Supporting Information for:

Distorted Copper(II) Complex with Unusually Short CF···Cu Distances

Claire C. Cody‡, H. Ray Kelly‡, Brandon Q. Mercado, Victor S. Batista, Robert H. Crabtree*, Gary W. Brudvig**

Department of Chemistry, and Yale Energy Sciences Institute, Yale University, New Haven, CT, 06520-8107, United States

TABLE OF CONTENTS

Experimental Details:

General methods: All materials were purchased from Sigma-Aldrich or Alfa-Aesar and were used without further purification.

Elemental analyses were performed by Roberson Microlit Laboratories, 1705 US-46 #1d, Ledgewood, NJ 07852.

NMR spectroscopy: ^{1}H, ^{19}F and ^{13}C NMR spectra were recorded on an Agilent DD2 400 MHz spectrometer and chemical shifts were referenced to residual solvent.

UV-Visible spectroscopy: Absorption spectra were collected using a Cary 50 spectrophotometer.

ATR-FTIR spectroscopy: ATR-FTIR spectra were taken on a Thermo Scientific Nicolet 6700 FT-IR spectrometer outfitted with a Smart Orbit diamond ATR cell. Samples were prepared as solid powders pressed directly onto the ATR crystal using a mechanical screw arm.

Mass spectrometry: Mass spectrometric measurements were performed with a Thermo Fisher QExactive Orbitrap LC-MS system, equipped with a Dionex UltraMate 3000 UHPLC, consisting of a LPG-3400SD pump unit, a WPS-3000 autosampler and a Column Oven TCC-3000. Mass spectra (MS and MS/MS) were subsequently recorded with the QExactive Orbitrap mass spectrometer. 1 µL of each solution was directly injected into the flow path of the LC system without column separation. Electrospray was used for desolvatization and ionization, with the electrospray needle held at +3.5 kV. Compressed air was used as desolvatization gas, capillary temperature was at 250 ºC, probe heater temperature at 400 ºC, sheath gas was at 47.5 L/min and aux gas flow at 11 L/min. Mass spectra were recorded in the range of 150 to 2000 m/z in positive

ion mode. Measurements and data post-processing were performed with Thermo Xcalibur 4.1.31.9.

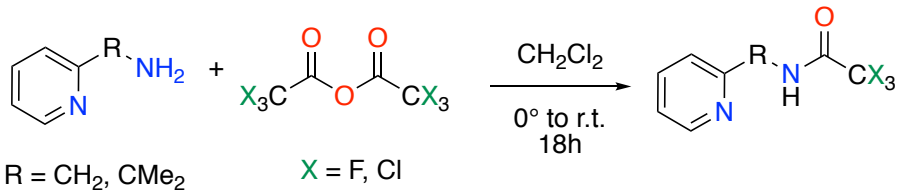
EPR spectroscopy: EPR spectra were measured on a Bruker EXELSYS E500 spectrometer utilizing a super-high Q resonator and a liquid nitrogen finger dewar at 77 K. Samples were prepared at 1 mM in a 1:1 CH_2Cl_2/toluene mixture. Simulations were performed using Matlab and the Easyspin package.[1]

Electrochemical measurements: Electrochemical measurements were made with a CHI 660E Potentiostat. Measurements were taken in 5 mL CH_2Cl_2, with 0.1 M $TBAPF_6$ electrolyte. The three-electrode set-up included a glassy carbon button working electrode, a Pt wire counter electrode, and a Ag wire pseudo-reference electrode. Potential was referenced to an internal ferrocene standard.

Single crystal X-ray diffraction: Low-temperature diffraction data (ω-scans) were collected on a Rigaku SCX Mini diffractometer coupled to a Rigaku Mercury275R CCD detector with Mo Kα (λ = 0.71073 Å) for the structure of **1** and **3**, and on a Rigaku MicroMax-007HF diffractometer coupled to a Dectris Pilatus3R detector with Mo Kα (λ = 0.71073 Å) for the structure of **2**. The diffraction images were processed and scaled using Rigaku Oxford Diffraction software (CrysAlisPro; Rigaku OD: The Woodlands, TX, 2015). The structures were solved with SHELXS or SHELXT and were refined against F^2 on all data by full-matrix least squares with SHELXL.[2] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the U value of the atoms to which they are linked (1.5 times for methyl groups). The full numbering scheme of compounds **1**, **2**, **3**, and **4**

can be found in the full details of the X-ray structure determinations (CIFs), which are included as Supporting Information. CCDC numbers 2082885 (**1**), 2082886 (**2**), 2082888 (**3**), and 2082887 (**4**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.

Synthetic Procedures:



Scheme S1. General procedure for ligand synthesis

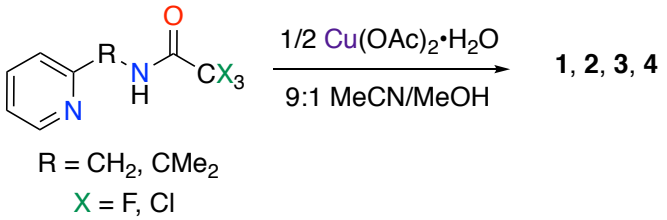
Synthesis of 2,2,2-trifluoro-*N*-[2-(pyridin-2-yl)propan-2-yl]acetamide (L-CF_3). A solution of 2-(pyridin-2-yl)isopropyl amine (0.20 mL, 1.4 mmol) and triethylamine (0.20 mL) in dry CH_2Cl_2 (3.0 mL) was cooled to 0 °C. Trifluoroacetic anhydride (0.40 mL, 2.9 mmol, 2.1 eq.) was added dropwise *via* syringe. The mixture was allowed to warm to room temperature, then stirred for 18 h. The reaction was quenched with the addition of water (3 mL), and basified with sat. aq. $NaHCO_3$ until the aqueous layer was pH 7. The resulting mixture was extracted with CH_2Cl_2 (3 × 10 mL). The organic layers were dried over Mg_2SO_4, filtered, and dried *in vacuo* to afford an amber oil. The product was purified by silica-gel column chromatography using hexanes:ethyl acetate (9:1), providing a colorless oil (321 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.44 (s, 1H, CON*H*), 8.52 (dd, *J* = 5.0, 1.8, 1H), 7.79 (td, *J* = 7.6, 1.8 Hz, 1H), 7.42 (d, *J* = 8.1 Hz, 1H), 7.27 (dd, *J* =

7.4, 5.0 Hz, 1H), 1.79 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.3, 147.2, 138.0, 122.6, 119.4, 56.9, 26.7. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -76.17. HRMS (ESI): m/z calcd. for $[M+H]^+$: 233.0902; found: 233.0896. Elemental analysis calculated for $C_{10}H_{11}F_3N_2O$: C, 51.73; H, 4.76; N, 12.06. Found: C, 51.78; H, 4.60; N, 11.79.

Synthesis of 2,2,2-trichloro-*N*-[2-(pyridin-2-yl)propan-2-yl]acetamide (L-CCl_3). A solution of 2-(pyridin-2-yl)isopropyl amine (0.40 mL, 3.5 mmol) and triethylamine (0.40 mL) in dry CH_2Cl_2 (6.0 mL) was cooled to 0 °C. Trichloroacetic anhydride (1.0 mL, 5.5 mmol, 1.6 eq.) was added dropwise *via* syringe. The mixture was allowed to warm to room temperature, then stirred for 18 h. The reaction was quenched with sat. aq. $NaHCO_3$ (10 mL) and extracted with CH_2Cl_2 (3 × 10 mL). The organic layers were dried over Mg_2SO_4, filtered, and dried *in vacuo* to afford a sticky brown solid. The product was purified by silica-gel column chromatography using hexanes:ethyl acetate (9:1), providing a white solid (861 mg, 87%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 9.77 (s, 1H, CON*H*), 8.54 (d, *J* = 4.9 Hz, 1H), 7.78 (t, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 8.1 Hz, 1H), 7.24-7.27 (m, 1H), 1.80 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 163.2, 147.5, 137.6, 122.4, 119.4, 57.5, 26.5. HRMS (ESI): m/z calcd. for $[M+H]^+$: 281.0015; found: 281.0015. Elemental analysis calculated for $C_{10}H_{11}F_3N_2O$: C, 42.66; H, 3.94; N, 9.95. Found: C, 43.22; H, 4.01; N, 9.77.

Synthesis of 2,2,2-trifluoro-*N*-(pyridin-2-ylmethyl)acetamide (L-CH_2-CF_3). The compound was synthesized according to a literature procedure.[3] Longer reaction times were found to afford higher yields of the hydrolyzed cyclic side product 3-(trifluoromethyl)-imidazo[1,5-a]pyridine,[4,5] so shorter reaction times than reported were used to afford higher yields of the desired amide

product. A solution of 2-picolylamine (707.8 mg, 6.54 mmol) in dry CH_2Cl_2 (20 mL) was cooled to 0 °C. Trifluoroacetic anhydride (1.8 mL, 12.9 mmol, 2.0 eq.) was added dropwise *via* syringe. After 5 minutes of stirring at 0 °C, the reaction was quenched with the addition of sat. aq. $NaHCO_3$ (20 mL) and extracted with CH_2Cl_2 (3 × 10 mL) to remove organic impurities. The organic extract was discarded. The aqueous layer was basified with sat. aq. $NaHCO_3$ until pH 7, and extracting again with CH_2Cl_2 (3 × 20 mL). The organic layers were dried over Mg_2SO_4, filtered, and dried *in vacuo* to afford a white solid (663 mg, 50%). ^{1}H NMR in $CDCl_3$ matched the reported values. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.56 (d, J = 4.7 Hz, 1H), 8.00 (s, 1H), 7.72 (t, J = 7.7 Hz, 1H), 7.28 (d, J = 7.7 Hz, 1H), 7.25 (d, J = 4.5 Hz, 1H), 4.64 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 153.5, 149.1, 137.2, 123.0, 122.0, 44.0. ^{19}F NMR (376 MHz, $CDCl_3$): δ = -75.81. HRMS (ESI): m/z calcd. for $[M+H]^+$: 205.0589; found: 205.0589.



Scheme S2. General procedure for complex synthesis

Synthesis of 1. To a solution of $Cu(OAc)_2{\cdot}H_2O$ (19.4 mg, 0.0972 mmol) in a 9:1 v/v acetonitrile:methanol mixture (~5 mL) was added ligand **L-CF$_3$** (50.8 mg, 0.219 mmol, 2.2 eq.). The mixture turned immediately from blue to teal. After stirring for 1 h at room temperature, the solvent was removed by rotary evaporation. The resulting solid was redissolved in dichloromethane and filtered through a cotton plug to remove unreacted $Cu(OAc)_2$.

Recrystallization by vapor diffusion with pentanes into the CH_2Cl_2 solution afforded crystals suitable for X-ray diffraction. Isolated yield: 14.2 mg, 28%. HRMS (ESI): m/z calcd for $[M+H]^+$: 526.0859; found: 526.0844. UV/Vis (CH_2Cl_2): λ_{max} (ε) = 643.0 nm (130 $M^{-1}cm^{-1}$), 982.0 nm (115 $M^{-1}cm^{-1}$). Elemental analysis calculated for $CuC_{20}H_{20}F_6N_4O_2$: C, 45.67; H, 3.83; N, 10.65. Found: C, 45.83; H, 3.67; N, 10.56.

Synthesis of 2. To a solution of $Cu(OAc)_2 \cdot H_2O$ (35.8 mg, 0.179 mmol) in a 9:1 v/v acetonitrile:methanol mixture (~6 mL) was added ligand **L-CCl$_3$** (100.1 mg, 0.356 mmol, 2.0 eq.). 1 M KOH in methanol (0.1 mL) was added to deprotonate the ligand. After stirring for 1 h at room temperature, the solvent was removed by rotary evaporation. The resulting solid was redissolved in dichloromethane and filtered through a cotton plug to remove a significant amount of pale blue solid (attributed to be $Cu(OH)_2$). Recrystallization by vapor diffusion with pentanes into the dichloromethane solution afforded a few teal crystals suitable for X-ray diffraction. Not enough material was able to be synthesized for bulk analysis.

Synthesis of 3. To a solution of $Cu(OAc)_2 \cdot H_2O$ (38.4 mg, 0.192 mmol) in a 9:1 v/v acetonitrile:methanol mixture (8 mL) was added ligand **L-CH$_2$-CF$_3$** (84.7 mg, 0.415 mmol, 2.2 eq). After stirring for 1 h at room temperature, the solvent was removed by rotary evaporation. The resulting teal solid was rinsed with minimal cold dichloromethane to remove excess ligand. Isolated yield: 54.2 mg (73%). Recrystallization by vapor diffusion with pentanes into a dichloromethane solution afforded teal crystals suitable for X-ray diffraction. UV/Vis (CH_2Cl_2): λ_{max} (ε) = 709.0 nm (~340 $M^{-1}cm^{-1}$). Elemental analysis calculated for $CuC_{24}H_{26}F_6N_4O_{10}$: C,

37.36; H, 3.40; N, 7.26. Found: C, 35.20; H, 3.14; N, 6.49. Found CHN analysis corresponds to calculated values when one molecule of dichloromethane is included (Calculated for $CuC_{24}H_{26}F_6N_4O_{10}\cdot CH_2Cl_2$: C, 35.06; H, 3.30; N, 6.54), which is reasonable since the crystal structure indicates CH_2Cl_2 in the lattice.

Synthesis of 4. A solution of $CuCl_2\cdot 4H_2O$ (23.7 mg, 0.139 mmol) and **L-CH$_2$-CF$_3$** (58.4 mg, 0.290 mmol, 2.1 eq.) in a 9:1 v/v acetonitrile:methanol mixture (~5 mL) was allowed to stir for 30 minutes at room temperature. 1 M KOH in methanol (0.18 mL) was added, and the teal solution stirred at room temperature for another 30 minutes. The solvent was removed by rotary evaporation, and the resulting solid was redissolved in dichloromethane, filtered through a cotton plug, and dried under a stream of compressed air. The teal solid was rinsed several times with diethyl ether to remove excess ligand. Isolated yield: 65.3 mg (89%). Recrystallization by vapor diffusion with pentanes into a dichloromethane solution afforded crystals suitable for X-ray diffraction. UV/Vis (CH_2Cl_2): λ_{max} (ε) = 635.0 nm (150 $M^{-1}cm^{-1}$). Elemental analysis calculated for $CuC_{16}H_{12}F_6N_4O_2$: C, 40.90; H, 2.57; N, 11.93. Found: C, 40.78; H, 2.37; N, 11.65.

Computational Details:

Density functional theory calculations were performed in Gaussian 16, Revision C.01.[6] All calculations used the default "ultrafine" integration grid (99 radial shells, 302 angular points per shell) and SCF convergence criterion. Geometry optimizations used the "tight" convergence criteria (maximum force of 0.000015 a.u., RMS force of 0.000010 a.u., maximum displacement of 0.000060 a.u., RMS displacement of 0.000040 a.u.), and were confirmed to be stationary points

using frequency calculations. Geometry optimizations were performed in the gas phase using the B3LYP functional[7,8] and 6-31+G(d,p) basis set.[9–13] Single point calculations used the B3LYP functional and 6-311+G(2df,p) basis set[14–19] in a solvation model based on density (SMD) continuum model for DCM.[20] As unrestricted DFT can suffer from spin contamination, the value of $<S^2>$ was checked for each doublet wavefunction. No corrections for spin contamination were needed, as $<S^2>$ never deviated by more than 5% (or even 0.5%) of the true value of S(S+1) = 0.750 (Table S3). Natural bond orbitals were visualized with the NBO Version 3.1 program implemented in Gaussian 16.[21] Structures and orbitals were visualized with GaussView, Version 6.[22] Orbitals were plotted with an isovalue of 0.04 a.u.

Computational Benchmarking. In order to identify a suitable DFT method, we performed benchmarking studies using three different hybrid functionals (B3LYP, ωB97X-D,[23] and M062X[24] and two different basis sets (6-31+G(d,p) and DEF2SVP;[25,26] Table S4 and S5). We found that B3LYP and ωB97X-D both showed similarly low deviations from the measured bond distances and angles (Table S6), so we performed further benchmarking via calculations of redox potentials (Table S7). To compare our computed redox potentials to the measured values, we used another redox couple measured in the same solvent conditions as a computational reference. To reduce systematic error in our redox potential calculations,[27] we chose a reference Cu redox couple for which the redox potential vs Fc/Fc^+ was previously measured in CH_2Cl_2 (LCuOH/[LCuOH]− in Zerk *et al.*; -0.074 V vs Fc/Fc^+).[28] B3LYP predicted the experimentally measured reduction potential of **1** (–1.00 V vs. Fc/Fc^+) with substantially more accuracy than ωB97X-D (Table S7). To ensure that both functionals were describing the Cu--F interaction similarly, the barrier for CF_3 rotation was computed at the B3LYP/6-31+G(d,p) and ωB97X-D /6-31+G(d,p) levels and determined to be +2.0 kcal/mol in both cases. Since B3LYP/6-31+G(d,p) showed the best

agreement with experimental bond distance/angles and redox potentials, it was considered the best candidate for subsequent analyses. To confirm that an accurate DFT description of the Cu···X interaction did not require dispersion effects or a larger basis set, further control calculations were performed incorporating the Grimme's D3 empirical dispersion correction with Becke-Johnson damping[29] and a larger aug-CC-PVDZ basis set[30–32] (Tables S8-S10). Adding dispersion had relatively minor effects on the bond lengths and angles, producing slightly better agreement with measured bond lengths but slightly worse agreement with measured angles. The barrier for CF_3 rotation in **1** was shifted slightly from +2.0 kcal/mol to +1.7 kcal/mol. Using the aug-CC-PVDZ basis set required much greater computational cost for very minor changes in bond lengths and angles, and resulted in no change in the +2.0 kcal/mol barrier for CF_3 rotation. Therefore, we proceeded with the B3LYP functional and 6-31+G(d,p) basis set for other calculations.

This method was further validated through calculations of the UV-vis spectra using TD-DFT as implemented in Gaussian 16 and calculations of EPR parameters as implemented in ORCA version 4.2.1.[33,34] The UV-vis spectrum shows peaks at 1003 nm and 675 nm, in good agreement with experiment (Figure S9, Table S11). The computed EPR parameters show fairly good agreement with the experimentally measured ones, with the exception of a much smaller predicted g_z value (Table S12). This underestimated g_z value is consistent with past studies with a variety of DFT functionals (including B3LYP), which have shown agreement between DFT-computed trends in g_z but similar deviations in their absolute value.[35,36]

Supplementary Figures:

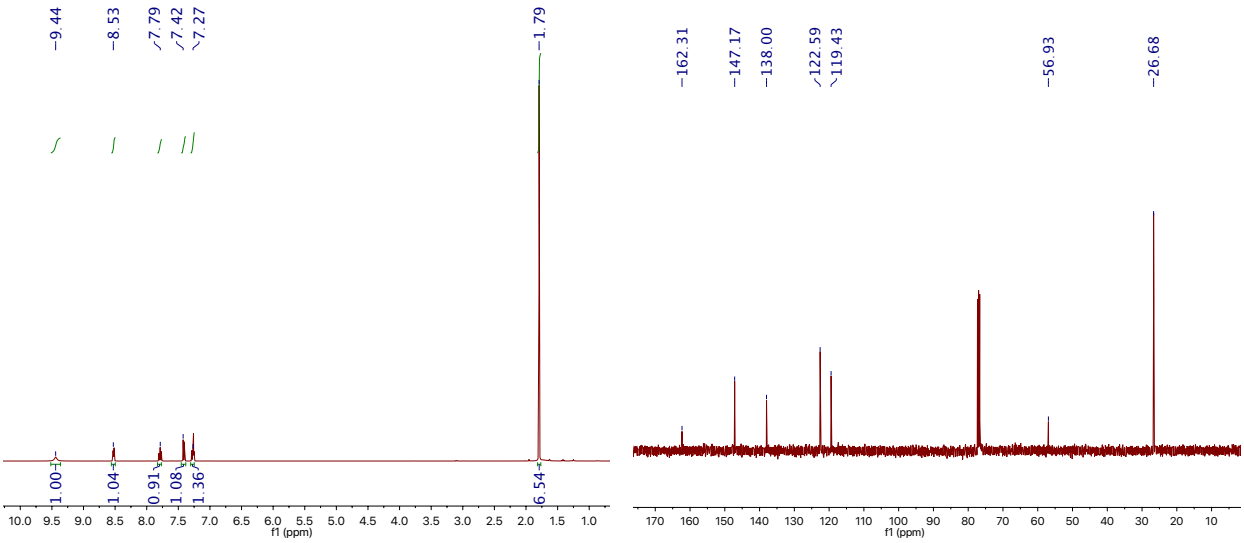


Figure S1. ^{1}H (left) and ^{13}C NMR (right) spectra of ligand **L-CF$_3$**.

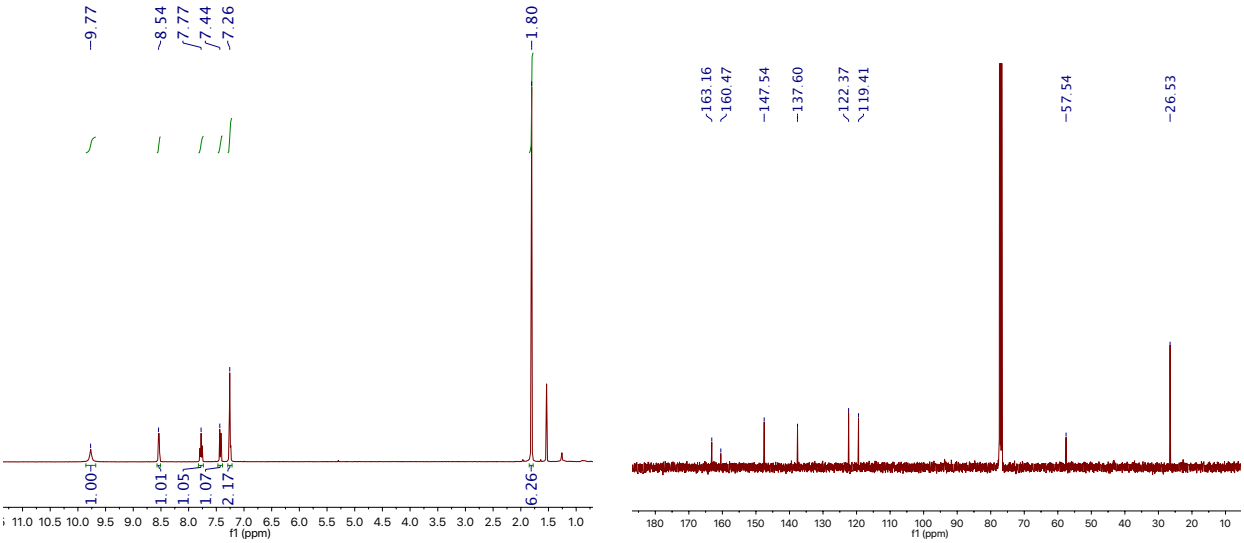


Figure S2. ^{1}H (left) and ^{13}C NMR (right) spectra of ligand **L-CCl$_3$**.

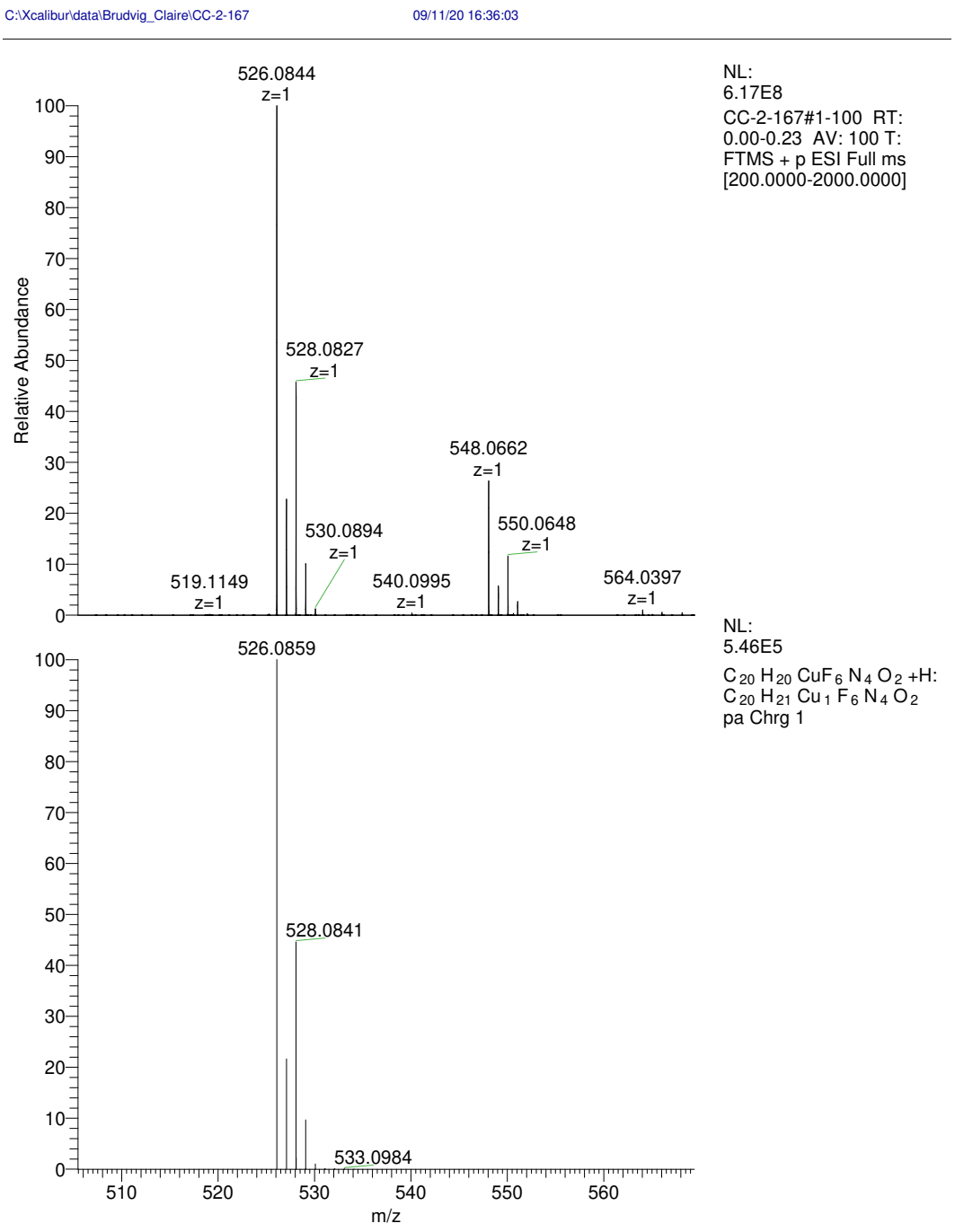


Figure S3. HRMS spectrum of complex **1** in positive mode, experimental (top) and theoretical (bottom). The experimental spectrum shows peaks of [**1** + H]$^+$ (m/z 526.0844) and [**1**+ Na]$^+$ (m/z 548.0662).

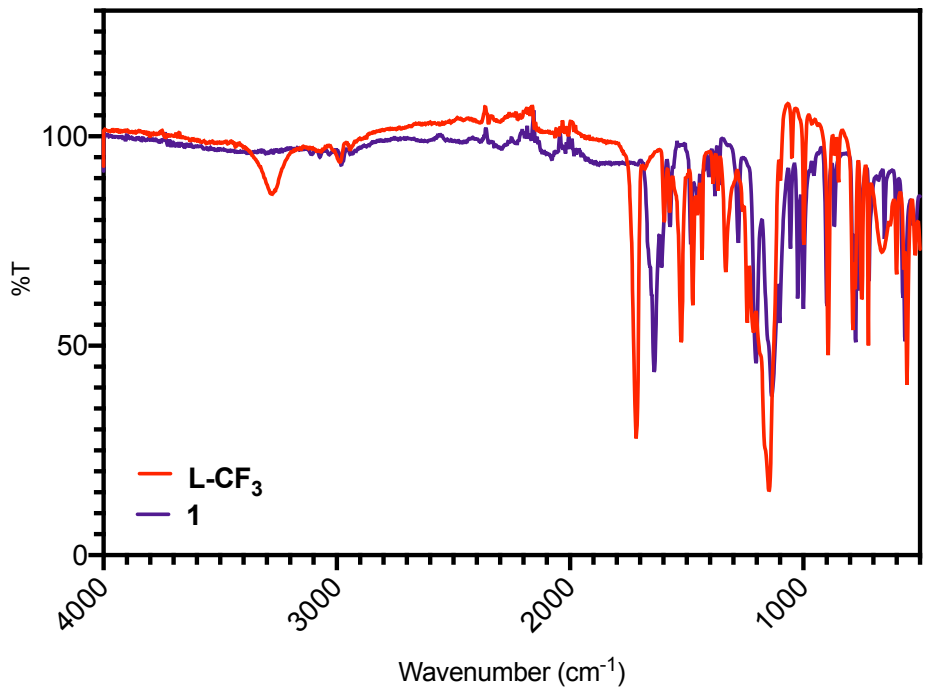


Figure S4. ATR-FTIR spectra of ligand **L-CF$_3$** and complex **1.**

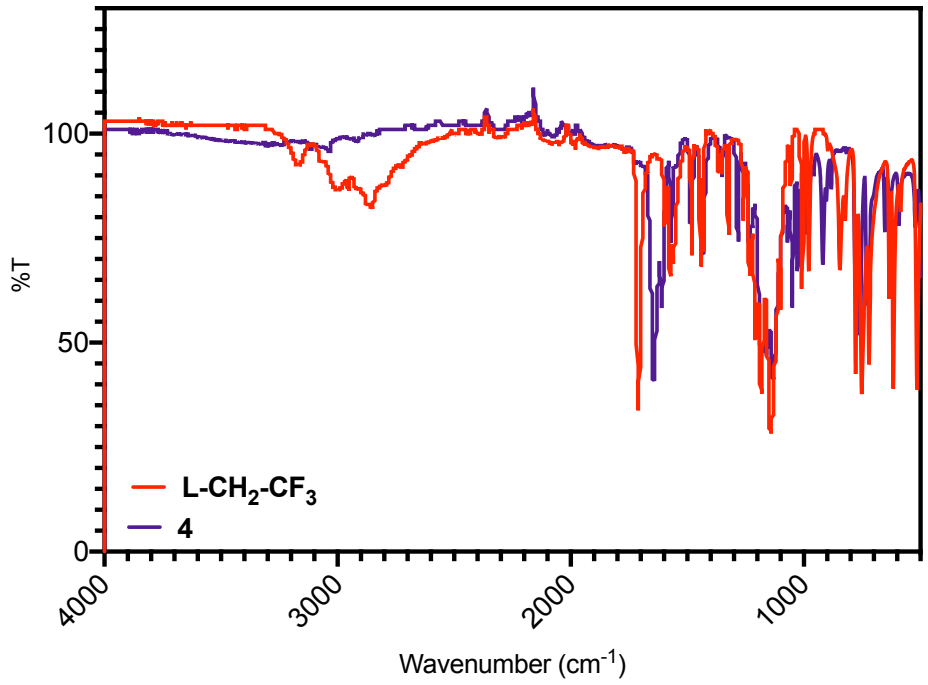


Figure S5. ATR-FTIR spectra of ligand **L-CH$_2$-CF$_3$** and complex **4.**

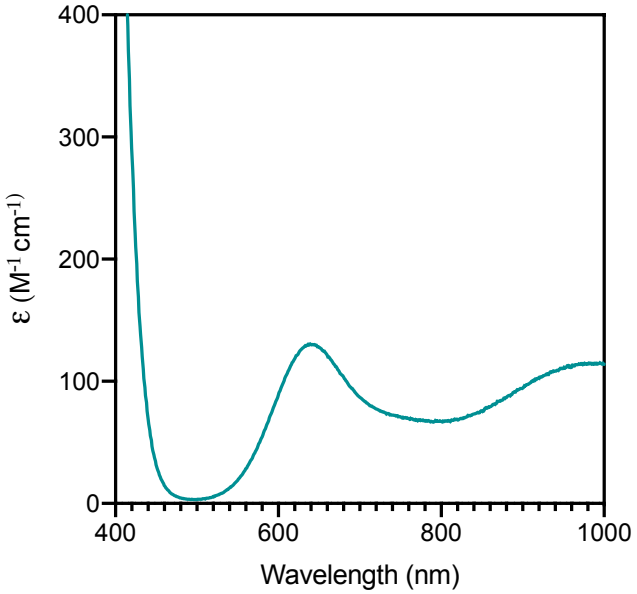


Figure S6. UV-visible spectrum of **1** in CH_2Cl_2.

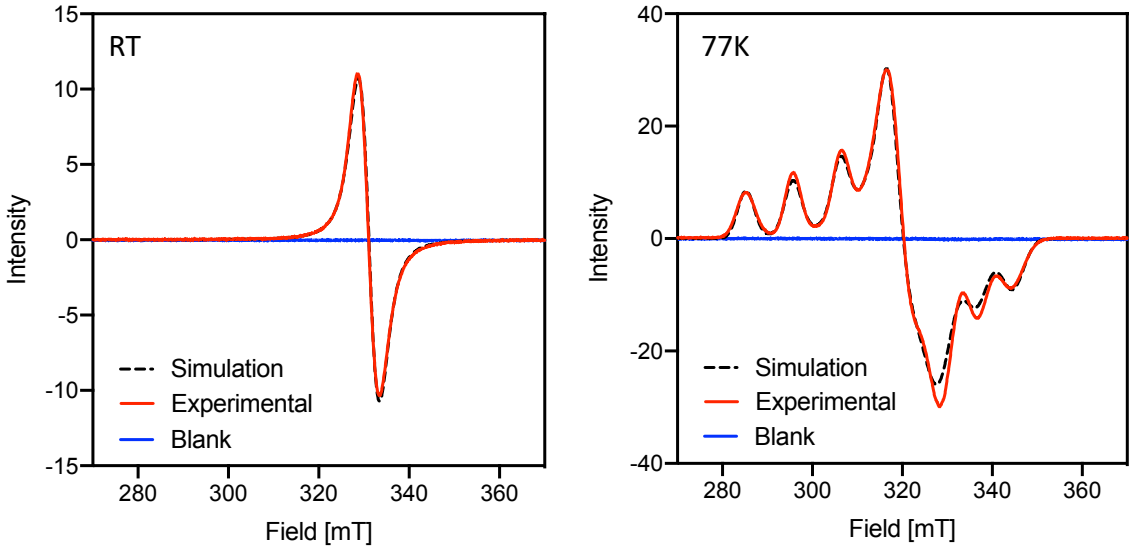


Figure S7. Continuous-wave X-band EPR spectra of **1** in a 1:1 toluene:CH_2Cl_2 mixture at (left) room temperature and (right) 77 K. Parameters: Microwave frequency: (left) 9.857 GHz, (right) 9.442 GHz; Microwave Power: 0.636 mW; Modulation Amplitude: 6.0 G; Modulation Frequency:

100 kHz; Time constant: 20.48 ms. Averaging of hyperfine splitting in the room temperature spectrum is potentially due to dynamics in solution, similar to what has been observed for other distorted complexes.[37]

Table S1. Modeled EPR parameters (hyperfine couplings in MHz).

g_x	g_y	g_z	g_{avg}	g_{iso}[a]	A_x	A_y	A_z
2.026	2.099	2.240	2.122	2.128	331	0	222

[a]Found from the room-temperature solution spectrum.

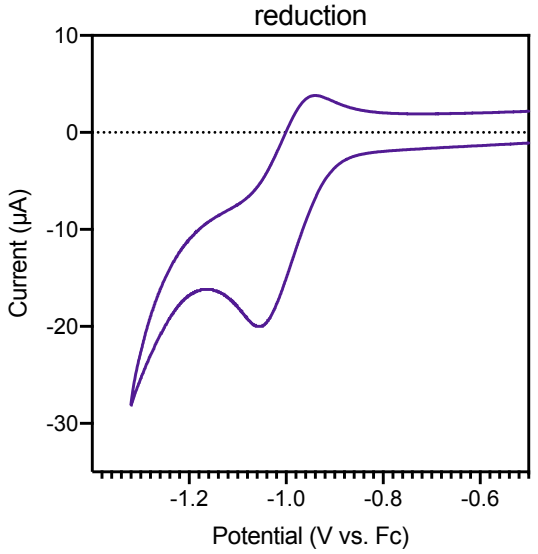


Figure S8. Cyclic voltammogram of **1** in CH_2Cl_2 with 0.1 M $TBAPF_6$. Scan rate: 100 mV/s. Electrodes: a glassy carbon working electrode, a Pt wire counter electrode, and a Ag wire pseudo-reference electrode. Potential referenced to an internal ferrocene/ferrocenium standard.

Table S2. Comparison of selected bond lengths (Å), distances (Å), and angles (º) for **1** and **2** from crystal structure to DFT-optimized values. Atom numbering is defined in Figure 1.

	1 (Crystal)	**1 (DFT)**	**2 (Crystal)**	**2 (DFT)**
Cu-N1 (py)	2.003(5)	2.059	2.049(3)	2.087
Cu-N2 (amide)	1.930(4)	1.955	1.947(3)	1.973
Cu-N3 (py)	1.999(4)	2.059	2.047(3)	2.087
Cu-N4 (amide)	1.913(4)	1.955	1.939(3)	1.973
Cu --- X1	2.569	2.581	2.708	2.768
Cu --- X4	2.530	2.579	2.707	2.766
N1-Cu-N2	83.71(18)	82.53	83.87(13)	82.72
N3-Cu-N4	83.39(18)	82.53	83.21(13)	82.72
N1-Cu-N3	125.88(18)	122.25	112.20(13)	110.67
N2-Cu-N4	162.45(18)	164.28	169.33(14)	171.12

Table S3. DFT-computed $<S^2>$ values for all species including transition states for CF_3/CCl_3 rotation (TS)

Complex	**$<S^2>$**
1	0.7525
1 TS	0.7526
2	0.7525
2 TS	0.7525
4	0.7526
4 TS	0.7526

Table S4. Comparison of selected bond lengths (Å), distances (Å), and angles (º) for **1** with three different hybrid functionals and two basis sets. **F1)** B3LYP, **F2)** ωB97X-D, **F3)** M062X; **BS1)** 6-31+G(d,p), **BS2)** DEF2SVP. Atom labels are shown in Figure 1.

	Crystal	**F1/BS1**	**F1/BS2**	**F2/BS1**	**F2/BS2**	**F3/BS1**	**F3/BS2**
Cu-N1 (py)	2.003(5)	2.059	2.079	2.038	2.057	2.091	2.083
Cu-N2 (amide)	1.930(4)	1.955	1.965	1.929	1.940	1.960	1.966
Cu-N3 (py)	1.999(4)	2.059	2.080	2.038	2.057	2.091	2.083
Cu-N4 (amide)	1.913(4)	1.955	1.964	1.929	1.940	1.961	1.966
Cu --- F1	2.569	2.581	2.523	2.532	2.476	2.431	2.441
Cu --- F4	2.530	2.579	2.521	2.530	2.474	2.432	2.438
N1-Cu-N2	83.71(18)	82.53	82.18	82.97	82.61	81.54	81.78
N3-Cu-N4	83.39(18)	82.53	82.17	82.97	82.61	81.53	81.77
N1-Cu-N3	125.88(18)	122.25	118.01	122.03	118.25	118.81	118.54
N2-Cu-N4	162.45(18)	164.28	165.14	166.42	167.58	168.93	167.28

Table S5. Comparison of selected bond lengths (Å), distances (Å), and angles (º) for **2** with three different hybrid functionals and two basis sets. **F1)** B3LYP, **F2)** ωB97X-D, **F3)** M062X; **BS1)** 6-31+G(d,p), **BS2)** DEF2SVP. Atom labels are shown in Figure 1.

	Crystal	**F1/BS1**	**F1/BS2**	**F2/BS1**	**F2/BS2**	**F3/BS1**	**F3/BS2**
Cu-N1 (py)	2.049(3)	2.087	2.109	2.057	2.080	2.113	2.104
Cu-N2 (amide)	1.947(3)	1.973	1.988	1.944	1.962	1.983	1.987
Cu-N3 (py)	2.047(3)	2.087	2.109	2.057	2.079	2.113	2.103
Cu-N4 (amide)	1.939(3)	1.973	1.988	1.944	1.962	1.983	1.987
Cu --- Cl1	2.708	2.768	2.700	2.787	2.669	2.668	2.659
Cu --- Cl4	2.707	2.766	2.699	2.789	2.671	2.670	2.658
N1-Cu-N2	83.87(13)	82.72	82.11	83.08	82.70	81.74	81.78
N3-Cu-N4	83.21(13)	82.72	82.11	83.11	82.71	81.75	81.80
N1-Cu-N3	112.20(13)	110.67	104.12	120.77	101.96	101.34	100.94
N2-Cu-N4	169.33(14)	171.12	171.59	172.13	172.30	172.27	171.52

Table S6. Root mean squared deviation between key DFT-computed bond lengths (Å), distances (Å), and angles (º) and those from the crystal structures of **1** and **2** (values in Tables S2 and S3). **F1)** B3LYP, **F2)** ωB97X-D, **F3)** M062X; **BS1)** 6-31+G(d,p), **BS2)** DEF2SVP.

RMSD	**F1/BS1**	**F1/BS2**	**F2/BS1**	**F2/BS2**	**F3/BS1**	**F3/BS2**
1 Bond Lengths	0.044	0.055	0.027	0.056	0.089	0.084
1 Angles	2.16	4.27	2.80	4.65	5.00	4.57
2 Bond Lengths	0.045	0.044	0.047	0.030	0.049	0.050
2 Angles	1.33	4.32	4.53	5.37	5.77	5.87
All Bond Lengths	0.044	0.050	0.038	0.045	0.072	0.069
All Angles	1.79	4.30	3.76	5.02	5.40	5.26

Table S7. DFT-computed reduction potentials (V vs Fc^+/Fc) of **1** and $\mathbf{1}^+$ for two different functionals and basis sets. The $\mathbf{1/1}^-$ redox couple was measured to be -1.00 V vs Fc^+/Fc, and no oxidative features were measured up to 1.5 V.

Redox Couple	**F1/BS1**	**F1/BS2**	**F2/BS1**	**F2/BS2**
$\mathbf{1/1}^-$	-0.89	-0.89	-1.45	-1.23
$\mathbf{1}^+\mathbf{/1}$	+1.80	+1.81	+1.52	+1.57

Table S8. Comparison of selected bond lengths (Å), distances (Å), and angles (º) for **1** with the B3LYP functional and the B3LYP functional with the D3 empirical dispersion correction. Optimizations were performed with the 6-31+G(d,p) and aug-cc-PVDZ basis sets.

	Crystal	**B3LYP/ 6-31+G(d,p)**	**B3LYP/ aug-cc-PVDZ**	**B3LYP-D3/ 6-31+G(d,p)**	**B3LYP-D3/ aug-cc-PVDZ**
Cu-N1 (py)	2.003(5)	2.059	2.062	2.039	2.043
Cu-N2 (amide)	1.930(4)	1.955	1.959	1.938	1.943
Cu-N3 (py)	1.999(4)	2.059	2.062	2.039	2.043
Cu-N4 (amide)	1.913(4)	1.955	1.959	1.938	1.943
Cu --- F1	2.569	2.581	2.579	2.555	2.556
Cu --- F4	2.530	2.579	2.578	2.555	2.555
N1-Cu-N2	83.71(18)	82.53	82.25	82.96	82.62
N3-Cu-N4	83.39(18)	82.53	82.25	82.96	82.60
N1-Cu-N3	125.88(18)	122.25	123.54	123.64	125.17
N2-Cu-N4	162.45(18)	164.28	165.26	166.16	167.30

Table S9. Comparison of selected bond lengths (Å), distances (Å), and angles (º) for **2** with the B3LYP functional and the B3LYP functional with the D3 empirical dispersion correction. Optimizations were performed with the 6-31+G(d,p) and aug-cc-PVDZ basis sets.

	Crystal	**B3LYP/ 6-31+G(d,p)**	**B3LYP/ aug-cc-PVDZ**	**B3LYP-D3/ 6-31+G(d,p)**	**B3LYP-D3/ aug-cc-PVDZ**
Cu-N1 (py)	2.049(3)	2.087	2.091	2.067	2.064
Cu-N2 (amide)	1.947(3)	1.973	1.977	1.938	1.954
Cu-N3 (py)	2.047(3)	2.087	2.092	2.039	2.064
Cu-N4 (amide)	1.939(3)	1.973	1.977	1.938	1.954
Cu --- Cl1	2.708	2.768	2.757	2.555	2.743
Cu --- Cl4	2.707	2.766	2.758	2.555	2.743
N1-Cu-N2	83.87(13)	82.72	82.39	82.96	83.00
N3-Cu-N4	83.21(13)	82.72	82.39	82.95	83.02
N1-Cu-N3	112.20(13)	110.67	111.59	123.64	118.47
N2-Cu-N4	169.33(14)	171.12	172.10	166.16	172.42

Table S10. Root mean squared deviation between key DFT-computed bond lengths (Å), distances (Å), and angles (º) and those from the crystal structures of **1** and **2**. Optimizations were performed with the B3LYP functional with and without the D3 empirical dispersion correction and the 6-31+G(d,p) and aug-cc-PVDZ basis sets.

RMSD	**B3LYP/ 6-31+G(d,p)**	**B3LYP/ aug-cc-PVDZ**	**B3LYP-D3/ 6-31+G(d,p)**	**B3LYP-D3/ aug-cc-PVDZ**
1 Bond Lengths	0.044	0.046	0.027	0.030
1 Angles	2.16	2.05	2.21	2.54
2 Bond Lengths	0.045	0.043	0.013	0.023
2 Angles	1.33	1.65	2.85	3.52
All Bond Lengths	0.044	0.045	0.021	0.027
All Angles	1.79	1.86	2.55	3.07

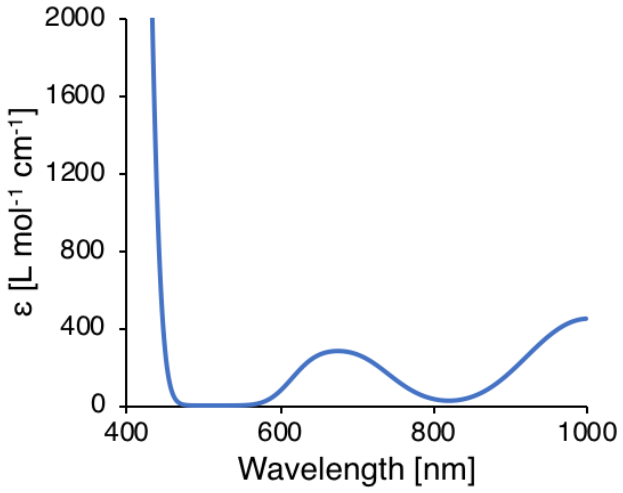


Figure S9. TD-DFT calculated UV-vis spectrum of **1**. Individual transitions and oscillator strengths are shown in Table S11.

Table S11. Ten lowest-energy TD-DFT excitation energies and oscillator strengths for **1**.

Wavelength (nm)	**Oscillator Strength**
1002	36901
708	16605
668	0
645	16605
418	6458
413	367160
397	179890
377.5	9225
351.9	1845
351.8	13838

Table S12. DFT-computed EPR parameters for **1** (hyperfine couplings in MHz). Note that the A_z value from the experimental modeling is reported as positive (Table S1), but the sign of A_z is ambiguous from fitting the solution-phase measurement.

g_x	g_y	g_z	g_a	g_{iso}	A_x	A_y	A_z
2.020	2.102	2.166	2.096	2.096	343	0	-265

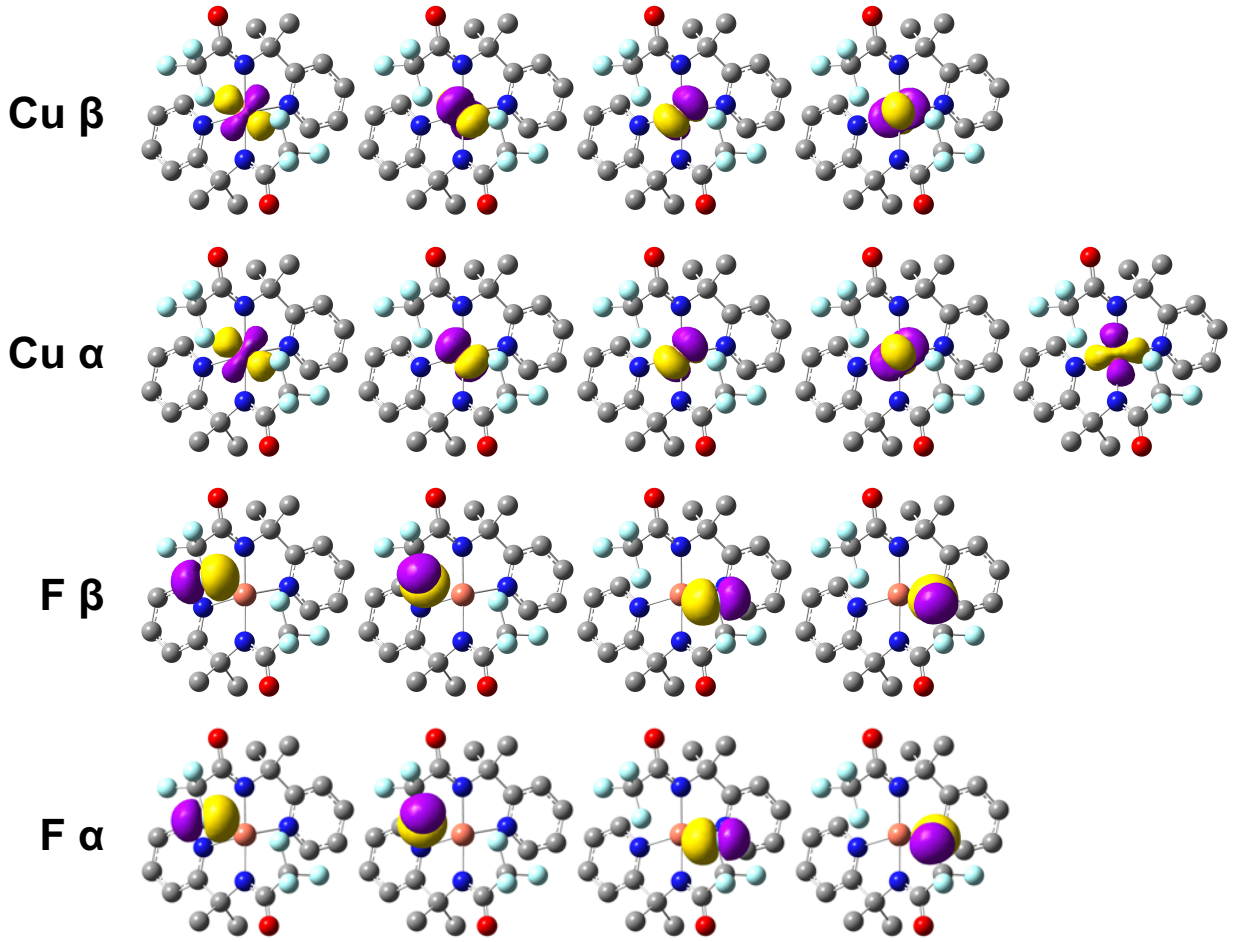


Figure S10. Complete set of occupied F *p* and Cu *d* one-center NBOs of **1**, showing that there is no covalent bond between F and Cu. Note that the Cu d_{xy} orbital is only singly occupied. Hydrogens are omitted for clarity.

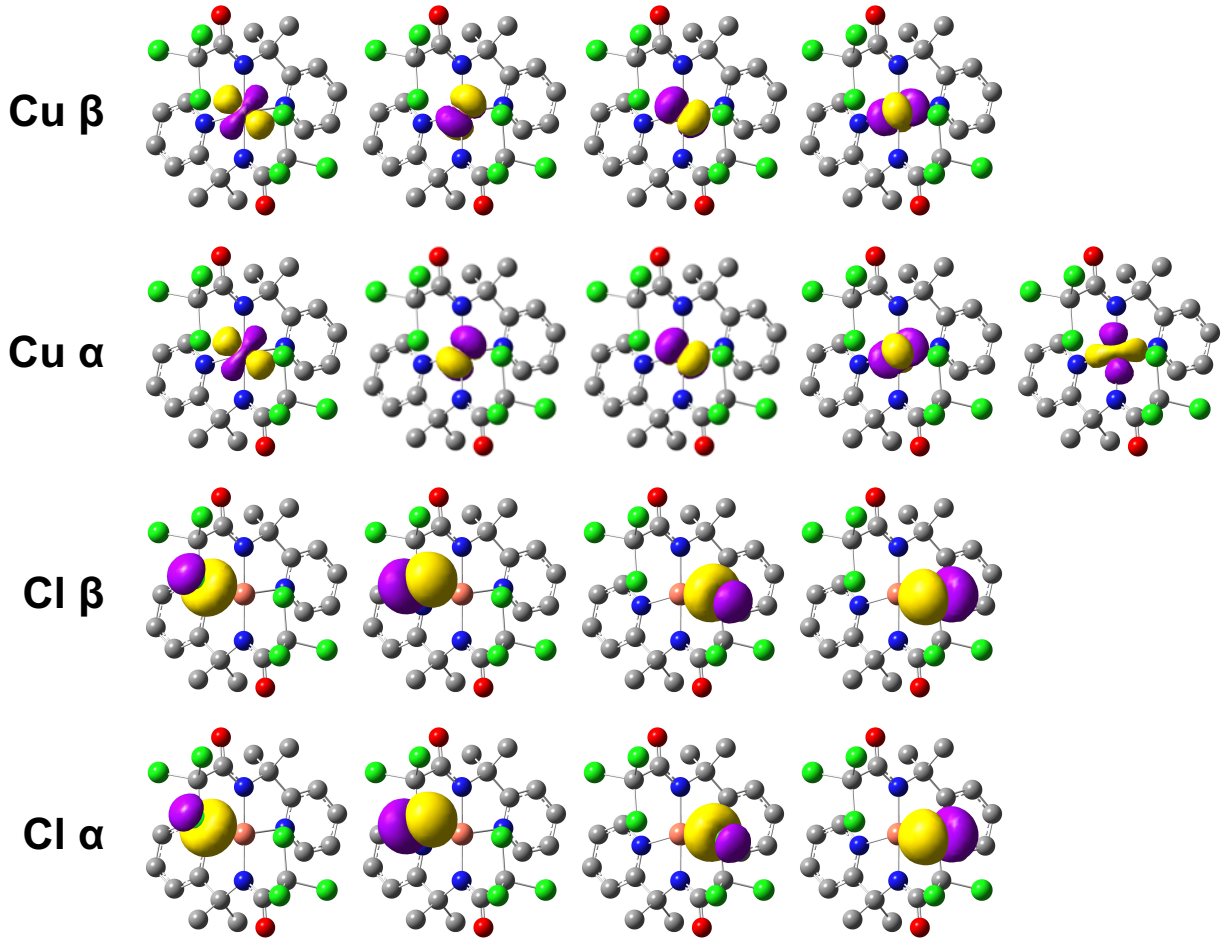


Figure S11. Complete set of occupied Cl *p* and Cu *d* one-center NBOs of **2**, showing that there is no covalent bond between Cl and Cu. Note that the Cu d_{xy} orbital is only singly occupied. Hydrogens are omitted for clarity.

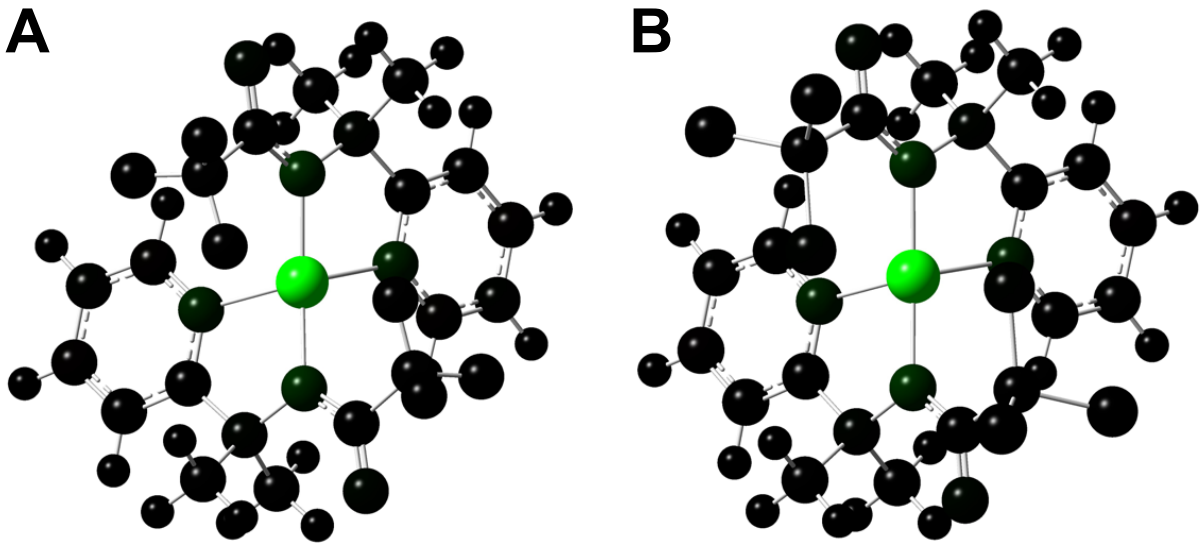
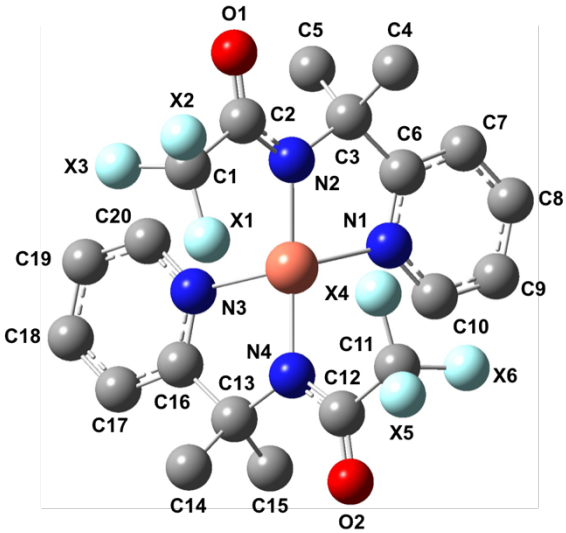


Figure S12. Plots of Mulliken spin population for A) **1** and B) **2**, where bright green indicates high α spin population and bright red indicates high β spin population. The green color is only visible on the Cu centers because the spin is mostly localized there (0.637 for **1,** 0.619 for **2**), with small populations on the N atoms (0.070 and 0.088 for **1**, 0.069 and 0.095 for **2**). A full list of the spin population on each heavy atom is provided in Table S13.

Table S13. Mulliken spin population for each heavy atom in **1** and **2**. Hydrogen atoms were excluded for clarity; no hydrogen has a spin population greater than 0.002. A labelled version of **1** shows the atom numbering scheme used in the table.

Atom	Spin Pop in 1	Spin Pop in 2
Cu	0.637	0.619
N1	0.070	0.069
N2	0.088	0.095
N3	0.070	0.069
N4	0.088	0.095
O1	0.013	0.014
O2	0.013	0.014
X1	0.001	0.005
X2	0.000	0.000
X3	0.000	0.001
X4	0.001	0.005
X5	0.000	0.000
X6	0.000	0.001
C1	0.002	0.001
C2	0.000	-0.001
C3	0.007	0.008
C4	0.002	0.002
C5	0.002	0.001
C6	-0.002	-0.002
C7	0.001	-0.001
C8	-0.005	-0.004
C8	0.004	0.003



C10	-0.006	-0.003
C11	0.002	0.001
C12	0.000	-0.001
C13	0.007	0.008
C14	0.002	0.002
C15	0.002	0.001
C16	-0.003	-0.002
C17	0.001	-0.001
C18	-0.005	-0.004
C19	0.004	0.003
C20	-0.006	-0.003

X-ray diffraction refinement details for CuL_2 complexes 1, 2, 3, and 4.

(**1**) Four small-angle reflections with high error:esd were omitted due to proximity to the beamstop. The hydrogen atoms were first found in the difference map, then generated geometrically and refined as riding atoms with C-H distances = 0.95 - 0.99 angstroms and Uiso(H) = 1.2 times Ueq for CH and CH2 groups and Uiso(H) = 1.5 times Ueq(C) for CH3 groups.

(**3**) Ultimately, the program SQUEEZE[38] was used to compensate for the contribution of disordered solvents contained in voids within the crystal lattice from the diffraction intensities. This procedure was applied to the data file and the submitted model is based on the solvent removed data. Based on the total electron density found in the voids (89 e/Å^3), it is likely that ~2 dichloromethane molecules are present in the unit cell. See "_platon_squeeze_details" in mini21003.cif for more information.

(**4**) Five small-angle reflections with high error:esd were omitted due to proximity to the beamstop. The CF3 group is positionally disordered over two positions. The site occupancies were freely refined as linked free variables, which converged at nearly equal occupancies. No additional restraints or constraints were needed for a stable refinement.

Table S14. Crystal data and structure refinement for complexes **1-2**.

Identification code	mini-19071 (**1**)	007c-21019 (**2**)
Empirical formula	C20 H20 Cu F6 N4 O2, C H2 Cl2	C20 H20 Cl6 Cu N4 O2
Formula weight	610.86	624.64
Temperature	93(2) K	93(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic
Space group	C2/c	Cc
Unit cell dimensions	a = 14.1596(8) Å	a = 8.4030(2) Å
	b = 33.7064(13) Å	b = 31.8691(6) Å
	c = 11.1616(7) Å	c = 10.1404(3) Å
	α = 90°.	α = 90°.
	β = 111.683(7)°.	β = 111.967(3)°.
	γ = 90°.	γ = 90°.
Volume	4950.1(5) $Å^3$	2518.41(12) $Å^3$
Z	8	4
Density (calculated)	1.639 Mg/m^3	1.647 Mg/m^3
Absorption coefficient	1.171 mm^{-1}	1.530 mm^{-1}
F(000)	2472	1260
Crystal size	0.200 x 0.100 x 0.100 mm^3	0.350 x 0.350 x 0.250 mm^3
Crystal color and habit	Green Block	Blue Block
Diffractometer	Rigaku SCX Mini	Dectris Pilatus 3R
Theta range for data collection	2.2860 to 26.2990°.	2.774 to 28.281°.

Index ranges	-17<=h<=17, -41<=k<=42, -13<=l<=13	-11<=h<=11, -42<=k<=42, -13<=l<=13
Reflections collected	39688	27094
Independent reflections	5070 [R(int) = 0.1736]	6203 [R(int) = 0.0300]
Observed reflections (I > 2sigma(I))	3213	6099
Completeness to theta = 25.242°	99.9 %	99.8 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.74277	1.00000 and 0.60568
Solution method	SHELXS	SHELXT-2014/5
Refinement method	SHELXL-2014/7	SHELXL-2014/7
Data / restraints / parameters	5070 / 0 / 330	6203 / 2 / 302
Goodness-of-fit on F^2	1.071	1.100
Final R indices [I>2sigma(I)]	R1 = 0.0739, wR2 = 0.1511	R1 = 0.0287, wR2 = 0.0775
R indices (all data)	R1 = 0.1306, wR2 = 0.1746	R1 = 0.0292, wR2 = 0.0777
Absolute structure parameter		0.014(5)
Largest diff. peak and hole	1.112 and -0.771 e.Å^{-3}	1.224 and -0.470 e.Å^{-3}

Table S15. Crystal data and structure refinement for complexes **3-4**.

Identification code	mini-21003 (**3**)	mini-21012 (**4**)
Empirical formula	C24 H26 Cu2 F6 N4 O10	C16 H12 Cu F6 N4 O2
Formula weight	771.57	469.84
Temperature	93(2) K	93(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	C2/c
Unit cell dimensions	a = 14.0192(13) Å	a = 13.2108(6) Å
	b = 13.1291(12) Å	b = 15.5086(7) Å
	c = 8.6829(7) Å	c = 17.4713(10) Å
	α = 90°.	α = 90°.
	β = 96.120(8)°.	β = 91.579(5)°.
	γ = 90°.	γ = 90°.
Volume	1589.1(2) Å^3	3578.2(3) Å^3
Z	2	8
Density (calculated)	1.613 Mg/m^3	1.744 Mg/m^3
Absorption coefficient	1.430 mm^{-1}	1.302 mm^{-1}
F(000)	780	1880

Crystal size	0.410 x 0.320 x 0.040 mm^3	0.340 x 0.240 x 0.120 mm^3
Crystal color and habit	Blue Plate	Blue Block
Diffractometer	Rigaku SCX Mini	Rigaku SCX Mini
Theta range for data collection	2.824 to 27.515°.	2.874 to 26.359°
Index ranges	-18<=h<=18, -17<=k<=17, -11<=l<=11	-16<=h<=16, -19<=k<=19, -21<=l<=21
Reflections collected	26556	28069
Independent reflections	3643 [R(int) = 0.0662]	3659 [R(int) = 0.0919]
Observed reflections (I > 2sigma(I))	3196	2753
Completeness to theta = 25.242°	99.9 %	99.8%
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.40856	1.00000 and 0.86486
Solution method	SHELXT-2018/2	SHELXT-2014/5
Refinement method	SHELXL-2014/7	SHELXL-2014/7
Data / restraints / parameters	3643 / 0 / 210	3659 / 36 / 299
Goodness-of-fit on F^2	1.046	1.095
Final R indices [I>2sigma(I)]	R1 = 0.0366, wR2 = 0.0947	R1 = 0.0584, wR2 = 0.1307
R indices (all data)	R1 = 0.0428, wR2 = 0.0983	R1 = 0.0867, wR2 = 0.1421
Absolute structure parameter	0.704 and -0.446 e.$Å^{-3}$	
Largest diff. peak and hole		1.503 and -0.658 e.$Å^{-3}$

DFT Coordinates:

Complex 1 - B3LYP/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
Cu	12.25988	21.183128	12.050199
N	12.747512	20.88038	10.07255
C	13.083052	21.835434	9.184234
H	12.99904	22.85873	9.532637
C	13.506302	21.537422	7.89769
H	13.762376	22.335417	7.209739
C	13.584223	20.191967	7.526954
H	13.909722	19.912256	6.529459
C	13.237827	19.210924	8.448853
H	13.29175	18.163788	8.176008
C	12.813844	19.580318	9.734894
C	12.422148	18.534969	10.784709
C	11.251217	17.697594	10.204688
H	10.394647	18.344443	9.992476
H	11.549853	17.203525	9.275508
H	10.951807	16.933646	10.92187
C	13.654175	17.636289	11.065458
H	14.494681	18.239087	11.425591
H	13.39444	16.893653	11.821088
H	13.975968	17.113866	10.159337
N	11.991348	19.247146	12.015751
C	11.520075	18.497954	13.024125
O	11.466178	17.267355	13.128318
C	10.946839	19.268938	14.251368
F	10.723366	20.599157	14.037909
F	9.775747	18.739378	14.63682
F	11.800652	19.186881	15.305572
N	13.688918	21.503931	13.497611
C	14.450359	20.559235	14.08211
H	14.217469	19.53291	13.821315
C	15.469551	20.870842	14.969382
H	16.05705	20.080812	15.423632

C	15.703194	22.219216	15.25411
H	16.490343	22.509409	15.943581
C	14.914723	23.189553	14.646593
H	15.082818	24.238774	14.85818
C	13.896355	22.806565	13.759764
C	13.001923	23.839731	13.066379
C	12.280424	24.657759	14.170577
H	11.666381	23.99631	14.78911
H	13.005213	25.161074	14.817113
H	11.641387	25.413099	13.713704
C	13.898051	24.760417	12.198178
H	14.445003	24.172499	11.453406
H	13.273586	25.495243	11.688282
H	14.630054	25.292184	12.813706
N	12.013064	23.114223	12.227249
C	11.077602	23.850517	11.60836
O	10.955553	25.079474	11.554598
C	9.97036	23.064472	10.843297
F	9.910347	21.731507	11.133807
F	8.758088	23.571937	11.113916
F	10.163222	23.15703	9.501067

Complex 1, Transition State for -CF_3 Rotation - B3LYP/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
Cu	12.251084	21.184109	12.077586
N	12.746544	20.884768	10.093242
C	13.086619	21.837051	9.203870
H	12.979662	22.862067	9.541048
C	13.543126	21.534772	7.929745
H	13.801467	22.330446	7.239906
C	13.652777	20.187270	7.574316
H	14.006813	19.903740	6.587664
C	13.300387	19.209187	8.496970
H	13.377590	18.160837	8.234734
C	12.838705	19.583567	9.768974
C	12.427831	18.540924	10.814717
C	11.276497	17.698789	10.201201

H	10.421280	18.341804	9.972609
H	11.601267	17.213934	9.276054
H	10.964103	16.926856	10.903809
C	13.655093	17.646235	11.126945
H	14.487434	18.251902	11.500973
H	13.379649	16.907712	11.881009
H	13.997785	17.118295	10.231645
N	11.960312	19.252060	12.035615
C	11.433483	18.495385	13.015622
O	11.389769	17.264931	13.107814
C	10.704149	19.290937	14.147128
F	9.623901	19.951405	13.659507
F	10.279260	18.477606	15.120543
F	11.499994	20.232372	14.736936
N	13.730613	21.499650	13.460158
C	14.501261	20.545253	14.015118
H	14.253933	19.523370	13.749082
C	15.542616	20.844351	14.880319
H	16.140643	20.048347	15.309863
C	15.785163	22.189237	15.176884
H	16.589516	22.469177	15.850540
C	14.981810	23.168229	14.604354
H	15.153468	24.214254	14.828626
C	13.942097	22.797188	13.736839
C	13.023797	23.834437	13.084137
C	12.330215	24.635788	14.217687
H	11.738558	23.963838	14.846632
H	13.070360	25.137322	14.848116
H	11.673497	25.391507	13.787163
C	13.891986	24.768646	12.202011
H	14.418045	24.191708	11.434018
H	13.253045	25.509827	11.720365
H	14.640892	25.292316	12.803974
N	12.013571	23.112888	12.266004
C	11.071593	23.856252	11.663521
O	10.948410	25.085374	11.628626
C	9.965347	23.079133	10.890035
F	9.917100	21.741644	11.155210
F	8.751233	23.574065	11.174089
F	10.154356	23.199596	9.549280

Complex [1]$^{+}$ - B3LYP/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
F	10.549286	22.870760	9.400288
N	12.946230	20.818887	10.040469
C	13.415220	21.725995	9.158182
H	13.485836	22.748780	9.509374
C	13.777313	21.376914	7.866688
H	14.143951	22.133663	7.182584
C	13.644298	20.040061	7.481223
H	13.911262	19.726887	6.476916
C	13.165614	19.109990	8.398209
H	13.062080	18.069817	8.113389
C	12.821246	19.523560	9.691346
C	10.955954	17.947369	10.227955
H	11.114204	17.461526	9.262556
H	10.210752	18.736667	10.097355
H	13.538228	16.898161	10.016186
F	8.881911	23.364324	10.712287
Cu	12.531523	21.185151	11.976068
F	10.047136	21.565820	11.081080
F	10.871852	20.765017	14.018688
F	10.086123	18.949051	14.920625
F	12.183044	19.470777	15.196023
O	10.820868	24.918380	11.635379
O	11.303765	17.423493	13.125688
N	13.875194	21.569788	13.425279
N	12.105524	23.066256	12.181792
N	12.093143	19.295967	12.007605
C	14.746780	20.676072	13.937885
H	14.644946	19.652614	13.596443
C	15.714730	21.038942	14.861126
H	16.394135	20.292670	15.256823
C	15.774931	22.375579	15.265139
H	16.514370	22.699236	15.990713
C	14.876631	23.291847	14.727971
H	14.915570	24.331731	15.029526
C	13.924256	22.864813	13.793931
C	12.918501	23.828882	13.166256
C	13.696061	24.967113	12.440638

H	14.341819	24.557477	11.658141
H	14.325946	25.499871	13.156687
H	12.995733	25.676059	12.001303
C	12.020459	24.405291	14.298042
H	11.323325	25.138419	13.894212
H	12.643400	24.899679	15.046775
H	11.462583	23.603957	14.790000
C	11.066586	23.721282	11.571476
C	10.114015	22.867682	10.682034
C	12.297781	18.544123	10.740902
H	10.578245	17.203303	10.928137
C	13.357177	17.422685	10.957149
H	14.306247	17.846698	11.298561
H	12.994595	16.703337	11.690049
C	11.526885	18.624980	13.061133
C	11.152442	19.464968	14.318544

Complex [1]$^{-}$ - B3LYP/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
F	10.718079	23.094596	9.447726
N	13.084685	20.678400	10.029107
C	13.603397	21.536657	9.132476
H	13.777330	22.545210	9.496971
C	13.889775	21.183571	7.819707
H	14.303066	21.915248	7.132434
C	13.617861	19.871090	7.423251
H	13.820754	19.543948	6.406739
C	13.074414	18.986812	8.349214
H	12.853977	17.966301	8.057196
C	12.808747	19.416303	9.662446
C	10.897290	17.870249	10.126974
H	11.065960	17.333374	9.186659
H	10.190308	18.684642	9.940065
H	13.476983	16.790047	9.973642
F	8.940495	23.683801	10.560060
Cu	12.546015	21.181717	11.977596
F	9.922709	21.812648	11.027749

F	10.797973	20.498120	14.138901
F	10.241372	18.606563	15.031553
F	12.325854	19.237046	15.060104
O	10.773551	25.124123	11.762416
O	11.193601	17.207980	13.029551
N	13.995377	21.712529	13.375806
N	11.999221	23.190894	12.291939
N	11.951293	19.162641	11.968873
C	14.915676	20.871347	13.880994
H	14.894844	19.861075	13.482097
C	15.829819	21.243045	14.858866
H	16.549922	20.524641	15.238140
C	15.777982	22.556244	15.334800
H	16.468813	22.897547	16.101448
C	14.821024	23.422799	14.817066
H	14.764819	24.443644	15.177649
C	13.925687	22.975050	13.828369
C	12.867616	23.925381	13.232742
C	13.641270	25.064973	12.510062
H	14.259306	24.644882	11.708525
H	14.299389	25.602952	13.202183
H	12.925672	25.766151	12.078428
C	12.024765	24.496578	14.405755
H	11.269436	25.173660	14.004186
H	12.645189	25.047723	15.121411
H	11.527477	23.677912	14.935392
C	11.053254	23.904494	11.696197
C	10.157243	23.104849	10.700175
C	12.218358	18.446774	10.705882
H	10.463427	17.179130	10.851094
C	13.264655	17.314511	10.912472
H	14.203335	17.738885	11.286152
H	12.880649	16.600414	11.642284
C	11.455387	18.431201	12.957866
C	11.194610	19.211998	14.283441

Complex 2 - B3LYP/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
Cu	12.054242	21.181057	12.107228
N	12.751879	20.886024	10.162138
C	13.110479	21.844501	9.287758
H	12.982013	22.866306	9.626161
C	13.605843	21.553500	8.025327
H	13.880013	22.355070	7.348432
C	13.729020	20.209163	7.663528
H	14.109896	19.932832	6.684831
C	13.355051	19.224265	8.570022
H	13.443953	18.178488	8.301848
C	12.860483	19.589605	9.833348
C	12.449346	18.532272	10.864174
C	11.352713	17.645587	10.216244
H	10.485701	18.255878	9.945591
H	11.727938	17.163178	9.309267
H	11.040395	16.868825	10.913229
C	13.714724	17.696690	11.197132
H	14.508578	18.342963	11.585889
H	13.471594	16.935554	11.938012
H	14.097274	17.200096	10.300443
N	11.908775	19.213241	12.085093
C	11.478084	18.389146	13.052729
O	11.545466	17.157345	13.091857
C	10.769577	18.991583	14.337452
Cl	10.476422	20.777796	14.342662
Cl	9.171976	18.189876	14.512880
Cl	11.800158	18.597111	15.769675
N	13.645053	21.498166	13.420210
C	14.419685	20.550597	13.980462
H	14.154673	19.525077	13.749997
C	15.487728	20.856601	14.810773
H	16.085610	20.063413	15.245816
C	15.754105	22.204605	15.066094
H	16.578282	22.492471	15.711958
C	14.949694	23.178198	14.485870
H	15.144516	24.226676	14.676151
C	13.883635	22.797931	13.653449

C	12.984039	23.842660	12.983574
C	12.361222	24.716218	14.104973
H	11.767247	24.094576	14.781827
H	13.141048	25.210874	14.690932
H	11.721889	25.483139	13.669327
C	13.885390	24.696031	12.050899
H	14.377321	24.059979	11.307647
H	13.284181	25.449243	11.542378
H	14.665968	25.203367	12.625617
N	11.905147	23.146083	12.210671
C	11.025302	23.957621	11.603960
O	11.042485	25.190112	11.539878
C	9.766758	23.337024	10.864902
Cl	9.548877	21.544542	10.993429
Cl	8.293486	24.102538	11.550578
Cl	9.898818	23.752016	9.110417

Complex 2, Transition State for -CCl_3 Rotation - B3LYP/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
Cu	12.040781	21.211090	12.122023
N	12.899601	20.836376	10.210810
C	13.401751	21.745231	9.356128
H	13.311782	22.782168	9.663027
C	13.987650	21.391128	8.149544
H	14.379145	22.153470	7.484906
C	14.044474	20.032316	7.825439
H	14.488754	19.705790	6.889798
C	13.522853	19.098048	8.712371
H	13.558903	18.043098	8.469192
C	12.947567	19.529147	9.921164
C	12.354734	18.524667	10.920235
C	11.183136	17.807234	10.194088
H	10.416872	18.532680	9.904459
H	11.537946	17.308775	9.287216
H	10.738102	17.057761	10.847324
C	13.477955	17.515662	11.283269
H	14.350304	18.038901	11.688170

H	13.112945	16.798634	12.017050
H	13.805203	16.963417	10.397637
N	11.851331	19.242759	12.143178
C	11.281155	18.442235	13.067199
O	11.191425	17.214117	13.037490
C	10.574874	19.122474	14.331275
Cl	9.148024	20.087239	13.792634
Cl	10.007584	17.859699	15.461799
Cl	11.693185	20.209868	15.253457
N	13.741598	21.544895	13.236183
C	14.624157	20.602576	13.616297
H	14.371314	19.584423	13.344337
C	15.773181	20.907949	14.328962
H	16.461922	20.121593	14.617368
C	15.998502	22.245695	14.669439
H	16.879673	22.530144	15.236734
C	15.079317	23.211111	14.278111
H	15.237066	24.250218	14.540294
C	13.942344	22.834282	13.542643
C	12.900093	23.858227	13.090859
C	12.252184	24.456064	14.368865
H	11.751269	23.669224	14.940736
H	13.012484	24.915646	15.007966
H	11.522233	25.216663	14.093528
C	13.637737	24.951818	12.274121
H	14.154664	24.505554	11.418178
H	12.926310	25.695082	11.916917
H	14.383742	25.460715	12.890929
N	11.871255	23.166129	12.248591
C	10.911140	23.967471	11.757542
O	10.761394	25.177153	11.942035
C	9.852803	23.363384	10.748960
Cl	9.713691	21.559838	10.764588
Cl	8.233693	24.028162	11.114249
Cl	10.351958	23.879709	9.085424

Complex 4 - B3LYP/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
Cu	12.352998	21.184003	12.024351
N	12.762929	20.865356	10.012173
C	13.003235	21.793541	9.067377
H	12.928136	22.827799	9.384526
C	13.320806	21.452931	7.759388
H	13.501938	22.230144	7.025366
C	13.389793	20.096944	7.423388
H	13.628943	19.792319	6.408978
C	13.143408	19.141028	8.403603
H	13.185055	18.080428	8.176148
C	12.829416	19.557515	9.702733
C	12.566972	18.574268	10.815707
H	11.830485	17.828213	10.489328
H	13.488474	18.002003	11.011168
N	12.099483	19.255639	12.017457
C	11.557548	18.427113	12.922168
O	11.475193	17.197482	12.853702
C	10.972416	19.089440	14.197810
F	10.777283	20.434417	14.083551
F	9.790742	18.547268	14.525199
F	11.813416	18.909798	15.251757
N	13.733515	21.519734	13.541181
C	14.441265	20.600707	14.224150
H	14.232200	19.563622	13.986014
C	15.379561	20.953437	15.184831
H	15.925599	20.183222	15.717998
C	15.587522	22.312107	15.443908
H	16.308398	22.626014	16.192786
C	14.855788	23.258560	14.733925
H	14.989642	24.320867	14.912610
C	13.926399	22.830080	13.778714
C	13.112045	23.803067	12.963566
H	12.634957	24.537599	13.625669
H	13.791881	24.390531	12.325145
N	12.105526	23.107773	12.169550
C	11.161237	23.922235	11.675954
O	11.103974	25.150506	11.783308

C	10.016273	23.243497	10.877969
F	9.929178	21.896362	11.072096
F	8.824960	23.765370	11.203140
F	10.196230	23.429937	9.542504

Complex 4, Transition State for -CF_3 Rotation - B3LYP/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
Cu	12.351318	21.180808	12.066230
N	12.772003	20.868440	10.048219
C	13.002169	21.793326	9.097827
H	12.906553	22.828867	9.405389
C	13.335307	21.448519	7.794732
H	13.507076	22.223131	7.055696
C	13.432161	20.091405	7.470197
H	13.683882	19.783332	6.459861
C	13.196070	19.138831	8.456201
H	13.258110	18.077434	8.237291
C	12.864268	19.560133	9.749498
C	12.610767	18.580710	10.868335
H	11.912622	17.803077	10.532864
H	13.550018	18.047753	11.090879
N	12.085954	19.254109	12.052214
C	11.470181	18.420436	12.908357
O	11.383230	17.193795	12.815461
C	10.733284	19.112398	14.090805
F	9.674431	19.836166	13.648694
F	10.279082	18.221461	14.979179
F	11.541001	19.980638	14.768930
N	13.772714	21.511127	13.531749
C	14.501431	20.583316	14.179164
H	14.278649	19.550002	13.936223
C	15.472665	20.925140	15.110125
H	16.038540	20.149580	15.614166
C	15.688299	22.281279	15.379002
H	16.434626	22.586379	16.106270
C	14.931178	23.235926	14.708171
H	15.068921	24.295931	14.897137

C	13.970654	22.817910	13.778954
C	13.122912	23.795752	13.006025
H	12.654596	24.510425	13.695921
H	13.775798	24.405716	12.361111
N	12.104421	23.101990	12.224968
C	11.174738	23.926502	11.718477
O	11.136449	25.155953	11.818364
C	10.025081	23.261385	10.917104
F	9.942687	21.911696	11.084083
F	8.835559	23.775562	11.262175
F	10.195409	23.476534	9.584844

Acetamide Complex - B3LYP/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
N	12.717395	20.888813	10.02625900
C	12.998681	21.846877	9.12233300
H	12.941058	22.868606	9.48306600
C	13.340988	21.550643	7.81131100
H	13.558868	22.348936	7.11039200
C	13.395237	20.204674	7.43440200
H	13.660650	19.926958	6.41856700
C	13.104480	19.221914	8.37335400
H	13.141643	18.174975	8.09666100
C	12.758937	19.588091	9.68440100
C	11.274528	17.661621	10.24077100
H	11.557468	17.143912	9.31883200
H	10.391766	18.275618	10.03546000
H	14.012158	17.167165	10.09519700
Cu	12.348647	21.184179	12.02540200
O	11.070980	25.032968	11.45579600
O	11.613668	17.316668	13.15287600
N	13.687334	21.495286	13.55210900
N	12.061482	23.086485	12.23023700
N	12.030263	19.276150	11.98816100
C	14.410396	20.546619	14.17767700
H	14.194286	19.522370	13.89202000
C	15.372152	20.854954	15.12829700

H	15.933617	20.063933	15.61314300
C	15.587889	22.203352	15.43145200
H	16.332343	22.490441	16.16824200
C	14.838347	23.176385	14.78076900
H	14.993391	24.225044	15.00504000
C	13.875148	22.798083	13.83130000
C	13.023542	23.825063	13.07708100
C	13.975180	24.704505	12.22236800
H	14.535569	24.084277	11.51422300
H	14.695822	25.239552	12.84985400
H	13.379720	25.432452	11.66943200
C	12.281163	24.694539	14.12691200
H	11.663710	25.430542	13.61243700
H	12.987884	25.221264	14.77586000
H	11.640020	24.065519	14.75273900
C	11.137315	23.792067	11.52329100
C	10.069286	22.980707	10.79310100
C	12.434467	18.550224	10.76432300
H	11.022126	16.917671	10.99607600
C	13.705933	17.693101	11.00568400
H	14.538739	18.327578	11.32832000
H	13.492135	16.958084	11.78303600
C	11.613245	18.558155	13.06623200
C	11.057377	19.354590	14.24474200
H	10.200022	21.897308	10.85382600
H	9.099329	23.236947	11.23155000
H	10.036596	23.284666	9.74244600
H	11.116312	20.439779	14.12873400
H	10.005537	19.076640	14.36747600
H	11.576386	19.058203	15.16133400

Acetamide Complex, Transition State for -CH_3 Rotation - B3LYP/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
N	12.735580	20.883594	10.038684
C	13.044750	21.837801	9.140078
H	12.980786	22.860750	9.496626
C	13.422008	21.536551	7.839746

H	13.661584	22.331811	7.142438
C	13.482954	20.189124	7.468920
H	13.776042	19.907312	6.461850
C	13.162422	19.210257	8.402269
H	13.203325	18.162367	8.129642
C	12.780923	19.581820	9.701859
C	11.252223	17.682052	10.216793
H	11.549405	17.163915	9.299548
H	10.385649	18.312216	9.992423
H	13.979203	17.131784	10.143670
Cu	12.329762	21.181666	12.034687
O	11.040078	25.034485	11.513856
O	11.489460	17.330909	13.134049
N	13.704599	21.486377	13.532076
N	12.056543	23.083700	12.241592
N	11.992748	19.279593	11.987429
C	14.452465	20.536693	14.126921
H	14.233323	19.513617	13.838129
C	15.438543	20.842259	15.052914
H	16.019294	20.050627	15.513423
C	15.651900	22.189256	15.365030
H	16.413630	22.474263	16.084754
C	14.878051	23.163157	14.745188
H	15.031216	24.210567	14.976529
C	13.892810	22.787672	13.817014
C	13.016802	23.816905	13.095134
C	13.945098	24.730173	12.250242
H	14.508824	24.134658	11.523783
H	14.662721	25.264313	12.881798
H	13.332262	25.459418	11.718659
C	12.273010	24.650468	14.173053
H	11.640523	25.389947	13.682194
H	12.979172	25.170664	14.828007
H	11.646635	23.997308	14.789023
C	11.123528	23.793401	11.550636
C	10.069864	22.986097	10.795769
C	12.414141	18.548851	10.773242
H	10.967728	16.939265	10.961684
C	13.662134	17.667121	11.044956
H	14.500125	18.285277	11.385373

H	13.415366	16.938522	11.818741
C	11.522286	18.571566	13.051879
C	10.962476	19.404488	14.205999
H	10.212375	21.903041	10.833763
H	9.093188	23.222753	11.230153
H	10.043634	23.311633	9.751358
H	10.185650	20.092700	13.855852
H	10.534349	18.725090	14.944441
H	11.738050	20.005299	14.690725

Formamide Complex - B3LYP/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
N	12.881533	20.826877	9.915681
C	13.170293	21.746836	8.973767
H	13.266104	22.768855	9.323372
C	13.334302	21.413815	7.637520
H	13.564997	22.183312	6.909195
C	13.190192	20.071979	7.270629
H	13.305557	19.767967	6.234463
C	12.898849	19.127504	8.247671
H	12.785817	18.082964	7.982451
C	12.750325	19.527502	9.584727
C	11.062073	17.879109	10.397128
H	11.082531	17.347470	9.440158
H	10.280923	18.644509	10.351962
H	13.596327	16.891126	9.801785
Cu	12.722565	21.187680	11.922289
O	11.193041	24.915525	11.231698
O	11.831920	17.437042	13.283298
N	13.882857	21.560538	13.564472
N	12.381324	23.085246	12.058299
N	12.391983	19.284018	11.971705
C	14.630625	20.650332	14.219714
H	14.549999	19.628164	13.866749
C	15.453412	20.992875	15.282269
H	16.039051	20.231035	15.784695
C	15.496100	22.333984	15.676632
H	16.123249	22.645168	16.506826

C	14.727373	23.268426	14.992960
H	14.749132	24.312252	15.283049
C	13.918753	22.859191	13.921290
C	13.056925	23.843440	13.128427
C	13.972845	24.943282	12.531794
H	14.732201	24.496737	11.881144
H	14.483081	25.511014	13.316674
H	13.360947	25.630699	11.945514
C	12.022326	24.470677	14.101350
H	11.392484	25.170923	13.551623
H	12.521307	25.006080	14.915742
H	11.389611	23.690368	14.535937
C	11.512717	23.718753	11.239362
C	12.436906	18.532124	10.703280
H	10.817621	17.171009	11.189632
C	13.550604	17.453728	10.739929
H	14.527335	17.918878	10.910248
H	13.340257	16.758370	11.554143
C	12.079179	18.639518	13.117675
H	12.051296	19.327621	13.985815
H	11.056228	23.026680	10.504120

Reference Complex LCuOH - B3LYP/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
Cu	8.249412	14.452183	11.454606
O	9.420400	14.742390	10.128957
H	8.944516	15.051518	9.342111
N	7.109082	14.121160	12.895421
O	4.317097	15.060987	10.986260
C	5.805575	14.331560	12.711658
C	4.921394	14.096460	13.760527
H	3.861597	14.268233	13.609175
C	5.449870	13.643472	14.976852
H	4.783686	13.451684	15.812510
C	6.827115	13.435189	15.127805
H	7.269894	13.085888	16.053844
C	7.650204	13.691654	14.034776
C	5.476361	14.818224	11.319233

N	6.603342	14.932162	10.555555
C	6.513188	15.377029	9.207097
C	6.616687	16.763383	8.922518
C	6.532375	17.172110	7.586823
C	6.359803	16.247977	6.557973
C	6.268657	14.888591	6.851364
H	6.130608	14.178199	6.041849
C	6.346327	14.424014	8.169091
H	6.974271	17.266751	10.956894
H	8.885799	18.213769	9.652770
C	6.203820	12.934031	8.458251
H	6.454204	12.779044	9.511785
C	4.743928	12.473194	8.259379
H	4.056511	13.064138	8.871730
H	4.636482	11.417841	8.536158
H	4.438859	12.577215	7.211655
C	7.176438	12.074117	7.629097
H	7.093786	11.022401	7.925131
H	8.214075	12.388528	7.779190
H	6.957476	12.129549	6.557087
N	9.613461	13.888486	12.716708
O	9.805664	13.158558	14.922821
C	9.152203	13.544339	13.954639
C	10.989111	13.835029	12.400208
C	11.798679	14.980404	12.615916
C	13.160480	14.893202	12.314862
H	13.802180	15.752981	12.483605
C	13.711641	13.720754	11.799593
H	14.773012	13.674217	11.571692
C	12.900586	12.610065	11.570893
H	13.341148	11.704516	11.164190
C	11.532617	12.643222	11.854466
C	11.230478	16.273894	13.184595
H	10.145381	16.154362	13.252534
C	11.496677	17.475691	12.257521
H	11.112890	17.284331	11.250955
H	12.567212	17.694835	12.176611
C	11.754227	16.537803	14.611680
H	11.536293	15.694507	15.274024
H	11.285775	17.436715	15.029628

H	12.838819	16.696209	14.612113
C	10.676598	11.409838	11.599104
H	9.637102	11.683782	11.800735
C	10.748557	10.955265	10.128446
H	10.475329	11.772571	9.454367
H	10.061744	10.118387	9.956746
H	11.754732	10.615015	9.859210
C	11.044195	10.261381	12.561544
H	10.962870	10.580057	13.605215
H	12.070836	9.916513	12.392723
H	10.375649	9.406133	12.407455
C	6.766370	17.803597	10.026746
H	6.598432	18.228960	7.346585
H	11.006535	18.373479	12.651564
C	5.448895	18.582331	10.229422
C	7.947256	18.762005	9.782017
H	4.616193	17.902648	10.432776
H	5.197988	19.167963	9.337393
H	5.543270	19.278304	11.071230
H	7.791832	19.381838	8.892140
H	8.064122	19.439459	10.635229
H	6.296480	16.587086	5.527794

Reference Complex [LCuOH]$^-$ - B3LYP/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
Cu	8.377313	14.465140	11.268202
O	9.531845	14.658020	9.836244
H	9.044467	14.952274	9.055377
N	7.183963	14.205735	12.808537
O	4.268898	15.051427	10.996286
C	5.874475	14.408722	12.641622
C	4.994848	14.224349	13.708507
H	3.935703	14.394503	13.552204
C	5.527449	13.825247	14.939948
H	4.866902	13.673226	15.789847
C	6.904244	13.622568	15.084519
H	7.360554	13.317105	16.019201

C	7.720397	13.827217	13.970870
C	5.473176	14.838829	11.242845
N	6.537161	14.934629	10.425984
C	6.337869	15.322026	9.075000
C	6.507141	16.680007	8.703761
C	6.351433	17.038334	7.358977
C	6.041654	16.087496	6.387692
C	5.889519	14.752845	6.759597
H	5.651060	14.012969	5.999623
C	6.037360	14.346305	8.091601
H	7.130798	17.218483	10.654414
H	8.856434	18.134977	9.104853
C	5.842302	12.881104	8.466220
H	6.182117	12.768599	9.499413
C	4.349341	12.493232	8.425675
H	3.762575	13.153490	9.070949
H	4.210994	11.458575	8.765386
H	3.952261	12.567296	7.405007
C	6.691007	11.928065	7.603949
H	6.580822	10.896643	7.960663
H	7.752082	12.192443	7.652539
H	6.383649	11.944906	6.551178
N	9.745626	13.919866	12.737989
O	9.808027	13.338326	15.009001
C	9.229820	13.665986	13.953082
C	11.153578	13.845281	12.565673
C	11.980274	14.923347	12.967793
C	13.361054	14.833307	12.755691
H	14.002661	15.654522	13.066824
C	13.930503	13.714614	12.149735
H	15.005156	13.663162	11.990974
C	13.107168	12.666659	11.742577
H	13.549299	11.798456	11.259513
C	11.721743	12.709832	11.939722
C	11.401380	16.173868	13.621182
H	10.313189	16.072821	13.605381
C	11.746140	17.450507	12.829250
H	11.419946	17.363185	11.788022
H	12.825046	17.648539	12.829574
C	11.830881	16.293992	15.097150

H	11.542615	15.396444	15.651942
H	11.353881	17.163803	15.567832
H	12.917522	16.421401	15.184690
C	10.856769	11.548268	11.463785
H	9.829295	11.683782	11.762774
C	10.870435	10.955265	9.926260
H	10.546427	11.772571	9.482234
H	10.194281	10.118387	9.593443
H	11.875506	10.615015	9.554191
C	11.249641	10.261381	12.134161
H	11.211666	10.580057	13.225642
H	12.264738	9.916513	11.854992
H	10.564556	9.406133	11.825021
C	6.805566	17.803597	9.753064
H	6.472332	18.228960	7.065678
H	11.250202	18.373479	13.274929
C	5.527199	18.582331	10.114865
C	7.946828	18.762005	9.345418
H	4.731403	17.902648	10.436855
H	5.159956	19.167963	9.250329
H	5.728313	19.278304	10.925489
H	7.682002	19.381838	8.475628
H	8.178343	19.439459	10.169541
H	5.923576	16.587086	5.348239

Complex 1 - B3LYP/DEF2SVP

Atom	x (Å)	y (Å)	z (Å)
F	10.450959	23.046947	9.444976
N	12.821323	20.841783	10.080884
C	13.242955	21.777783	9.215171
H	13.174002	22.813112	9.555773
C	13.729765	21.454847	7.955179
H	14.062201	22.241270	7.275486
C	13.773664	20.103876	7.594810
H	14.147109	19.803213	6.612653
C	13.334607	19.142392	8.499696
H	13.359743	18.085606	8.233006

C	12.855758	19.538871	9.760472
C	11.069819	17.867025	10.177134
H	11.299617	17.362569	9.226299
H	10.306574	18.637420	9.988478
H	13.681134	16.899242	10.127310
F	8.819280	23.489380	10.794208
Cu	12.251766	21.183887	12.051610
F	9.981565	21.688412	11.073953
F	10.812178	20.647573	14.050958
F	9.987483	18.829152	14.879280
F	12.071523	19.306778	15.206776
O	10.778015	25.029310	11.695580
O	11.241064	17.315811	13.100553
N	13.746626	21.543594	13.451626
N	12.012883	23.127911	12.204195
N	12.001238	19.235542	12.034849
C	14.569606	20.618598	13.971623
H	14.352786	19.580831	13.709489
C	15.630263	20.955109	14.802637
H	16.278579	20.177385	15.209812
C	15.830636	22.308134	15.096068
H	16.651472	22.619285	15.747150
C	14.972032	23.258142	14.551700
H	15.112995	24.316285	14.773098
C	13.919075	22.848231	13.715426
C	12.930599	23.851882	13.110277
C	13.720385	24.934577	12.335719
H	14.334812	24.473168	11.546301
H	14.387596	25.504213	13.000141
H	13.010936	25.633842	11.875942
C	12.140552	24.480155	14.288938
H	11.419066	25.208797	13.899761
H	12.816072	24.990305	14.992369
H	11.596838	23.693735	14.834440
C	11.019997	23.827049	11.631920
C	10.053025	23.003975	10.732629
C	12.338961	18.521569	10.784501
H	10.665694	17.128823	10.880426
C	13.437429	17.461623	11.041366
H	14.359875	17.942247	11.404300

H	13.079810	16.752850	11.798661
C	11.456850	18.522890	13.033751
C	11.070913	19.335361	14.303472

Complex [1]$^{+}$ - B3LYP/DEF2SVP

Atom	x (Å)	y (Å)	z (Å)
F	10.710058	22.857846	9.395632
N	12.974370	20.794045	10.045502
C	13.486827	21.687404	9.179069
H	13.550815	22.721739	9.521745
C	13.902759	21.320844	7.906400
H	14.309652	22.070475	7.225890
C	13.774774	19.979801	7.530478
H	14.085071	19.650404	6.536116
C	13.246673	19.063876	8.436877
H	13.143816	18.015261	8.156863
C	12.851298	19.497273	9.711083
C	10.871069	18.064962	10.199883
H	11.000402	17.581102	9.221738
H	10.196234	18.924559	10.076732
H	13.352832	16.795429	10.002799
F	8.939915	23.318105	10.551275
Cu	12.497971	21.184761	11.985603
F	10.105848	21.557288	11.030822
F	10.941103	20.774358	14.028041
F	10.215997	18.995926	15.028857
F	12.319926	19.492424	15.117131
O	10.697550	24.880376	11.733514
O	11.149064	17.458273	13.106335
N	13.895366	21.594587	13.408137
N	12.090387	23.087699	12.183181
N	12.079491	19.274241	12.014252
C	14.795982	20.715284	13.884684
H	14.691977	19.679878	13.555311
C	15.801542	21.096871	14.762365
H	16.513627	20.358413	15.134143
C	15.862493	22.438160	15.153906

H	16.634963	22.779099	15.847155
C	14.927304	23.339454	14.651470
H	14.965268	24.388071	14.947318
C	13.939779	22.891387	13.761657
C	12.877412	23.832979	13.189728
C	13.571403	25.053689	12.524271
H	14.242162	24.727196	11.714986
H	14.169994	25.600513	13.265846
H	12.818164	25.738682	12.119291
C	11.964022	24.284759	14.366483
H	11.209289	24.995562	14.009939
H	12.568933	24.775687	15.141540
H	11.464023	23.413777	14.814655
C	11.025025	23.716608	11.592457
C	10.168822	22.852135	10.623204
C	12.250983	18.538966	10.742310
H	10.419779	17.342405	10.889983
C	13.210387	17.334274	10.949727
H	14.195582	17.676639	11.301332
H	12.784747	16.637329	11.680286
C	11.480362	18.628752	13.064853
C	11.226417	19.482740	14.339981

Complex $[1]^-$ - B3LYP/DEF2SVP

Atom	x (Å)	y (Å)	z (Å)
F	11.156333	23.035147	9.402598
N	13.170122	20.617577	10.029227
C	13.779590	21.424536	9.149208
H	13.966974	22.445998	9.494584
C	14.137978	21.013243	7.869482
H	14.634614	21.704097	7.184020
C	13.830939	19.700489	7.496476
H	14.085445	19.328712	6.499652
C	13.186446	18.871828	8.411627
H	12.930362	17.848288	8.134648
C	12.862811	19.357378	9.693513
C	10.697006	18.221755	10.142970

H	10.734374	17.716151	9.163514
H	10.175088	19.183176	10.023914
H	12.950464	16.586059	9.912753
F	9.215951	23.668431	10.107363
Cu	12.580128	21.186633	11.961392
F	10.028041	21.789361	10.780727
F	10.985826	20.548342	14.273737
F	10.681558	18.660472	15.267458
F	12.692104	19.346526	14.880839
O	10.531960	24.951077	11.922293
O	10.913465	17.385928	13.033162
N	14.070278	21.774341	13.317338
N	12.052263	23.195606	12.212173
N	12.030407	19.169012	12.008539
C	15.059985	20.982156	13.753217
H	15.060440	19.962536	13.355428
C	16.019522	21.405415	14.667255
H	16.810383	20.726515	14.995012
C	15.925806	22.714185	15.152094
H	16.651117	23.094861	15.877117
C	14.887449	23.527209	14.704465
H	14.792987	24.547204	15.079431
C	13.957989	23.030400	13.770120
C	12.775201	23.892628	13.282463
C	13.339506	25.244630	12.772144
H	14.047943	25.068977	11.946393
H	13.863142	25.803491	13.564544
H	12.504937	25.853596	12.402898
C	11.845988	24.115253	14.507143
H	10.991666	24.728846	14.192028
H	12.370614	24.621990	15.334423
H	11.478226	23.142135	14.865833
C	11.021102	23.835140	11.674890
C	10.351189	23.067848	10.494419
C	12.117510	18.476363	10.717497
H	10.139466	17.594860	10.851329
C	12.894774	17.141478	10.862953
H	13.922329	17.340112	11.208322
H	12.382248	16.518823	11.606828
C	11.434372	18.514264	12.996969

C	11.443293	19.281287	14.354408

Complex 2 - B3LYP/DEF2SVP

Atom	x (Å)	y (Å)	z (Å)
N	12.825625	20.849724	10.205018
C	13.297082	21.794188	9.376657
H	13.159740	22.827669	9.701362
C	13.909501	21.483877	8.168819
H	14.280352	22.278101	7.518508
C	14.025274	20.134098	7.821039
H	14.496644	19.841012	6.879487
C	13.531141	19.163308	8.686448
H	13.611463	18.107698	8.426815
C	12.926987	19.550461	9.896837
C	11.178600	17.810068	10.141356
H	11.523262	17.324259	9.215967
H	10.405043	18.546520	9.875192
H	13.810380	16.957072	10.315232
Cu	12.006606	21.180667	12.120114
O	10.775585	25.159307	11.799845
O	11.185126	17.182372	13.006592
N	13.687337	21.536021	13.344286
N	11.861935	23.161390	12.214001
N	11.870292	19.197220	12.104245
C	14.533479	20.604267	13.809327
H	14.267181	19.566894	13.596322
C	15.673067	20.931559	14.533549
H	16.338978	20.147394	14.898067
C	15.926872	22.284971	14.778756
H	16.809190	22.591199	15.346514
C	15.041627	23.242445	14.293836
H	15.225078	24.300614	14.480411
C	13.909100	22.838429	13.563024
C	12.898743	23.860068	13.025683
C	13.670430	24.888451	12.160292
H	14.211111	24.379578	11.346830
H	14.406698	25.443698	12.760227

H	12.964708	25.609020	11.730855
C	12.253532	24.547793	14.258399
H	11.526265	25.297488	13.925525
H	13.015883	25.046235	14.876062
H	11.741046	23.799856	14.882524
C	10.900274	23.943646	11.701738
C	9.791962	23.276172	10.785227
C	12.353911	18.513479	10.871199
H	10.739381	17.047936	10.795607
C	13.477883	17.502031	11.211232
H	14.351068	18.023491	11.633904
H	13.105470	16.771159	11.938432
C	11.322259	18.400351	13.033622
C	10.832068	19.051467	14.393565
Cl	9.317449	18.267243	14.904994
Cl	12.114112	18.738880	15.624811
Cl	10.518340	20.837727	14.344851
Cl	9.574890	21.486518	10.987763
Cl	8.217631	24.036299	11.123034
Cl	10.256095	23.596318	9.070740

Reference Complex LCuOH - B3LYP/DEF2SVP

Atom	**x (Å)**	**y (Å)**	**z (Å)**
Cu	8.226530	14.449074	11.454158
O	9.387672	14.733462	10.099813
H	8.881698	14.940823	9.297776
N	7.092849	14.114782	12.921675
O	4.260783	14.889362	10.999326
C	5.785322	14.271643	12.733554
C	4.909308	14.026607	13.790110
H	3.837329	14.155238	13.631199
C	5.455701	13.620632	15.016524
H	4.794059	13.421379	15.863257
C	6.841353	13.466374	15.167846
H	7.305340	13.152126	16.104292
C	7.652526	13.729927	14.064727
C	5.422497	14.708527	11.328370

N	6.539718	14.852740	10.552682
C	6.446266	15.243640	9.196065
C	6.635655	16.609870	8.850736
C	6.569095	16.970050	7.498882
C	6.319963	16.019400	6.509745
C	6.138903	14.681054	6.858967
H	5.942196	13.946038	6.075076
C	6.203337	14.263656	8.193967
H	6.812336	17.190627	10.888634
H	9.080898	17.330322	9.907837
C	5.974710	12.798067	8.545836
H	6.268256	12.668107	9.598119
C	4.480534	12.436573	8.437554
H	3.868599	13.101892	9.064364
H	4.308409	11.396354	8.760966
H	4.126436	12.526165	7.396973
C	6.849908	11.844054	7.716430
H	6.711691	10.805408	8.058419
H	7.918339	12.092830	7.813505
H	6.591893	11.870160	6.645320
N	9.617793	13.965508	12.750718
O	9.821909	13.290990	14.965018
C	9.162938	13.631596	13.994875
C	10.980859	13.982925	12.416650
C	11.765674	15.134896	12.707984
C	13.122820	15.113797	12.373236
H	13.747715	15.980237	12.601221
C	13.696416	14.004164	11.749894
H	14.759436	14.011203	11.494513
C	12.914257	12.890120	11.446573
H	13.373816	12.031332	10.951208
C	11.552524	12.855796	11.763958
C	11.170262	16.349543	13.408932
H	10.075789	16.245797	13.361570
C	11.525767	17.672807	12.711729
H	11.240271	17.655194	11.648675
H	12.603871	17.894150	12.769711
C	11.567325	16.372719	14.898389
H	11.280181	15.436423	15.399316
H	11.076240	17.212231	15.418724

H	12.656871	16.499520	15.012933
C	10.723516	11.626924	11.416287
H	9.694870	11.824012	11.751199
C	10.665850	11.398720	9.895521
H	10.277266	12.297804	9.394415
H	10.007529	10.546892	9.656354
H	11.661788	11.174325	9.479224
C	11.214246	10.378867	12.171574
H	11.213278	10.548327	13.259703
H	12.238996	10.100535	11.875078
H	10.562165	9.515792	11.957503
C	6.922813	17.672000	9.906086
H	6.712493	18.015007	7.213654
H	10.997267	18.511261	13.194380
C	5.912233	18.830006	9.854975
C	8.377103	18.170841	9.808083
H	4.879074	18.460488	9.947759
H	5.984628	19.398843	8.913586
H	6.098321	19.537471	10.679620
H	8.567760	18.667355	8.842151
H	8.593037	18.899889	10.606554
H	6.269285	16.322106	5.460593

Reference Complex [LCuOH]$^-$ - B3LYP/DEF2SVP

Atom	**x (Å)**	**y (Å)**	**z (Å)**
Cu	8.340760	14.490844	11.274850
O	9.478328	14.783367	9.829597
H	8.934031	14.887269	9.036330
N	7.150173	14.147686	12.825195
O	4.199493	14.784732	10.995766
C	5.835107	14.268231	12.650312
C	4.962664	14.025245	13.714106
H	3.889683	14.128732	13.546222
C	5.514981	13.657299	14.947960
H	4.858284	13.460511	15.800636
C	6.902562	13.539278	15.095676
H	7.383284	13.256101	16.033161

C	7.707664	13.798973	13.982900
C	5.403987	14.669535	11.247981
N	6.465430	14.852415	10.437582
C	6.264869	15.219957	9.088805
C	6.484421	16.565735	8.688494
C	6.336927	16.905861	7.336756
C	5.973766	15.954405	6.384351
C	5.766114	14.633754	6.781352
H	5.486611	13.887132	6.032413
C	5.911576	14.242481	8.119247
H	6.822173	17.167486	10.692667
H	9.022559	17.145895	9.582261
C	5.682603	12.786968	8.513564
H	6.028330	12.683369	9.552028
C	4.184665	12.432078	8.490840
H	3.623971	13.115270	9.145536
H	4.021078	11.397626	8.840725
H	3.772363	12.508507	7.469414
C	6.517300	11.809587	7.669433
H	6.387422	10.776371	8.034127
H	7.589361	12.056384	7.725811
H	6.222219	11.820434	6.606494
N	9.731767	14.017486	12.762282
O	9.813595	13.402542	15.016070
C	9.226942	13.717682	13.973312
C	11.131249	14.002488	12.567587
C	11.930239	15.098418	12.989570
C	13.312029	15.060354	12.760159
H	13.933253	15.898045	13.090281
C	13.911757	13.978228	12.116806
H	14.992249	13.967645	11.944509
C	13.119335	12.914428	11.687968
H	13.587290	12.070524	11.172327
C	11.734779	12.903822	11.902355
C	11.312140	16.302140	13.693900
H	10.222657	16.212164	13.573575
C	11.721996	17.638656	13.053300
H	11.490391	17.649791	11.976697
H	12.800457	17.840665	13.169105
C	11.612392	16.280838	15.204331

H	11.268437	15.334577	15.646821
H	11.104104	17.115791	15.718710
H	12.695583	16.381742	15.393854
C	10.902015	11.727679	11.403450
H	9.872968	11.902204	11.748766
C	10.859871	11.690056	9.865375
H	10.471951	12.649615	9.487633
H	10.205622	10.872836	9.512394
H	11.864181	11.519949	9.439040
C	11.362591	10.390324	12.007420
H	11.352245	10.428159	13.108615
H	12.386179	10.126556	11.690120
H	10.698315	9.569231	11.686292
C	6.900702	17.630658	9.698701
H	6.509616	17.939468	7.023255
H	11.181858	18.475691	13.528427
C	5.962092	18.848269	9.688400
C	8.374454	18.033573	9.503975
H	4.915745	18.545348	9.853892
H	6.006570	19.396620	8.731851
H	6.242742	19.558713	10.484727
H	8.534999	18.501211	8.516669
H	8.685544	18.761880	10.273193
H	5.858703	16.239790	5.334524

Complex 1 - B3LYP/aug-CC-PVDZ

Atom	**x (Å)**	**y (Å)**	**z (Å)**
F	10.105169	23.194614	9.518833
N	12.709949	20.888441	10.067199
C	13.013645	21.848246	9.173078
H	12.916315	22.874765	9.519836
C	13.424124	21.558218	7.879757
H	13.655360	22.364066	7.185687
C	13.523613	20.213791	7.507494
H	13.841771	19.938644	6.501723
C	13.209235	19.227569	8.436175
H	13.280763	18.178274	8.161300

C	12.796481	19.590264	9.727995
C	11.308313	17.652786	10.213005
H	11.628378	17.157805	9.288053
H	10.428016	18.268779	9.990986
H	14.051720	17.175869	10.160222
F	8.763906	23.611530	11.186203
Cu	12.244575	21.183046	12.054462
F	9.898422	21.758744	11.150613
F	10.704310	20.571255	14.029488
F	9.745704	18.698599	14.573094
F	11.743938	19.149001	15.319352
O	11.016372	25.095454	11.504172
O	11.544028	17.252810	13.139868
N	13.659377	21.495318	13.521755
N	12.015123	23.119773	12.234698
N	11.989632	19.241712	12.008345
C	14.396945	20.545352	14.127178
H	14.153879	19.515582	13.874235
C	15.408791	20.848808	15.026809
H	15.978657	20.050539	15.498629
C	15.661234	22.196525	15.302305
H	16.446347	22.482073	16.002709
C	14.896334	23.172557	14.672862
H	15.080213	24.224245	14.877495
C	13.884698	22.796432	13.775130
C	13.022956	23.838227	13.055386
C	13.949964	24.703610	12.165450
H	14.483832	24.073909	11.441340
H	14.696467	25.230576	12.772949
H	13.350040	25.443962	11.628763
C	12.324128	24.704323	14.133955
H	11.701944	25.463954	13.654842
H	13.065013	25.209170	14.765767
H	11.694044	24.073740	14.773487
C	11.101941	23.866817	11.596217
C	9.962320	23.094765	10.867121
C	12.446031	18.537051	10.783379
H	11.034450	16.884775	10.940228
C	13.714017	17.693305	11.067024
H	14.532646	18.336461	11.416441

H	13.488377	16.945763	11.832761
C	11.547434	18.482201	13.021868
C	10.928763	19.238271	14.235109

Complex 1, Transition State for -CF_3 Rotation - B3LYP/aug-CC-PVDZ

Atom	x (Å)	y (Å)	z (Å)
F	10.120299	23.220872	9.562009
N	12.719225	20.889634	10.089535
C	13.039351	21.844504	9.196011
H	12.919959	22.873052	9.530184
C	13.492499	21.547231	7.918709
H	13.735356	22.348847	7.223584
C	13.620632	20.200299	7.564030
H	13.974638	19.919198	6.571945
C	13.287904	19.219424	8.491818
H	13.379901	18.168637	8.229035
C	12.827997	19.589906	9.765905
C	11.312870	17.671117	10.204665
H	11.653986	17.186452	9.281854
H	10.442828	18.296031	9.967818
H	14.043814	17.156100	10.235926
F	8.753427	23.604774	11.216666
Cu	12.238074	21.184969	12.079140
F	9.904113	21.761919	11.172187
F	9.621131	19.938140	13.636786
F	10.244142	18.444597	15.091733
F	11.478850	20.200447	14.754670
O	10.983994	25.098826	11.600842
O	11.430771	17.253901	13.112020
N	13.709533	21.493838	13.475825
N	12.014741	23.118632	12.270344
N	11.954998	19.248087	12.030097
C	14.466401	20.536092	14.043119
H	14.212199	19.510412	13.783403
C	15.505738	20.829572	14.913798
H	16.094318	20.026823	15.354192
C	15.761446	22.174314	15.203684

H	16.567441	22.451418	15.883452
C	14.971693	23.157090	14.617605
H	15.154746	24.206019	14.836822
C	13.934040	22.790382	13.745339
C	13.036627	23.834758	13.076888
C	13.924299	24.733764	12.180344
H	14.444986	24.128791	11.426252
H	14.681232	25.256230	12.778717
H	13.299874	25.478572	11.679344
C	12.357531	24.664654	14.195727
H	11.710469	25.425420	13.752660
H	13.109554	25.165764	14.817457
H	11.755814	24.009816	14.838179
C	11.085585	23.869734	11.658179
C	9.959115	23.101078	10.907217
C	12.441583	18.542111	10.814628
H	11.014741	16.895247	10.913343
C	13.691637	17.683748	11.131369
H	14.511353	18.317226	11.495596
H	13.438060	16.943073	11.894863
C	11.442525	18.482987	13.011299
C	10.691666	19.267830	14.136018

Complex 2 - B3LYP/aug-CC-PVDZ

Atom	**x (Å)**	**y (Å)**	**z (Å)**
N	12.724493	20.891468	10.154399
C	13.056722	21.852644	9.273176
H	12.918457	22.878085	9.608755
C	13.540771	21.567395	8.004222
H	13.794101	22.375171	7.320092
C	13.681212	20.223906	7.642484
H	14.055982	19.950416	6.655915
C	13.333507	19.235904	8.556901
H	13.436375	18.187908	8.287884
C	12.848541	19.596893	9.825372
C	11.401794	17.611702	10.223735
H	11.796788	17.125217	9.323844

H	10.519077	18.197821	9.939176
H	14.158276	17.253012	10.303949
Cu	12.041832	21.181107	12.110376
O	11.086918	25.195496	11.495970
O	11.605266	17.153328	13.106603
N	13.625616	21.492191	13.439997
N	11.911105	23.151012	12.216799
N	11.910148	19.208731	12.076408
C	14.381127	20.541235	14.019399
H	14.109446	19.512010	13.795693
C	15.442623	20.840971	14.861572
H	16.026375	20.041025	15.313273
C	15.723570	22.188353	15.108768
H	16.546329	22.473044	15.764957
C	14.937732	23.165736	14.508435
H	15.144775	24.216621	14.692879
C	13.877519	22.790315	13.666129
C	13.003303	23.840813	12.974040
C	13.925150	24.649195	12.024127
H	14.404322	23.981371	11.296344
H	14.718267	25.150715	12.592421
H	13.341916	25.406999	11.495869
C	12.398567	24.750329	14.073622
H	11.766490	25.517024	13.620399
H	13.191419	25.250019	14.643053
H	11.798600	24.152122	14.770640
C	11.046818	23.966694	11.594375
C	9.764256	23.353399	10.897334
C	12.470640	18.534567	10.862482
H	11.105511	16.834821	10.931832
C	13.761959	17.745063	11.200806
H	14.536440	18.423661	11.581566
H	13.544782	16.980920	11.950726
C	11.500864	18.380963	13.049632
C	10.750971	18.975777	14.310925
Cl	9.135947	18.186679	14.411945
Cl	11.711701	18.558880	15.785850
Cl	10.467221	20.767004	14.335999
Cl	9.544936	21.555855	11.002119
Cl	8.315646	24.104873	11.658262

Cl	9.811548	23.791248	9.143210

Complex 1 - B3LYP-D3/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
F	10.091608	23.137469	9.523089
N	12.668833	20.926793	10.092319
C	12.946667	21.903828	9.210535
H	12.842454	22.918473	9.575887
C	13.340218	21.632407	7.909312
H	13.549236	22.444942	7.223138
C	13.451698	20.294467	7.521024
H	13.756155	20.037465	6.511310
C	13.168267	19.291411	8.440890
H	13.252688	18.249483	8.157883
C	12.770420	19.634005	9.739836
C	11.395798	17.614401	10.241790
H	11.745086	17.125472	9.328471
H	10.484138	18.172928	10.011488
H	14.171658	17.321940	10.205028
F	8.773449	23.624877	11.189255
Cu	12.211630	21.182977	12.063121
F	9.877203	21.754048	11.194519
F	10.660091	20.576639	14.000088
F	9.751173	18.686277	14.564763
F	11.726716	19.209999	15.322355
O	11.071492	25.078057	11.428818
O	11.630772	17.273201	13.178125
N	13.610860	21.455689	13.521206
N	12.000193	23.101780	12.239424
N	11.972956	19.260046	12.011547
C	14.319695	20.487569	14.129268
H	14.059467	19.469587	13.864989
C	15.322573	20.771627	15.043175
H	15.868985	19.965930	15.519645
C	15.595426	22.113045	15.325064
H	16.372129	22.379832	16.034871
C	14.861680	23.106877	14.687512

H	15.062072	24.151379	14.891767
C	13.857570	22.751614	13.777262
C	13.038106	23.802320	13.027571
C	13.997877	24.583083	12.098066
H	14.482694	23.897605	11.395385
H	14.778045	25.088541	12.674722
H	13.430191	25.330011	11.541750
C	12.382753	24.741334	14.066931
H	11.792816	25.501038	13.555613
H	13.142433	25.240885	14.674012
H	11.730538	24.165196	14.729346
C	11.116471	23.850722	11.570207
C	9.958386	23.078212	10.873218
C	12.472882	18.573382	10.800051
H	11.168490	16.846923	10.980652
C	13.789105	17.817656	11.102050
H	14.552611	18.517331	11.457270
H	13.602771	17.064961	11.869121
C	11.572477	18.500005	13.037059
C	10.920007	19.256627	14.231033

Complex 1, Transition State for -CF_3 Rotation - B3LYP-D3/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
F	10.025609	23.172348	9.607825
N	12.641047	20.944560	10.119053
C	12.906736	21.925084	9.237489
H	12.759528	22.938057	9.592315
C	13.343091	21.660014	7.948625
H	13.540379	22.475144	7.262005
C	13.515036	20.324501	7.574021
H	13.857131	20.072102	6.575242
C	13.242377	19.317962	8.493199
H	13.372341	18.278190	8.219852
C	12.794969	19.654449	9.777959
C	11.464709	17.601519	10.237373
H	11.855877	17.130446	9.331855
H	10.544166	18.134528	9.983254

H	14.238883	17.372503	10.295653
F	8.755888	23.653207	11.313440
Cu	12.179391	21.183124	12.100273
F	9.851785	21.777279	11.273906
F	9.575785	19.864277	13.551565
F	10.198553	18.413057	15.049407
F	11.372035	20.215052	14.737202
O	11.084743	25.088370	11.479188
O	11.573864	17.260043	13.158860
N	13.626093	21.440619	13.502122
N	11.994981	23.102129	12.286303
N	11.934239	19.262115	12.027958
C	14.324083	20.457344	14.097443
H	14.027836	19.446048	13.844612
C	15.355654	20.721717	14.984612
H	15.896570	19.905824	15.450018
C	15.665230	22.058073	15.255657
H	16.465575	22.308958	15.944686
C	14.935192	23.066451	14.637549
H	15.159587	24.106872	14.837668
C	13.901423	22.730314	13.753068
C	13.074735	23.791253	13.028081
C	14.014968	24.545939	12.057770
H	14.460701	23.846043	11.343693
H	14.825160	25.038442	12.603444
H	13.443757	25.301103	11.516505
C	12.475774	24.751114	14.081782
H	11.878811	25.514886	13.584830
H	13.266362	25.244953	14.653120
H	11.840541	24.193097	14.775448
C	11.110338	23.861741	11.628981
C	9.928445	23.102488	10.960274
C	12.495588	18.589196	10.833541
H	11.237776	16.820957	10.962161
C	13.820607	17.867555	11.177108
H	14.559140	18.586621	11.545771
H	13.629864	17.117007	11.945360
C	11.478701	18.483294	13.020777
C	10.648055	19.244393	14.102933

Complex 2 - B3LYP-D3/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
N	12.802067	20.892680	10.207296
C	13.221277	21.851835	9.365579
H	13.130432	22.868767	9.727904
C	13.724775	21.560775	8.106881
H	14.050502	22.359538	7.450380
C	13.784812	20.219487	7.718646
H	14.165391	19.945681	6.739568
C	13.351688	19.234063	8.598407
H	13.394083	18.190381	8.312486
C	12.859740	19.599770	9.859704
C	11.244024	17.745492	10.222965
H	11.579970	17.260682	9.302314
H	10.415080	18.415330	9.976692
H	13.957483	17.135669	10.284267
Cu	12.046926	21.181122	12.108971
O	10.940810	25.143472	11.586728
O	11.438241	17.202422	13.106403
N	13.666204	21.492372	13.355169
N	11.896191	23.123319	12.193800
N	11.908884	19.236208	12.104120
C	14.474457	20.544997	13.858476
H	14.227600	19.524684	13.590582
C	15.548101	20.851414	14.680645
H	16.178417	20.061886	15.073659
C	15.776343	22.195722	14.987518
H	16.601280	22.481308	15.632749
C	14.935919	23.168901	14.459062
H	15.101382	24.214732	14.686486
C	13.871998	22.787962	13.628619
C	12.934543	23.822645	13.004811
C	13.797966	24.748705	12.113825
H	14.320420	24.159076	11.353933
H	14.550367	25.269819	12.712112
H	13.163497	25.488776	11.627725
C	12.266726	24.610860	14.156941
H	11.597387	25.367129	13.748969
H	13.019568	25.107562	14.775030

H	11.696405	23.927162	14.792369
C	10.995861	23.911095	11.597030
C	9.842913	23.234084	10.747093
C	12.394906	18.551495	10.871342
H	10.894968	16.978251	10.912815
C	13.610164	17.645701	11.186977
H	14.437981	18.248482	11.573515
H	13.329320	16.896461	11.926092
C	11.457726	18.435534	13.074988
C	10.891912	19.095669	14.399332
Cl	9.367564	18.272806	14.842459
Cl	12.121524	18.831895	15.698446
Cl	10.537148	20.870378	14.321640
Cl	9.605263	21.455498	10.993818
Cl	8.293531	24.032630	11.145210
Cl	10.232019	23.505327	9.002192

Complex 1 - B3LYP-D3/aug-CC-PVDZ

Atom	**x (Å)**	**y (Å)**	**z (Å)**
F	10.015045	23.185074	9.554645
N	12.622052	20.937885	10.085853
C	12.857792	21.919513	9.197535
H	12.739136	22.936893	9.561440
C	13.230073	21.657119	7.887309
H	13.406278	22.477521	7.194874
C	13.364717	20.321615	7.495696
H	13.654858	20.070109	6.475824
C	13.123673	19.313341	8.422970
H	13.227162	18.270432	8.136250
C	12.746319	19.647993	9.730145
C	11.487071	17.558044	10.253142
H	11.872577	17.067981	9.351609
H	10.547535	18.064970	10.002541
H	14.275363	17.431620	10.210669
F	8.786447	23.683259	11.286229
Cu	12.191506	21.183088	12.068051
F	9.856687	21.792123	11.225799

F	10.623782	20.539709	13.980772
F	9.712244	18.628840	14.473993
F	11.643197	19.165503	15.333796
O	11.151051	25.087271	11.364496
O	11.732738	17.267832	13.194489
N	13.574398	21.443181	13.549416
N	12.001884	23.108057	12.251505
N	11.967228	19.254360	11.999894
C	14.250559	20.469252	14.184006
H	13.978280	19.448497	13.928141
C	15.240524	20.743191	15.116200
H	15.762045	19.928676	15.614347
C	15.535616	22.082368	15.389426
H	16.305810	22.342866	16.115041
C	14.834317	23.082625	14.724495
H	15.053407	24.128288	14.922483
C	13.842743	22.736387	13.797069
C	13.067746	23.794478	13.012442
C	14.060621	24.495062	12.056386
H	14.514687	23.760224	11.378991
H	14.864482	24.984401	12.619815
H	13.526780	25.249076	11.471315
C	12.452940	24.796743	14.013285
H	11.884402	25.556263	13.472381
H	13.236743	25.296765	14.593982
H	11.785583	24.269545	14.705542
C	11.147384	23.867241	11.556930
C	9.947137	23.118421	10.909273
C	12.506121	18.581763	10.798485
H	11.293687	16.792675	11.007772
C	13.863898	17.909841	11.107975
H	14.585010	18.659757	11.458168
H	13.722380	17.150648	11.882230
C	11.605415	18.485695	13.032922
C	10.890578	19.218286	14.204789

Complex 1, Transition State for -CF_3 Rotation - B3LYP-D3/aug-CC-PVDZ

Atom	x (Å)	y (Å)	z (Å)
F	9.980557	23.212555	9.625774
N	12.607293	20.950723	10.112347
C	12.844292	21.933006	9.225182
H	12.685883	22.949029	9.577687
C	13.267108	21.673159	7.929878
H	13.442089	22.493612	7.237079
C	13.455526	20.339492	7.553971
H	13.789165	20.089859	6.546998
C	13.211346	19.330826	8.479811
H	13.354914	18.289696	8.204122
C	12.776918	19.663008	9.770279
C	11.528299	17.562930	10.246392
H	11.947203	17.089890	9.350806
H	10.589635	18.060181	9.974173
H	14.308731	17.451591	10.303473
F	8.768188	23.698910	11.372377
Cu	12.164497	21.184753	12.100149
F	9.838448	21.808154	11.288785
F	9.568304	19.840619	13.518880
F	10.162723	18.371140	15.010134
F	11.336683	20.182760	14.751552
O	11.138085	25.098743	11.438938
O	11.637861	17.258408	13.171524
N	13.599593	21.431445	13.520934
N	11.998194	23.108937	12.291618
N	11.925752	19.258873	12.017585
C	14.276085	20.444237	14.133676
H	13.971249	19.430185	13.886852
C	15.300023	20.700721	15.033078
H	15.824957	19.877615	15.513405
C	15.624955	22.035135	15.299391
H	16.422387	22.281266	16.000176
C	14.916182	23.048040	14.662870
H	15.153723	24.089896	14.859855
C	13.890418	22.718642	13.766293
C	13.094369	23.786240	13.018331
C	14.056588	24.488920	12.033035
H	14.482836	23.757043	11.334858
H	14.882194	24.968622	12.572799

H	13.508296	25.251182	11.472749
C	12.520149	24.783527	14.047724
H	11.936992	25.549795	13.532461
H	13.326446	25.275104	14.604529
H	11.874587	24.254374	14.758882
C	11.132946	23.877198	11.619327
C	9.924373	23.135920	10.980569
C	12.516444	18.595447	10.833060
H	11.323030	16.784818	10.984273
C	13.869333	17.934947	11.184763
H	14.577385	18.690682	11.548358
H	13.710063	17.180143	11.959893
C	11.494457	18.473367	13.015939
C	10.631951	19.216999	14.085238

Complex 2 - B3LYP-D3/aug-CC-PVDZ

Atom	x (Å)	y (Å)	z (Å)
N	12.633211	20.947585	10.124195
C	12.829193	21.928657	9.227425
H	12.728642	22.946472	9.594518
C	13.136747	21.667686	7.899860
H	13.282180	22.488978	7.201365
C	13.240413	20.332755	7.499459
H	13.476355	20.080835	6.465817
C	13.037039	19.323818	8.435706
H	13.117355	18.281824	8.139700
C	12.729137	19.659525	9.761102
C	11.635585	17.480336	10.318679
H	12.079139	16.980322	9.450198
H	10.669341	17.906325	10.023245
H	14.428999	17.629085	10.246221
Cu	12.083504	21.181401	12.099510
O	11.383864	25.117317	11.181588
O	12.020978	17.235170	13.222046
N	13.568263	21.436091	13.510496
N	11.964008	23.128051	12.222074
N	11.954148	19.232301	12.046007

C	14.214168	20.463422	14.175021
H	13.960187	19.442120	13.904287
C	15.151435	20.736792	15.160941
H	15.649413	19.921927	15.682076
C	15.418357	22.075410	15.460747
H	16.143858	22.336915	16.230689
C	14.745387	23.075705	14.766064
H	14.944990	24.120432	14.986322
C	13.810493	22.727590	13.781764
C	13.092572	23.782039	12.939842
C	14.142577	24.340443	11.949030
H	14.530546	23.531190	11.317258
H	14.985966	24.779595	12.495839
H	13.685177	25.108201	11.320435
C	12.550769	24.887291	13.869528
H	12.003035	25.628387	13.284198
H	13.369513	25.400549	14.386445
H	11.881257	24.449413	14.619458
C	11.209508	23.929617	11.463592
C	9.851968	23.353133	10.893483
C	12.562321	18.595423	10.845520
H	11.477948	16.730995	11.096818
C	13.980160	18.055211	11.151808
H	14.625930	18.871290	11.500457
H	13.921978	17.280866	11.920422
C	11.709208	18.419588	13.078770
C	10.830998	18.974400	14.270826
Cl	9.245312	18.121908	14.175399
Cl	11.638918	18.574244	15.830417
Cl	10.483610	20.750525	14.286056
Cl	9.577232	21.571463	11.054104
Cl	8.528474	24.180363	11.795951
Cl	9.732383	23.756725	9.141959

Complex 1 - ωB97X-D/6-31+G(d,p)

Atom	**x (Å)**	**y (Å)**	**z (Å)**
F	10.125432	23.108442	9.529105

N	12.689199	20.922422	10.102623
C	12.992000	21.892563	9.227014
H	12.890334	22.909225	9.591504
C	13.404329	21.618822	7.936789
H	13.633216	22.428422	7.254333
C	13.509021	20.282680	7.552860
H	13.828643	20.022018	6.549084
C	13.201132	19.285944	8.465174
H	13.281551	18.242833	8.183508
C	12.785024	19.633922	9.753816
C	11.356649	17.655547	10.236549
H	11.695758	17.162159	9.321597
H	10.462096	18.241026	10.005979
H	14.116820	17.280884	10.211697
F	8.772971	23.578317	11.155303
Cu	12.204978	21.182917	12.064859
F	9.894428	21.733481	11.188574
F	10.683859	20.598271	13.999746
F	9.765483	18.735660	14.590907
F	11.750627	19.233448	15.302391
O	11.022259	25.057695	11.470536
O	11.567752	17.292044	13.167931
N	13.624448	21.460604	13.500650
N	11.997540	23.093580	12.235623
N	11.972927	19.268116	12.016501
C	14.351486	20.499904	14.090565
H	14.095743	19.480033	13.823789
C	15.363434	20.786605	14.986887
H	15.924976	19.984263	15.450044
C	15.626880	22.126083	15.269833
H	16.412490	22.396831	15.967825
C	14.876235	23.113135	14.651087
H	15.071706	24.158738	14.857018
C	13.863033	22.752097	13.757791
C	13.018758	23.799170	13.030203
C	13.956902	24.612679	12.114313
H	14.455558	23.948870	11.400143
H	14.726726	25.128650	12.695711
H	13.372853	25.356560	11.570077
C	12.353462	24.700432	14.090528

H	11.747169	25.461444	13.599650
H	13.105549	25.202371	14.705357
H	11.714638	24.098715	14.743220
C	11.096184	23.834950	11.586788
C	9.962536	23.049868	10.866563
C	12.454552	18.576169	10.807621
H	11.102844	16.887595	10.966974
C	13.745684	17.786548	11.108070
H	14.527648	18.464399	11.466396
H	13.539230	17.035849	11.872529
C	11.547347	18.515020	13.033752
C	10.927606	19.284350	14.235441

Complex 1, Transition State for -CF_3 Rotation - ωB97X-D/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
F	10.043196	23.181120	9.607384
N	12.656449	20.941638	10.126077
C	12.939968	21.915353	9.248012
H	12.797994	22.930903	9.601861
C	13.385330	21.647463	7.967583
H	13.596723	22.459719	7.282613
C	13.548474	20.313137	7.597695
H	13.898643	20.056605	6.603072
C	13.258919	19.312959	8.512081
H	13.384361	18.271715	8.240409
C	12.802316	19.655318	9.788918
C	11.440266	17.628434	10.239375
H	11.824829	17.152695	9.333296
H	10.528943	18.177071	9.985189
H	14.203449	17.350192	10.302795
F	8.760500	23.608545	11.301126
Cu	12.175009	21.185282	12.099287
F	9.882670	21.763942	11.238315
F	9.594941	19.897088	13.572455
F	10.198332	18.431887	15.045710
F	11.391330	20.207303	14.744384
O	11.053855	25.075180	11.508775

O	11.541098	17.276512	13.152622
N	13.629412	21.444352	13.488341
N	11.995723	23.096775	12.278996
N	11.933706	19.271133	12.033212
C	14.337660	20.466475	14.072637
H	14.040456	19.453479	13.822601
C	15.376820	20.731318	14.943718
H	15.925914	19.917161	15.401269
C	15.684469	22.065388	15.210394
H	16.493221	22.318401	15.888308
C	14.945472	23.068796	14.604905
H	15.170577	24.110024	14.802528
C	13.903412	22.729280	13.736189
C	13.060723	23.788873	13.027558
C	13.987644	24.567176	12.070394
H	14.443870	23.882751	11.347450
H	14.790465	25.066640	12.620817
H	13.406804	25.321959	11.538025
C	12.454585	24.719146	14.097725
H	11.846593	25.485608	13.617624
H	13.239273	25.214518	14.676093
H	11.828066	24.141252	14.783015
C	11.100014	23.852553	11.637383
C	9.936169	23.087163	10.947702
C	12.482521	18.593377	10.842311
H	11.197878	16.846899	10.958755
C	13.793783	17.854631	11.183103
H	14.544131	18.563627	11.548593
H	13.595262	17.107066	11.952818
C	11.465013	18.495873	13.020027
C	10.652476	19.260607	14.111310

Complex $[1]^+$ - ωB97X-D/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
F	10.253426	22.716523	9.559122
N	12.862138	20.919845	10.093140
C	13.125319	21.903631	9.217441

H	13.241992	22.897966	9.634548
C	13.223936	21.669019	7.857521
H	13.430197	22.489093	7.180904
C	13.036880	20.370121	7.396416
H	13.096965	20.147248	6.336676
C	12.773002	19.353972	8.308011
H	12.633532	18.335793	7.963685
C	12.694865	19.661421	9.661216
C	11.128778	17.826621	10.437230
H	11.190858	17.328760	9.468131
H	10.280450	18.513090	10.424145
H	13.736403	17.149685	9.740271
F	8.999458	23.219479	11.252226
Cu	12.718928	21.212441	12.068880
F	10.243600	21.453457	11.321044
F	9.703961	18.978868	13.023655
F	10.468597	18.275945	14.928541
F	10.920884	20.290412	14.258655
O	11.219085	24.845038	11.220616
O	12.687026	17.613732	13.615512
N	13.827684	21.557714	13.668679
N	12.223532	23.034137	12.261235
N	12.389468	19.237053	12.017694
C	14.511613	20.647996	14.388103
H	14.391297	19.608569	14.101428
C	15.333379	21.007248	15.436441
H	15.864679	20.247482	15.996400
C	15.455525	22.363442	15.740118
H	16.094156	22.688315	16.554520
C	14.753781	23.295282	14.992068
H	14.843126	24.351727	15.212902
C	13.927911	22.869023	13.950540
C	13.154411	23.845086	13.066660
C	14.167766	24.587055	12.171403
H	14.737632	23.875399	11.563671
H	14.876997	25.160810	12.774201
H	13.632199	25.275817	11.515600
C	12.375454	24.829164	13.959689
H	11.807624	25.522506	13.340204
H	13.057111	25.416643	14.578782

H	11.687094	24.286929	14.613382
C	11.314999	23.656724	11.487704
C	10.190286	22.752815	10.899794
C	12.445495	18.579674	10.713328
H	10.961214	17.053553	11.191892
C	13.649671	17.595155	10.733658
H	14.578187	18.121727	10.964908
H	13.492879	16.801511	11.463570
C	12.019732	18.502743	13.163356
C	10.734529	19.018909	13.873316

Complex $[1]^-$ - ωB97X-D/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
F	9.929721	23.216893	9.747769
N	12.701246	20.933313	9.996386
C	12.733058	21.904681	9.081847
H	12.790165	22.919670	9.466732
C	12.674917	21.654172	7.716662
H	12.691350	22.476232	7.009797
C	12.574101	20.330839	7.303790
H	12.514580	20.083742	6.247493
C	12.538854	19.320152	8.259175
H	12.452073	18.285753	7.950773
C	12.602411	19.652646	9.613989
C	12.063978	17.270183	10.274605
H	12.675008	16.821246	9.483564
H	11.043199	17.406405	9.903236
H	14.717623	18.111722	10.233526
F	8.988551	24.315478	11.364561
Cu	12.200284	21.182992	12.065976
F	9.563550	22.256042	11.650215
F	10.176839	20.069936	13.775009
F	9.859978	18.002358	14.303102
F	11.481490	19.119353	15.213975
O	11.621850	25.062391	11.026321
O	12.307789	17.299846	13.239073
N	13.688623	21.450376	13.585842

N	11.984192	23.205781	12.409373
N	11.874357	19.154552	11.873869
C	14.202577	20.483411	14.348598
H	14.070144	19.467882	13.984088
C	14.850948	20.738550	15.550387
H	15.242370	19.919894	16.143905
C	14.954969	22.061701	15.962997
H	15.443487	22.312142	16.900547
C	14.416200	23.067723	15.167301
H	14.483524	24.101603	15.482164
C	13.778918	22.730767	13.971229
C	13.217796	23.766028	12.984363
C	14.312154	23.959986	11.906468
H	14.505942	23.006829	11.403868
H	15.246453	24.309734	12.361870
H	13.968333	24.693790	11.174374
C	12.934144	25.100056	13.694649
H	12.472959	25.786019	12.983271
H	13.856210	25.563538	14.062922
H	12.251033	24.946570	14.536223
C	11.335675	23.961899	11.542073
C	9.956215	23.408578	11.090172
C	12.647266	18.613166	10.744409
H	12.045744	16.579905	11.118655
C	14.143298	18.445423	11.106126
H	14.549480	19.404528	11.443496
H	14.238341	17.708634	11.906567
C	11.777835	18.392335	12.948186
C	10.817909	18.924923	14.047263

Complex 2 - ωB97X-D/6-31+G(d,p)

Atom	**x (Å)**	**y (Å)**	**z (Å)**
N	12.598215	20.959843	10.118090
C	12.754002	21.937440	9.213340
H	12.633790	22.952647	9.575989
C	13.049688	21.677891	7.888096
H	13.160426	22.495131	7.185646

C	13.192577	20.347877	7.498666
H	13.424746	20.096937	6.468707
C	13.034152	19.342646	8.440048
H	13.148429	18.305107	8.152295
C	12.727465	19.677021	9.762594
C	11.754816	17.447321	10.341288
H	12.236410	16.952706	9.494000
H	10.772219	17.808485	10.024764
H	14.533152	17.759365	10.292111
Cu	12.088536	21.181134	12.098160
O	11.443072	25.080054	11.128393
O	12.103963	17.273798	13.238638
N	13.538247	21.423475	13.537292
N	11.966710	23.117004	12.229572
N	11.953298	19.242508	12.037736
C	14.153705	20.454165	14.230190
H	13.884384	19.434813	13.975261
C	15.080864	20.726782	15.218699
H	15.551257	19.915814	15.761509
C	15.377254	22.061468	15.486603
H	16.098879	22.322562	16.253934
C	14.740064	23.058222	14.763905
H	14.965499	24.099338	14.957875
C	13.806332	22.710561	13.782969
C	13.120189	23.758377	12.905165
C	14.183994	24.231675	11.888786
H	14.530613	23.385437	11.286073
H	15.049167	24.655997	12.407529
H	13.756163	24.991660	11.234349
C	12.634733	24.920225	13.792159
H	12.107433	25.654731	13.184626
H	13.474064	25.429190	14.272715
H	11.961081	24.544863	14.567676
C	11.221266	23.919388	11.463799
C	9.803755	23.392997	10.994313
C	12.607197	18.620052	10.861508
H	11.626981	16.704401	11.127582
C	14.049701	18.168816	11.184458
H	14.642008	19.022734	11.530204
H	14.031533	17.402586	11.959959

C	11.720494	18.428767	13.072054
C	10.732518	18.929133	14.203654
Cl	9.163345	18.139206	13.858863
Cl	11.345151	18.393312	15.789058
Cl	10.449281	20.694370	14.301806
Cl	9.539363	21.623316	11.062440
Cl	8.614480	24.168336	12.084771
Cl	9.517091	23.916026	9.314821

Reference Complex LCuOH - ωB97X-D/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
Cu	8.186675	14.461531	11.530961
O	9.347141	14.803750	10.233534
H	8.870870	15.108236	9.449154
N	7.054878	14.097932	12.942009
O	4.294847	14.945126	10.973650
C	5.751659	14.261664	12.742124
C	4.868665	14.004747	13.777987
H	3.805438	14.138445	13.616015
C	5.400937	13.582079	14.999532
H	4.733681	13.373622	15.829366
C	6.779030	13.423854	15.168005
H	7.222853	13.096168	16.100885
C	7.599140	13.698790	14.085449
C	5.441772	14.736420	11.340704
N	6.589647	14.889324	10.627791
C	6.549253	15.362667	9.289777
C	6.478728	16.749992	9.052924
C	6.481745	17.186922	7.729095
C	6.561175	16.281857	6.675845
C	6.644722	14.918686	6.929232
H	6.710982	14.224904	6.097492
C	6.645501	14.432121	8.237489
H	5.988555	17.235360	11.061307
H	8.489558	17.229210	10.852738
C	6.704713	12.940784	8.519797
H	7.086607	12.814462	9.537777

C	5.290532	12.341197	8.481899
H	4.619287	12.866814	9.167243
H	5.315549	11.281283	8.757270
H	4.868442	12.421016	7.473782
C	7.659648	12.185053	7.591560
H	7.760785	11.148796	7.928956
H	8.655320	12.638953	7.592649
H	7.293582	12.156960	6.559737
N	9.525837	13.938423	12.748547
O	9.777876	13.227341	14.945938
C	9.105023	13.593302	13.994314
C	10.889754	13.849533	12.387251
C	11.685450	15.006179	12.429972
C	13.029946	14.892479	12.076488
H	13.670492	15.768855	12.113700
C	13.559580	13.674985	11.670139
H	14.607949	13.604038	11.396293
C	12.747886	12.546570	11.601672
H	13.173362	11.606243	11.266034
C	11.401615	12.611185	11.951363
C	11.115805	16.347640	12.851155
H	10.033298	16.229110	12.955291
C	11.350640	17.421070	11.781643
H	10.970700	17.082640	10.813660
H	12.415265	17.654883	11.672290
C	11.664518	16.774104	14.219601
H	11.461428	16.010928	14.976758
H	11.205505	17.715675	14.540388
H	12.748837	16.926398	14.176508
C	10.495454	11.401224	11.802342
H	9.635102	11.547523	12.461531
C	9.966092	11.323705	10.360766
H	9.513309	12.272150	10.056501
H	9.223881	10.523232	10.262340
H	10.785739	11.115719	9.663640
C	11.157892	10.086128	12.223109
H	11.569620	10.157659	13.233943
H	11.966416	9.799128	11.542276
H	10.420952	9.276481	12.207840
C	6.455409	17.736759	10.209058

H	6.423548	18.248391	7.512511
H	10.834598	18.347877	12.055066
C	5.621734	18.989369	9.923687
C	7.889866	18.112776	10.614274
H	4.617208	18.727303	9.579245
H	6.089553	19.630402	9.168676
H	5.526310	19.585436	10.836672
H	8.394696	18.638297	9.795808
H	7.883825	18.772451	11.488783
H	6.562468	16.643064	5.652016

Reference Complex [LCuOH]$^-$ - ωB97X-D/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
Cu	8.324907	14.553707	11.389185
O	9.491290	14.924535	10.006592
H	9.016351	15.232550	9.228429
N	7.123708	14.187308	12.893575
O	4.247197	15.057728	11.064054
C	5.819954	14.379263	12.723421
C	4.937611	14.134706	13.768035
H	3.876987	14.294974	13.612964
C	5.468308	13.686613	14.979389
H	4.804726	13.486518	15.815872
C	6.842239	13.488656	15.124204
H	7.293442	13.135879	16.044340
C	7.657199	13.755090	14.030361
C	5.440878	14.855495	11.332026
N	6.522784	14.991743	10.557049
C	6.377732	15.413066	9.216184
C	6.211607	16.779624	8.915890
C	6.141550	17.166138	7.577352
C	6.245684	16.231127	6.552658
C	6.432434	14.888872	6.860736
H	6.527820	14.166112	6.055809
C	6.505594	14.459303	8.187027
H	5.761565	17.319379	10.915422
H	8.254912	17.352705	10.610849

C	6.683457	12.991547	8.535833
H	7.204051	12.956021	9.497727
C	5.314319	12.321876	8.727355
H	4.709291	12.866408	9.458142
H	5.434700	11.287244	9.070297
H	4.761492	12.306641	7.779769
C	7.547150	12.219620	7.536247
H	7.740739	11.211013	7.916639
H	8.512302	12.714048	7.389529
H	7.056463	12.112264	6.561262
N	9.651586	13.903161	12.775181
O	9.756514	13.169453	14.989150
C	9.166107	13.579236	13.979629
C	11.040503	13.753573	12.543630
C	11.910466	14.829415	12.792249
C	13.266772	14.676537	12.503062
H	13.949647	15.503089	12.681839
C	13.758379	13.487971	11.975766
H	14.817357	13.384907	11.753909
C	12.885010	12.436457	11.720880
H	13.271016	11.515997	11.290715
C	11.522407	12.550169	11.996809
C	11.365411	16.160186	13.279564
H	10.374352	15.969180	13.699303
C	11.185930	17.111293	12.085818
H	10.603132	16.627766	11.293744
H	12.162951	17.382715	11.665686
C	12.212002	16.794573	14.387573
H	12.350118	16.099315	15.221586
H	11.718216	17.696773	14.766967
H	13.202070	17.095088	14.024272
C	10.558656	11.432261	11.637390
H	9.644334	11.598146	12.213396
C	10.188329	11.522083	10.148229
H	9.851563	12.532841	9.891482
H	9.397058	10.802939	9.900961
H	11.061998	11.294660	9.524137
C	11.077624	10.038350	12.004075
H	11.361986	9.990561	13.059977
H	11.948927	9.754678	11.401796

H	10.299286	9.288492	11.820950
C	6.192906	17.805393	10.036990
H	6.011112	18.214665	7.326190
H	10.679949	18.034243	12.396287
C	5.324375	19.030649	9.738068
C	7.630552	18.222462	10.385829
H	4.313655	18.734639	9.440165
H	5.750752	19.653120	8.942323
H	5.248819	19.658492	10.632730
H	8.090681	18.749146	9.540872
H	7.642187	18.892277	11.253912
H	6.191211	16.550656	5.515507

Complex 1 - ωB97X-D/DEF2SVP

Atom	x (Å)	y (Å)	z (Å)
F	10.324733	23.021842	9.483871
N	12.752345	20.889675	10.109367
C	13.123210	21.847913	9.252323
H	13.033701	22.874762	9.613840
C	13.586438	21.557337	7.980801
H	13.877056	22.361003	7.303892
C	13.662744	20.215824	7.603363
H	14.019996	19.940162	6.608921
C	13.280788	19.231289	8.503137
H	13.335659	18.178739	8.224473
C	12.822469	19.598509	9.774782
C	11.200154	17.777727	10.213704
H	11.480142	17.273083	9.277675
H	10.372096	18.471216	10.005400
H	13.895473	17.077725	10.184464
F	8.804080	23.498470	10.930403
Cu	12.195692	21.182448	12.067776
F	9.955460	21.696562	11.146683
F	10.754350	20.635315	14.003219
F	9.908919	18.815299	14.772962
F	11.947477	19.326487	15.236631
O	10.883868	25.033941	11.577777

O	11.391136	17.311696	13.145567
N	13.674041	21.494224	13.464340
N	12.000299	23.106925	12.212454
N	11.986437	19.254375	12.034325
C	14.449130	20.546899	14.004841
H	14.204114	19.516694	13.736931
C	15.495358	20.852031	14.858094
H	16.106355	20.057014	15.286076
C	15.732240	22.196671	15.147568
H	16.545514	22.483568	15.817498
C	14.925197	23.169854	14.576279
H	15.097697	24.224684	14.791044
C	13.884215	22.788150	13.720244
C	12.964496	23.817656	13.060941
C	13.828979	24.771726	12.213796
H	14.395208	24.203058	11.460023
H	14.545870	25.328943	12.834373
H	13.174000	25.491350	11.706965
C	12.232987	24.574727	14.188522
H	11.559555	25.321400	13.751491
H	12.944460	25.088010	14.851511
H	11.642429	23.865910	14.787531
C	11.051083	23.822937	11.603196
C	10.018277	22.998573	10.786967
C	12.391743	18.556119	10.808432
H	10.861303	17.021744	10.931788
C	13.587515	17.624751	11.087515
H	14.448561	18.209565	11.446389
H	13.300337	16.895819	11.855498
C	11.498520	18.525308	13.041925
C	11.015802	19.336661	14.275244

Complex $[1]^+$ - ωB97X-D/DEF2SVP

Atom	**x (Å)**	**y (Å)**	**z (Å)**
F	10.256843	22.570320	9.585301
N	12.878428	20.904587	10.091337
C	13.131964	21.890711	9.220005

H	13.264175	22.890637	9.639048
C	13.207412	21.662097	7.855352
H	13.410275	22.488315	7.173955
C	13.003990	20.365060	7.391900
H	13.045549	20.144533	6.323660
C	12.747276	19.346347	8.304925
H	12.592140	18.324578	7.956468
C	12.694266	19.650182	9.663046
C	11.078233	17.882816	10.474449
H	11.077064	17.401153	9.488164
H	10.263822	18.617864	10.508883
H	13.623718	17.078728	9.676024
F	9.002251	23.071299	11.261551
Cu	12.723173	21.204851	12.092357
F	10.311121	21.365719	11.373655
F	11.076013	20.265604	14.270410
F	9.816863	18.921521	13.140316
F	10.670569	18.280093	15.015243
O	11.164484	24.772634	11.166118
O	12.811708	17.578750	13.606872
N	13.854406	21.601454	13.688283
N	12.210602	23.029479	12.264527
N	12.444060	19.197949	12.024245
C	14.539673	20.715095	14.428780
H	14.451233	19.661932	14.151225
C	15.332502	21.104199	15.492011
H	15.873186	20.358844	16.075441
C	15.417918	22.467392	15.781792
H	16.035453	22.818228	16.610863
C	14.710219	23.375817	15.007382
H	14.769308	24.442864	15.219988
C	13.915658	22.917050	13.952598
C	13.138896	23.862789	13.036416
C	14.149326	24.570532	12.112275
H	14.730479	23.831790	11.537582
H	14.856321	25.184677	12.688299
H	13.603428	25.222981	11.417736
C	12.361321	24.879407	13.891067
H	11.778437	25.540222	13.239641
H	13.044061	25.506162	14.480378

H	11.677265	24.359182	14.576662
C	11.289607	23.602821	11.468511
C	10.196813	22.643720	10.913567
C	12.441353	18.564805	10.713653
H	10.896775	17.100616	11.225638
C	13.595544	17.527581	10.677919
H	14.561550	18.012145	10.874321
H	13.436017	16.732003	11.414797
C	12.130231	18.462849	13.182380
C	10.876727	18.989383	13.935818

Complex $[1]^-$ - ωB97X-D/DEF2SVP

Atom	x (Å)	y (Å)	z (Å)
F	11.133072	22.953062	9.433705
N	13.164515	20.640357	10.056359
C	13.764353	21.460824	9.191907
H	13.949453	22.475678	9.556468
C	14.112584	21.071638	7.906910
H	14.601422	21.772300	7.227844
C	13.803291	19.767469	7.518157
H	14.048915	19.412816	6.513853
C	13.170273	18.924847	8.420940
H	12.911159	17.905821	8.130730
C	12.858564	19.391758	9.708683
C	10.725002	18.218238	10.148520
H	10.775678	17.715435	9.169267
H	10.189523	19.171532	10.031452
H	13.013576	16.638679	9.920518
F	9.219987	23.636112	10.129733
Cu	12.542509	21.183063	11.976597
F	10.001132	21.774267	10.847132
F	10.920827	20.549953	14.236179
F	10.679833	18.677754	15.250505
F	12.655279	19.423909	14.862687
O	10.563774	24.940590	11.897895
O	10.947148	17.391765	13.034914
N	14.051518	21.749410	13.306455

N	12.052007	23.175587	12.213893
N	12.026135	19.184301	12.008698
C	15.024403	20.944856	13.738259
H	15.010144	19.928688	13.332939
C	15.980803	21.350969	14.657177
H	16.761097	20.663005	14.987170
C	15.897054	22.655152	15.146865
H	16.620968	23.022761	15.878667
C	14.875554	23.481049	14.699363
H	14.787780	24.499669	15.079484
C	13.950439	22.997743	13.759214
C	12.786022	23.872238	13.264426
C	13.376781	25.195816	12.732029
H	14.076583	24.985739	11.908076
H	13.914987	25.755545	13.512816
H	12.554900	25.816562	12.354599
C	11.870980	24.124773	14.483634
H	11.025160	24.747213	14.164426
H	12.406990	24.633578	15.301059
H	11.491341	23.160997	14.852788
C	11.031560	23.816731	11.673210
C	10.341629	23.029076	10.522350
C	12.130646	18.496970	10.726284
H	10.175972	17.580233	10.852807
C	12.938923	17.189225	10.871300
H	13.957172	17.418906	11.222244
H	12.440370	16.551522	11.611448
C	11.440612	18.526243	12.993063
C	11.419308	19.309947	14.337134

Complex 2 - ωB97X-D/DEF2SVP

Atom	**x (Å)**	**y (Å)**	**z (Å)**
N	13.678312	20.324384	10.355815
C	14.657803	20.917599	9.657868
H	15.081045	21.825390	10.095531
C	15.099550	20.426688	8.443751
H	15.897059	20.933921	7.900383

C	14.481186	19.278691	7.941029
H	14.793380	18.856373	6.983673
C	13.458624	18.685188	8.662687
H	12.956963	17.797295	8.278621
C	13.059788	19.237010	9.889392
C	10.659399	18.587153	9.837032
H	10.802588	17.927577	8.968086
H	10.396868	19.590620	9.479656
H	12.580855	16.599874	10.200614
Cu	12.721829	21.186951	11.923106
O	10.009646	24.265795	12.609798
O	10.098956	18.054710	12.709360
N	14.330603	22.073820	12.782973
N	11.858645	22.908605	12.418890
N	11.756353	19.448788	11.930864
C	15.539828	21.501608	12.877443
H	15.693689	20.597030	12.283462
C	16.534164	22.009157	13.692275
H	17.506301	21.518817	13.747819
C	16.242194	23.151402	14.442613
H	16.994660	23.586292	15.103687
C	14.983846	23.722860	14.350180
H	14.735413	24.605793	14.938602
C	14.020895	23.154980	13.502524
C	12.613431	23.731570	13.379437
C	12.775730	25.168038	12.829554
H	13.247262	25.137664	11.835804
H	13.397447	25.782562	13.496469
H	11.791880	25.642812	12.742454
C	11.977911	23.759204	14.784230
H	10.952088	24.134847	14.697752
H	12.537416	24.422914	15.460300
H	11.953056	22.752063	15.218443
C	10.654657	23.381955	12.073602
C	9.988286	22.771625	10.770295
C	11.926371	18.634988	10.714817
H	9.831626	18.195354	10.439069
C	12.376039	17.204906	11.095582
H	13.289232	17.249914	11.707832
H	11.585387	16.710650	11.671237

C	10.909972	18.954213	12.843003
C	10.994266	19.559770	14.306600
Cl	10.545004	18.299558	15.474660
Cl	12.661937	20.094813	14.735905
Cl	9.864092	20.921374	14.470903
Cl	8.953579	21.392524	11.201177
Cl	8.986647	24.020270	10.001054
Cl	11.209991	22.259751	9.546828

Reference Complex LCuOH - ωB97X-D/DEF2SVP

Atom	x (Å)	y (Å)	z (Å)
Cu	8.192678	14.449444	11.516422
O	9.352776	14.779988	10.197369
H	8.858749	15.047030	9.409512
N	7.060367	14.106840	12.951629
O	4.289094	14.919825	10.985270
C	5.759714	14.271553	12.752767
C	4.879308	14.032677	13.798774
H	3.809209	14.167094	13.636103
C	5.418003	13.628644	15.025696
H	4.750763	13.434007	15.867963
C	6.798577	13.471545	15.189297
H	7.253247	13.159574	16.130382
C	7.613265	13.727020	14.094579
C	5.432164	14.728599	11.344393
N	6.574085	14.880407	10.619352
C	6.542936	15.333898	9.281455
C	6.525021	16.721781	9.022792
C	6.530764	17.142093	7.691794
C	6.567294	16.220374	6.649505
C	6.609646	14.856985	6.920693
H	6.649231	14.146439	6.093049
C	6.603078	14.387383	8.236257
H	6.142577	17.230498	11.048497
H	8.633010	17.152796	10.670009
C	6.622886	12.900330	8.544485
H	7.043332	12.788314	9.555459

C	5.190840	12.349736	8.579497
H	4.557711	12.924804	9.270712
H	5.185954	11.293742	8.892325
H	4.731306	12.410157	7.579837
C	7.516988	12.095643	7.601174
H	7.597507	11.056268	7.953478
H	8.532431	12.517119	7.557644
H	7.113962	12.060522	6.576845
N	9.541644	13.923735	12.749023
O	9.796054	13.303224	14.965826
C	9.123807	13.622852	14.008143
C	10.892258	13.870958	12.366069
C	11.662038	15.051188	12.400213
C	13.003505	14.974889	12.024318
H	13.626437	15.871221	12.054772
C	13.557846	13.770901	11.602703
H	14.609813	13.728884	11.311259
C	12.774259	12.622021	11.535239
H	13.219775	11.690519	11.180585
C	11.429908	12.649948	11.904807
C	11.049171	16.359967	12.861975
H	9.958332	16.252332	12.769738
C	11.450501	17.545351	11.983480
H	11.242059	17.330919	10.925013
H	12.519424	17.791812	12.082740
C	11.362929	16.604170	14.343525
H	11.042935	15.751548	14.960689
H	10.855868	17.511910	14.707564
H	12.446384	16.737594	14.494114
C	10.545541	11.425621	11.744894
H	9.686849	11.552211	12.419900
C	9.994805	11.370686	10.312109
H	9.532474	12.328811	10.032366
H	9.251432	10.564309	10.205836
H	10.808125	11.180538	9.593308
C	11.233099	10.117761	12.137808
H	11.646498	10.175783	13.155579
H	12.052879	9.859247	11.449340
H	10.512376	9.286188	12.106770
C	6.575639	17.721970	10.165708

H	6.513131	18.208878	7.461449
H	10.881811	18.442767	12.272282
C	5.751359	18.983975	9.910495
C	8.036602	18.060805	10.497209
H	4.715041	18.735124	9.638338
H	6.179392	19.602074	9.105758
H	5.727207	19.608252	10.816559
H	8.506479	18.604415	9.661770
H	8.099944	18.697207	11.393854
H	6.572254	16.569684	5.614690

Reference Complex [LCuOH]$^-$ - ωB97X-D/DEF2SVP

Atom	x (Å)	y (Å)	z (Å)
Cu	8.310344	14.550206	11.335892
O	9.449543	14.924836	9.921474
H	8.922603	15.075022	9.128950
N	7.111134	14.203345	12.875372
O	4.211017	14.873829	11.005561
C	5.804716	14.339734	12.694479
C	4.928943	14.109390	13.751033
H	3.857366	14.223090	13.583307
C	5.475707	13.739269	14.983257
H	4.815610	13.552364	15.834278
C	6.857947	13.603601	15.135972
H	7.330189	13.315203	16.075734
C	7.663060	13.848385	14.026747
C	5.401998	14.744320	11.282736
N	6.481533	14.904042	10.506210
C	6.340386	15.274772	9.156748
C	6.367006	16.639265	8.797450
C	6.285079	16.981978	7.445742
C	6.188037	16.004421	6.460399
C	6.194719	14.660602	6.821451
H	6.138466	13.895995	6.042714
C	6.279416	14.275022	8.161528
H	6.350356	17.239549	10.827305
H	8.703153	17.223285	9.995530

C	6.288138	12.810373	8.563468
H	6.765793	12.767770	9.553774
C	4.853657	12.289770	8.720447
H	4.279847	12.929310	9.407056
H	4.849288	11.257967	9.109250
H	4.335972	12.288409	7.746134
C	7.116223	11.928244	7.628702
H	7.189733	10.907623	8.036501
H	8.137610	12.322395	7.518757
H	6.666456	11.845853	6.625449
N	9.652874	13.989583	12.766069
O	9.782177	13.433470	15.023613
C	9.181831	13.734747	13.993048
C	11.036695	13.912945	12.519500
C	11.874504	15.002196	12.832079
C	13.241180	14.903977	12.560998
H	13.899874	15.740339	12.812116
C	13.776670	13.764799	11.969384
H	14.848021	13.704280	11.760400
C	12.935368	12.709809	11.629601
H	13.353313	11.825685	11.139970
C	11.565556	12.763829	11.894883
C	11.300376	16.264861	13.450703
H	10.207367	16.187699	13.360502
C	11.719494	17.525216	12.689560
H	11.462229	17.434443	11.623695
H	12.803350	17.712714	12.766780
C	11.636603	16.345202	14.943860
H	11.283295	15.439333	15.457745
H	11.161051	17.225005	15.409074
H	12.726088	16.429751	15.096848
C	10.649429	11.633746	11.455251
H	9.682889	11.800454	11.951602
C	10.401828	11.713883	9.943070
H	10.044634	12.722083	9.674968
H	9.655485	10.965540	9.626302
H	11.334011	11.519773	9.385298
C	11.151394	10.254432	11.887664
H	11.319513	10.217485	12.974947
H	12.097401	9.986020	11.388884

H	10.414351	9.477762	11.625977
C	6.579818	17.704906	9.858984
H	6.309342	18.035806	7.155735
H	11.203602	18.410481	13.096062
C	5.652232	18.910382	9.701239
C	8.059788	18.111789	9.891589
H	4.597902	18.595610	9.676144
H	5.862321	19.476006	8.778518
H	5.783720	19.606802	10.544881
H	8.341166	18.626688	8.957212
H	8.263466	18.796645	10.731320
H	6.123103	16.289966	5.407348

Complex 1 - M062X/6-31+G(d,p)

Atom	**x (Å)**	**y (Å)**	**z (Å)**
F	10.272627	23.079120	9.518063
N	12.719190	20.887308	10.084238
C	13.056072	21.845410	9.207321
H	12.961268	22.867593	9.563588
C	13.490081	21.554844	7.925900
H	13.747306	22.354381	7.241564
C	13.578371	20.212674	7.554303
H	13.913588	19.939034	6.558817
C	13.232948	19.227458	8.466833
H	13.296597	18.180036	8.194947
C	12.797369	19.594475	9.746298
C	11.262184	17.694663	10.198133
H	11.573736	17.209228	9.269176
H	10.401534	18.335608	9.985240
H	13.983843	17.152680	10.170165
F	8.796228	23.540682	11.027134
Cu	12.162847	21.181147	12.078768
F	9.969235	21.734261	11.187673
F	10.742889	20.590522	13.963077
F	9.865866	18.762190	14.706271
F	11.900774	19.268845	15.228388
O	10.948877	25.085165	11.545775

O	11.458652	17.257726	13.133226
N	13.658189	21.497010	13.505890
N	11.994009	23.127013	12.247822
N	11.966610	19.231671	12.008417
C	14.415399	20.550530	14.081444
H	14.169657	19.524617	13.820901
C	15.440292	20.856732	14.959299
H	16.027321	20.066124	15.411046
C	15.681740	22.202474	15.238403
H	16.475276	22.488126	15.921737
C	14.898648	23.175725	14.636591
H	15.073633	24.225760	14.841292
C	13.874997	22.793161	13.760683
C	12.989947	23.833671	13.069693
C	13.889981	24.721351	12.187908
H	14.418940	24.105897	11.452438
H	14.634202	25.249266	12.791245
H	13.271957	25.456617	11.669995
C	12.294561	24.667538	14.164328
H	11.664631	25.427585	13.701862
H	13.031194	25.164090	14.801849
H	11.675459	24.016507	14.788571
C	11.078339	23.865643	11.620330
C	10.015684	23.049071	10.837886
C	12.409162	18.540533	10.786417
H	10.969850	16.925234	10.912877
C	13.647124	17.668700	11.074018
H	14.469356	18.293509	11.438790
H	13.393409	16.923659	11.829836
C	11.513883	18.479050	13.011644
C	10.994172	19.280454	14.234721

Complex 2 – M062X/6-31+G(d,p)

Atom	x (Å)	y (Å)	z (Å)
N	12.862935	20.837452	10.227053
C	13.368829	21.771162	9.409111
H	13.292483	22.795572	9.763133

C	13.935136	21.454807	8.186567
H	14.332439	22.234832	7.547894
C	13.965007	20.111177	7.810545
H	14.392067	19.816532	6.857046
C	13.445613	19.150737	8.664925
H	13.463648	18.103513	8.386357
C	12.896070	19.545115	9.893012
C	11.129979	17.833169	10.162336
H	11.453020	17.363861	9.228689
H	10.364637	18.578538	9.924362
H	13.753553	16.975178	10.276459
Cu	11.996143	21.180465	12.122998
O	10.783896	25.158302	11.773195
O	11.194619	17.184612	13.020134
N	13.710035	21.548834	13.302870
N	11.862264	23.157250	12.210491
N	11.872605	19.200921	12.107426
C	14.582214	20.629099	13.739122
H	14.357069	19.602206	13.464622
C	15.686594	20.961513	14.504050
H	16.370581	20.192467	14.843019
C	15.875923	22.306380	14.825142
H	16.723400	22.613062	15.430196
C	14.973495	23.252535	14.364190
H	15.109545	24.300661	14.604105
C	13.882606	22.842530	13.584705
C	12.871186	23.857478	13.044648
C	13.656855	24.884952	12.203365
H	14.202855	24.374211	11.403472
H	14.383969	25.418650	12.821327
H	12.971377	25.612514	11.769973
C	12.200547	24.527588	14.262035
H	11.488839	25.281232	13.926380
H	12.948343	25.009237	14.898420
H	11.677875	23.772929	14.858064
C	10.922169	23.944064	11.681012
C	9.860826	23.264672	10.720456
C	12.320323	18.515233	10.868971
H	10.701959	17.068073	10.809372
C	13.439522	17.500580	11.182435

H	14.311872	18.020209	11.592008
H	13.082523	16.764600	11.902240
C	11.347590	18.400401	13.038519
C	10.928107	19.064739	14.414777
Cl	9.513166	18.232025	15.068686
Cl	12.309196	18.861844	15.533284
Cl	10.528142	20.814653	14.323104
Cl	9.601409	21.507311	10.993025
Cl	8.296554	24.065677	10.907708
Cl	10.452140	23.492359	9.047705

Complex 1 – M062X/DEF2SVP

Atom	x (Å)	y (Å)	z (Å)
F	10.545550	22.993862	9.445887
N	12.798149	20.843937	10.079702
C	13.204910	21.781778	9.215660
H	13.138125	22.814458	9.566292
C	13.670639	21.462903	7.950619
H	13.991404	22.248789	7.268175
C	13.708082	20.114865	7.588146
H	14.064284	19.818526	6.600256
C	13.288101	19.151293	8.494064
H	13.308599	18.094676	8.228833
C	12.832091	19.547547	9.759321
C	11.073901	17.870748	10.198754
H	11.294104	17.380311	9.239959
H	10.307410	18.641907	10.033537
H	13.680313	16.929390	10.098579
F	8.886899	23.460853	10.729568
Cu	12.237411	21.183006	12.056701
F	10.053651	21.691107	11.091127
F	10.879744	20.643190	14.008829
F	10.073723	18.857154	14.894577
F	12.150068	19.339630	15.163745
O	10.808694	25.029205	11.653112
O	11.287286	17.313831	13.117187
N	13.728211	21.542026	13.466598

N	12.031288	23.133715	12.193518
N	12.023492	19.228558	12.034813
C	14.537367	20.616052	13.995198
H	14.318154	19.580385	13.724663
C	15.581649	20.949871	14.841934
H	16.221120	20.173291	15.259368
C	15.777153	22.300397	15.138213
H	16.585613	22.608260	15.803218
C	14.934609	23.251645	14.580717
H	15.070344	24.309978	14.801428
C	13.899653	22.840620	13.728799
C	12.931077	23.848173	13.105693
C	13.740724	24.912517	12.343916
H	14.357415	24.434327	11.568203
H	14.403165	25.473797	13.017707
H	13.044258	25.615868	11.872283
C	12.134249	24.480897	14.264635
H	11.428690	25.217031	13.862823
H	12.806300	24.979592	14.977380
H	11.576203	23.695540	14.795024
C	11.055732	23.834948	11.611877
C	10.116966	22.989497	10.712253
C	12.340280	18.525690	10.786702
H	10.689233	17.123928	10.902568
C	13.446879	17.481701	11.019636
H	14.364818	17.976501	11.370786
H	13.105392	16.767930	11.778669
C	11.498231	18.512674	13.031421
C	11.138303	19.343991	14.290159

Complex 2 – M062X/DEF2SVP

Atom	**x (Å)**	**y (Å)**	**z (Å)**
N	12.883819	20.821356	10.237893
C	13.435404	21.748926	9.448795
H	13.348327	22.780623	9.798770
C	14.057574	21.421974	8.254508
H	14.497575	22.198819	7.630419

C	14.090937	20.075925	7.884219
H	14.562125	19.772278	6.947977
C	13.523170	19.122278	8.717250
H	13.543205	18.068142	8.443368
C	12.922506	19.527975	9.918948
C	11.055620	17.931057	10.141912
H	11.354685	17.457279	9.195940
H	10.342801	18.737660	9.915496
H	13.600687	16.875697	10.254346
Cu	12.011206	21.181198	12.117324
O	10.663279	25.106183	11.877983
O	11.054285	17.233811	13.003955
N	13.719371	21.564281	13.283727
N	11.862106	23.160701	12.197619
N	11.878081	19.198857	12.118070
C	14.614428	20.650095	13.671702
H	14.378736	19.615732	13.408970
C	15.755315	20.992900	14.379605
H	16.467093	20.226677	14.684340
C	15.949929	22.340664	14.689065
H	16.829292	22.656369	15.252811
C	15.018257	23.280523	14.271519
H	15.157172	24.335853	14.503068
C	13.893256	22.859279	13.546011
C	12.836352	23.856628	13.063351
C	13.558519	24.970112	12.280723
H	14.133951	24.536037	11.449449
H	14.253191	25.524122	12.926769
H	12.820616	25.675818	11.884628
C	12.149125	24.419819	14.324518
H	11.392592	25.156958	14.034029
H	12.883635	24.901473	14.985760
H	11.667921	23.600909	14.879307
C	10.877487	23.920007	11.710896
C	9.892820	23.220754	10.683206
C	12.282559	18.514886	10.872399
H	10.569626	17.183123	10.778006
C	13.325252	17.419783	11.168128
H	14.237224	17.869295	11.588587
H	12.908928	16.702323	11.883048

C	11.298983	18.425346	13.039668
C	10.965749	19.115667	14.427949
Cl	9.620006	18.288006	15.204013
Cl	12.421727	18.974196	15.451016
Cl	10.528755	20.856694	14.299789
Cl	9.615162	21.471130	11.001333
Cl	8.325512	24.020677	10.712043
Cl	10.617818	23.390833	9.060514

REFERENCES

(1) Stoll, S.; Schweiger, A. EasySpin, a Comprehensive Software Package for Spectral Simulation and Analysis in EPR. *J. Magn. Reson.* **2006**, *178* (1), 42–55. https://doi.org/10.1016/j.jmr.2005.08.013.

(2) Sheldrick, G. M. Crystal Structure Refinement with SHELXL. *Acta Crystallogr. Sect. C Struct. Chem.* **2015**, *71*, 3–8. https://doi.org/10.1107/S2053229614024218.

(3) Davis, H. J.; Genov, G. R.; Phipps, R. J. Meta-Selective C–H Borylation of Benzylamine-, Phenethylamine-, and Phenylpropylamine-Derived Amides Enabled by a Single Anionic Ligand. *Angew. Chem. Int. Ed.* **2017**, *56* (43), 13351–13355. https://doi.org/10.1002/anie.201708967.

(4) Schäfer, G.; Ahmetovic, M.; Abele, S. Scalable Synthesis of Trifluoromethylated Imidazo-Fused N-Heterocycles Using TFAA and Trifluoroacetamide as CF_3-Reagents. *Org. Lett.* **2017**, *19* (24), 6578–6581. https://doi.org/10.1021/acs.orglett.7b03291.

(5) Amini-Rentsch, L.; Vanoli, E.; Richard-Bildstein, S.; Marti, R.; Vilé, G. A Novel and Efficient Continuous-Flow Route to Prepare Trifluoromethylated N-Fused Heterocycles for Drug Discovery and Pharmaceutical Manufacturing. *Ind. Eng. Chem. Res.* **2019**, *58* (24), 10164–10171. https://doi.org/10.1021/acs.iecr.9b01906.

(6) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; et al. *Gaussian 16,* Revision C.01; Gaussian Inc: Wallingford, CT, 2016.

(7) Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti Correlation-Energy

Formula into a Functional of the Electron Density. *Phys. Rev. B* **1988**, *37* (2), 785–789. https://doi.org/10.1103/PhysRevB.37.785.

(8) Becke, A. D. Density-Functional Thermochemistry. III. The Role of Exact Exchange. *J. Chem. Phys.* **1993**, *98* (7), 5648–5652. https://doi.org/10.1063/1.464913.

(9) Hehre, W. J.; Ditchfield, R.; Pople, J. A. Self-Consistent Molecular Orbital Methods. XII. Further Extensions of Gaussian-Type Basis Sets for Use in Molecular Orbital Studies of Organic Molecules. *J. Chem. Phys.* **1972**, *56* (5), 2257–2261. https://doi.org/10.1063/1.1677527.

(10) Hariharan, P. C.; Pople, J. A. The Influence of Polarization Functions on Molecular Orbital Hydrogenation Energies. *Theor. Chim. Acta* **1973**, *28* (3), 213–222. https://doi.org/10.1007/BF00533485.

(11) Clark, T.; Chandrasekhar, J.; Spitznagel, G. W.; Schleyer, P. V. R. Efficient Diffuse Function-Augmented Basis Sets for Anion Calculations. III. The 3-21+G Basis Set for First-Row Elements, Li-F. *J. Comput. Chem.* **1983**, *4* (3), 294–301. https://doi.org/10.1002/jcc.540040303.

(12) Francl, M. M.; Pietro, W. J.; Hehre, W. J.; Binkley, J. S.; Gordon, M. S.; DeFrees, D. J.; Pople, J. A. Self-Consistent Molecular Orbital Methods. XXIII. A Polarization-Type Basis Set for Second-Row Elements. *J. Chem. Phys.* **1982**, *77* (7), 3654–3665. https://doi.org/10.1063/1.444267.

(13) Rassolov, V. A.; Pople, J. A.; Ratner, M. A.; Windus, T. L. 6-31G* Basis Set for Atoms K through Zn. *J. Chem. Phys.* **1998**, *109* (4), 1223–1229. https://doi.org/10.1063/1.476673.

(14) Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. Self-Consistent Molecular Orbital Methods. XX. A Basis Set for Correlated Wave Functions. *J. Chem. Phys.* **1980**, *72* (1), 650–654. https://doi.org/10.1063/1.438955.

(15) McLean, A. D.; Chandler, G. S. Contracted Gaussian Basis Sets for Molecular Calculations. I. Second Row Atoms, Z=11-18. *J. Chem. Phys.* **1980**, *72* (10), 5639–5648. https://doi.org/10.1063/1.438980.

(16) Wachters, A. J. H. Gaussian Basis Set for Molecular Wavefunctions Containing Third-Row Atoms. *J. Chem. Phys.* **1970**, *52* (3), 1033–1036. https://doi.org/10.1063/1.1673095.

(17) Hay, P. J. Gaussian Basis Sets for Molecular Calculations. The Representation of 3d Orbitals in Transition-Metal Atoms. *J. Chem. Phys.* **1977**, *66* (10), 4377–4384. https://doi.org/10.1063/1.433731.

(18) Raghavachari, K.; Trucks, G. W. Highly Correlated Systems. Excitation Energies of First Row Transition Metals Sc-Cu. *J. Chem. Phys.* **1989**, *91* (2), 1062–1065. https://doi.org/10.1063/1.457230.

(19) Frisch, M. J.; Pople, J. A.; Binkley, J. S. Self-Consistent Molecular Orbital Methods 25. Supplementary Functions for Gaussian Basis Sets. *J. Chem. Phys.* **1984**, *80* (7), 3265–3269. https://doi.org/10.1063/1.447079.

(20) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B* **2009**, *113* (18), 6378–6396. https://doi.org/10.1021/jp810292n.

(21) Glendening, E. D.; Reed, A. E.; Carpenter, J. E.; Weinhold, F. *NBO,* Version 3.1; University of Wisconsin: Madison, WI, 2016.

(22) Dennington, R.; Keith, T. A.; Millam, J. M. GaussView, Version 6; Semichem Inc.: Shawnee Mission, KS, 2016.

(23) Chai, J.-D.; Head-Gordon, M. Long-Range Corrected Hybrid Density Functionals with Damped Atom–Atom Dispersion Corrections. *Phys. Chem. Chem. Phys.* **2008**, *10* (44), 6615–6620. https://doi.org/10.1039/b810189b.

(24) Zhao, Y.; Truhlar, D. G. The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements: Two New Functionals and Systematic Testing of Four M06-Class Functionals and 12 Other Function. *Theor. Chem. Acc.* **2008**, *120*, 215–241. https://doi.org/10.1007/s00214-007-0310-x.

(25) Weigend, F. Accurate Coulomb-Fitting Basis Sets for H to Rn. *Phys. Chem. Chem. Phys.* **2006**, *8* (9), 1057–1065. https://doi.org/10.1039/b515623h.

(26) Weigend, F.; Ahlrichs, R. Balanced Basis Sets of Split Valence, Triple Zeta Valence and Quadruple Zeta Valence Quality for H to Rn: Design and Assessment of Accuracy. *Phys. Chem. Chem. Phys.* **2005**, *7* (18), 3297–3305. https://doi.org/10.1039/b508541a.

(27) Konezny, S. J.; Doherty, M. D.; Luca, O. R.; Crabtree, R. H.; Soloveichik, G. L.; Batista, V. S. Reduction of Systematic Uncertainty in DFT Redox Potentials of Transition-Metal Complexes. *J. Phys. Chem. C* **2012**, *116* (10), 6349–6356. https://doi.org/10.1021/jp300485t.

(28) Zerk, T. J.; Saouma, C. T.; Mayer, J. M.; Tolman, W. B. Low Reorganization Energy for Electron Self-Exchange by a Formally Copper(III,II) Redox Couple. *Inorg. Chem.* **2019**, *58* (20), 14151–14158. https://doi.org/10.1021/acs.inorgchem.9b02185.

(29) Grimme, S.; Ehrlich, S.; Goerigk, L. Effect of the Damping Function in Dispersion Corrected Density Functional Theory. *J. Comput. Chem.* **2011**, *32* (7), 1456–1465. https://doi.org/10.1002/jcc.21759.

(30) Dunning, T. H. Gaussian Basis Sets for Use in Correlated Molecular Calculations. I. The Atoms Boron through Neon and Hydrogen. *J. Chem. Phys.* **1989**, *90* (2), 1007–1023. https://doi.org/10.1063/1.456153.

(31) Kendall, R. A.; Dunning, T. H.; Harrison, R. J. Electron Affinities of the First-Row Atoms Revisited. Systematic Basis Sets and Wave Functions. *J. Chem. Phys.* **1992**, *96* (9), 6796–6806. https://doi.org/10.1063/1.462569.

(32) Woon, D. E.; Dunning, T. H. Gaussian Basis Sets for Use in Correlated Molecular Calculations. III. The Atoms Aluminum through Argon. *J. Chem. Phys.* **1993**, *98* (2), 1358–1371. https://doi.org/10.1063/1.464303.

(33) Neese, F. The ORCA Program System. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, *2* (1), 73–78. https://doi.org/10.1002/wcms.81.

(34) Neese, F. Software Update: The ORCA Program System, Version 4.0. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2018**, *8* (1), e1327. https://doi.org/10.1002/wcms.1327.

(35) Ames, W. M.; Larsen, S. C. DFT Calculations of the EPR Parameters for Cu(II) DETA

Imidazole Complexes. *Phys. Chem. Chem. Phys.* **2009**, *11* (37), 8266–8274. https://doi.org/10.1039/b905750a.

(36) Sciortino, G.; Lubinu, G.; Maréchal, J.-D.; Garribba, E. DFT Protocol for EPR Prediction of Paramagnetic Cu(II) Complexes and Application to Protein Binding Sites. *Magnetochemistry* **2018**, *4* (4), 55. https://doi.org/10.3390/magnetochemistry4040055.

(37) Flores, J. A.; Andino, J. G.; Lord, R. L.; Wolfe, R. J.; Park, H.; Pink, M.; Telser, J.; Caulton, K. G. Probing Redox Noninnocence of Copper and Zinc Bis-Pyridylpyrrolides. *Eur. J. Inorg. Chem.* **2018**, *2018* (45), 4893–4904. https://doi.org/10.1002/ejic.201800935.

(38) Spek, A. L. PLATON SQUEEZE: A Tool for the Calculation of the Disordered Solvent Contribution to the Calculated Structure Factors. *Acta Crystallogr. Sect. C Struct. Chem.* **2015**, *71*, 9–18. https://doi.org/10.1107/S2053229614024929.