu\textsuperscript{II}Cu\textsuperscript{II}Cu\textsuperscript{II}) at BP86/def2-TZVP(Cu)/def2-TZVP(C, N, O, H) level of theory to determine the ground state (Table S3). To estimate the reorganization energy (\( \lambda \)), single-point calculations of the one-electron oxidized or reduced species at their redox counterpart’s geometry were performed. The implication of reorganization energy for the oxidized complex (\( \lambda_{\text{ox}} \)) and the reduced complex (\( \lambda_{\text{red}} \)) of a redox couple is clarified in Fig. S21. The total inner-sphere reorganization energy for a self-exchange reaction (\( \lambda_s \)) is the sum of \( \lambda_{\text{ox}} \) and \( \lambda_{\text{red}} \). Solvated single-point energies were calculated at TPSSH/def2-TZVP(Cu)/def2-SVP(C, N, O, H) level\(^{10}\) with a continuum solvation model (SMD, acetonitrile).\(^{11}\) Dispersion corrections with Becke-Johnson damping were applied for single-point calculation.\(^{12,13}\) The Gibbs free energy of each species was determined by adding the solvated single point SCF energy to the thermal correction from the respective frequency calculation.\(^{14}\) The results are shown in Table S4. Time-dependent density-functional theory (TD-DFT) calculation for complex 4b and 4c were performed at TPSSH/def2-TZVP level using 50 roots.
Table S3: Ground state determination of complex 3 and 4 at the Cu$^{I}$Cu$^{II}$Cu$^{II}$ and Cu$^{II}$Cu$^{II}$Cu$^{II}$ oxidation states. The isolated [TREN$_3$Cu$_3$OH] in Cu$^{I}$Cu$^{II}$Cu$^{II}$ oxidation has a paramagnetic $^1$H NMR, which suggests its triplet ground state.

| Oxidation state | Spin state | [TREN$_3$Cu$_3$O]/Ha | [TREN$_4$Cu$_3$OH]/Ha |
|-----------------|------------|----------------------|-----------------------|
| I II II          | Singlet    | $-6598.60730064^{a,b}$ | $-$                   |
|                 | Triplet    | $-6598.63490810^{a,b}$ | Exp. Ground state     |
|                 | Triplet Broken-symmetry | $-6598.62889281^{a,b}$ | $-$                   |
| II II II         | Doublet    | $-6598.15449969^{a,b}$ | $-7284.95586835^{a,b}$ |
|                 | Quartet    | $-6598.15523773^{a,b}$ | $-7284.96125714^{a,b}$ |
|                 | Quartet Broken-symmetry | $-6598.15451636^{a,b}$ | $-7284.95890205^{a,b}$ |

a: TPSSH/SVP; b: SCF single point energy

FIG. S21. The potential energy of a general electron transfer. The reorganization energy of the reduction and the oxidation ($\lambda_{\text{ox}}$ and $\lambda_{\text{red}}$) are indicated.

SCHEME S3. Computed inner-sphere reorganization energy of (A) 4 and (B) 3. $\lambda_{\text{ox}}$ and $\lambda_{\text{red}}$ can be computationally estimated by the energy required to distort the equilibrium geometries to
their redox-partners’ geometries. For example, $\lambda_{\text{ox}}$ of 4a/4b couple is the energy of 4b calculated at 4a’s optimal geometry minus the energy of 4b at its optimal geometry. Similarly, the $l_{\text{red}}$ of 4a/4b couple is the energy of 4a calculated at 4b’s optimal geometry minus the energy of 4a at its optimal geometry.

| Complex | Redox couple | $\lambda_{\text{ox}}$ | $\lambda_{\text{red}}$ | $\lambda_i$ |
|---------|--------------|-----------------------|------------------------|-------------|
| Complex 4 | I,II – I,II | 0.047 | 0.65 | 0.70 |
|          | I,II – I,II,II | 0.027 | 0.39 | 0.42 |
|          | I,II,II – II,II,II | 0.13 | 0.046 | 0.18 |
| Complex 3 | I,II – I,II | 1.1 | 0.95 | 2.1 |
|          | I,II – I,II,II | 0.15 | 0.53 | 0.68 |
|          | I,II,II – II,II,II | 0.084 | 0.26 | 0.34 |

**Table S4.** The calculated $\lambda_{\text{ox}}$, $\lambda_{\text{red}}$, and $\lambda_i$ (eV) for complex 3 and 4.

**Fig. S22.** Experimental and simulated UV-vis spectrum of complex 4b (A) and 4c (B).
Table S5: Selected TD-DFT transitions for 4b. Orbitals plotted at a 0.048 isosurface value.
Table S6: Selected TD-DFT transitions for 4c. Orbitals plotted at a 0.048 isosurface value.

Table S7: Comparison of geometry of optimized 3 and 4 at different oxidation states.
Fig. S23. Selected average bond distances from the optimized geometries of (A) 3 and (B) 4 at different oxidation states.

Cartesian coordinates of complexes used in computations

Complex – Level of theory optimized (Calculations used for) Charge, spin multiplicity

\[ \text{[TREN]}\text{Cu}^1\text{Cu}^1\text{Cu}^1(\mu-\text{OH})] \rightarrow \text{BP86/def2-SVP (C, H, O, N)/def2-TZVP (Cu)} \]

2, 2

\[ \begin{array}{ccc}
29 & 9.73391000 & -0.179256000 \\
6 & 10.982866000 & 2.011531000 \\
1 & 11.025418000 & 2.878547000 \\
1 & 12.009104000 & 1.913309000 \\
6 & 8.394227000 & -1.447503000 \\
1 & 7.985615000 & -2.246915000 \\
1 & 8.085973000 & -0.488172000 \\
7 & 7.805923000 & -1.495428000 \\
6 & 9.919155000 & -1.572553000 \\
1 & 10.265463000 & -1.593725000 \\
1 & 10.208664000 & -2.549079000 \\
7 & 10.642610000 & -0.508729000 \\
7 & 11.791656000 & -1.584373000 \\
7 & 12.160309000 & -0.182954000 \\
7 & 11.009843000 & -2.284928000 \\
6 & 10.621100000 & 0.765416000 \\
1 & 11.315256000 & 0.693894000 \\
1 & 9.607250000 & 0.884495000 \\
6 & 11.554433000 & -2.725960000 \\
1 & 10.826684000 & -3.402991000 \\
1 & 12.509034000 & -3.313851000 \\
6 & 7.797845000 & -2.849105000 \\
1 & 7.209979000 & -3.545175000 \\
1 & 8.837605000 & -3.232061000 \\
6 & 12.060197000 & -0.937458000 \\
1 & 12.484165000 & -1.318461000 \\
1 & 12.653522000 & -0.038392000 \\
6 & 11.916571000 & -1.311899000 \\
1 & 11.444677000 & -0.951305000 \\
1 & 12.892217000 & -1.815181000 \\
\end{array} \]

10.360415000
12.156563000
12.864461000
11.746150000
12.936769000
13.606288000
13.402451000
11.593444000
12.945956000
14.006910000
12.510799000
12.190831000
9.582177000
7.675744000
7.415317000
12.970879000
13.841371000
13.400234000
8.702771000
9.196248000
8.540103000
11.039747000
11.985616000
12.944471000
11.728707000
6.791432000
5.856688000
6.504521000
|   |        |          |          |          |
|---|--------|----------|----------|----------|
| 6 | 12.7159 | -0.648 | 8.93496 | 60000    |
| 1 | 12.8739 | 0.226 | 9.59681 | 30000    |
| 1 | 13.7259 | -1.145 | 5.92780 | 80000    |
| 6 | 12.3653 | 1.643 | 5.11904 | 20000    |
| 1 | 12.0661 | 0.948 | 5.11904 | 20000    |
| 1 | 13.1703 | 2.282 | 5.47575 | 00000    |
| 6 | 12.2546 | -2.006 | 10.906 | 26600    |
| 1 | 13.3349 | -2.299 | 10.907 | 35300    |
| 1 | 11.6990 | -2.927 | 11.179 | 93000    |
| 6 | 13.0137 | 0.840 | 7.85897 | 00000    |
| 1 | 13.3256 | 1.529 | 7.87589 | 70000    |
| 1 | 13.9659 | 2.283 | 5.47575 | 00000    |
| 6 | 12.2501 | -2.848 | 9.68525 | 70000    |
| 1 | 13.1739 | -4.200 | 7.57188 | 50000    |
| 1 | 13.7502 | -5.261 | 7.22534 | 00000    |
| 6 | 16.1982 | -3.764 | 7.28142 | 10000    |
| 1 | 18.2394 | -3.447 | 6.84959 | 20000    |
| 7 | 17.1676 | -0.837 | 5.69958 | 70000    |
| 7 | 8.5714 | 1.068 | 5.33241 | 90000    |
| 7 | 6.4685 | 1.330 | 6.48066 | 70000    |
| 6 | 9.5126 | -4.228 | 6.87245 | 60000    |
| 1 | 9.4409 | -5.098 | 6.17810 | 80000    |
| 1 | 9.6300 | -4.657 | 7.8864 | 00000    |
| 6 | 6.0267 | 0.043 | 5.9357 | 08000    |
| 1 | 5.3489 | -0.449 | 6.6628 | 54000    |
| 1 | 5.4398 | 0.206 | 4.9805 | 74000    |
| 6 | 5.8971 | -2.293 | 9.6916 | 39000    |
| 1 | 5.1994 | -2.965 | 10.2785 | 59000    |
| 1 | 5.5156 | -2.243 | 8.6513 | 68000    |
| 6 | 7.8123 | -3.241 | 5.4315 | 68000    |
| 1 | 7.4308 | -4.199 | 5.0071 | 76000    |
| 1 | 8.7123 | -2.985 | 4.8391 | 86000    |
| 6 | 7.4430 | 1.953 | 5.5690 | 96000    |
| 1 | 7.8040 | 2.887 | 6.0470 | 85000    |
| 1 | 6.9411 | 2.240 | 4.5987 | 02000    |
| 6 | 8.1048 | -0.190 | 4.7762 | 15000    |
| 1 | 8.9794 | -0.853 | 4.6190 | 68000    |
| 1 | 7.6092 | -0.045 | 3.7658 | 10000    |
| 6 | 10.4000 | 2.814 | 5.1294 | 37000    |
| 1 | 9.7053 | 3.623 | 5.4279 | 49000    |
| 6 | 11.0404 | 3.265 | 4.3251 | 45000    |
| 1 | 6.7449 | -2.160 | 5.2306 | 01000    |
| 1 | 6.4532 | -2.161 | 4.1554 | 58000    |
| 1 | 5.8226 | -2.433 | 5.7906 | 02000    |
| 6 | 9.5966 | 1.679 | 4.4800 | 24000    |
| 1 | 10.2846 | 0.866 | 4.1687 | 76000    |
| 1 | 9.1607 | 2.080 | 3.5275 | 69000    |
| 29 | 7.1337 | 0.985 | 8.9213 | 74000    |
| 8  | 8.864795000 | 0.114946000 | 8.628418000 |
| 6  | 5.338977000 | 2.234920000 | 6.729351000 |
| 1  | 4.631238000 | 2.277421000 | 5.862207000 |
| 1  | 5.750538000 | 3.260785000 | 6.826652000 |
| 6  | 4.555278000 | -0.349247000 | 10.191094000 |
| 1  | 3.885707000 | -0.756137000 | 10.990790000 |
| 1  | 4.089734000 | -0.658122000 | 9.232121000 |
| 7  | 5.898404000 | -0.938916000 | 10.239760000 |
| 6  | 4.548128000 | 1.175837000 | 10.314442000 |
| 1  | 3.487539000 | 2.570607000 | 8.046523000 |
| 1  | 4.093660000 | 0.861886000 | 7.857809000 |
| 7  | 8.793068000 | 2.807526000 | 11.466465000 |
| 1  | 8.298766000 | 2.080822000 | 12.144011000 |
| 1  | 8.956602000 | 3.762412000 | 12.053660000 |
| 6  | 6.452076000 | -0.946087000 | 11.593432000 |
| 1  | 5.778675000 | -1.532507000 | 12.290326000 |
| 1  | 6.502607000 | 0.094087000 | 11.975118000 |
| 7  | 11.190650000 | 2.436277000 | 6.304654000 |
| 6  | 5.510863000 | 3.315137000 | 9.673080000 |
| 1  | 4.552460000 | 3.740484000 | 10.057906000 |
| 1  | 5.768349000 | 3.907361000 | 8.777676000 |
| 6  | 10.704600000 | 3.164960000 | 10.052210000 |
| 1  | 11.639265000 | 2.693447000 | 9.692246000 |
| 1  | 10.992563000 | 4.142349000 | 10.554636000 |
| 6  | 8.562235000 | 3.967362000 | 9.388103000 |
| 1  | 7.900606000 | 4.125176000 | 8.512814000 |
| 1  | 8.707665000 | 4.977604000 | 9.883931000 |
| 6  | 11.569065000 | 3.611045000 | 7.096077000 |
| 1  | 12.377493000 | 3.311640000 | 7.791626000 |
| 1  | 12.022140000 | 4.414918000 | 6.456272000 |
| 6  | 6.590379000 | 3.509413000 | 10.745946000 |
| 1  | 6.590425000 | 4.589988000 | 11.037810000 |
| 1  | 6.316022000 | 2.954997000 | 11.667822000 |
| 6  | 10.434820000 | 4.261588000 | 7.898321000 |
| 1  | 9.622012000 | 4.573522000 | 7.209407000 |
| 1  | 10.836021000 | 5.213710000 | 8.334511000 |
| 1  | 9.434252000 | 0.683367000 | 8.059623000 |

\[ \text{TREN} \text{Cu}^{I}\text{Cu}^{I}\text{Cu}^{II}((\text{H}_2\text{-OH})) \] – BP86/def2-SVP (C, H, O, N)/def2-TZVP (Cu)

| 3, 2 | 9.867699000 | -0.252278000 | 10.297176000 |
| 6 | 11.003535000 | 1.970426000 | 12.057747000 |
| 1 | 11.027273000 | 2.896362000 | 12.683653000 |
| 1 | 12.024885000 | 1.869689000 | 11.635057000 |
| 6 | 8.397633000 | -1.340594000 | 12.894941000 |
| 7 | 7.894433000 | -2.111376000 | 13.528052000 |
| 1 | 8.098392000 | -0.362154000 | 13.324360000 |
| 7 | 7.909043000 | -1.372691000 | 11.499656000 |
|   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|
| 6 | 9.907769000 | -1.530610000 | 13.016478000 |
| 1 | 10.185168000 | -1.512097000 | 14.095906000 |
| 1 | 10.190410000 | -2.537853000 | 12.651056000 |
| 7 | 10.696260000 | -0.522880000 | 12.255915000 |
| 7 | 11.658692000 | -1.548835000 | 9.652030000 |
| 7 | 12.068763000 | -0.138308000 | 7.751116000 |
| 7 | 10.860800000 | -2.234046000 | 7.451121000 |
| 6 | 10.699457000 | 0.785005000 | 12.971991000 |
|   | 11.440417000 | 0.775505000 | 13.804403000 |
| 1 | 9.713253000 | 0.918153000 | 13.456622000 |
| 6 | 11.408508000 | -2.684620000 | 8.746904000 |
| 1 | 10.690420000 | -3.373686000 | 9.232315000 |
| 1 | 12.365930000 | -3.249670000 | 8.576350000 |
| 6 | 7.897300000 | -2.740753000 | 10.972960000 |
| 1 | 7.256819000 | -3.402649000 | 11.623795000 |
| 1 | 8.924484000 | -3.155875000 | 10.987740000 |
| 6 | 12.091369000 | -1.009883000 | 12.057090000 |
| 1 | 12.498026000 | -1.443772000 | 12.999191000 |
| 1 | 12.732425000 | -0.137420000 | 11.822924000 |
| 6 | 11.785443000 | -1.238275000 | 6.845599000 |
| 1 | 11.309599000 | -0.844782000 | 5.928537000 |
| 1 | 12.734381000 | -1.767282000 | 6.538720000 |
| 6 | 12.629431000 | -0.645323000 | 8.987490000 |
| 1 | 12.860459000 | 0.205856000 | 9.658056000 |
| 1 | 13.593307000 | -1.210179000 | 8.821449000 |
| 6 | 12.375517000 | 1.654369000 | 5.969708000 |
| 1 | 12.108602000 | 0.953654000 | 5.154203000 |
| 1 | 13.204196000 | 2.280823000 | 5.548643000 |
| 6 | 12.195466000 | -2.049727000 | 10.942542000 |
| 1 | 13.257632000 | -2.374651000 | 10.846843000 |
| 1 | 11.622521000 | -2.960662000 | 11.213506000 |
| 6 | 12.966919000 | 0.863844000 | 7.142286000 |
| 1 | 13.263991000 | 1.560859000 | 7.952600000 |
| 1 | 13.918938000 | 0.393563000 | 6.787675000 |
| 29 | 8.693098000 | -1.653489000 | 7.762670000 |
| 6 | 10.734697000 | -3.376168000 | 6.505207000 |
| 1 | 11.657575000 | -4.003152000 | 6.497111000 |
| 1 | 10.654784000 | -2.945198000 | 5.486202000 |
| 6 | 7.408799000 | -4.161876000 | 9.099819000 |
| 1 | 6.620123000 | -4.776454000 | 9.597903000 |
| 1 | 8.376452000 | -4.613473000 | 9.402750000 |
| 7 | 7.404152000 | -2.765305000 | 9.589209000 |
| 6 | 7.221567000 | -4.269832000 | 7.589235000 |
| 1 | 7.220524000 | -5.346285000 | 7.300868000 |
| 1 | 6.224394000 | -3.880469000 | 7.306773000 |
| 7 | 8.245960000 | -3.517862000 | 6.815302000 |
| 7 | 7.207595000 | -0.861474000 | 5.842430000 |
| 7 | 8.616212000 | 1.027267000 | 5.412652000 |
| 7 | 6.542923000 | 1.340993000 | 6.650146000 |
| 6 | 9.532085000 | -4.272614000 | 6.791161000 |
| 6 | 9.5000306000 | -5.087777000 | 6.031746000 |
| 1 | 9.656925000 | -4.779218000 | 7.767849000 |
| 6 | 6.083012000 | 0.035820000 | 6.120847000 |
| 1 | 5.422322000 | -0.448092000 | 6.867709000 |
| 1 | 5.474328000 | 0.209777000 | 5.187999000 |
| 6 | 6.044128000 | -2.207727000 | 9.560324000 |
|---|-------------|---------------|-------------|
| 1 | 5.347658000 | -2.870012000 | 10.152354000 |
| 1 | 5.672842000 | -2.187900000 | 8.516808000 |
| 6 | 7.757923000 | -3.271289000 | 5.427238000 |
| 1 | 7.327802000 | -4.204184000 | 4.995779000 |
| 1 | 8.632342000 | -3.020866000 | 4.794885000 |
| 7 | 7.521173000 | 1.935401000 | 5.701109000 |
| 1 | 7.919352000 | 2.861565000 | 6.155790000 |
| 6 | 6.975306000 | 2.227476000 | 4.755882000 |
| 6 | 8.095749000 | -0.211396000 | 4.628726000 |
| 1 | 8.943494000 | -0.884700000 | 4.278590000 |
| 1 | 7.530433000 | -0.040758000 | 3.897952000 |
| 6 | 10.413946000 | 2.787609000 | 5.096288000 |
| 1 | 9.725676000 | 3.616420000 | 5.351278000 |
| 1 | 11.060921000 | 3.194888000 | 4.275908000 |
| 6 | 7.133569000 | -2.157303000 | 5.337840000 |
| 1 | 6.366249000 | -2.087150000 | 4.785900000 |
| 7 | 6.100044000 | 1.626828000 | 4.503998000 |
| 6 | 10.296094000 | 0.810506000 | 4.196426000 |
| 1 | 9.135869000 | 1.989436000 | 3.556522000 |
| 29 | 7.153099000 | 1.134582000 | 8.851469000 |
| 8 | 8.852851000 | 0.142821000 | 8.617909000 |
| 6 | 5.395216000 | 2.279248000 | 6.765410000 |
| 1 | 4.781077000 | 2.285510000 | 5.833640000 |
| 1 | 5.815684000 | 3.301998000 | 6.856736000 |
| 6 | 4.616964000 | -0.351698000 | 10.058400000 |
| 1 | 3.987080000 | -0.862990000 | 10.827099000 |
| 1 | 4.186235000 | -0.645259000 | 9.078350000 |
| 6 | 7.013546000 | -0.838080000 | 10.086433000 |
| 6 | 4.464690000 | 1.155570000 | 10.260945000 |
| 1 | 3.405054000 | 1.424722000 | 10.263047000 |
| 1 | 4.868105000 | 1.433780000 | 11.267140000 |
| 6 | 5.222904000 | 1.957218000 | 9.246379000 |
| 7 | 7.358852000 | 2.892031000 | 10.236735000 |
| 7 | 9.761280000 | 3.354026000 | 8.853719000 |
| 7 | 10.073115000 | 2.108180000 | 10.914385000 |
| 6 | 4.483128000 | 1.977992000 | 7.952198000 |
| 1 | 3.656961000 | 2.727357000 | 7.978183000 |
| 1 | 3.989868000 | 0.996219000 | 7.817485000 |
| 6 | 8.762336000 | 2.598128000 | 11.367512000 |
| 1 | 8.280965000 | 1.827063000 | 12.001725000 |
| 8 | 8.891879000 | 3.526435000 | 11.993690000 |
| 6 | 6.544982000 | -0.831439000 | 11.454951000 |
| 1 | 5.868848000 | -1.424741000 | 12.137154000 |
| 1 | 6.569121000 | 0.208091000 | 11.837911000 |
| 7 | 11.189520000 | 2.451746000 | 6.295688000 |
| 6 | 5.445366000 | 3.344641000 | 9.746261000 |
| 1 | 4.514042000 | 3.754980000 | 10.199241000 |
| 1 | 5.673587000 | 3.992072000 | 8.876993000 |
| 6 | 10.665487000 | 3.064931000 | 9.954255000 |
| 1 | 11.595177000 | 2.616441000 | 9.556937000 |
| 1 | 10.953696000 | 4.013902000 | 10.497746000 |
| 6 | 8.521133000 | 3.894837000 | 9.369944000 |
| 1 | 7.853624000 | 4.152110000 | 8.523929000 |
|     |        |          |            |            |
|-----|--------|----------|------------|------------|
| 1   | 8.682614000 | 4.840931000 | 9.967295000 |
| 6   | 11.532594000 | 3.651025000 | 7.067082000 |
| 1   | 12.352925000 | 4.474788000 | 11.115915000 |
| 1   | 11.952146000 | 3.392721000 | 7.765211000 |
| 6   | 6.578374000  | 2.830500000 | 11.670706000 |
| 1   | 12.352925000 | 3.392721000 | 7.765211000 |
| 1   | 11.952146000 | 4.474788000 | 6.420426000 |
| 1   | 6.317423000  | 2.830500000 | 11.670706000 |
| 6   | 10.368209000 | 4.256558000 | 7.859115000 |
| 1   | 9.558553000  | 4.562678000 | 7.164755000 |
| 1   | 10.732632000 | 5.204324000 | 8.330877000 |
| 1   | 9.437600000  | 0.695093000 | 8.040209000 |

\[\text{TREN}_4\text{Cu}^{II}\text{Cu}^{II}(\mu_3-\text{OH})\] – BP86/def2-SVP (C, H, O, N)/def2-TZVP (Cu)

4, 3
|   |        |        |        |        |
|---|--------|--------|--------|--------|
| 6 | 10.09622000 | 2.91480000 | 5.741302000 |
| 6 | 8.38721300 | 8.55961600 | 1.824149000 |
| 6 | 6.68772100 | 9.73689000 | 4.222430000 |
| 6 | 10.71388500 | 2.65477600 | 4.373085000 |
| 6 | 13.07098700 | 3.20829900 | 4.797203000 |
| 6 | 14.80389300 | 9.04591800 | 5.967806000 |
| 6 | 9.99905800 | 8.64634700 | 9.949359000 |
| 6 | 13.38064700 | 10.81747000 | 2.646942000 |
| 6 | 10.50061100 | 9.80185800 | 9.093397000 |
| 6 | 12.78374400 | 6.16318400 | 9.291537000 |
| 6 | 11.61600300 | 11.67298000 | 4.787665000 |
| 6 | 11.97224700 | 7.18260300 | 10.08272000 |
| 6 | 6.52670600 | 5.97195100 | 4.652861000 |
| 1 | 13.12456000 | 11.40959300 | 4.747042000 |
| 6 | 7.05830300 | 8.10473300 | 2.414860000 |
| 1 | 8.50661600 | 10.80041500 | 7.754380000 |
| 1 | 8.22706400 | 9.02388600 | 7.791557000 |
| 1 | 15.34367700 | 6.42606800 | 5.667487000 |
| 1 | 14.26160500 | 6.98091600 | 4.334870000 |
| 1 | 12.57482000 | 4.47907600 | 7.271503000 |
| 1 | 14.28788000 | 4.97923000 | 7.486616000 |
| 1 | 14.83302100 | 7.23579000 | 7.996032000 |
| 1 | 13.55135200 | 8.48146900 | 8.166584000 |
| 1 | 8.84531000 | 5.91458300 | 2.369506000 |
| 1 | 9.65320700 | 6.48901900 | 0.865855000 |
| 1 | 10.73857000 | 8.81817700 | 0.928580000 |
| 1 | 10.71252000 | 9.68501900 | 2.508925000 |
| 1 | 5.75795500 | 7.80758900 | 5.525189000 |
| 1 | 5.06045400 | 7.39572800 | 3.951232000 |
| 1 | 8.54308900 | 4.37979300 | 4.091310000 |
| 1 | 7.60256400 | 3.74794000 | 5.488227000 |
| 1 | 12.04607900 | 6.68188200 | 0.791766000 |
| 1 | 13.04404000 | 6.23467500 | 2.219560000 |
| 1 | 6.80450400 | 5.33934500 | 7.197215000 |
| 1 | 7.20987200 | 7.08291900 | 7.021368000 |
| 1 | 8.62684400 | 3.75514500 | 7.725237000 |
| 1 | 10.30306600 | 4.38404000 | 7.903980000 |
| 1 | 7.84562200 | 6.92903000 | 9.138998000 |
| 1 | 7.89844200 | 5.18225100 | 9.430852000 |
| 1 | 13.08609400 | 4.05126800 | 2.413061000 |
| 1 | 12.07466000 | 2.61933800 | 2.151296000 |
| 1 | 14.09241700 | 8.18402100 | 2.193298000 |
| 1 | 13.18191700 | 8.96311800 | 0.885876000 |
| 1 | 12.15668600 | 10.34383000 | 7.060260000 |
| 1 | 10.91740500 | 11.61340500 | 7.383054000 |
| 1 | 9.19896100 | 10.96238800 | 4.177053000 |
| 1 | 9.06799600 | 11.88914600 | 5.711576000 |
| 1 | 10.33978000 | 5.28019000 | 9.298711000 |
| 1 | 9.39545500 | 6.32936000 | 10.995940000 |
| 1 | 15.16118500 | 8.88308200 | 3.803120000 |
| 1 | 15.59127100 | 10.43686000 | 4.542670000 |
| 1 | 10.02260500 | 4.04001600 | 1.959712000 |
| 1 | 11.25842000 | 4.51902100 | 0.783092000 |
| 1 | 6.55207800 | 9.49477000 | 6.381694000 |
| 1 | 6.87250100 | 11.15635200 | 5.847511000 |
|    | 14.388944000 | 4.730429000 | 3.974436000 |
|---|---|---|---|
| 1  | 14.930444000 | 4.044831000 | 5.910135000 |
| 1  | 10.841042000 | 2.722993000 | 6.541054000 |
| 1  | 9.275600000  | 9.653926000 | 1.956454000 |
| 1  | 8.379043000  | 8.382026000 | 0.723993000 |
| 1  | 7.154140000  | 10.389454000 | 3.486818000 |
| 1  | 5.985540000  | 9.349330000 | 4.107727000 |
| 1  | 9.943000000  | 2.745980000 | 3.578558000 |
| 1  | 11.066117000 | 1.599279000 | 4.329151000 |
| 1  | 12.775500000 | 2.805487000 | 5.876229000 |
| 1  | 13.599010000 | 2.377566000 | 4.276849000 |
| 1  | 14.518910000 | 9.825346000 | 6.704656000 |
| 1  | 15.850410000 | 8.770031000 | 6.218640000 |
| 1  | 8.966704000  | 8.565930000 | 9.868370000 |
| 1  | 10.226546000 | 8.853989000 | 11.018822000 |
| 1  | 12.528515000 | 10.843787000 | 2.380281000 |
| 1  | 14.268442000 | 10.667286000 | 2.162961000 |
| 1  | 11.592815000 | 9.936321000 | 9.229864000 |
| 1  | 10.029899000 | 10.748472000 | 9.445195000 |
| 1  | 12.339611000 | 5.151680000 | 9.388175000 |
| 1  | 13.805940000 | 6.087200000 | 9.727725000 |
| 1  | 11.217674000 | 11.752276000 | 3.754436000 |
| 1  | 11.461699000 | 12.683710000 | 5.241020000 |
| 1  | 12.470747000 | 8.170875000 | 10.666564000 |
| 1  | 11.931360000 | 6.876909000 | 11.151928000 |
| 1  | 6.685303000  | 5.328711000 | 3.646291000 |
| 1  | 5.735261000  | 5.347644000 | 5.130849000 |
| 1  | 13.537194000 | 11.423297000 | 5.775666000 |
| 1  | 13.593600000 | 12.292980000 | 4.244279000 |
| 1  | 6.888120000  | 7.030500000 | 2.206111000 |
| 1  | 6.227002000  | 8.643700000 | 1.907658000 |
| 1  | 11.389142000 | 8.004095000 | 5.055192000 |

$[\text{TREN}]_{2}\text{Cu}^{+}\text{Cu}^{+}\text{Cu}^{+}((\mu_{2}-\text{OH})) \rightarrow \text{BP86/def2-SVP (C, H, O, N)/def2-TZVP (Cu)}$
|   | 7       | 10.970441000       | 5.882876000       | 2.466246000       |
|---|----------|---------------------|---------------------|---------------------|
|   | 6        | 8.832210000         | 9.810266000         | 7.303379000         |
|   | 6        | 14.276423000        | 6.720493000         | 5.392861000         |
|   | 6        | 13.272453000        | 5.319934000         | 7.094490000         |
|   | 6        | 13.794148000        | 7.611253000         | 7.560150000         |
|   | 6        | 9.707930000         | 6.497074000         | 1.960570000         |
|   | 6        | 10.747170000        | 8.685337000         | 2.051032000         |
|   | 6        | 5.993844000         | 7.419421000         | 4.552460000         |
|   | 6        | 8.351822000         | 4.541503000         | 5.160791000         |
|   | 6        | 12.096001000        | 6.720507000         | 1.970371000         |
|   | 6        | 7.607095000         | 6.720507000         | 6.852980000         |
|   | 6        | 9.371399000         | 4.523443000         | 7.331839000         |
|   | 6        | 8.521362000         | 6.007407000         | 9.069474000         |
|   | 6        | 12.098979000        | 3.650799000         | 2.591252000         |
|   | 6        | 13.168953000        | 8.855754000         | 1.997821000         |
|   | 6        | 11.097638000        | 10.584347000        | 6.931801000         |
|   | 6        | 9.442770000         | 10.856371000        | 5.234520000         |
|   | 6        | 9.745860000         | 6.173060000         | 9.953586000         |
|   | 6        | 14.861752000        | 9.636736000         | 4.520959000         |
|   | 6        | 11.065947000        | 4.507318000         | 1.873209000         |
|   | 6        | 7.144991000         | 10.11131000         | 5.607377000         |
|   | 6        | 14.019940000        | 4.359063000         | 4.982068000         |
|   | 6        | 10.072126000        | 2.901686000         | 5.710231000         |
|   | 6        | 8.357212000         | 8.523320000         | 1.806312000         |
|   | 6        | 6.706545000         | 9.747078000         | 4.195734000         |
|   | 6        | 10.701046000        | 2.646225000         | 4.348936000         |
|   | 6        | 13.059690000        | 3.190254000         | 4.819488000         |
|   | 6        | 14.820357000        | 9.026721000         | 5.927756000         |
|   | 6        | 9.967253000         | 8.633301000         | 9.962204000         |
|   | 6        | 13.369843000        | 10.240530000        | 2.621560000         |
|   | 6        | 10.463476000        | 9.796155000         | 9.117080000         |
|   | 6        | 12.797496000        | 6.202098000         | 9.288918000         |
|   | 6        | 11.654795000        | 11.665491000        | 4.830718000         |
|   | 6        | 11.977964000        | 7.210170000         | 10.081040000        |
|   | 6        | 6.495219000         | 5.989398000         | 4.686737000         |
|   | 6        | 13.171351000        | 11.444951000        | 4.789617000         |
|   | 6        | 7.037636000         | 8.069668000         | 2.413013000         |
|   | 1        | 8.508926000         | 10.800196000        | 7.718658000         |
|   | 1        | 8.205312000         | 9.031985000         | 7.778967000         |
|   | 1        | 15.324063000        | 6.418063000         | 5.670081000         |
|   | 1        | 14.267870000        | 6.935830000         | 4.307913000         |
|   | 1        | 12.566117000        | 4.490464000         | 7.287448000         |
|   | 1        | 14.272463000        | 5.008625000         | 7.493584000         |
|   | 1        | 14.792968000        | 7.297930000         | 7.969270000         |
|   | 1        | 13.491015000        | 8.525300000         | 8.103278000         |
|   | 1        | 8.856022000         | 5.888043000         | 2.355199000         |
|   | 1        | 9.687398000         | 6.477461000         | 0.874920000         |
|   | 1        | 10.722124000        | 8.795172000         | 0.931401000         |
|   | 1        | 10.650298000        | 9.699159000         | 2.483289000         |
|   | 1        | 5.751346000         | 7.845699000         | 5.544398000         |
|   | 1        | 5.038547000         | 7.422826000         | 3.980881000         |
|   | 1        | 8.519672000         | 4.409830000         | 4.075362000         |
|   | 1        | 7.595161000         | 3.776211000         | 5.479077000         |
|   | 1        | 12.085309000        | 6.698181000         | 0.845552000         |
|   | 1        | 13.055827000        | 6.275007000         | 2.295823000         |
|   | 6.829393000 | 5.348723000 | 7.214110000 |
|---|-------------|-------------|-------------|
|   | 7.224807000 | 7.093123000 | 7.051299000 |
|   | 8.637174000 | 3.757307000 | 7.699446000 |
|   | 10.319427000| 4.361321000 | 7.878288000 |
|   | 7.846732000 | 6.881055000 | 9.169936000 |
|   | 7.933085000 | 5.130380000 | 9.426988000 |
|   | 13.117751000| 4.055839000 | 2.436761000 |
|   | 12.108880000| 2.627988000 | 2.151809000 |
|   | 14.070634000| 8.232444000 | 2.166606000 |
|   | 13.119539000| 9.006193000 | 0.891484000 |
|   | 12.158634000| 10.339851000| 7.127607000 |
|   | 10.893751000| 11.593098000| 7.386678000 |
|   | 9.273697000  | 10.880769000 | 4.140515000 |
|   | 9.113031000  | 11.852484000 | 5.641268000 |
|   | 10.373639000 | 5.265448000  | 9.939820000 |
|   | 9.420168000  | 6.300170000  | 11.011338000|
|   | 15.181275000 | 8.887131000  | 3.771731000 |
|   | 15.680225000 | 10.400246000 | 4.529983000 |
|   | 10.060435000 | 4.042998000  | 1.929688000 |
|   | 11.315294000 | 4.555066000  | 0.789218000 |
|   | 6.553782000  | 9.549425000  | 6.358418000 |
|   | 6.932536000  | 11.187571000 | 5.795587000 |
|   | 14.401587000 | 4.690220000  | 3.995369000 |
|   | 14.913651000 | 4.024610000  | 5.555624000 |
|   | 10.806544000 | 2.689537000  | 6.519089000 |
|   | 9.231874000  | 2.186190000  | 5.863830000 |
|   | 8.472834000  | 9.621884000  | 1.905980000 |
|   | 8.350827000  | 8.315235000  | 0.712243000 |
|   | 7.223312000  | 10.377372000 | 3.447123000 |
|   | 5.620611000  | 9.958379000  | 4.074671000 |
|   | 9.948116000  | 2.741403000  | 3.542121000 |
|   | 11.055734000 | 1.591824000  | 4.301400000 |
|   | 12.752499000 | 2.792506000  | 5.806355000 |
|   | 13.579453000 | 2.351309000  | 4.305175000 |
|   | 14.569007000 | 9.809911000  | 6.671527000 |
|   | 15.865850000 | 8.715084000  | 6.172608000 |
|   | 8.866719000  | 8.535853000  | 9.894758000 |
|   | 10.187271000 | 8.382129000  | 11.034864000|
|   | 12.509626000 | 10.903013000 | 2.404534000 |
|   | 14.234751000 | 10.709961000 | 2.087121000 |
|   | 11.550175000 | 9.951083000  | 9.270589000 |
|   | 9.970505000  | 10.735050000 | 9.455059000 |
|   | 12.385645000 | 5.179515000  | 9.407572000 |
|   | 13.830363000 | 6.158489000  | 9.702668000 |
|   | 11.260870000 | 11.777634000 | 3.799891000 |
|   | 11.488434000 | 12.659937000 | 5.313237000 |
|   | 12.455598000 | 8.208480000  | 10.060456000|
|   | 11.945307000 | 6.909351000  | 11.151773000|
|   | 6.623884000  | 5.526484000  | 3.687065000 |
|   | 5.717458000  | 5.378624000  | 5.200412000 |
|   | 13.599856000 | 11.417236000 | 5.809515000 |
|   | 13.612769000 | 12.359634000 | 4.319886000 |
|   | 6.868105000  | 6.991516000  | 2.226900000 |
|   | 6.196751000  | 8.596785000  | 1.909255000 |
|   | 11.353151000 | 7.971043000  | 5.077297000 |
\[ \text{TREN}_3\text{Cu}^+\text{Cu}^+\text{Cu}^+\{\mu_3\text{-O}\} \text{ – BP86/def2-SVP (C, H, O, N)/def2-TZVP (Cu)} \]

|   | 5.142650000 | 1.378498000 | -2.485868000 |
|---|-------------|-------------|-------------|
| 3 | 3.599546000 | 0.008147000 | -3.843059000 |
| 6 | 3.990698000 | -1.387176000 | -4.160881000 |
| 1 | 3.978414000 | -1.951726000 | -3.207630000 |
| 1 | 3.219284000 | -1.865609000 | -4.818215000 |
| 6 | 5.376240000 | -1.559008000 | -4.822788000 |
| 7 | 6.541422000 | -1.138282000 | -4.048112000 |
| 7 | 4.964341000 | 2.630356000 | -4.157060000 |
| 6 | 6.092672000 | 2.376963000 | -4.438305000 |
| 29 | 3.599546000 | 0.008147000 | -3.843059000 |
| 7 | 7.357690000 | 2.669300000 | -4.438305000 |
| 29 | 7.828430000 | 1.225693000 | -2.215122000 |
| 29 | 6.425283000 | 2.750381000 | -0.553633000 |
| 7 | 8.102290000 | 2.913058000 | 1.158071000 |
| 6 | 9.397202000 | 2.523003000 | 0.606058000 |
| 7 | 9.590117000 | 3.168400000 | -0.690685000 |
| 7 | 8.019221000 | -1.650082000 | -2.143390000 |
| 6 | 6.992811000 | -2.122506000 | -3.028362000 |
| 1 | 7.365468000 | -3.018277000 | -3.577272000 |
| 6 | 9.378642000 | -1.464116000 | -2.607531000 |
| 1 | 10.038602000 | -1.381079000 | -1.715100000 |
| 1 | 9.702238000 | -2.399383000 | -3.117526000 |
| 6 | 9.704348000 | -0.330805000 | -3.615446000 |
| 7 | 9.615471000 | 1.088967000 | -3.108933000 |
| 7 | 3.431167000 | 0.968776000 | -0.963684000 |
| 6 | 2.670818000 | -0.161950000 | -1.502907000 |
| 6 | 2.382393000 | 0.024713000 | -2.999854000 |
| 6 | 3.436626000 | 0.839124000 | -5.048152000 |
| 6 | 3.657952000 | 2.337684000 | -4.792640000 |
| 6 | 5.024547000 | 4.052453000 | -3.727967000 |
| 7 | 6.306979000 | 4.333104000 | -3.109331000 |
| 6 | 6.019713000 | 4.703153000 | 0.000640000 |
| 6 | 7.288307000 | 5.213551000 | 0.610700000 |
| 6 | 7.928909000 | 4.281807000 | 1.653748000 |
| 1 | 7.307731000 | 4.248954000 | 2.572124000 |
| 1 | 8.898871000 | 4.742375000 | 1.953238000 |
| 8 | 8.018073000 | 5.352614000 | -0.209391000 |
| 1 | 7.102698000 | 6.210630000 | 1.079788000 |
| 6 | 5.859128000 | 5.639778000 | -1.082133000 |
| 6 | 7.507636000 | 5.421776000 | -1.315712000 |
| 1 | 5.614007000 | 6.687429000 | -0.698321000 |
| 6 | 6.398842000 | 5.597468000 | -2.387776000 |
| 6 | 7.409534000 | 4.064221000 | -4.018247000 |
| 6 | 8.523139000 | 2.167299000 | -5.156171000 |
| 6 | 9.763411000 | 2.022637000 | -4.266181000 |
| 6 | 10.720835000 | 1.335230000 | -2.118604000 |
| 6 | 11.701259000 | 1.177405000 | -2.631137000 |
| 6 | 10.636943000 | 0.550397000 | -1.342453000 |
| 6 | 10.757520000 | 2.732853000 | -1.449388000 |
| 1 | 10.989795000 | 3.508161000 | -2.211220000 |
| 1 | 11.640614000 | 2.728210000 | -0.773416000 |
| 6 | 10.042187000 | 3.016056000 | -3.865870000 |
| 1 | 10.618544000 | 1.697192000 | -4.904163000 |
|   | 1     | 2     | 3     | 4     | 5     |
|---|-------|-------|-------|-------|-------|
|   |       |       |       |       |       |
|   | 8.245291000 | 1.181218000 | -5.580434000 |       |       |
|   | 8.810377000 | 2.814214000 | -6.024716000 |       |       |
|   | 7.387733000 | 4.748832000 | -4.921638000 |       |       |
|   | 8.361956000 | 4.255848000 | -3.484554000 |       |       |
|   | 7.473168000 | 5.781890000 | -2.181307000 |       |       |
|   | 6.057572000 | 6.471722000 | -3.002010000 |       |       |
|   | 4.948621000 | 4.583566000 | 1.049449000   |       |       |
|   | 6.520463000 | 4.291071000 | 0.527384000   |       |       |
|   | 3.443022000 | 3.315145000 | -0.551065000 |       |       |
|   | 2.673733000 | 2.083071000 | -0.389903000 |       |       |
|   | 1.697903000 | 2.137872000 | -0.927489000 |       |       |
|   | 3.041779000 | 5.253656000 | 1.410304000   |       |       |
|   | 5.268681000 | 4.583566000 | 1.049449000   |       |       |
|   | 4.903468000 | 4.291071000 | 1.735068000   |       |       |
|   | 4.206825000 | 4.217132000 | -2.998028000 |       |       |
|   | 2.876471000 | 2.733702000 | -4.111734000 |       |       |
|   | 3.548452000 | 2.883444000 | -5.761841000 |       |       |
|   | 4.156277000 | 0.487475000 | -5.812418000 |       |       |
|   | 2.427052000 | 0.714672000 | -5.513324000 |       |       |
|   | 1.877988000 | 1.004620000 | -3.130216000 |       |       |
|   | 1.653247000 | -0.750199000 | -3.345697000 |       |       |
|   | 3.266505000 | -1.084458000 | -1.347266000 |       |       |
|   | 1.705363000 | -0.325737000 | -0.970150000 |       |       |
|   | 8.996217000 | -0.425977000 | -4.460843000 |       |       |
|   | 10.739428000 | -0.490171000 | -4.006190000 |       |       |
|   | 9.378883000 | 1.405135000 | 0.559092000  |       |       |
|   | 5.942230000 | 3.005764000 | -6.017285000 |       |       |
|   | 6.088833000 | 1.313699000 | -5.390434000 |       |       |
|   | 5.381959000 | -1.047005000 | -5.812345000 |       |       |
|   | 5.484248000 | -2.637526000 | -5.071007000 |       |       |
|   | 6.145900000 | -2.475116000 | -2.387543000 |       |       |
|   | 2.421810000 | 1.915663000 | 0.692100000  |       |       |
|   | 10.254150000 | 2.816707000 | 1.264903000  |       |       |
|   | 6.313646000 | -0.256422000 | -3.539311000 |       |       |
|   | 7.681873000 | -0.940863000 | -1.473599000 |       |       |
|   | 7.801250000 | 2.218795000 | 1.847391000  |       |       |
|   | 4.387904000 | 3.047541000 | -0.904278000 |       |       |
|   | 4.187634000 | 0.661089000 | -0.356840000 |       |       |
|   | 8.721686000 | 2.981075000 | -1.242204000 |       |       |
|   | 6.405816000 | 0.936532000 | -1.057821000 |       |       |

\[\text{TREN}_3\text{Cu}^1\text{Cu}^1\text{Cu}^1\text{Cu}^1(\mu_2\text{O})] - \text{BP86/def2-SVP(C, H, O, N)/def2-TZVP(Cu)}\]

2, 2

9

[488x51]S35
|      |                |                |                |
|-----|----------------|----------------|----------------|
| 29  | 8.041408000    | 0.982797000    | -2.282325000   |
| 29  | 6.197588000    | 2.922971000    | -0.652406000   |
| 7   | 7.960702000    | 3.116538000    | 0.816342000    |
| 6   | 9.332713000    | 3.219660000    | 0.287810000    |
| 6   | 9.685306000    | 2.091716000    | -0.551806000   |
| 7   | 8.177109000    | -1.228943000   | -2.634919000   |
| 7   | 7.221777000    | -1.808268000   | -3.587275000   |
| 1   | 7.423134000    | -1.369017000   | -4.586354000   |
| 6   | 9.579668000    | -1.467009000   | -3.031345000   |
| 1   | 10.195712000   | -1.518237000   | -2.112721000   |
| 1   | 9.715593000    | -2.445852000   | -3.547367000   |
| 6   | 10.077503000   | -0.543070000   | -3.949800000   |
| 7   | 7.966616000    | 0.993277000    | -3.125550000   |
| 7   | 9.247547000    | 0.661011000    | -0.804892000   |
| 6   | 2.182785000    | -0.053394000   | -1.518208000   |
| 7   | 2.141107000    | 0.349639000    | -2.998236000   |
| 6   | 3.499469000    | 0.867347000    | -4.971369000   |
| 6   | 3.823667000    | 2.352022000    | -4.775912000   |
| 6   | 5.167724000    | 3.974925000    | -3.598192000   |
| 7   | 6.412325000    | 4.201743000    | -2.857734000   |
| 7   | 6.704960000    | 0.661011000    | -0.804892000   |
| 6   | 7.613920000    | 4.510806000    | 0.783833000    |
| 6   | 6.869512000    | 3.961764000    | 2.407415000    |
| 1   | 8.488825000    | 4.668101000    | 2.224485000    |
| 1   | 7.816652000    | 5.722979000    | 0.048223000    |
| 1   | 6.836477000    | 6.307252000    | 1.411893000    |
| 6   | 5.589354000    | 5.854755000    | -1.140211000   |
| 1   | 4.351337000    | 0.5723427000   | -1.444106000   |
| 5   | 6.490811000    | 6.931529000    | -0.863213000   |
| 6   | 6.506316000    | 5.574413000    | -2.334178000   |
| 6   | 7.564875000    | 3.914160000    | -3.715853000   |
| 6   | 8.665976000    | 2.242506000    | -5.101902000   |
| 6   | 9.981924000    | 2.069900000    | -4.337590000   |
| 6   | 11.097106000   | 1.177532000    | -2.358460000   |
| 1   | 12.049648000   | 1.348278000    | -2.913336000   |
| 1   | 11.229850000   | 0.227371000    | -1.802579000   |
| 6   | 10.893408000   | 2.303608000    | -1.347499000   |
| 1   | 10.790457000   | 3.279942000    | -1.869720000   |
| 1   | 11.827555000   | 2.388276000    | -0.739229000   |
| 1   | 10.242536000   | 3.017880000    | -3.827836000   |
| 1   | 10.795971000   | 1.894090000    | -5.080196000   |
| 1   | 8.426684000    | 1.311063000    | -5.657815000   |
| 1   | 8.829908000    | 3.025997000    | -5.885052000   |
| 1   | 7.619776000    | 4.659223000    | -4.567470000   |
| 1   | 8.482997000    | 4.032831000    | -3.107042000   |
| 1   | 7.564608000    | 5.742334000    | -2.042938000   |
| 1   | 6.285718000    | 6.337727000    | -3.122611000   |
| 1   | 4.666726000    | 5.005429000    | 0.955084000    |
| 1   | 3.500727000    | 4.151070000    | 0.474930000    |
| 1   | 3.916938000    | 2.763691000    | 0.228313000    |
| 1   | 2.831496000    | 1.993803000    | -0.382548000   |
| 1   | 2.504994000    | 2.554544000    | -1.284050000   |
| 1   | 3.091050000    | 4.551674000    | -0.476791000   |
| 1   | 2.671396000    | 4.237765000    | 1.217762000    |
|   |   |   |   |   |   |   |   |   |   |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 4.999807000 | 4.627422000 | 1.941980000 |
| 1 | 4.319338000 | 6.050867000 | -2.918109000 |
| 1 | 5.073846000 | 4.727580000 | -2.932943000 |
| 1 | 4.305885000 | 4.127217000 | -2.946384000 |
| 1 | 3.760639000 | 2.847610000 | -2.986870000 |
| 1 | 4.270325000 | 0.401324000 | -3.072406000 |
| 1 | 2.542922000 | 0.791906000 | -3.148111000 |
| 1 | 1.932577000 | 1.435111000 | -3.153281000 |
| 1 | 1.289200000 | -0.164334000 | -3.158782000 |
| 1 | 2.364921000 | -1.142484000 | -3.163281000 |
| 1 | 1.169362000 | 0.125532000 | -3.172406000 |
| 1 | 9.470602000 | -0.337442000 | -3.177848000 |
| 1 | 11.126403000 | 0.552993000 | -3.182866000 |
| 1 | 10.057667000 | 3.375725000 | -3.187848000 |
| 1 | 6.221299000 | 3.014399000 | -3.192866000 |
| 1 | 6.226661000 | 1.299093000 | -3.197848000 |
| 1 | 5.287989000 | -1.362486000 | -3.202866000 |
| 1 | 4.878045000 | -2.943684000 | -3.207848000 |
| 1 | 7.385530000 | -2.913843000 | -3.212866000 |
| 1 | 1.933267000 | 1.948144000 | -3.217848000 |
| 1 | 9.392372000 | 4.135648000 | -3.222866000 |
| 1 | 1.933267000 | 1.948144000 | -3.227848000 |
| 1 | 9.392372000 | 4.135648000 | -3.232866000 |
| 1 | 1.933267000 | 1.948144000 | -3.237848000 |
| 1 | 9.392372000 | 4.135648000 | -3.242866000 |
| 1 | 1.933267000 | 1.948144000 | -3.247848000 |

[TREN]_\text{Cu}^I\text{Cu}^\text{II}(\mu_3-O)\text{I} – \text{BP}86/\text{def2-SVP (C, H, O, N)/def2-TZVP (Cu)}

\[3, 3\]

29 | 5.013514000 | 0.642931000 | -2.445526000 |
7  | 3.370342000 | 0.079773000 | -3.764293000 |
6  | 3.501299000 | -1.362486000 | -4.095789000 |
1  | 3.095849000 | -1.957383000 | -3.249704000 |
1  | 2.879667000 | -1.632801000 | -4.981157000 |
6  | 4.947675000 | -1.768680000 | -4.339857000 |
7  | 5.804839000 | -1.386192000 | -3.189495000 |
7  | 5.091639000 | 2.552374000 | -4.021035000 |
6  | 6.245253000 | 2.285569000 | -4.893939000 |
7  | 7.515811000 | 2.492293000 | -4.178846000 |
29 | 8.129092000 | 1.094591000 | -2.239055000 |
29 | 6.158894000 | 2.985397000 | -0.669338000 |
7  | 7.848373000 | 3.055874000 | 0.768780000 |
6  | 9.206555000 | 3.135575000 | 0.207034000 |
7  | 9.548084000 | 2.012951000 | -0.674142000 |
7  | 8.163024000 | -1.107790000 | -2.530103000 |
6  | 7.210131000 | -1.677776000 | -3.496610000 |
7  | 7.431122000 | -1.242985000 | -4.492092000 |
6  | 9.559760000 | -1.424091000 | -2.932943000 |
1  | 10.184184000 | -1.449687000 | -2.018900000 |
1  | 9.641192000 | -2.436850000 | -3.387548000 |
6  | 10.080029000 | -0.379666000 | -3.922754000 |
7  | 10.003054000 | 0.991123000 | -3.346917000 |
|    | 3.412823000 | 0.649856000 | -0.913602000 |
|----|-------------|-------------|--------------|
| 6  | 2.279685000 | -0.092213000| -1.531313000|
| 6  | 2.114014000 | 0.311263000 | -2.998331000|
| 6  | 3.435506000 | 0.910444000 | -4.998465000|
| 6  | 3.804537000 | 2.370954000 | -4.735709000|
| 6  | 5.174391000 | 3.936186000 | -3.527525000|
| 7  | 6.427832000 | 4.168431000 | -2.793195000|
| 7  | 5.841734000 | 5.025905000 | 0.038130000 |
| 6  | 7.058573000 | 5.406559000 | 0.807650000 |
| 6  | 3.435506000 | 0.910444000 | -4.998465000|
| 6  | 7.572982000 | 2.279685000 | -0.092213000|
| 6  | 7.832220000 | 5.732491000 | -1.531313000|
| 6  | 8.503235000 | 6.282835000 | 1.465305000 |
| 6  | 5.624528000 | 5.905070000 | -1.142721000|
| 1  | 4.561784000 | 5.813446000 | -1.445503000|
| 1  | 5.767582000 | 6.977212000 | -0.872694000|
| 6  | 6.534230000 | 5.573267000 | -2.325734000|
| 6  | 7.567537000 | 3.874199000 | -3.679061000|
| 6  | 8.642661000 | 2.200630000 | -5.098749000|
| 6  | 9.994158000 | 2.041859000 | -4.401431000|
| 6  | 11.131424000| 1.203009000 | -2.396269000|
| 1  | 12.019650000| 1.447057000 | -2.939978000|
| 1  | 11.323269000| 0.248960000 | -1.865269000|
| 6  | 10.826726000| 2.289992000 | -1.376996000|
| 6  | 10.728574000| 3.278753000 | -1.873656000|
| 1  | 11.685202000| 2.382145000 | -0.673824000|
| 1  | 10.291930000| 2.999374000 | -3.930569000|
| 1  | 10.768294000| 1.834094000 | -5.175101000|
| 1  | 8.386878000 | 1.267730000 | -5.643960000|
| 1  | 8.748180000 | 2.987625000 | -5.885016000|
| 1  | 7.581846000 | 4.597607000 | -4.544747000|
| 1  | 8.503235000 | 4.024259000 | -3.105280000|
| 1  | 7.595405000 | 5.743057000 | -2.048142000|
| 1  | 6.317330000 | 6.296997000 | -3.148327000|
| 6  | 4.652553000 | 5.043282000 | 0.936061000 |
| 6  | 3.532622000 | 4.151002000 | 0.424859000 |
| 7  | 4.025623000 | 2.772988000 | 0.175498000 |
| 6  | 2.958390000 | 1.961154000 | -0.421814000|
| 1  | 2.549764000 | 2.528165000 | -1.282423000|
| 1  | 3.124636000 | 4.537550000 | -0.532027000|
| 1  | 2.688102000 | 4.173858000 | 1.150617000 |
| 1  | 4.967881000 | 4.691614000 | 1.938149000 |
| 1  | 4.275369000 | 6.080751000 | 1.079045000 |
| 1  | 5.092128000 | 4.661534000 | -4.387558000|
| 1  | 4.314540000 | 4.120652000 | -2.854685000|
| 1  | 3.019451000 | 2.851748000 | -4.115877000|
| 1  | 3.795480000 | 2.915223000 | -5.710641000|
| 1  | 4.175108000 | 0.448996000 | -5.683908000|
| 1  | 2.464351000 | 0.882760000 | -5.543858000|
| 1  | 1.856954000 | 1.387002000 | -3.064887000|
| 1  | 1.259035000 | -0.239822000| -3.451257000|
| 1  | 2.486983000 | -1.177104000| -1.439252000|
| 1  | 1.323469000 | 0.082224000 | -0.988341000|
| 1  | 9.472386000 | -0.401251000| -4.848106000|
|   |       |                  |                  |                  |
|---|-------|------------------|------------------|------------------|
| 1 | 11.12068200 | -0.628703000 | -4.229877000 |
| 1 | 9.957506000 | 3.233142000 | 1.031664000 |
| 1 | 6.202706000 | 2.947919000 | -5.806356000 |
| 1 | 6.208420000 | 1.236498000 | -5.245300000 |
| 1 | 5.350376000 | -1.256318000 | -5.238473000 |
| 1 | 4.992159000 | -2.859465000 | -4.557940000 |
| 1 | 7.371091000 | -2.781430000 | -3.589660000 |
| 1 | 2.113625000 | 1.828312000 | 0.300599000 |
| 1 | 9.276376000 | 4.065018000 | -0.393501000 |
| 1 | 5.527432000 | 2.355677000 | 1.087239000 |
| 1 | 3.777301000 | -0.119625000 | 0.300599000 |
| 1 | 9.685699000 | 1.174129000 | -0.088048000 |
| 8 | 2.113625000 | 1.828312000 | -3.589660000 |

[TREN]$_3^{-}$Cu$_{11}$Cu$_{11}$Cu$_{11}$($\mu_2$=O) – BP86/def2-SVP (C, H, O, N)/def2-TZVP (Cu)
|   |   |   |   |   |
|---|---|---|---|---|
| 1 | 6.865153000 | 6.289859000 | 1.460130000 |
| 6 | 5.600324000 | 5.925512000 | -1.139444000 |
| 1 | 4.532025000 | 5.839666000 | -1.422757000 |
| 1 | 5.752081000 | 6.994164000 | -0.863670100 |
| 6 | 6.495937000 | 5.587361000 | -2.325577000 |
| 6 | 7.561578000 | 3.863118000 | -3.629591000 |
| 6 | 8.671955000 | 2.227075000 | -5.090859000 |
| 6 | 10.023304000 | 2.060775000 | -4.404950000 |
| 6 | 11.135486000 | 1.187118000 | -2.390486000 |
| 12 | 12.078290000 | 1.424421000 | 2.931149000 |
| 1 | 11.315107000 | 0.226253000 | -1.869107000 |
| 6 | 10.824376000 | 2.268200000 | -1.372722000 |
| 1 | 10.777473000 | 3.269904000 | -1.848200000 |
| 1 | 11.648458000 | 1.187118000 | -2.390486000 |
| 1 | 12.078290000 | 1.424421000 | 2.931149000 |
| 1 | 8.414814000 | 1.310790000 | -5.660913000 |
| 1 | 8.744287000 | 3.045514000 | -5.843959000 |
| 1 | 7.552158000 | 4.577135000 | -4.495465000 |
| 1 | 8.494454000 | 4.039840000 | -3.061843000 |
| 1 | 7.558578000 | 5.782570000 | -2.076057000 |
| 1 | 6.251243000 | 6.267679000 | -3.173623000 |
| 6 | 4.656717000 | 5.040651000 | 0.950034000 |
| 6 | 3.546300000 | 4.147445000 | 0.432035000 |
| 7 | 4.077745000 | 2.785531000 | 0.136409000 |
| 6 | 2.999232000 | 1.946778000 | -0.407843000 |
| 1 | 2.503092000 | 2.513329000 | -1.221357000 |
| 1 | 3.108016000 | 4.549100000 | -0.504640000 |
| 1 | 2.717611000 | 4.120496000 | 1.174515000 |
| 1 | 4.982692000 | 4.687040000 | 1.947242000 |
| 1 | 4.283502000 | 6.077770000 | 1.098287000 |
| 1 | 5.083376000 | 4.600381000 | -4.358770000 |
| 1 | 4.287418000 | 4.069033000 | -2.836476000 |
| 1 | 3.022627000 | 2.848546000 | 0.416862000 |
| 7 | 3.858859000 | 2.895662000 | 0.416862000 |
| 1 | 2.163500000 | 0.416862000 | 0.416862000 |
| 2 | 2.457853000 | 0.867828000 | 0.416862000 |
| 1 | 1.850174000 | 1.403217000 | -3.076060000 |
| 1 | 1.253552000 | -0.225191000 | -3.459512000 |
| 1 | 2.489422000 | -1.166851000 | -1.452353000 |
| 1 | 1.357666000 | 0.106814000 | -0.977096000 |
| 1 | 9.470191000 | 0.400319000 | -4.867268000 |
| 1 | 11.117317000 | -0.628500000 | -4.245072000 |
| 1 | 9.915816000 | 3.132291000 | 1.033007000 |
| 1 | 6.231795000 | 2.920808000 | 0.920808000 |
| 1 | 6.250301000 | 1.204315000 | -5.222756000 |
| 1 | 5.339786000 | -1.305145000 | 5.248854000 |
| 1 | 5.000579000 | -2.869352000 | 4.476467000 |
| 1 | 7.321063000 | -2.769903000 | 3.455305000 |
| 1 | 2.221383000 | 1.767054000 | 0.373925000 |
| 1 | 9.302692000 | 4.063020000 | -0.362481000 |
| 1 | 5.494365000 | -1.839555000 | 2.346599000 |
| 1 | 7.986327000 | -1.418029000 | -1.580642000 |
| 1 | 7.706695000 | 2.193015000 | 1.281877000 |
| 1 | 4.373186000 | 2.368071000 | 1.034752000 |
|    |                    |                  |                   |                   |
|----|--------------------|------------------|-------------------|-------------------|
| 1  | 3.850507000        | 0.092839000      | -0.191869000      |
| 1  | 9.598273000        | 1.144987000      | -0.168339000      |
| 8  | 6.450609000        | 1.284085000      | -1.417582000      |

\[\text{TREN}_2\text{Cu}^+\text{Cu}^+\text{Cu}^{II}(\mu_2\text{-OH})] - \text{TPSSH/def2-TZVP (TD-DFT)}

|    |                    |                  |                   |                   |
|----|--------------------|------------------|-------------------|-------------------|
| 29 | 9.863709000        | -0.255723000     | 10.292554000      |
| 6  | 10.996198000       | 1.975354000      | 12.070077000      |
| 1  | 11.009247000       | 2.886877000      | 12.700143000      |
| 1  | 12.011053000       | 1.879665000      | 11.655274000      |
| 6  | 8.394522000        | -1.357951000     | 13.329232000      |
| 1  | 7.912575000        | -2.129739000     | 13.534778000      |
| 1  | 8.092595000        | -0.389376000     | 13.329232000      |
| 7  | 7.892816000        | -1.394897000     | 11.512450000      |
| 6  | 9.905498000        | -1.535335000     | 13.002691000      |
| 1  | 10.196914000       | -1.512594000     | 14.068425000      |
| 1  | 10.188046000       | -2.529058000     | 12.628443000      |
| 7  | 10.678965000       | -0.518770000     | 12.233411000      |
| 7  | 11.664062000       | -1.539717000     | 9.645162000       |
| 7  | 12.065839000       | -0.142993000     | 7.738207000       |
| 7  | 10.868347000       | -2.238593000     | 7.454234000       |
| 6  | 10.681852000       | 0.782202000      | 12.966313000      |
| 1  | 11.415535000       | 0.755193000      | 13.792111000      |
| 1  | 9.700541000        | 0.909767000      | 13.440207000      |
| 6  | 11.427041000       | -2.684149000     | 8.746803000       |
| 1  | 10.721391000       | -3.370771000     | 9.232890000       |
| 1  | 12.383882000       | -3.230268000     | 8.573150000       |
| 6  | 7.869488000        | -2.766267000     | 10.993029000      |
| 7  | 7.216418000        | -3.409952000     | 11.633127000      |
| 1  | 8.883266000        | -3.188673000     | 11.014811000      |
| 6  | 12.082067000       | -0.995383000     | 12.046313000      |
| 1  | 12.475399000       | -1.422054000     | 12.986130000      |
| 1  | 12.708463000       | -0.122883000     | 11.817099000      |
| 6  | 11.802554000       | -1.255963000     | 6.841092000       |
| 1  | 11.341095000       | -0.880102000     | 5.920946000       |
| 1  | 12.749456000       | -1.783781000     | 6.563662000       |
| 6  | 12.638072000       | -0.643691000     | 8.975244000       |
| 1  | 12.868770000       | 0.204208000      | 9.632619000       |
| 1  | 13.587265000       | -1.211572000     | 8.803081000       |
| 6  | 12.363314000       | 1.645696000      | 5.957453000       |
| 1  | 12.087599000       | 0.954393000      | 5.150228000       |
| 1  | 13.178325000       | 2.273903000      | 5.537934000       |
| 6  | 12.204642000       | -2.034433000     | 10.937301000      |
| 1  | 13.263140000       | -2.338398000     | 10.844876000      |
| 1  | 11.645727000       | -2.944036000     | 11.203832000      |
| 6  | 12.966250000       | 0.856304000      | 7.122064000       |
| 1  | 13.266756000       | 1.545121000      | 7.925146000       |
| 1  | 13.902905000       | 0.384603000      | 6.759948000       |
| 29 | 8.702366000        | -1.652336000     | 7.771688000       |
| 6  | 10.739917000       | -3.388253000     | 6.516339000       |
| 1  | 11.649199000       | -4.017716000     | 6.522337000       |
| 1  | 10.668836000       | -2.964932000     | 5.503717000       |
| 6  | 7.394857000        | -4.168657000     | 9.101675000       |
| 1  | 6.604674000        | -4.779748000     | 9.579532000       |
| 1  | 8.352281000        | -4.618290000     | 9.405667000       |

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|   |   |   |   |   |
|---|---|---|---|---|
|   |   |   |   |   |
| 7 | 7.388331000 | -2.776360000 | 9.604639000 |
| 6 | 7.218453000 | -4.253454000 | 7.590769000 |
| 1 | 7.220178000 | -5.315876000 | 7.287668000 |
| 1 | 6.235404000 | -3.853949000 | 7.310640000 |
| 7 | 8.252059000 | -3.494233000 | 6.832302000 |
| 7 | 7.214861000 | -0.850763000 | 5.830471000 |
| 7 | 8.609598000 | 1.040664000 | 5.406815000 |
| 7 | 6.541636000 | 1.340543000 | 6.642776000 |
| 6 | 9.529505000 | -4.267559000 | 6.806790000 |
| 6 | 9.481000000 | -5.071846000 | 6.050631000 |
| 6 | 9.646750000 | -4.768952000 | 7.776325000 |
| 6 | 6.082530000 | 0.039031000 | 6.102565000 |
| 1 | 5.428087000 | -0.446095000 | 6.840381000 |
| 1 | 5.487319000 | 0.217436000 | 5.173478000 |
| 6 | 6.024859000 | -2.225177000 | 9.583361000 |
| 1 | 5.342101000 | -2.879762000 | 10.181194000 |
| 6 | 5.651344000 | -2.060240000 | 8.550520000 |
| 7 | 7.774170000 | -3.256183000 | 5.436355000 |
| 1 | 7.355140000 | -4.187551000 | 5.015129000 |
| 1 | 8.648212000 | -3.005856000 | 4.820058000 |
| 6 | 7.504236000 | 1.941928000 | 5.681483000 |
| 1 | 7.888163000 | 2.869412000 | 6.122072000 |
| 1 | 6.956656000 | 2.207012000 | 4.741098000 |
| 6 | 8.089357000 | -0.193984000 | 4.843498000 |
| 1 | 8.930023000 | -0.856679000 | 4.598821000 |
| 6 | 7.514700000 | -0.012626000 | 3.897536000 |
| 6 | 10.407617000 | 2.797693000 | 5.103654000 |
| 1 | 9.729009000 | 3.619106000 | 5.368236000 |
| 1 | 11.056322000 | 3.203153000 | 4.297868000 |
| 6 | 6.726711000 | -2.150674000 | 5.329262000 |
| 1 | 6.395559000 | -2.088928000 | 4.274503000 |
| 1 | 5.829874000 | -2.419329000 | 5.908369000 |
| 6 | 9.601100000 | 1.648027000 | 4.497327000 |
| 1 | 10.276769000 | 0.838359000 | 4.183313000 |
| 1 | 9.126301000 | 2.022479000 | 3.566691000 |
| 29 | 7.158111000 | 1.128257000 | 8.846880000 |
| 8 | 8.851378000 | 0.136057000 | 8.622385000 |
| 6 | 5.387653000 | 2.271853000 | 6.762782000 |
| 1 | 4.771943000 | 2.267856000 | 5.843496000 |
| 1 | 5.801486000 | 3.287524000 | 6.849266000 |
| 6 | 4.613268000 | -0.354338000 | 10.070969000 |
| 1 | 3.984521000 | -0.847535000 | 10.838310000 |
| 1 | 4.188648000 | -0.648092000 | 9.098945000 |
| 7 | 6.006374000 | -0.852643000 | 10.104899000 |
| 6 | 4.505395000 | 1.153132000 | 10.265351000 |
| 1 | 3.437766000 | 1.437399000 | 10.267220000 |
| 1 | 4.899720000 | 1.428169000 | 11.252638000 |
| 7 | 5.248070000 | 1.941203000 | 9.241585000 |
| 7 | 7.869196000 | 2.897880000 | 10.228261000 |
| 7 | 9.777036000 | 3.353388000 | 8.859463000 |
| 7 | 10.074835000 | 2.120060000 | 10.919291000 |
| 6 | 4.490892000 | 1.963103000 | 7.955470000 |
| 1 | 3.675900000 | 2.707542000 | 7.998122000 |
| 1 | 4.005410000 | 0.987623000 | 7.826170000 |
| 6 | 8.767107000 | 2.621324000 | 11.368701000 |
|   |    |    |     |
|---|---|---|-----|
|1  | 8.286735000 | 1.864398000 | 12.004481000 |
|1  | 8.899749000 | 3.552346000 | 11.972786000 |
|6  | 6.524587000 | -0.862005000 | 11.479286000 |
|1  | 5.855095000 | -1.468687000 | 12.139473000 |
|7  | 11.178739000 | 2.441302000 | 6.302162000 |
|6  | 5.459492000 | 3.336250000 | 9.732359000 |
|1  | 4.530342000 | 3.733246000 | 10.178285000 |
|1  | 5.682589000 | 3.969852000 | 8.863544000 |
|7  | 11.178739000 | 2.441302000 | 6.302162000 |
|6  | 5.459492000 | 3.336250000 | 9.732359000 |
|1  | 4.530342000 | 3.733246000 | 10.178285000 |
|1  | 5.682589000 | 3.969852000 | 8.863544000 |
|6  | 10.672572000 | 3.089564000 | 9.975105000 |
|1  | 11.608257000 | 2.660712000 | 9.597428000 |
|1  | 10.924299000 | 4.037686000 | 10.517402000 |
|6  | 8.535482000 | 3.903527000 | 9.367139000 |
|1  | 7.879577000 | 4.155901000 | 8.523339000 |
|1  | 8.698406000 | 4.837310000 | 9.964318000 |
|6  | 11.542249000 | 3.638522000 | 7.071755000 |
|1  | 12.354632000 | 3.369750000 | 7.759526000 |
|1  | 11.960118000 | 4.438051000 | 6.423372000 |
|6  | 6.586956000 | 3.429677000 | 10.753219000 |
|1  | 6.688198000 | 4.480456000 | 11.081520000 |
|1  | 6.330941000 | 2.853114000 | 11.655149000 |
|6  | 10.388442000 | 4.256360000 | 7.865101000 |
|1  | 9.584375000 | 4.565586000 | 7.180776000 |
|1  | 9.434888000 | 0.686981000 | 8.049087000 |

$|\text{TREN}_2\text{Cu}^{II}\text{Cu}^{II}(\mu_2\text{-OH})|$ – TPSSh/def2-TZVP (TD-DFT)

4, 3

|   |    |    |     |
|---|---|---|-----|
|29 | 11.335532000 | 5.561258000 | 4.697933000 |
|29 | 8.965119000 | 7.918370000 | 4.633196000 |
|29 | 10.784921000 | 7.414099000 | 7.401208000 |
|8  | 10.730231000 | 7.342440000 | 5.391752000 |
|7  | 9.601658000 | 4.305787000 | 5.913186000 |
|7  | 7.029813000 | 8.308150000 | 3.899175000 |
|7  | 13.401160000 | 5.595030000 | 5.643785000 |
|7  | 9.568134000 | 7.902492000 | 2.447341000 |
|8  | 8.587901000 | 9.829380000 | 5.860954000 |
|7  | 13.898960000 | 7.892815000 | 6.169954000 |
|7  | 10.817242000 | 10.653486000 | 5.504129000 |
|7  | 11.824082000 | 3.613733000 | 4.072882000 |
|7  | 8.827917000 | 5.861894000 | 7.608814000 |
|7  | 12.843888000 | 6.511488000 | 7.830235000 |
|7  | 12.003851000 | 8.060406000 | 2.439214000 |
|7  | 10.259138000 | 9.604626000 | 7.637565000 |
|7  | 7.809035000 | 5.863488000 | 5.401357000 |
|7  | 10.593006000 | 7.343613000 | 9.503238000 |
|7  | 13.484446000 | 10.128058000 | 4.116902000 |
|7  | 10.964562000 | 5.887885000 | 2.440322000 |
|7  | 8.832687000 | 9.837020000 | 7.319098000 |
|7  | 14.318335000 | 6.717565000 | 5.422672000 |
|7  | 13.302045000 | 5.311170000 | 7.100235000 |
|7  | 13.849989000 | 7.579865000 | 7.586690000 |
|7  | 9.703921000 | 6.505471000 | 1.974771000 |
|7  | 10.762776000 | 8.676379000 | 1.997320000 |
|6  | 6.025334000 | 7.408828000 | 4.542013000 |
|   | 8.337969000 | 4.504391000 | 5.181463000 |
|---|-------------|-------------|-------------|
| 6 | 12.085941000 | 6.710405000 | 9.926836000 |
| 6 | 7.577710000 | 6.025135000 | 9.054182000 |
| 6 | 9.335141000 | 4.505255000 | 7.038135000 |
| 6 | 8.505515000 | 6.025135000 | 9.054182000 |
| 6 | 12.080056000 | 3.659203000 | 2.600672000 |
| 6 | 13.137558000 | 10.102151000 | 5.628197000 |
| 6 | 14.026838000 | 4.371006000 | 4.977902000 |
| 6 | 10.082301000 | 2.906945000 | 5.732732000 |
| 6 | 8.372672000 | 8.539775000 | 4.368416000 |
| 6 | 6.712916000 | 9.735270000 | 4.213219000 |
| 6 | 10.708835000 | 2.665130000 | 4.812072000 |
| 6 | 13.058429000 | 3.210634000 | 4.812072000 |
| 6 | 14.821937000 | 9.034936000 | 5.946933000 |
| 6 | 9.985465000 | 8.636213000 | 9.944026000 |
| 6 | 13.356230000 | 10.198890000 | 2.657310000 |
| 6 | 10.481005000 | 9.803457000 | 9.106326000 |
| 6 | 12.792143000 | 6.181799000 | 9.287073000 |
| 6 | 11.635329000 | 11.684212000 | 4.816715000 |
| 6 | 11.969865000 | 7.196163000 | 10.067759000 |
| 6 | 6.517466000 | 5.974820000 | 4.664162000 |
| 6 | 13.136110000 | 11.396799000 | 4.766973000 |
| 6 | 7.058219000 | 8.087045000 | 2.421944000 |
| 6 | 8.514891000 | 10.817908000 | 7.739130000 |
| 6 | 8.220684000 | 9.053524000 | 7.857590000 |
| 6 | 15.351169000 | 6.402646000 | 5.708833000 |
| 6 | 14.315674000 | 6.947249000 | 4.350434000 |
| 6 | 12.596182000 | 4.490984000 | 7.285384000 |
| 6 | 14.297583000 | 5.003360000 | 7.490710000 |
| 6 | 14.835861000 | 7.234382000 | 7.982888000 |
| 6 | 13.569739000 | 8.484940000 | 8.142602000 |
| 6 | 8.860627000 | 5.910864000 | 2.350337000 |
| 6 | 9.673569000 | 6.485746000 | 0.861765000 |
| 6 | 10.727366000 | 8.757807000 | 0.883665000 |
| 6 | 10.685612000 | 9.688059000 | 2.412661000 |
| 6 | 5.787257000 | 7.817501000 | 5.531771000 |
| 6 | 5.082215000 | 7.418837000 | 3.968611000 |
| 6 | 8.511656000 | 4.363880000 | 4.107223000 |
| 6 | 7.588524000 | 3.745599000 | 5.508546000 |
| 6 | 12.043824000 | 6.687767000 | 0.796576000 |
| 6 | 13.041290000 | 6.265379000 | 2.220610000 |
| 6 | 6.809579000 | 5.306759000 | 7.197120000 |
| 6 | 7.193915000 | 7.047363000 | 7.038135000 |
| 6 | 8.597280000 | 3.748676000 | 7.708946000 |
| 6 | 10.271630000 | 4.350479000 | 7.900881000 |
| 6 | 7.850100000 | 6.903510000 | 9.140753000 |
| 6 | 7.918495000 | 5.168319000 | 9.435427000 |
| 6 | 13.086689000 | 4.066012000 | 2.438914000 |
| 6 | 12.084114000 | 2.640194000 | 2.176174000 |
| 1 | 14.067532000 | 8.212812000 | 2.168207000 |
| 1 | 13.153162000 | 9.004748000 | 0.886060000 |
| 1 | 12.138306000 | 10.390408000 | 7.106983000 |
| 1 | 12.138306000 | 10.390408000 | 7.106983000 |
| 1 | 10.872417000 | 11.626756000 | 7.399653000 |
| 1 | 9.9081751000 | 11.890768000 | 5.726309000 |
| 1 | 10.352290000 | 5.285700000 | 9.904579000 |
| 1 | 9.4191950000 | 6.323458000 | 10.976024000 |
| 1 | 15.135178000 | 8.874194000 | 3.811287000 |
| 1 | 15.573156000 | 10.420366000 | 4.509497000 |
| 1 | 10.046680000 | 4.052990000 | 1.951180000 |
| 1 | 11.288508000 | 4.532363000 | 0.798059000 |
| 1 | 6.568520000 | 9.518445000 | 6.366143000 |
| 1 | 6.894262000 | 11.162363000 | 5.817872000 |
| 1 | 14.396504000 | 4.709210000 | 3.999400000 |
| 1 | 14.913033000 | 4.026151000 | 5.539297000 |
| 1 | 10.813615000 | 2.711052000 | 6.530863000 |
| 1 | 9.264050000 | 2.178391000 | 5.881825000 |
| 1 | 8.495408000 | 9.627179000 | 1.917568000 |
| 1 | 8.353116000 | 8.339270000 | 0.720454000 |
| 1 | 7.225948000 | 10.369979000 | 3.479735000 |
| 1 | 5.633189000 | 9.927657000 | 4.091020000 |
| 1 | 9.953885000 | 2.764675000 | 3.577114000 |
| 1 | 11.069051000 | 1.623228000 | 4.316679000 |
| 1 | 12.757884000 | 2.818857000 | 5.792964000 |
| 1 | 13.568807000 | 2.381607000 | 4.292760000 |
| 1 | 14.546663000 | 9.805766000 | 6.682281000 |
| 1 | 15.868821000 | 8.753437000 | 6.179382000 |
| 1 | 8.893964000 | 8.546432000 | 9.875441000 |
| 1 | 10.212950000 | 8.826539000 | 11.006903000 |
| 1 | 12.502164000 | 10.845663000 | 2.412754000 |
| 1 | 14.233613000 | 10.689342000 | 2.186552000 |
| 1 | 11.561902000 | 9.946232000 | 9.247141000 |
| 1 | 9.997378000 | 10.732914000 | 9.455837000 |
| 1 | 12.361262000 | 5.175022000 | 9.385649000 |
| 1 | 13.806751000 | 6.125678000 | 9.719026000 |
| 1 | 11.234816000 | 11.770676000 | 3.795318000 |
| 1 | 11.496337000 | 12.681731000 | 5.279522000 |
| 1 | 12.453938000 | 8.181040000 | 10.047821000 |
| 1 | 11.921870000 | 6.893481000 | 11.127633000 |
| 1 | 6.670163000 | 5.368826000 | 3.666579000 |
| 1 | 5.726963000 | 5.368833000 | 5.144445000 |
| 1 | 13.550766000 | 11.393785000 | 5.784266000 |
| 1 | 13.612618000 | 12.264046000 | 4.265301000 |
| 1 | 6.893461000 | 7.018939000 | 2.230208000 |
| 1 | 6.223248000 | 8.618437000 | 1.933931000 |
| 1 | 11.389742000 | 8.002306000 | 5.060312000 |

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