Electronic Supplementary Material (ESI) for ChemComm.

Probing Cu^{I} in Homogeneous Catalysis using High-Energy-Resolution Fluorescence-Detected X-ray Absorption Spectroscopy

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Supporting Information

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Experimental Methods

General Considerations:
Tetrahydrofuran (THF), benzene, dichloromethane, acetonitrile, n-pentane, and diethyl ether were dried via the method of Grubbs,[1] using a custom-built solvent purification system. 2,2′-bipyridine and 4,4′-dimethoxy-2,2′-bipyridine were purchased from Sigma Aldrich and used as received. Deuterated NMR solvents were purchased from Cambridge Isotope Laboratories or Sigma-Aldrich and were used as received. 2-(2-pyridyl)-1,8-naphthyridine was prepared according using a literature procedure.[2] Where required, compounds were maintained under inert N_2 atmosphere using an Mbraun glovebox or standard Schlenk techniques. The following model compounds were prepared using literature procedures: (N,N′-bis-2,6-diisopropylphenyl-2,4-dimethyl-1,5-diketamide)Cu($NCCH_3$) (**1**),[3] [(tris-(2-dimethylaminoethyl)-amine)Cu](BPh_4) (**2**),[4] [$(CH_3CN)_4$Cu](PF_6) (**3**),[5] [(2,2′- bipyridine)$_2$Cu](PF_6) **(4)**,[6] [(N,N,N′,N′-tetramethylethylenediamine)Cu(OH)]$_2$ (**7**),[7] [(tris-(2-dimethylaminoethyl)-amine)CuO]$_2$(BPh_4)$_2$ (**8**),[4] and (N,N′-bis-2,6-diisopropylphenyl-2,4-dimethyl-1,5-diketamide)Cu(O_2) (**9**).[3] ^{1}H NMR spectra were measured at room temperature using a Varian 400 MHz instrument. Chemical shifts are reported in ppm relative to $SiMe_4$ and were referenced internally with respect to the protio solvent impurity (δ = 2.50 for DMSO, 5.32 for CH_2Cl_2). NMR coupling constants are given in Hz. UV-visible spectra were recorded in dry, degassed acetonitrile at room temperature using an Agilent Technologies Cary 60 spectrophotometer. High-resolution mass spectra were measured using a Bruker Solarix XR 74 ESI/MALDI-FT-ICR-MS using MALDI ionization with a dithranol matrix.

Syntheses:

[(4,4′-dimethoxy-2,2′-bipyridine)$_2$Cu](PF_6) (**5**): To a 20 mL scintillation vial charged with a stir bar and 5 mL THF was added solid **3** (98.3 mg, 264 mmol). With stirring, two equivalents of 4,4′-dimethoxy-2,2′-bipyridine (118 mg, 547 mmol) were added as a solid, immediately forming an orange precipitate. The solution was allowed to stir for 10 minutes before collecting the precipitate on a fritted glass funnel. The orange solid (162 mg, 96%) was washed with THF and pentane, then dried under vacuum. ^{1}H NMR (400 MHz, DMSO-d_6): δ 7.63 (m, 2H), 6.56 (s, 1H), 1.83 (s, 3H). HR-MS: calculated *m/z*: 495.108804; experimental *m/z*: 495.108343. UV/visible cm^{-1}, ($M^{-1}cm^{-1}$): 18,600 (2,700); 23,800 (9,560).

[(2-(2-pyridyl)-1,8-naphthyridine)$_2$Cu)](PF_6) (**6**): To a 20 mL scintillation vial charged with a stir bar and 5 mL THF was added solid **3** (112 mg, 301 mmol). With stirring, two equivalents of (2-(2-pyridyl)-1,8-naphthyridine (126 mg, 607 mmol) were added as a solid, immediately forming a purple precipitate. The solution was allowed to stir for 10 minutes before collecting the precipitate on a fritted glass funnel. The purple solid (176 mg, 94%) was washed with THF and pentane, then dried under vacuum. ^{1}H NMR (400 MHz, CD_2Cl_2): δ 8.65 (d, 1H, J = 8.60), 8.58 (s, 1H), 8.50 (m, 3H, ^3J = 8.60, ^4J = 11.60), 8.35 (d, 1H, J = 7.89), 8.14 (t, 1H, J = 7.59); 7.58 (m, 1H, J = 6.23); 7.46 (d/d, 1H, ^3J = 4.09, ^4J = 7.89). HR-MS: calculated *m/z*: 477.088344; experimental *m/z*: 477.088203. UV/visible cm^{-1}, ($M^{-1}cm^{-1}$): 14,800 (1500); 18,800 (3,700); 24,700 (8,970).

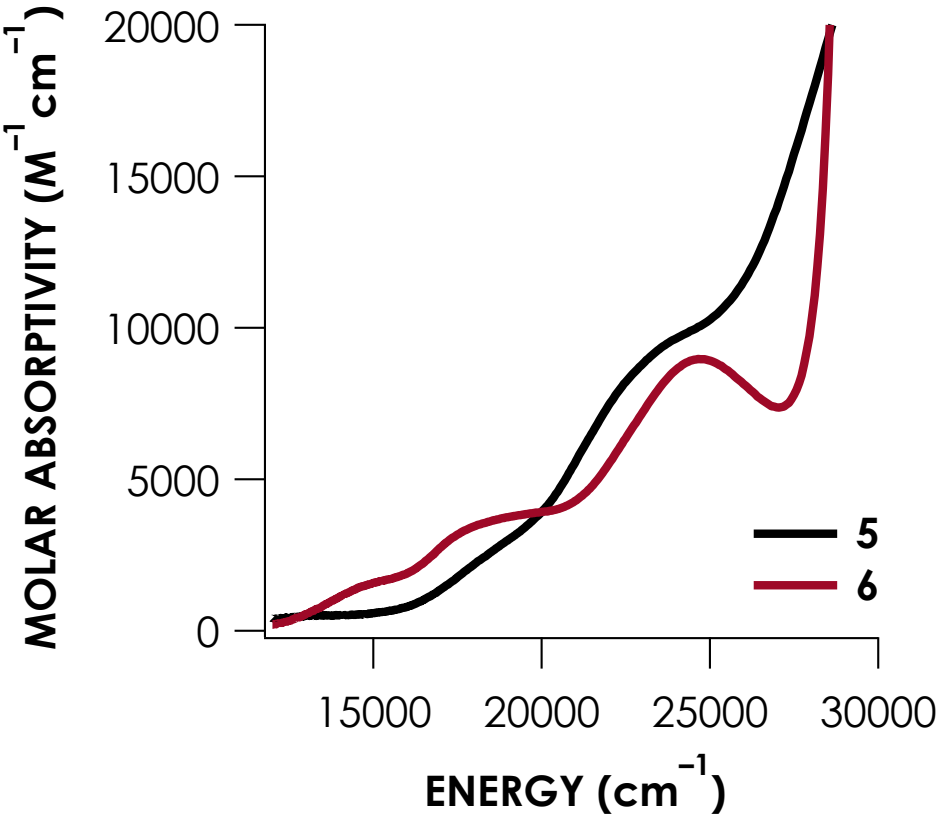

Figure S1. Electronic absorption spectra of **5** and **6** in acetonitrile.

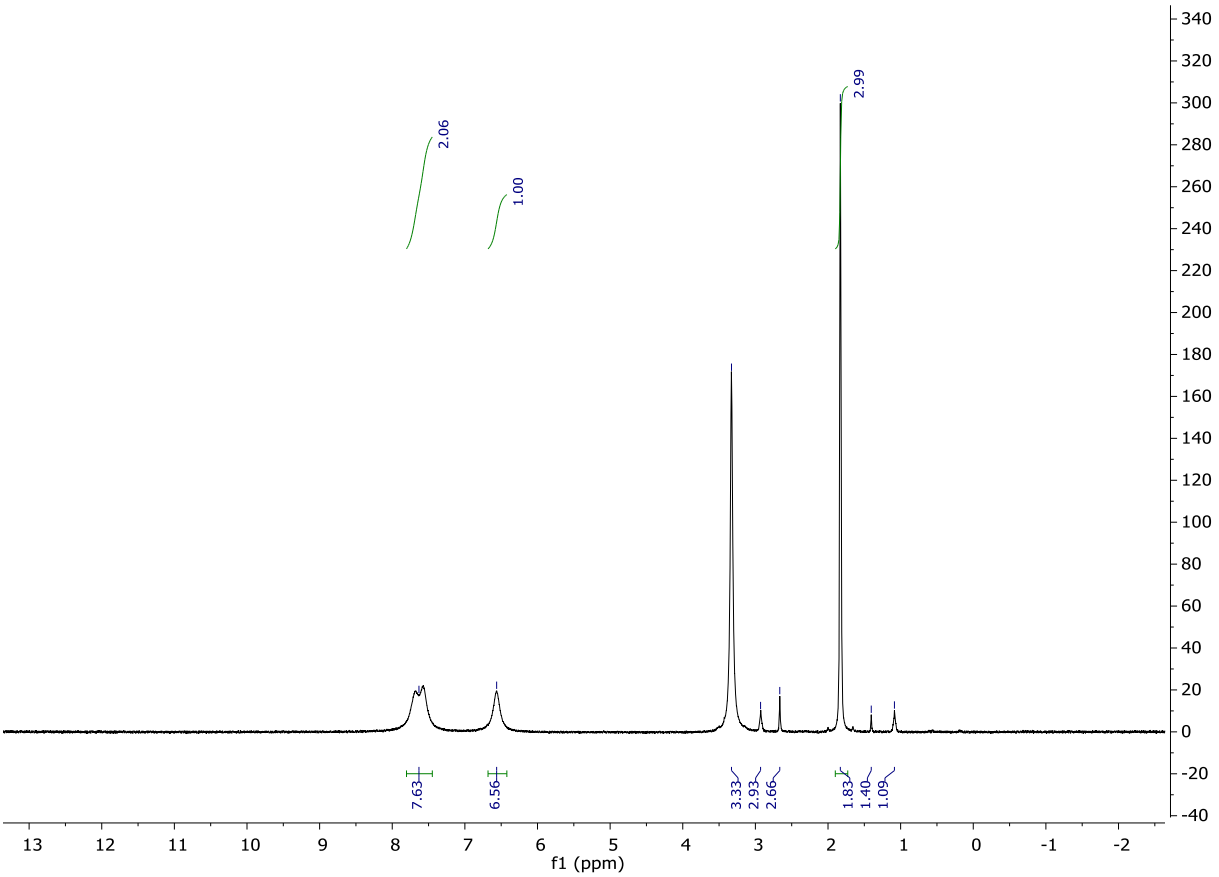

Figure S2. ^{1}H NMR spectrum of **5** in DMSO-d_6. Peaks at 2.93 and 2.66 ppm correspond to THF. Peaks at 1.40 and 1.09 ppm correspond to pentane. The peak at 3.33 ppm corresponds to H_2O.

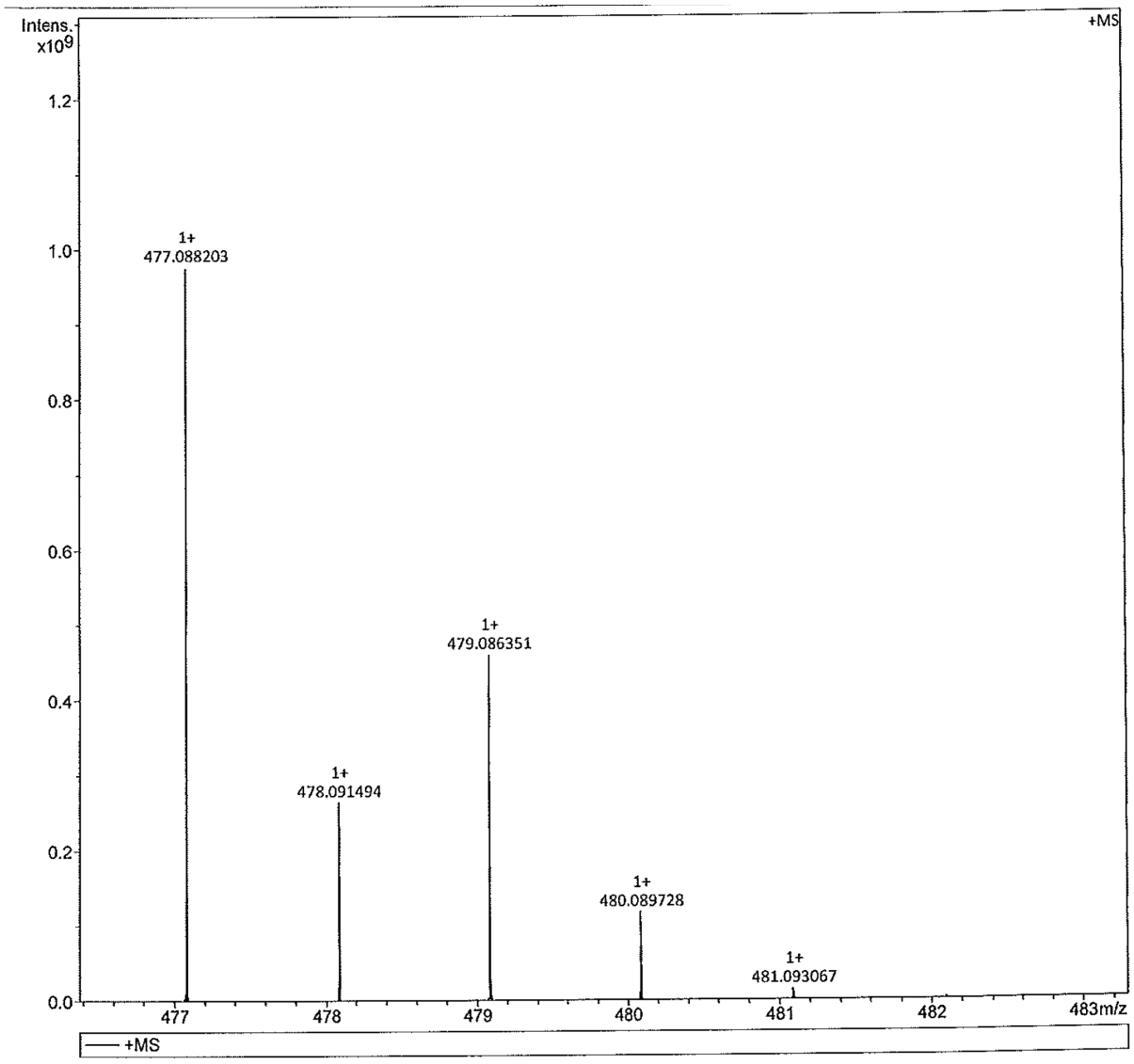

Figure S3. MALDI–MS spectrum of **5** prepared in a dithranol matrix.

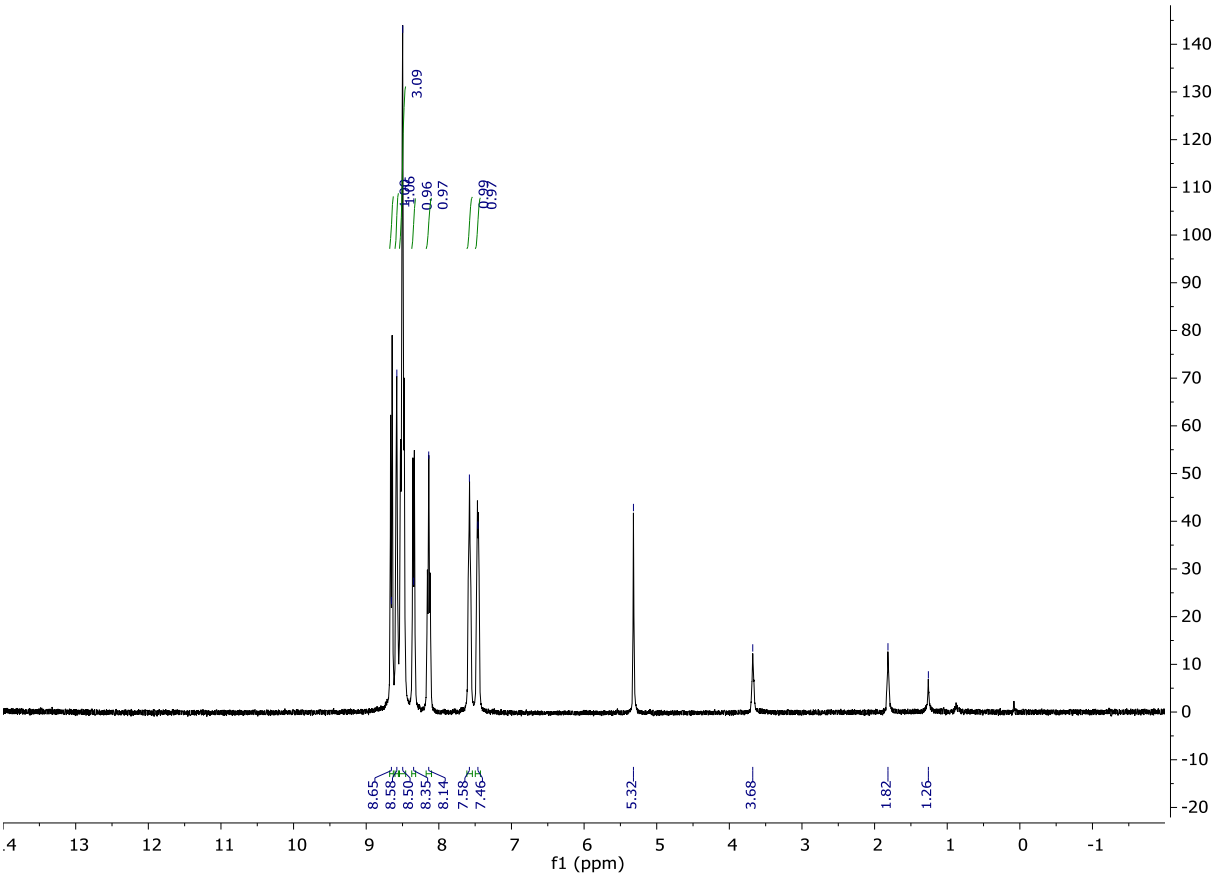

Figure S4. ^{1}H NMR spectrum of **6** in CD_2Cl_2. The peaks at 3.68 and 1.82 ppm correspond to THF. The peaks at 1.26 and 0.88 ppm correspond to pentane. The peak at 5.32 ppm is the solvent residual peak arising from CH_2Cl_2.

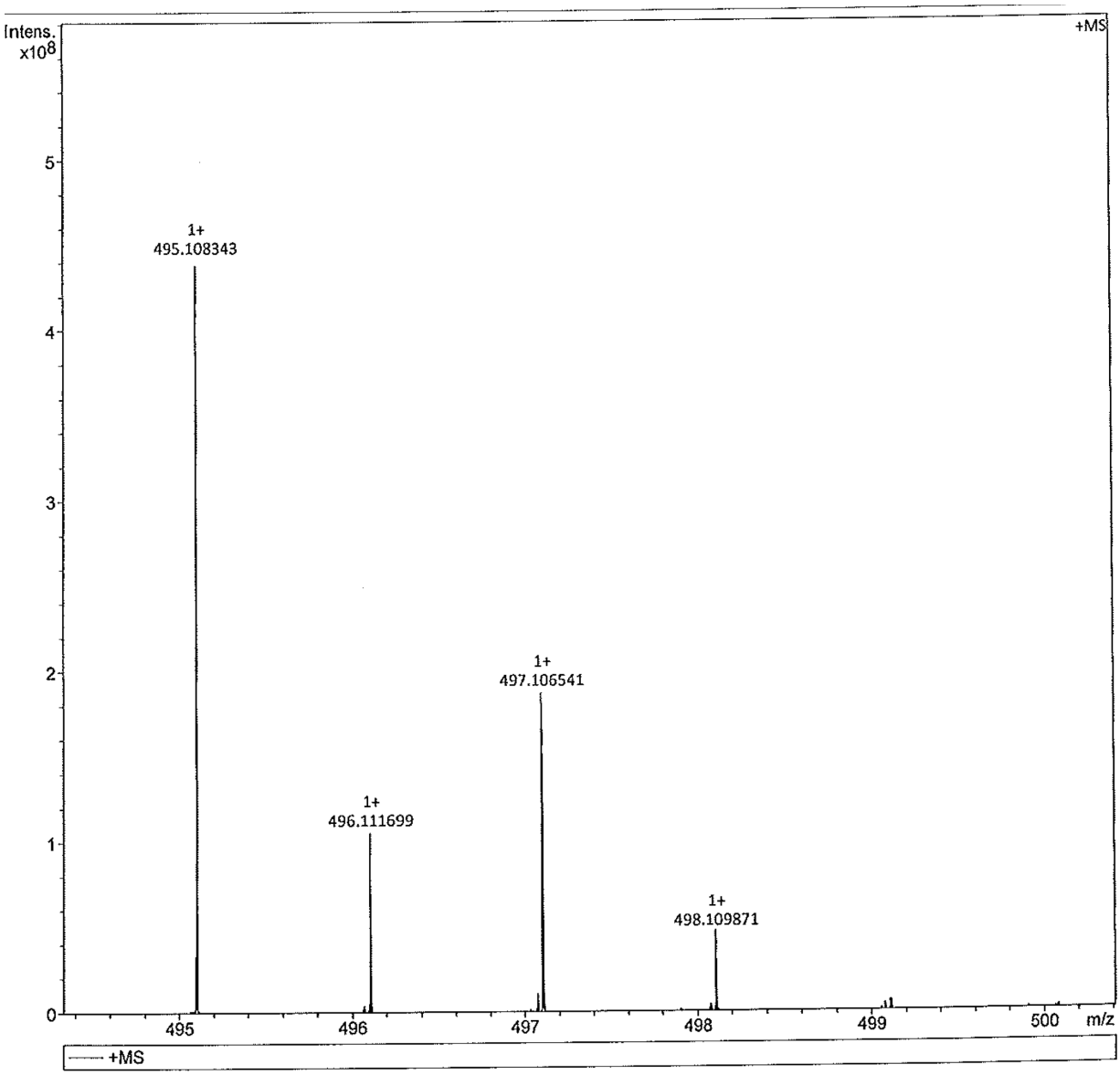

Figure S5. MALDI-MS spectrum of **6** prepared in a dithranol matrix.

X-ray Sample Preparation:
Samples were prepared as ~10 mM solutions in MiteGen MicroRT tubes and kept frozen in liquid N_2 until data collection. During data collection the samples were kept at a temperature of ~170 K using a stream of cold N_2 gas. Temperature was monitored with a diode at the base of the sample holder.

For the Cu/TEMPO catalytic cycle, the procedure outlined by Stahl *et al.* was followed.[8] To a solution of benzyl alcohol (20 eq.) in acetonitrile in a test tube with a stir bar was added 2,2′-bipyridine (1 eq.), **3** (1 eq.), and TEMPO (1 eq.) as solids under ambient conditions. Once all components had dissolved, a 100 μL sample was collected and placed in a MiteGen MicroRT tube, then frozen in liquid nitrogen. N-methylimidazole (2 eq.) was then added, and ten minutes later another sample collected and frozen in liquid N_2. After 6 hours of stirring, the solution turned from dark red to green signifying depletion of the benzyl alcohol substrate. A final sample was collected and frozen in liquid N_2.

X-ray Spectroscopy:
High energy resolution fluorescence detected X-ray absorption spectra (HERFD-XAS) were collected at the C1 beamline of the Cornell High Energy Synchrotron Source (CHESS) under ring conditions of 5 GeV and 200 mA. Incident X-rays were monochromated using a double Si(111) crystal monochromator. Incident energy was calibrated using Cu foil downstream of the samples as an internal standard. The first inflection point of the Cu foil scan was set to 8980.3 eV. X-ray emission was monochromated using a set of five spherically bent Si crystals (444 reflection) maintained in a Rowland circle geometry with a Pilatus Area Detector.[9] He filled plastic bags were positioned in the beam flight path to minimize X-ray fluorescence attenuation. HERFD-XAS was collected with the X-ray emission detector positioned at the $K\alpha_1$ maximum. Data were collected from 8850 to 9200 eV. A step size of 5 eV was used from 8850 to 8965 eV and from 9010 to 9200 eV. Higher point density data (0.15 eV) were collected from 8965 to 9010 eV.

Experimental spectra were averaged and normalized using PyMCA. For normalization, the post-edge region (E > 9000 eV) was set to an absorbance of 1.0. Peaks were fit to the experimental spectra using the BlueprintXAS Matlab software package.[10]

DFT Calculations:
DFT calculations were performed using the ORCA 3.0 software package.[11] All spectra were calculated from geometry optimized coordinates. Optimizations were carried out with the BP86 functional,[12,13] zeroth order regular approximation (ZORA) for relativistic effects,[14,15] and the scalar-relativistically recontracted def2-TZVP(-f) basis set.[16,17] Solvation was modeled using the conductor like screening model (COSMO).[18]

XAS spectra were calculated using a previously described TD-DFT protocol.[19] Spectral predictions employed the B3LYP functional.[20] The CP(PPP) basis set was used for Cu with an

integration accuracy of 7. The def2-TZVP-ZORA basis set was used for all other atoms. Solvation was again modeled using COSMO dielectric.

Fitted Experimental Data and TD-DFT Calculated Spectra

(N,N′-bis-2,6-diisopropylphenyl-2,4-dimethyl-1,5-diketamide)Cu(NCCH$_3$) (1)

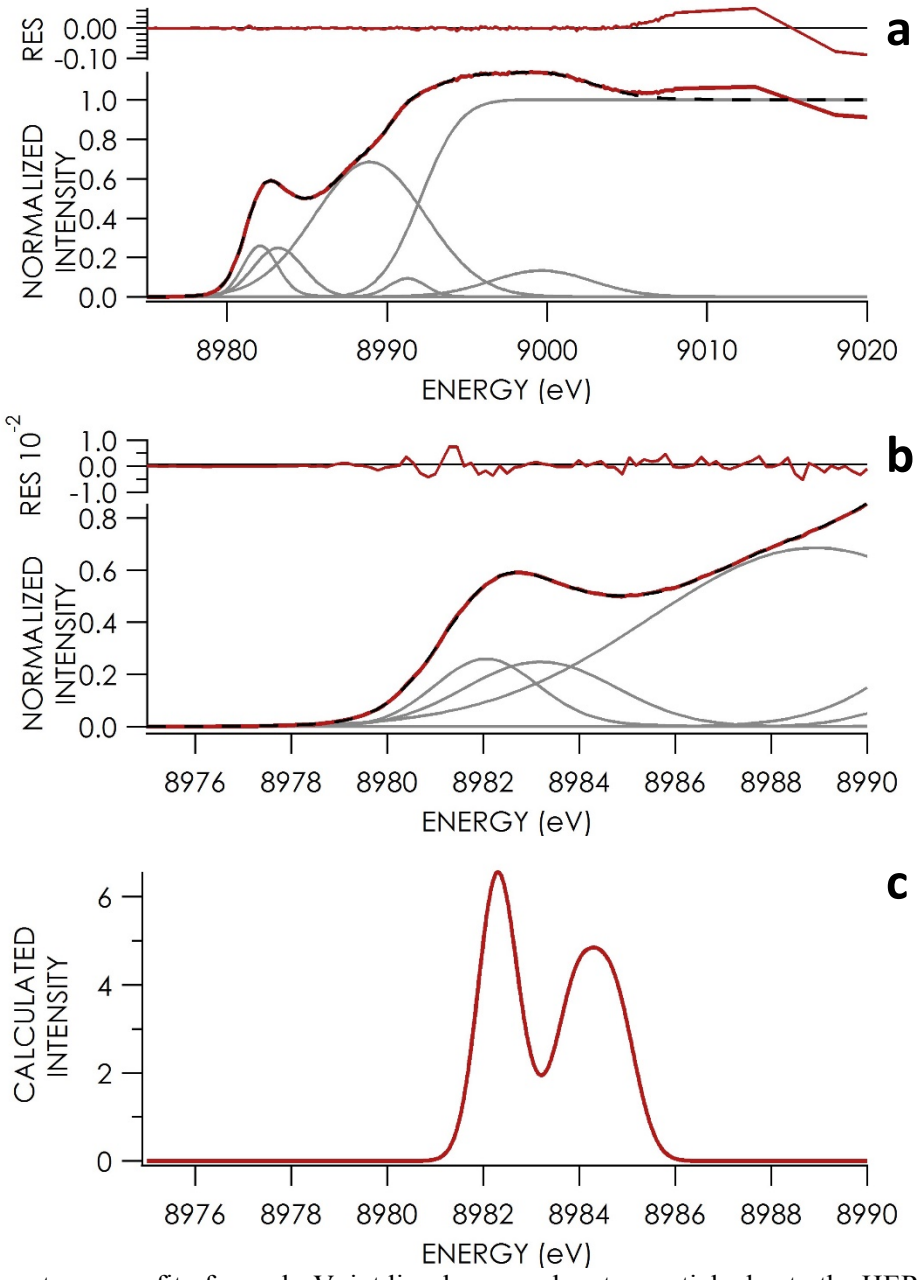

Figure S6. (a) Least-squares fit of pseudo-Voigt lineshapes and arctangential edge to the HERFD-XAS spectrum of (N,N′-bis-2,6-diisopropylphenyl-2,4-dimethyl-1,5-diketamide)Cu(NCCH$_3$) (**1**). Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks and the arctangential edge are gray. (b) Zoomed in look at pre-edge features. (c) TD-DFT calculated HERFD-XAS spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

[(tris-(2-dimethylaminoethyl)-amine)Cu](BPh$_4$) (2)

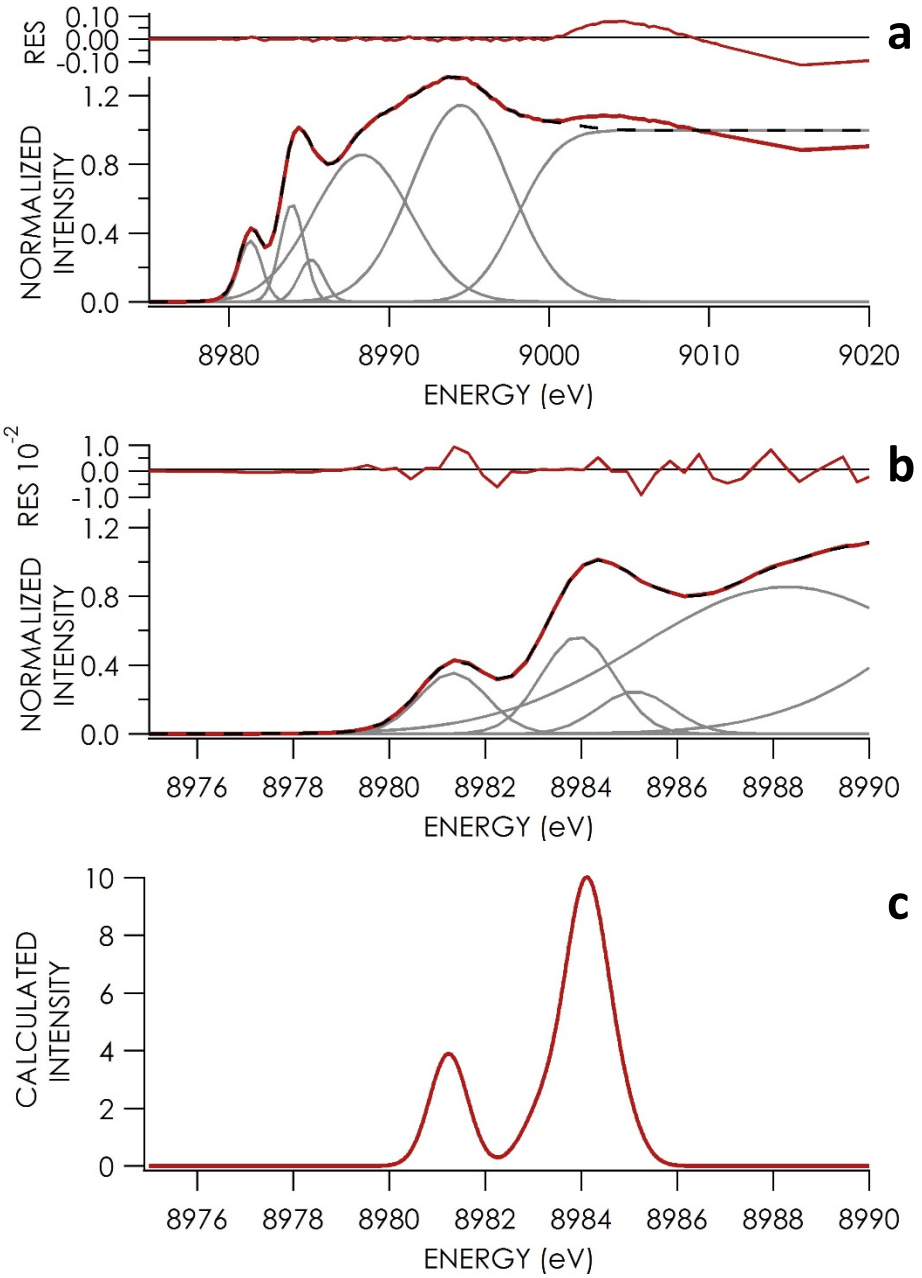

Figure S7. (a) Least-squares fit of pseudo-Voigt lineshapes and arctangential edge to the HERFD-XAS spectrum of [(tris-(2-dimethylaminoethyl)-amine)Cu](BPh$_4$) (**2**). Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks and the arctangential edge are gray. (b) Zoomed in look at pre-edge features. (c) TD-DFT calculated HERFD-XAS spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

[(CH$_3$CN)$_4$Cu](PF$_6$) (3)

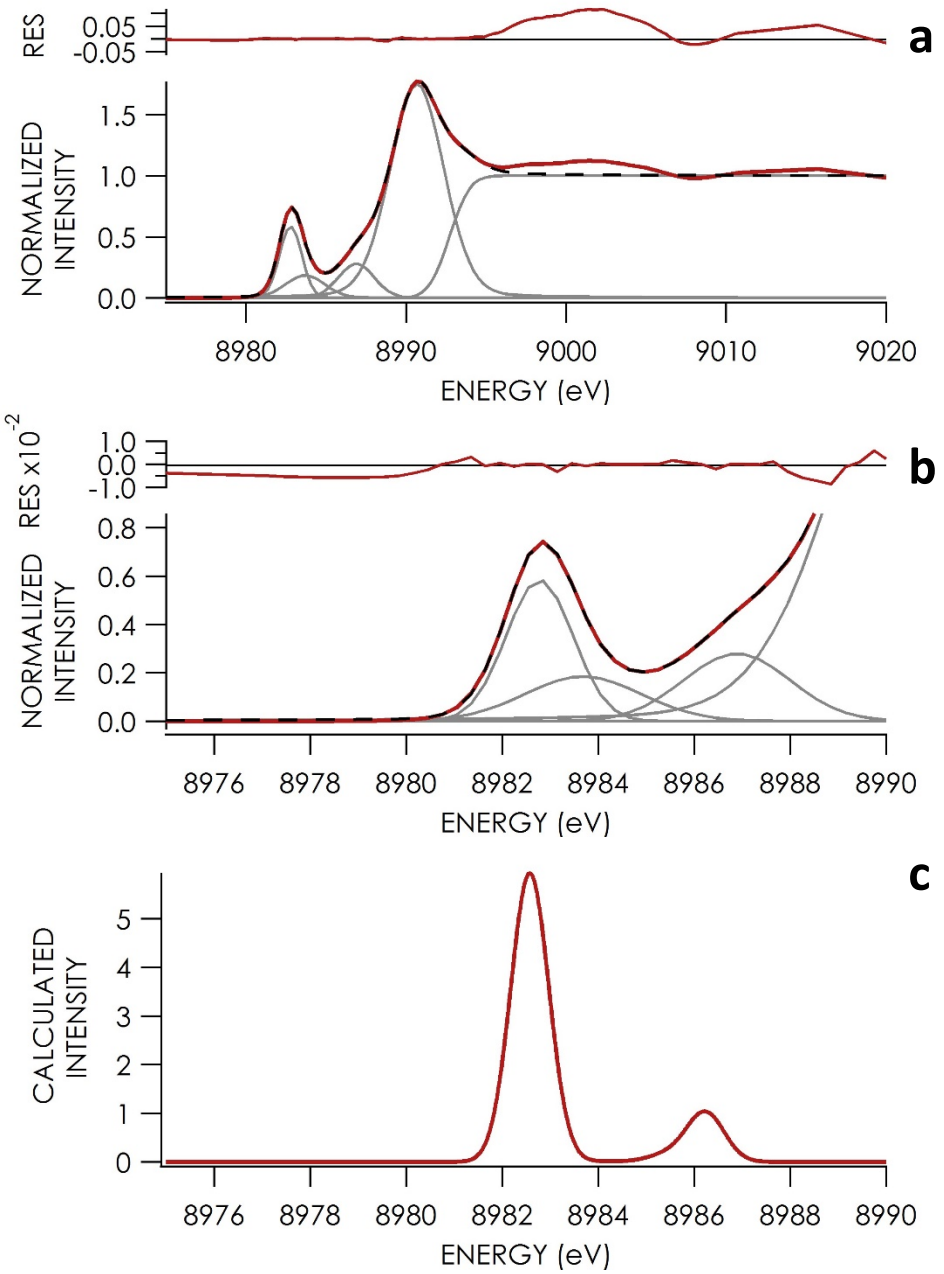

Figure S8. (a) Least-squares fit of pseudo-Voigt lineshapes and arctangential edge to the HERFD-XAS spectrum of [(CH$_3$CN)$_4$Cu](PF$_6$) (**3**). Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks and the arctangential edge are gray. (b) Zoomed in look at pre-edge features. (c) TD-DFT calculated HERFD-XAS spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

[(2,2′-bipyridine)$_2$Cu](PF$_6$) (4)

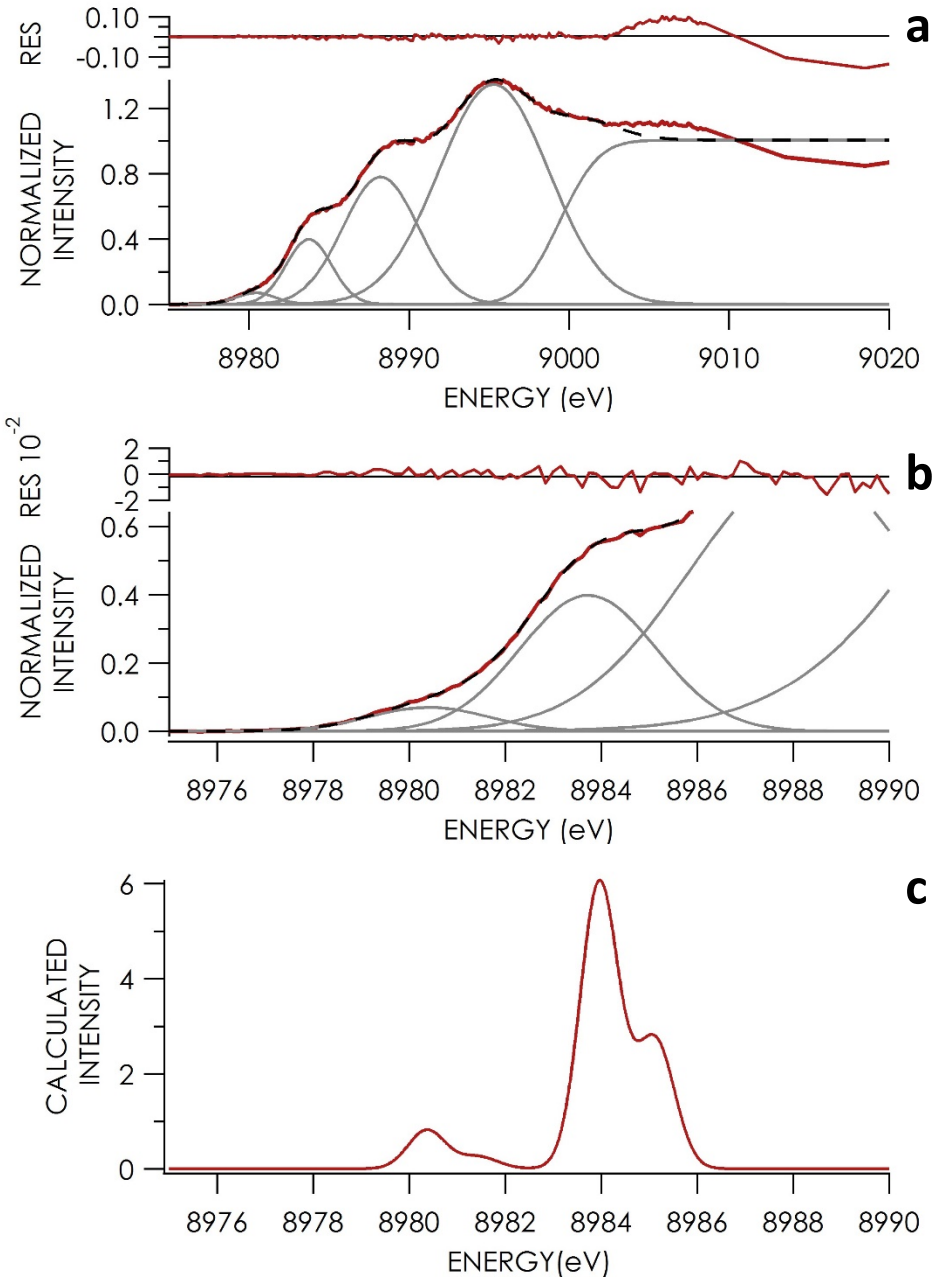

Figure S9. (a) Least-squares fit of pseudo-Voigt lineshapes and arctangential edge to the HERFD-XAS spectrum of [(2,2′-bipyridine)$_2$Cu](PF$_6$) (**4**). Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks and the arctangential edge are gray. (b) Zoomed in look at pre-edge features. (c) TD-DFT calculated HERFD-XAS spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

[(4,4′-dimethoxy-2,2′-bipyridine)$_2$Cu](PF$_6$) (5)

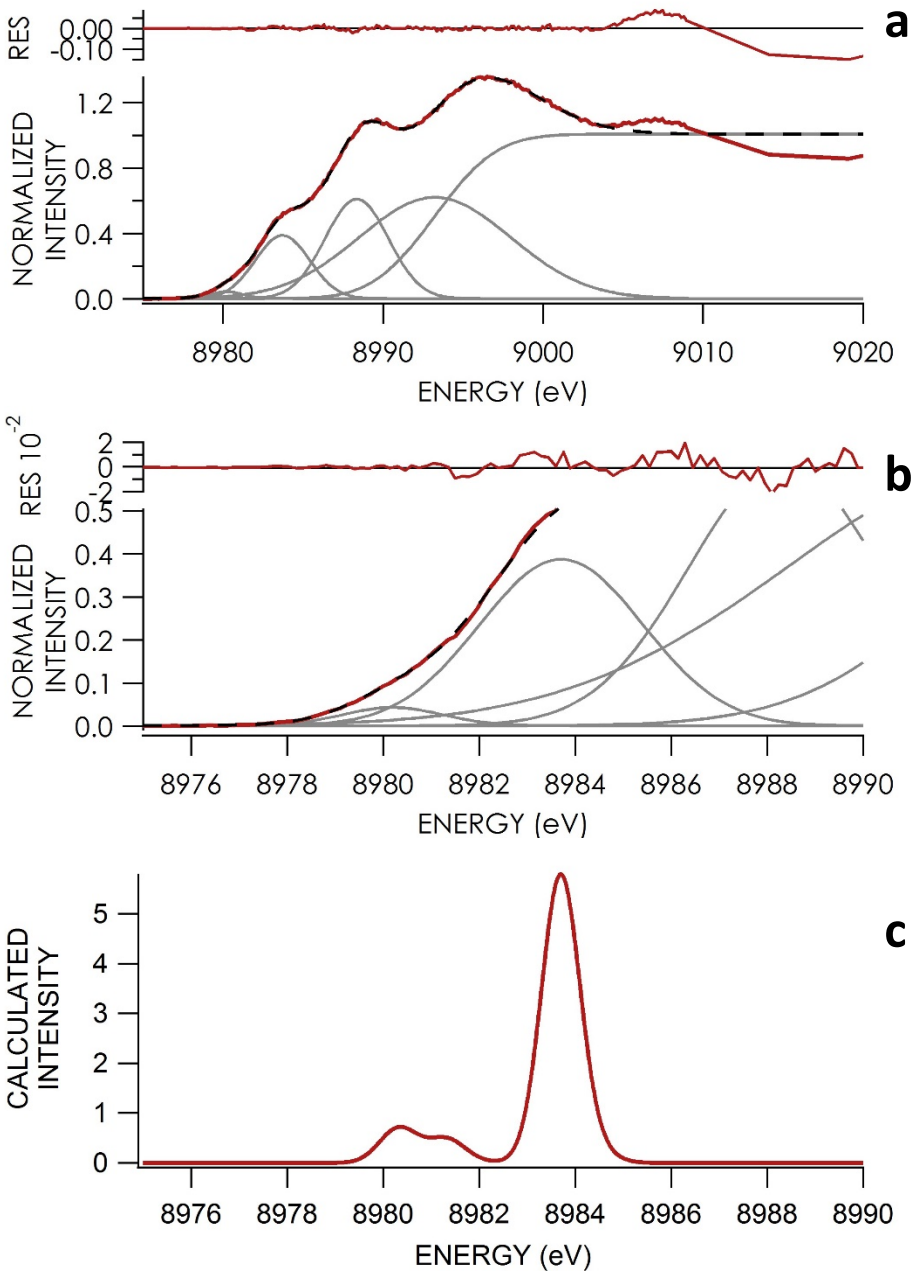

Figure S10. (a) Least-squares fit of pseudo-Voigt lineshapes and arctangential edge to the HERFD-XAS spectrum of [(4,4′-dimethoxy-2,2′-bipyridine)$_2$Cu](PF$_6$) (**5**). Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks and the arctangential edge are gray. (b) Zoomed in look at pre-edge features. (c) TD-DFT calculated HERFD-XAS spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

[(2-(2-pyridyl)-1,8-naphthyridine)Cu)](PF_6) (6)

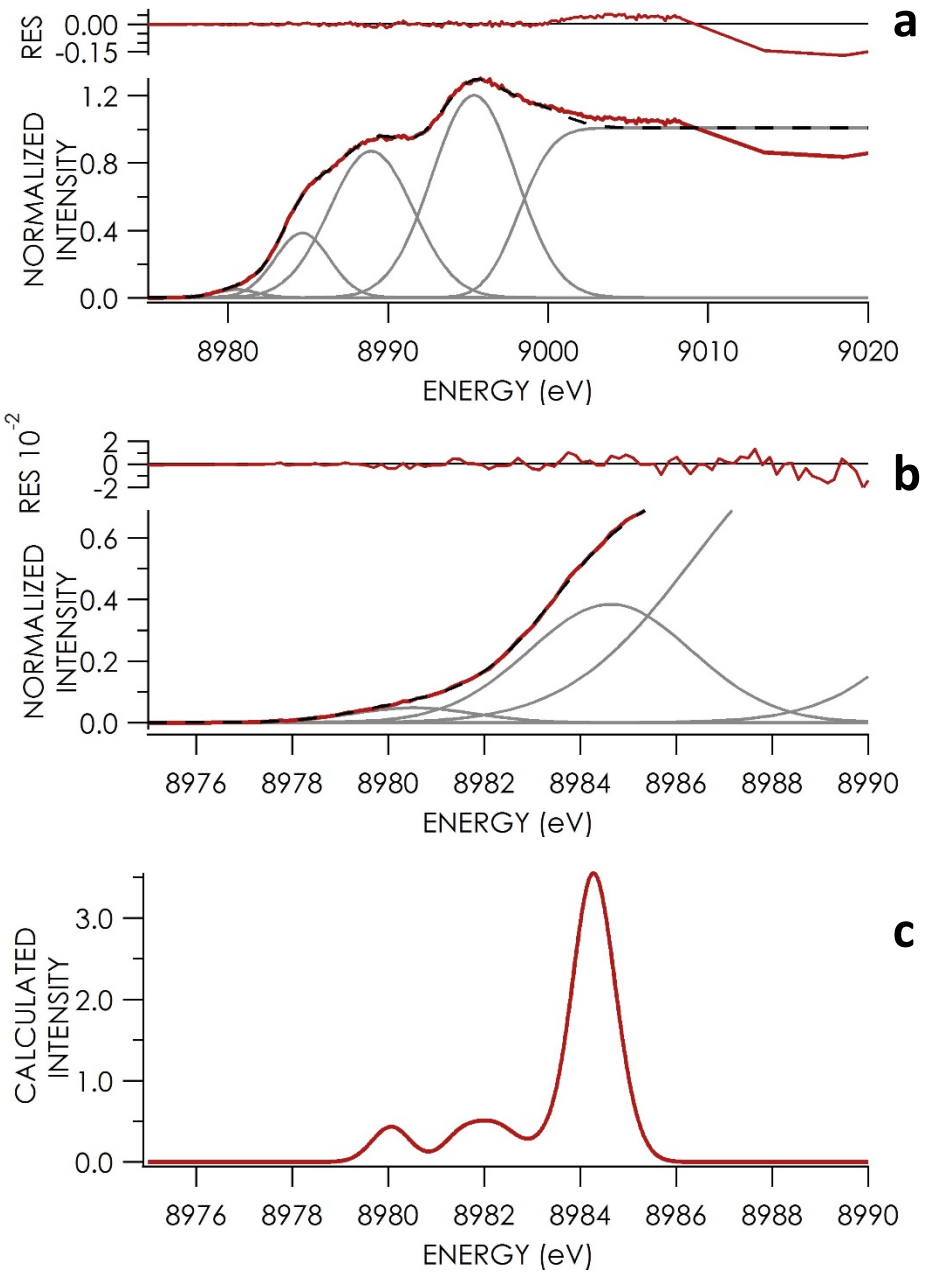

Figure S11. (a) Least-squares fit of pseudo-Voigt lineshapes and arctangential edge to the HERFD-XAS spectrum of [(2-(2-pyridyl)-1,8-naphthyridine)Cu)](PF_6) (**6**). Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks and the arctangential edge are gray. (b) Zoomed in look at pre-edge features. (c) TD-DFT calculated HERFD-XAS spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

[(N,N,N′,N′-tetramethylethylenediamine)Cu(OH)]$_2$ (7)

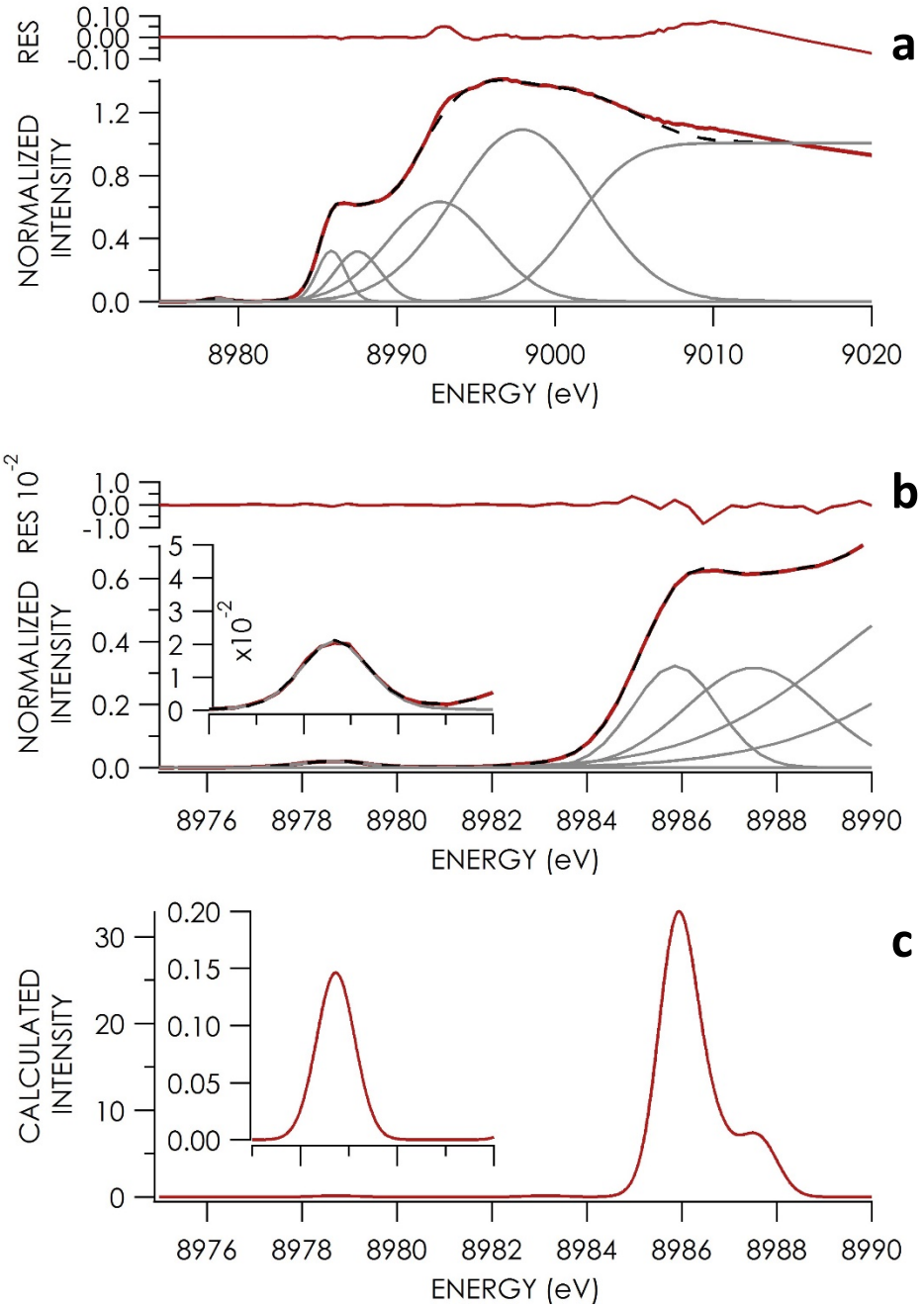

Figure S12. (a) Least-squares fit of pseudo-Voigt lineshapes and arctangential edge to the HERFD-XAS spectrum of [(TMED)Cu(OH)]$_2$ (**7**). Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks and the arctangential edge are gray. (b) Zoomed in look at pre-edge features. (c) TD-DFT calculated HERFD-XAS spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

[(tris-(2-dimethylaminoethyl)-amine)CuO]$_2$(BPh$_4$)$_2$ (8)

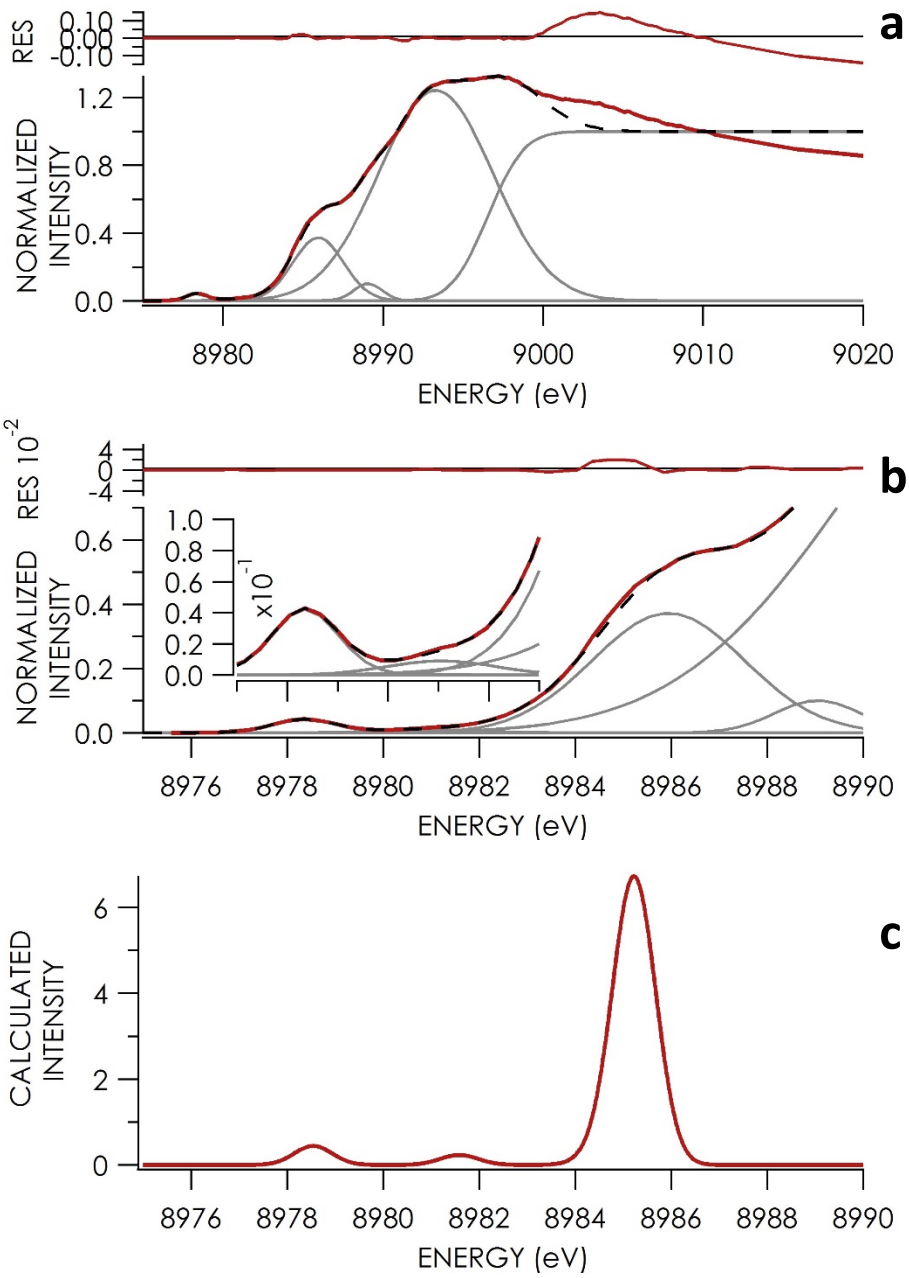

Figure S13. (a) Least-squares fit of pseudo-Voigt lineshapes and arctangential edge to the HERFD-XAS spectrum of [(tris-(2-dimethylaminoethyl)-amine)CuO]$_2$(BPh$_4$)$_2$ (**8**). Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks and the arctangential edge are gray. (b) Zoomed in look at pre-edge features. (c) TD-DFT calculated HERFD-XAS spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

(N,N′-bis-2,6-diisopropylphenyl-2,4-dimethyl-1,5-diketamide)Cu(O_2) (9)

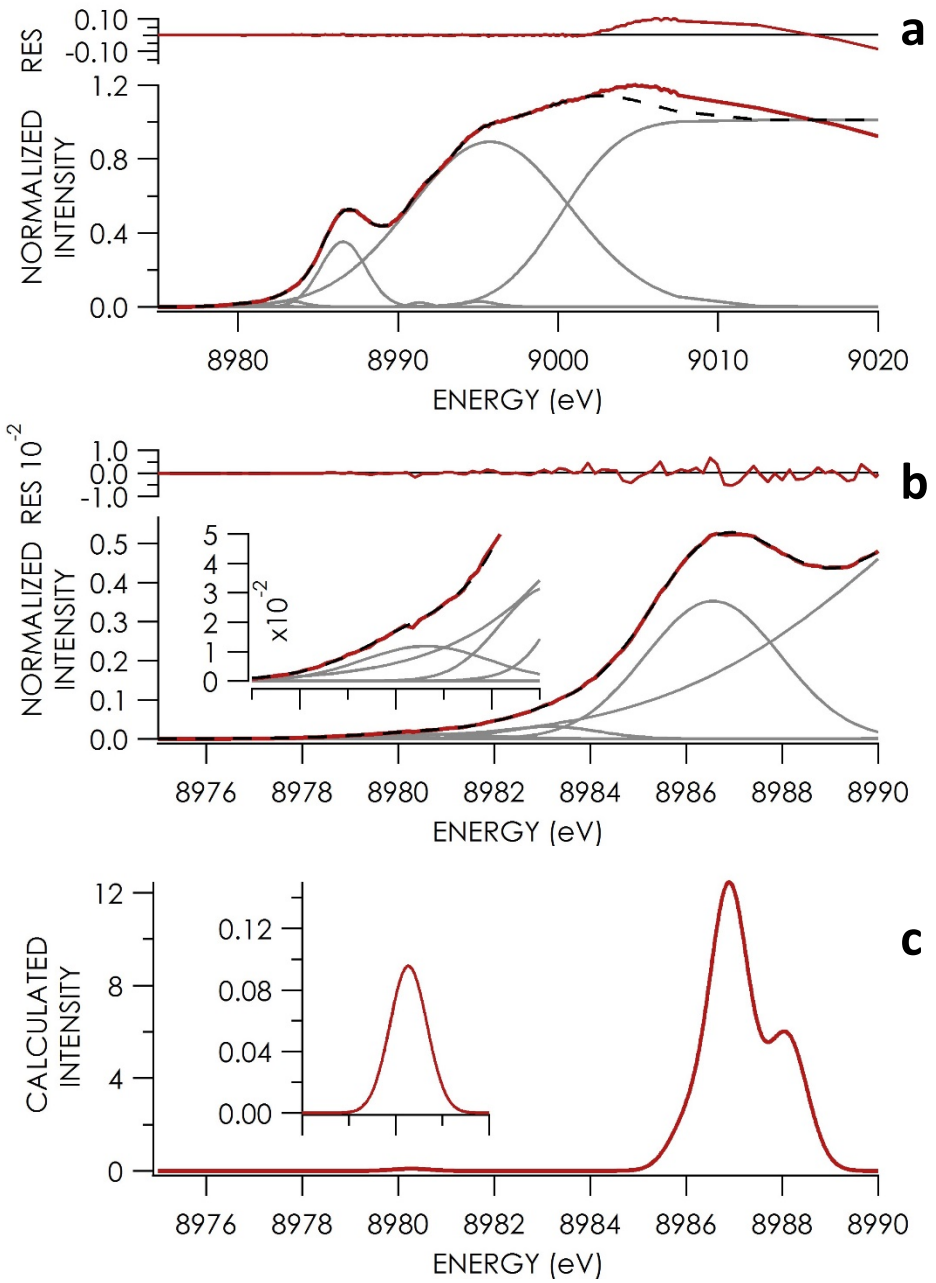

Figure S14. (a) Least-squares fit of pseudo-Voigt lineshapes and arctangential edge to the HERFD-XAS spectrum of (N,N′-bis-2,6-diisopropylphenyl-2,4-dimethyl-1,5-diketamide)Cu(O_2) (**9**). Experimental data are red, fitted data are dashed black. Individual pseudo-Voigt peaks and the arctangential edge are gray. (b) Zoomed in look at pre-edge features. (c) TD-DFT calculated HERFD-XAS spectrum using the B3LYP functional with the energy domain empirically corrected as discussed in the text.

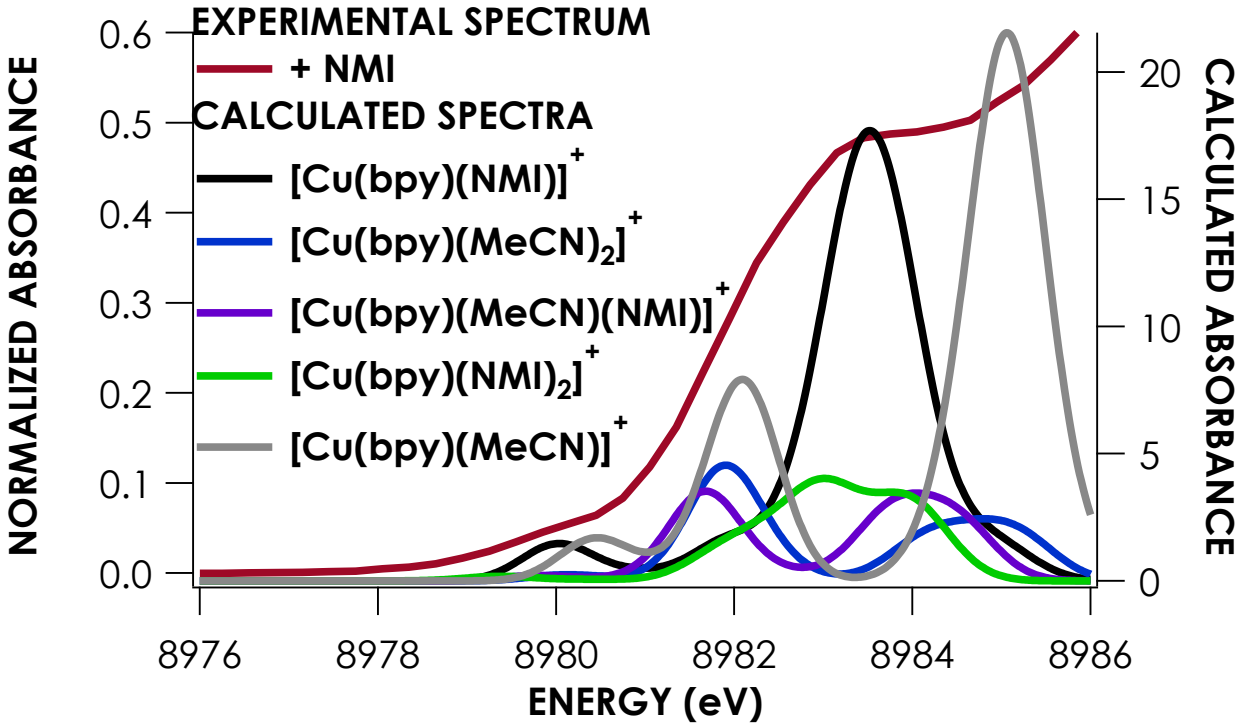

Figure S15. TD-DFT calculated HERFD-XAS spectra of putative Cu^{I} species formed during Cu/bpy/TEMPO/NMI aerobic alcohol oxidations. Spectra were calculated using the B3LYP functional with the energy domain empirically corrected as discussed in the text. On the basis of comparison to data collected of the steady-state reaction mixture, we propose $[Cu(bpy)(NMI)]^{+}$ as the major species present under steady state reaction conditions.

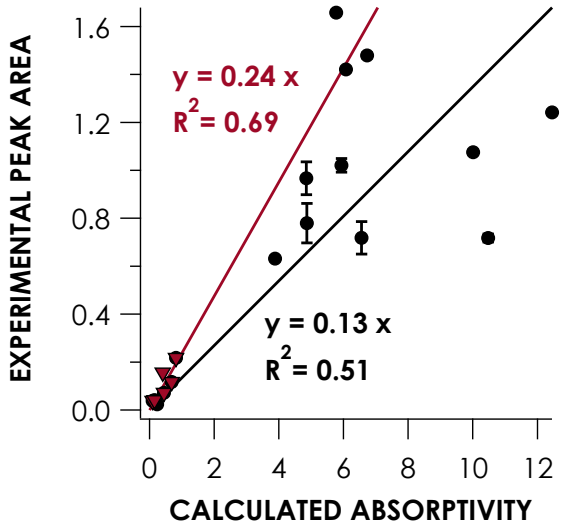

Figure S16. Plot of experimental HERFD Cu K-edge XAS pre- and rising-edge peak areas vs TD-DFT (B3LYP/def2-TZVP-ZORA) calculated peak areas. The black line ($R^2 = 0.51$) corresponds to the global fit, while the red line ($R^2 = 0.69$) represents a fit solely to pre-edge features. The poor correlation between calculated and experimental rising-edge peak areas can partially be attributed to substantial correlation between amplitude and linewidth parameters used for rising edge features and the edge jump. Further errors arise due to the inability of TD-DFT to model shakedown transitions and near-edge X-ray scattering.

Example ORCA Input Files

Geometry Optimization

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! Normalprint OPT
! PAL4 UKS

%SCF   Directresetfreq 1
     DIIS MaxEq 15
         end
     Shift Shift 0.5
          Erroff 0.1
          end
     MaxIter 500
     end

%maxcore 4000

* xyz CHARGE SPIN_MULTIPLICITY
COORDINATES
*
```

Single Point and TD-DFT X-ray Absorption Spectrum

```
!B3LYP RIJCOSX def2-TZVP(-f) def2-TZVP/J ZORA COSMO UKS PAL4
!NormalPrint VeryTightSCF SlowConv Grid4 NoFinalGrid UNO UCO

%basis newgto Cu "CP(PPP)" end
            end

%tddft   NRoots 40
        MaxDim 400
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HIGHEST_ENERGY_DONOR_ORBITAL, -1, -1
        OrbWin[1] = LOWEST_ENERGY_DONOR_ORBITAL,
HIGHEST_ENERGY_DONOR_ORBITAL, -1, -1
        DoQuad true
        end

%method SpecialGridAtoms 29
       SpecialGridIntAcc 7
       end

%MaxCore 4000

%SCF
    MaxIter 500
    end

* xyz CHARGE SPIN_MULTIPLICITY
COORDINATES
*
```

Geometry Optimized Coordinates

(counterions omitted from input coordinates)

(N,N′-bis-2,6-diisopropylphenyl-2,4-dimethyl-1,5-diketamide)Cu($NCCH_3$) (1)

Charge: 0 Spin Multiplicity: 1

C	-2.44782487219799	1.43449041429619	1.21009768801165
C	-1.16973939529275	0.90931837999006	1.52369172162422
C	0.11767208450563	1.27054749019591	1.07053463280659
C	-3.61209810929372	0.74476155442852	1.90326256883195
C	1.28107491643021	0.47038811743299	1.62393483229614
N	0.35496518945251	2.26070367491633	0.20121276166019
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C	1.69061263953478	2.56291797035265	-0.20546647008235
C	-3.96931446318528	2.93505254789570	0.10273338919539
C	2.42714590886197	3.56847814410808	0.47718619680670
C	3.70264286161827	3.91077244157488	0.00835270117549
C	4.26080540690664	3.28451982171843	-1.10684895334343
C	3.53148517052279	2.29734345214575	-1.77068000785885
C	2.25262850223327	1.91758002947440	-1.33978928884404
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C	1.03919362351860	1.40277372290561	-3.49252078850856
C	2.28036840908023	-0.44756441173747	-2.29025316434866
C	-4.51141617779712	3.98292355248026	0.90545602520185
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C	-5.99712921838107	2.94734197173489	-1.24195581661147
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C	-4.21800764061190	1.38670102836594	-2.01433075956013
C	-3.90395371596821	-0.01029305988220	-1.45104314792292
C	-3.05815041409456	1.89337075001502	-2.88932578302030
Cu	-1.12509022516969	3.31079984079266	-0.53527872456297
H	-1.18650103839834	0.08729669513198	2.24004453575438
H	-3.35120948539546	0.51050224052438	2.94373141125903
H	-3.84216834171880	-0.20651595461694	1.40111386593625
H	-4.52005722418330	1.35697306960704	1.89384545787116
H	0.94140495554332	-0.26327208632167	2.36513477139040
H	2.02529879953855	1.12847654573756	2.09688325807252
H	1.80625496080414	-0.06657770394205	0.81954936309470

H	4.27332365773178	4.68424303313628	0.52824989002282
H	5.25633204192663	3.56405871759629	-1.45614233218005
H	3.96653404163021	1.81029811788359	-2.64649141495256
H	0.91060026699798	3.79652567198461	1.95031491623497
H	3.05163313702481	3.22896065452042	3.16958330147398
H	2.28396306984443	4.71536485404792	3.77749030139694
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H	0.78566957689573	5.79434948620478	0.47814459437180
H	2.40300863664645	6.31462854079757	1.01528751800337
H	0.57284488053154	0.62618299045138	-1.54813758173812
H	0.43115807090776	0.65682219509626	-4.02796453340377
H	1.91136747022672	1.64368140144299	-4.12008709361459
H	0.43882990285139	2.31680469002355	-3.37803901928067
H	1.66340695509796	-1.21002096193872	-2.79027363147802
H	2.60236747313925	-0.85364981004923	-1.32004658333433
H	3.18048556127158	-0.29363073182879	-2.90472852931797
H	-6.21720255771193	5.25265017451372	1.23190834331458
H	-7.55460136034187	4.32652007650905	-0.64903197674104
H	-6.56813561396941	2.55261451032549	-2.08667707637905
H	-4.53010427305535	5.41695310178944	2.43469701084280
H	-3.06110990955544	4.47451506614113	4.08421222407638
H	-2.57316109142784	3.13814085524508	3.02110459973810
H	-4.24890178146816	3.23632658605873	3.62398736436627
H	-2.19964373659037	6.14421611544173	2.41245780722012
H	-2.88022365464779	6.22573002099691	0.76674099546002
H	-1.76985382397950	4.90776109878160	1.20808147004561
H	-5.07351750358887	1.24552006349562	-2.69653664671490
H	-3.73769288495632	-0.70990189279078	-2.28485685445234
H	-4.74007183247654	-0.39854154873713	-0.85040734933004
H	-2.99670904669436	-0.00793104873867	-0.83177875868088
H	-2.85912551021294	1.17574142376019	-3.69991485578268
H	-2.13153866506500	2.00473522910855	-2.30408483642418
H	-3.29249513436479	2.86818254137240	-3.33989364659819
N	-1.05949574910186	4.73555394534030	-1.73795772604120
C	-1.00423315887003	5.61989980894277	-2.49398068258300
C	-0.93239580977200	6.71969804111132	-3.43504055337311
H	-0.04365908994693	6.61582091869524	-4.07356837086817
H	-0.86791648330539	7.67192212087698	-2.89032482900178
H	-1.83006314267017	6.73583799188892	-4.06944611717427

[(tris-(2-dimethylaminoethyl)-amine)Cu](BPh$_4$) (2)

Charge: 1 Spin Multiplicity: 1

C	-0.435133	1.911869	10.826279
H	-1.311118	1.269122	10.617199

H	-0.692914	2.498207	11.719025
C	0.771893	1.011594	11.123625
H	0.518687	0.326483	11.955012
H	0.985636	0.380330	10.248976
C	1.961158	2.292052	12.821998
H	1.879010	1.465991	13.553616
H	1.096957	2.954469	12.949801
H	2.874457	2.860039	13.037500
C	3.185218	0.854144	11.348345
H	4.103626	1.411773	11.569062
H	3.259383	0.438324	10.337734
H	3.096575	0.021571	12.070529
C	-0.267010	2.263109	8.374812
H	-1.282893	2.373894	7.948926
H	-0.088770	1.182846	8.462773
C	0.741982	2.881692	7.398247
H	0.624794	2.406400	6.405148
H	0.519367	3.949780	7.264073
C	2.661506	1.401848	7.646635
H	2.643328	1.136188	6.573424
H	2.047753	0.677300	8.193976
H	3.694545	1.329904	8.007114
C	3.004884	3.699350	7.061346
H	4.042123	3.635643	7.411777
H	2.654336	4.730587	7.181184
H	2.979357	3.437148	5.987081
C	-0.822894	4.167992	9.866367
H	-1.870524	4.071332	10.209083
H	-0.867810	4.635243	8.873248
C	-0.071294	5.083234	10.841455
H	-0.602054	6.051642	10.914647
H	-0.084765	4.639967	11.847500
C	1.453034	6.271939	9.356645
H	1.024010	7.249561	9.645600
H	0.913401	5.902578	8.477472
H	2.505252	6.416973	9.086906
C	2.082652	5.880404	11.635084
H	3.135107	6.032581	11.367857
H	2.030529	5.195151	12.488218
H	1.649864	6.853183	11.932027
Cu	1.975442	3.311296	9.936907
N	-0.163061	2.854831	9.723341
N	2.020547	1.770862	11.434550
N	2.157821	2.780175	7.862435
N	1.360513	5.299876	10.473881

$[(CH_3CN)_4Cu](PF_6)$ (3)

Charge: 1 Spin Multiplicity: 1

C	-7.99447427794018	1.86997896498432	-1.28664136388098
N	-7.04248747127276	1.55653118800098	-0.70030985844713
C	-9.18202937714588	2.26097250238687	-2.01851481936257
H	-9.76271917498329	1.36846070051578	-2.28838064737406
H	-8.89439558481681	2.79454855316784	-2.93458076617052
H	-9.80179959091459	2.92069182819651	-1.39548548734844
H	-6.67082473885241	-1.14538623070502	4.70929656289118
C	-6.53909567499224	-0.05832803593829	4.62090388963775
C	-6.18655219875027	0.28286458968589	3.25768298062004
N	-5.90311656701904	0.55625236278573	2.16534111545014
H	-7.47611527814389	0.44255584096122	4.89878424008297
H	-5.74084710979975	0.26551382636247	5.30282344305576
H	-2.58838557445732	5.14606193356580	-0.55047474873811
H	-3.40732258845253	-2.43034436164678	-2.82234731219671
C	-2.42960936688804	4.51313485014340	0.33350757485361
C	-3.49015088288908	-2.61248175760388	-1.74193988886225
C	-4.09692407865145	-1.46568348291059	-1.09723300956449
N	-4.58368615529500	-0.54650808652978	-0.58105622020276
H	-1.40310173419981	4.12240639992207	0.31825583511364
C	-3.37199385399863	3.41327315888765	0.32366109430945
H	-2.57275309469970	5.11678973251001	1.24032557250468
H	-4.10929005259972	-3.50404792714951	-1.57222998999215
H	-2.48799748321656	-2.78480556599241	-1.32725564622933
N	-4.12726334616466	2.53137701099591	0.31570509973300
Cu	-5.41580474385641	1.02288200540381	0.30071235011729

[(2,2′-bipyridine)$_2$Cu](PF$_6$) (4)

Charge: 1 Spin Multiplicity: 1

C	-1.06794492416096	-2.33829928732427	-0.23410574762532
C	-0.32500872704554	-1.15587098228115	-0.28513910699044
H	-2.15779482360894	-2.32630153741727	-0.24408589263227
H	-0.82190356132095	-0.18676966102039	-0.33663669543586
C	1.06543155858087	-1.23175607145715	-0.26958061346213
C	1.68771557059409	-2.48530689868049	-0.20357882248276
N	0.95905108586164	-3.63518231121522	-0.15363876840554
C	-0.38698628376039	-3.55067587165298	-0.16941938603833
C	3.15709916211735	-2.66294418450402	-0.18213871417035
C	4.06337495582867	-1.59527554779117	-0.22892513747866
C	5.43179509974298	-1.85500300079731	-0.20327293289053
C	5.86819476350515	-3.18057581667369	-0.13107623937164
C	4.91485873280878	-4.19368489930190	-0.08822672183052
N	3.58798638521233	-3.95325209521955	-0.11267570141495

H	1.66029214039106	-0.32060415401320	-0.30901006791508
H	-0.92801070233612	-4.49690298638118	-0.12796528429709
H	3.70728095106589	-0.56804566312224	-0.28535955526694
H	6.14703409547898	-1.03293365650104	-0.23912446649752
H	6.92868721853161	-3.43041872472116	-0.10806399965060
H	5.21197439694533	-5.24162843996032	-0.03182229145846
C	1.94568549316563	-6.87941818186400	-2.65641604546719
C	1.82379240996600	-8.03319062622186	-3.42550051907452
C	1.64253987749348	-9.28219503031444	-1.37981164630957
C	1.88292004048328	-6.61299046534875	2.67658256436907
C	1.77017973546600	-8.08321364569618	-0.66584535690300
C	1.66948689431159	-9.25871404024452	-2.77215891591769
C	1.73857271011529	-7.68399753025590	3.55375881864600
C	1.59630870288284	-8.96859653646408	3.02241140454407
C	1.75191402352273	-8.00935032856955	0.81247931121905
C	1.60331850692350	-9.13106012818433	1.63910601471467
N	1.89067318701849	-6.75933654221275	1.33596550745467
N	1.92134795528590	-6.89131994553097	-1.30797484848257
H	2.06927890532613	-5.90257328174334	-3.12574871917455
H	1.85020694441450	-7.96736135697587	-4.51314253101101
H	1.52124664280492	-10.22884173738068	-0.85587828439649
H	1.57085670858807	-10.18475204173546	-3.33897319112816
H	1.99855397306546	-5.59437643285985	3.04906234109000
H	1.49304980939932	-10.12530960895370	1.20985845992721
H	1.48086293906527	-9.83343530614424	3.67602101545310
H	1.73813139658257	-7.50941988190054	4.62962195643435
Cu	2.08942604968718	-5.30970556136328	-0.05949119067243

[(4,4′-dimethoxy-2,2′-bipyridine)$_2$Cu](PF$_6$) (5)

Charge: 1 Spin Multiplicity: 1

C	-1.11022485816054	-2.48332865064319	-0.47638811707326
C	-0.40611607756931	-1.26567029436668	-0.52235906293599
H	-2.19894914896037	-2.49385885234825	-0.52644881835491
C	0.99276749866650	-1.30103248356282	-0.45925683938919
C	1.64097680699905	-2.53767146582057	-0.34745193905234
N	0.95823270414310	-3.71173727275057	-0.29819964639799
C	-0.39197525147600	-3.66037564765772	-0.36529336371083
C	3.11823726030328	-2.66409975951167	-0.26986406916749
C	3.97616476779088	-1.55789817573405	-0.31404061070487
C	5.35958477001768	-1.76126031349153	-0.23148079833229
C	5.83736395559244	-3.07899488093399	-0.10465169583071
C	4.92119198893778	-4.11469117874630	-0.07014159945228
N	3.58266231414084	-3.93571409330235	-0.15038000736505
H	-0.91087506884053	-4.61902914852390	-0.32583368473873
H	3.57119117183433	-0.55469321743094	-0.41183373498839

O	6.28974022928592	-0.77965104551094	-0.26351134524304
H	6.90713156594308	-3.27468955604070	-0.03574675877416
H	5.26193489193650	-5.14625980175805	0.02694242958101
C	2.13265361342661	-7.02477640930344	-2.67128961977874
C	2.07780214936671	-8.19346008091050	-3.40911413576323
C	1.86582813910277	-9.39521010725862	-1.32766265560567
C	1.87262852568617	-6.62186300017762	2.64580209959478
C	1.92868114449261	-8.16651053267742	-0.65920993065552
C	1.94177920458643	-9.41660573759750	-2.72620032882175
C	1.73702912097259	-7.66695564783597	3.55315670962842
C	1.65828429795959	-8.97506877189894	3.04793059184283
C	1.85550795980731	-8.05595576541987	0.81949653281165
C	1.71844115702560	-9.15960200775281	1.65748533525690
N	1.93318355398232	-6.78428035320131	1.31058775481437
N	2.06208905321664	-6.98686580447356	-1.32050364728708
H	2.23958555605570	-6.06229924912829	-3.17303849504797
H	2.14010507242093	-8.17260204760128	-4.49702504154996
H	1.75900681294300	-10.31814435846759	-0.76419308559760
O	1.89517245196486	-10.53343140226491	-3.48772564288623
H	1.93739828135199	-5.59448466582441	3.00712610124521
H	1.65551149237214	-10.17298932420225	1.26502401370399
O	1.52791149956678	-10.09367116266483	3.79660914446217
H	1.69544780890946	-7.44941611180952	4.61844158239351
Cu	2.13377786668024	-5.35620161515284	-0.11605303337834
O	-1.14903601171922	-0.13986812053901	-0.62469574098895
H	1.57074751871686	-0.38148629996208	-0.49519261197770
C	1.47243425623988	-9.93847440942412	5.23238420056901
H	1.38130131496730	-10.95339728841407	5.63017381592613
H	0.59582935317125	-9.34299525575425	5.52674524836117
H	2.39355829952470	-9.47134886619524	5.60929616496327
C	1.76114986220567	-11.80530805749564	-2.81519365281812
H	1.75259302410849	-12.55452395057808	-3.61242174403007
H	0.81865765521007	-11.85027737790003	-2.25095738936913
H	2.61474291600878	-11.98330433025015	-2.14513561807344
C	-0.45512527735736	1.12650916792038	-0.66510038690598
H	-1.24073405648565	1.88512473149552	-0.72957413255588
H	0.19441405596126	1.18686069640512	-1.55026347137760
H	0.13449104695203	1.27729385384792	0.25093727514147
C	5.83042449308905	0.58337549883686	-0.39685351045353
H	6.73751410665582	1.19462949332190	-0.40822179261141
H	5.19997352588179	0.86812777493484	0.45832404392392
H	5.27801963439419	0.71829273350788	-1.33809528517439

[(2-(2-pyridyl)-1,8-naphthyridine)Cu)](PF_6) (6)

Charge: 1 Spin Multiplicity: 1

C	-0.63523411096053	-2.95209284241843	-1.07239507946835
C	-0.02917157685116	-1.67071792330437	-1.05706383584376
C	-1.99705906356047	-3.17789816801579	-1.38908643001746
C	1.30348047452329	-1.55828144036404	-0.73601601383951
C	2.05168691178308	-2.72359142366694	-0.42979419820668
N	1.50043663000731	-3.94996998837971	-0.43953442427258
C	0.17370444391068	-4.08797929654781	-0.75060709384612
C	3.48617780556964	-2.68008027532920	-0.07519467869415
C	4.23200905444302	-1.49464465172841	-0.01075377413111
C	5.57947165508326	-1.55134373381921	0.33786206934179
C	6.15476500750922	-2.79382671311445	0.61607092303504
C	5.35652310063411	-3.93229786175355	0.53121649792967
N	4.05340528271165	-3.88881546702216	0.19371637155727
N	-0.31248819812803	-5.35571752793409	-0.73309916774801
H	7.20392402100004	-2.88573250543001	0.89533299798636
H	5.76648483037228	-4.92152825261152	0.73866047491350
C	3.45611462617397	-7.19082531795118	-2.37855401122637
C	3.66954239400446	-8.44465797293593	-3.03536439651524
C	3.20663661536190	-9.54601618068443	-0.94036225190954
C	2.18347865559246	-6.57552629936001	2.77327515815820
C	3.00753509807080	-8.27233311822818	-0.34863161680673
C	3.53441669761082	-9.63262896659808	-2.27341566627024
C	2.00329557918581	-7.59226807363645	3.70807394964619
C	2.15969080307907	-8.91747015670076	3.29414808569429
C	2.65618055477278	-8.10241729530328	1.07727503659248
C	2.49024828764056	-9.17385465765738	1.96557907767102
N	2.50128363244923	-6.81265764752043	1.48628943396138
N	3.12722216442520	-7.13106532504106	-1.05000984669143
N	3.56491941187509	-5.99780363439742	-3.01832376589392
C	4.00523220859213	-8.42197248353675	-4.41121626851258
H	2.06889634048588	-5.52793546891939	3.05530810462410
H	1.74376089669636	-7.34362950702631	4.73667438012313
Cu	2.76403145827387	-5.45186791507430	-0.00558400509568
H	2.02531190927366	-9.74129616871433	3.99543696048265
H	-0.62325881001213	-0.78800911665774	-1.29920491155909
H	6.17102820753821	-0.63723966845428	0.39229265616540
H	1.78005969765269	-0.58025701624457	-0.71900749130032
H	3.76893775410542	-0.53413093491917	-0.23016462197296
H	3.10146900330926	-10.45091576951645	-0.34494099054379
H	3.69244231680350	-10.60191383404849	-2.74927974865638
H	2.61564530598336	-10.20044949586706	1.62608651578523
C	4.11250350197033	-7.20613737718108	-5.05207956125175
C	3.88226244270547	-6.02357739794699	-4.30788570994404
H	3.96551633029912	-5.05132351784437	-4.80288560778976
H	4.37050156018002	-7.14040540590605	-6.10895750791906

H	4.17495072098991	-9.36183201938831	-4.93953085069526
C	-2.48057194849725	-4.46886112108649	-1.37192775755634
C	-1.59488970579083	-5.52120060726967	-1.03519966871603
H	-2.63885057914872	-2.33165439834234	-1.64127819256671
H	-3.52059806292580	-4.69119014989224	-1.61019257424752
H	-1.96585133677401	-6.55032790870928	-1.01386697395922

[(N,N,N′,N′-tetramethylethylenediamine)Cu(OH)]$_2$ (7)

Charge: 2 Spin Multiplicty: 3

Cu	-0.923058	13.659669	6.565042
O	-0.730029	13.807688	4.602910
H	-0.989890	12.973151	4.170207
N	0.487019	12.167335	6.794288
N	-1.138377	13.595932	8.619401
C	0.322870	11.654633	8.188228
H	-0.498418	10.925369	8.178231
H	1.233539	11.121673	8.506949
C	0.018327	12.801286	9.133072
H	-0.198626	12.422620	10.144835
H	0.876777	13.481591	9.214389
C	1.813796	12.816262	6.605943
H	1.950030	13.626440	7.331412
H	1.865648	13.230949	5.593187
H	2.617850	12.074208	6.741985
C	0.340099	11.054019	5.823597
H	-0.667661	10.626889	5.895314
H	1.081392	10.266298	6.036674
H	0.515646	11.429891	4.809208
C	-1.158050	14.935830	9.258488
H	-0.244764	15.485884	9.000040
H	-1.217993	14.831106	10.354268
H	-2.038497	15.490226	8.913950
C	-2.432089	12.904901	8.878867
H	-2.426800	11.903013	8.434551
H	-3.242863	13.490360	8.430769
H	-2.598685	12.814606	9.964551
Cu	-2.105894	15.196732	4.304520
O	-2.295114	15.052873	6.267851
N	-3.518972	16.685604	4.074745
C	-3.358491	17.195156	2.679208
H	-2.538074	17.925441	2.685643
H	-4.270489	17.726207	2.361112
C	-3.054420	16.046588	1.736554
N	-1.895108	15.255167	2.249421
C	-1.875226	13.913471	1.614095

H	-2.786681	13.362582	1.877170
H	-1.819122	14.015154	0.517838
H	-0.992638	13.361535	1.957156
C	-0.603173	15.947412	1.984441
H	-0.608723	16.950565	2.425886
H	0.209725	15.364503	2.432031
H	-0.439689	16.034803	0.898045
H	-2.840678	16.423037	0.723269
H	-3.912008	15.364712	1.659130
C	-4.844390	16.035275	4.267648
H	-4.980925	15.222742	3.544886
H	-4.893518	15.623565	5.281743
H	-5.649787	16.775766	4.131057
C	-3.371436	17.801362	5.042544
H	-2.364650	18.230180	4.967106
H	-4.114753	18.587257	4.829759
H	-3.543321	17.427329	6.058240
H	-2.029687	15.887188	6.697656

[(tris-(2-dimethylaminoethyl)-amine)CuO]$_2$(BPh$_4$)$_2$ (8)

Charge: 2 Spin Multiplicity: 3

Cu	10.565862	6.099114	11.141952
N	8.621757	5.454473	11.969957
N	10.027003	8.023531	12.160427
N	11.314203	4.384809	12.276035
N	9.444525	5.626895	9.163734
O	12.175696	6.891470	10.270435
C	8.212865	6.498877	12.947260
H	8.720680	6.294102	13.899376
H	7.129419	6.446410	13.154123
C	8.574048	7.895106	12.451252
H	8.029976	8.119033	11.521951
H	8.251832	8.647481	13.194751
C	10.266910	9.216622	11.317530
H	9.695821	9.137565	10.385629
H	11.334426	9.268570	11.071856
H	9.971613	10.145777	11.838018
C	10.791310	8.181647	13.419281
H	10.489654	9.100053	13.956889
H	11.860606	8.246876	13.186606
H	10.628574	7.324829	14.083168
C	8.855722	4.146107	12.636565
H	8.749918	3.354941	11.882131
H	8.088885	3.946912	13.406066
C	10.244410	4.084995	13.266686

H	10.327999	4.824796	14.075810
H	10.400089	3.091586	13.726699
C	12.580032	4.699825	12.972597
H	12.948433	3.834507	13.553237
H	12.430149	5.544540	13.655444
H	13.329352	4.973056	12.218913
C	11.549744	3.220888	11.389569
H	12.290984	3.498645	10.631383
H	10.623473	2.926302	10.883321
H	11.923688	2.353591	11.963903
C	7.639665	5.333755	10.859653
H	7.212994	6.328018	10.672619
H	6.795271	4.682916	11.149086
C	8.288945	4.798527	9.586089
H	8.655359	3.774610	9.749266
H	7.525476	4.734231	8.787486
C	8.981197	6.870556	8.509721
H	8.419537	6.651154	7.582614
H	9.848573	7.491923	8.256520
H	8.328951	7.442944	9.179672
C	10.282558	4.881138	8.201645
H	10.605904	3.931777	8.644102
H	11.172931	5.476644	7.965570
H	9.735105	4.664863	7.265774
Cu	14.984616	6.892643	9.422537
N	16.931711	7.569146	8.623197
N	15.653365	4.935167	8.496008
N	14.252671	8.575051	8.000004
N	15.855442	7.505469	11.341060
O	13.189853	6.115499	9.804848
C	17.455181	6.491687	7.742009
H	17.014734	6.626864	6.745659
H	18.548907	6.579778	7.615070
C	17.112851	5.106142	8.280730
H	17.610910	4.941060	9.247933
H	17.506413	4.336918	7.590098
C	15.409587	3.757611	9.357493
H	15.922754	3.881552	10.318604
H	14.331909	3.667904	9.538896
H	15.769353	2.826050	8.883469
C	14.954354	4.720008	7.208642
H	15.294494	3.788076	6.719467
H	13.875514	4.650120	7.394375
H	15.137214	5.556000	6.524222
C	16.728293	8.832998	7.865421
H	16.742184	9.666835	8.580895

H	17.563100	9.011383	7.164451
C	15.407195	8.823132	7.103310
H	15.414217	8.027099	6.343706
H	15.293336	9.777941	6.555851
C	13.073359	8.169677	7.207285
H	12.756797	8.969028	6.512014
H	13.304486	7.269917	6.624705
H	12.249735	7.943299	7.894888
C	13.905390	9.794392	8.759878
H	13.090368	9.559350	9.455398
H	14.766750	10.152816	9.337007
H	13.578118	10.610382	8.088277
C	17.805026	7.783746	9.806296
H	18.243462	6.818024	10.091081
H	18.651877	8.449641	9.561161
C	17.015958	8.365815	10.974673
H	16.621161	9.356159	10.709981
H	17.685828	8.510715	11.841848
C	16.318482	6.336340	12.127474
H	16.792931	6.658489	13.071901
H	15.463838	5.692716	12.364243
H	17.046541	5.750137	11.555324
C	14.897869	8.275668	12.165950
H	14.580415	9.174313	11.624641
H	14.014806	7.654871	12.359027
H	15.346752	8.579375	13.128540

(N,N′-bis-2,6-diisopropylphenyl-2,4-dimethyl-1,5-diketamide)Cu(O_2) (9)

Charge: 0 Spin Multiplicity: 1

C	-2.40692405352206	1.43043916380960	1.28227975473983
C	-1.14875563013550	0.88767497452511	1.61451321208501
C	0.12072777013449	1.25013361809261	1.13819157085698
C	-3.60182455920053	0.77875622059982	1.94905490357830
C	1.30680183684419	0.47429435847246	1.66583644769257
N	0.33568855286488	2.23356502625059	0.25415231336605
N	-2.57198123969960	2.43901048961507	0.42487893874438
C	1.66354353653958	2.56568106811123	-0.18284269988471
C	-3.86738300034819	2.96884821426406	0.09684905873018
C	2.42165413354187	3.51812080369345	0.54642098450932
C	3.70566990236255	3.83918946615233	0.08652205135249
C	4.23265882057625	3.25102475851577	-1.06301718281188
C	3.47032806985031	2.32827257743104	-1.77741055438246
C	2.18089786070188	1.96876176054411	-1.36049513826619
C	1.86722228957498	4.22441786248366	1.77774999495150

C	2.81903566370688	4.15172707861648	2.98561501489077
C	1.52235063729734	5.68975671133729	1.44352555548405
C	1.37738573870686	0.97907310179662	-2.19479098112922
C	0.99918270485014	1.59466265349466	-3.55665285175633
C	2.11768187600849	-0.35803133730627	-2.38738704859399
C	-4.39600145565837	4.04578034493032	0.86115301270425
C	-5.66372336705636	4.53932196636585	0.51164367147655
C	-6.39031528428414	4.01546875637741	-0.55375800737445
C	-5.83908195243353	2.98458018932309	-1.30996270699691
C	-4.57591576582285	2.44450386257691	-1.02009074461860
C	-3.71830369525763	4.73473175184918	2.05289226262295
C	-3.72541908150801	3.90336977083795	3.35055118165569
C	-2.31599483545141	5.30592887595851	1.78570063060826
C	-4.08241855722784	1.34756706691443	-1.97249268000278
C	-3.90152442648978	-0.04578821278771	-1.34396879373557
C	-2.84224143487956	1.73627864028397	-2.79566460606434
Cu	-1.09417706302885	3.27110154620483	-0.44536381738118
H	-1.16899800253240	0.06771506747124	2.33073575305749
H	-3.44132373964489	0.72491714573790	3.03414425444288
H	-3.71058646386169	-0.25223148323832	1.58428876431952
H	-4.53445452076962	1.31539042402361	1.75158500469497
H	0.98139698657290	-0.29329143844974	2.37678651818566
H	2.01968258059456	1.14339689027454	2.16936960737324
H	1.85425899458081	-0.01137355699789	0.84520833162502
H	4.30413558046522	4.56830636638678	0.63677204702586
H	5.23419366885773	3.51714255185521	-1.40487394021381
H	3.88402929148751	1.87876663474094	-2.68214108153286
H	0.93393955852650	3.71657356879205	2.05949018591215
H	3.09584696887226	3.11454228101660	3.22350264393803
H	2.33615653708636	4.58666153346081	3.87327875845420
H	3.74557524193292	4.71632448540214	2.80503536841397
H	1.07011704343034	6.18864870253815	2.31386023443031
H	0.81712553852906	5.74800988104375	0.60096651461993
H	2.42994606257931	6.24790530469373	1.16647015428456
H	0.44347465951537	0.76711428743998	-1.65335383751004
H	0.37133054360045	0.89708333587067	-4.13194196655880
H	1.89876565820922	1.81072076212939	-4.15274672671082
H	0.44361170768963	2.53446020492916	-3.42362329169053
H	1.48192292484039	-1.06824554535105	-2.93732100556354
H	2.38476876570058	-0.81621996676708	-1.42375884670800
H	3.04482713742635	-0.22389295199444	-2.96480941190724
H	-6.08080013848745	5.36362550599523	1.09438427004502
H	-7.37230014321178	4.41960222989410	-0.80412129825761
H	-6.39394416435868	2.58279573330447	-2.16081208858183
H	-4.36341215699562	5.60616441405535	2.25069401628541
H	-3.45280468903438	4.54968347378484	4.19919066643343

H	-2.99441735567028	3.08414155573991	3.31429291641557
H	-4.71671130801116	3.47567483869164	3.55664275504512
H	-2.04431839397317	6.00087278458129	2.59496713014555
H	-2.26800135780381	5.84904901445545	0.83242988883395
H	-1.55196956740743	4.51389162653839	1.76636447682448
H	-4.90386596508638	1.24220646019353	-2.70016000172189
H	-3.76050273475512	-0.78837685528401	-2.14375329700738
H	-4.78343593281315	-0.34485336254618	-0.75925715283704
H	-3.01607173349256	-0.09122134220874	-0.69439798816241
H	-2.70468845146951	1.01516866441126	-3.61541458698760
H	-1.92379311580366	1.71268557131188	-2.18862800847184
H	-2.93585291737522	2.74075864589042	-3.22790542202156
O	-0.34411528282640	4.55140699178422	-1.59269508416324
O	-1.72716130666954	4.68682643506437	-1.52896797124881

[Cu(2,2′-bipyridine)(N-methylimidazole)]$^{+}$

Charge: 1 Spin Multiplicity: 1

H	1.38449726278425	-0.00686198581688	-0.39406718503955
C	0.53939882578773	0.67331461800116	-0.29436281703899
C	-0.77266860398139	0.20387155444409	-0.22128545882906
H	-0.98624573011133	-0.86455192134006	-0.26602024087865
C	-1.81428741874317	1.12144369633113	-0.09362031189679
H	-2.84366562158826	0.77158780295624	-0.04408945745985
C	-1.52269984809551	2.48916492993410	-0.04094892744319
N	-0.24325843097268	2.94155315988956	-0.11645469293152
C	0.75749729063054	2.04892365151065	-0.23998251740701
H	1.76583963436277	2.46025059386018	-0.29617111926094
C	-2.56816559550225	3.53690452903638	0.09026764122602
C	-3.92135418683827	3.24589270239198	0.29880423634415
H	-4.26350151925177	2.21567263920753	0.37794236970994
C	-4.83455464577702	4.29281700253931	0.41606067338814
H	-5.89125637392863	4.08133336366144	0.58234894829212
C	-4.37595331740744	5.60738630408624	0.32233524651125
H	-5.05403597772413	6.45578677354932	0.40774590735461
C	-3.01400562401645	5.82273548142466	0.11659830806766
H	-2.61109533709542	6.83333880454907	0.03783810304266
N	-2.12655025970240	4.81783541440947	0.00260588194423
Cu	-0.08288214442350	4.96132274166695	-0.15983644491000
N	1.18461072338289	6.38205595431729	-0.29125511683433
C	1.16663827731675	7.43048891528392	-1.20142673167192
C	2.22571340676465	8.26509662241410	-0.94389567004007
N	2.89532991125340	7.72500425025534	0.13497370790687
C	2.24536201870734	6.59256160220954	0.49973655776482
H	2.55664587444787	9.18004543835985	-1.42098040095239

H	0.40595473747660	7.51220537283452	-1.96958946589792
H	2.56100544447317	5.96309098803625	1.32465458857403
C	4.09402069617114	8.27332119246389	0.77390304548638
H	4.37482068332731	9.19232401850640	0.25146303443716
H	4.91854137425828	7.55298251603905	0.70766357477538
H	3.88719447401486	8.50445127298737	1.82553473366676

[Cu(2,2′-bipyridine)(acetonitrile)$_2$]$^+$

Charge: 1 Spin Multiplicity: 1

H	2.09432191370880	0.36953225350636	1.65885041660580
C	1.40866559323587	1.03950292669926	1.14082374609585
C	0.03969781410496	0.77410411145650	1.07254919154636
H	-0.38032735893542	-0.11672061055479	1.54012475559734
C	-0.78860584342700	1.66612239492712	0.39511724810939
H	-1.85825002384246	1.47082450591003	0.33546864625547
C	-0.23357566161269	2.80633996064703	-0.20271584364892
N	1.09972728812299	3.05967161609558	-0.13162592707188
C	1.89219398782536	2.19224594098971	0.52569078311941
H	2.95457725535748	2.43959787350745	0.55492706403831
C	-1.04424630935975	3.80658564848392	-0.94308455457718
C	-2.42784226689020	3.67957321666432	-1.12961946111689
H	-2.96614331517077	2.82185133849906	-0.73040174662202
C	-3.11826266823013	4.66124844570490	-1.83688429770788
H	-4.19414853788347	4.57200442387332	-1.99100177751458
C	-2.41179742275756	5.75359009426274	-2.34363287028239
H	-2.91012446348318	6.54607836920763	-2.90150235965431
C	-1.03769398444974	5.81539388007159	-2.12222140588983
H	-0.44633422615965	6.65008105506367	-2.50170449176970
N	-0.36181618969785	4.87063169586399	-1.44174067676002
N	2.77434384212753	4.57165635608066	-2.65579014428694
C	3.43362068761012	4.41239252624763	-3.59956912569827
C	4.25566949644949	4.21581816122954	-4.77603689455758
H	4.94608344422752	5.06253452288986	-4.89429009843789
H	3.61876585018973	4.14363674568950	-5.66823342204570
H	4.83707409519366	3.28907044569008	-4.67388798048909
N	2.36447443761750	6.19346627751214	0.09481205014719
C	2.79667339027239	7.01732063207063	0.79149245009889
C	3.33268685156147	8.04489995426832	1.66083981515687
H	2.56887197289997	8.35437125036705	2.38752497946509
H	3.63679141377155	8.91617528160596	1.06457271425440
H	4.20705819892609	7.65647416093347	2.20103592990915
Cu	1.67997073869742	4.81432454453576	-1.07459671226846

[Cu(2,2′-bipyridine)(acetonitrile)(N-methylimidazole)]$^+$

Charge: 1 Spin Multiplicity: 1

H	1.96498048244322	0.45330482678484	1.63592874042124
C	1.25072748247070	1.04640034556680	1.06532068404038
C	-0.10968605015981	0.72994596036710	1.04415496767193
H	-0.49304879409725	-0.12519718277411	1.60150384759707
C	-0.97550244105269	1.52457427915256	0.29679556424059
H	-2.03890439594818	1.29052921850250	0.27135989888058
C	-0.46649748757748	2.61888984783059	-0.41723498575448
N	0.85871810304285	2.92119455712202	-0.39538113395101
C	1.68705777984297	2.14787250266229	0.33279071123315
H	2.74094401789897	2.43119452960147	0.32122313623747
C	-1.31859273322188	3.51732137785929	-1.23511281422004
C	-2.70418705904724	3.34448041112312	-1.36716892946160
H	-3.21166641051002	2.52409254343201	-0.86258576267915
C	-3.43471658273336	4.23291187455908	-2.15253044408600
H	-4.51238663775504	4.10831386082540	-2.26532363835566
C	-2.76549426286751	5.28055560500744	-2.78982013978175
H	-3.29602477429462	6.00076494582059	-3.41250846360294
C	-1.38812585878072	5.39219261650825	-2.61456419035446
H	-0.82558293025027	6.19516598328015	-3.09356580499500
N	-0.67156296681800	4.53660571067937	-1.86005860059450
Cu	1.37743036665796	4.58251683188728	-1.52718930600638
N	1.95993823248343	6.15346709518776	-0.39381451267505
C	1.35006069635973	6.62073657804509	0.75799094243481
C	2.04971011970123	7.70019412205309	1.24209815860996
N	3.10412094509307	7.89506325004663	0.37124982075801
C	3.01417722401800	6.94657733112452	-0.59629010960226
H	1.89769268100300	8.33323206063833	2.10909568058853
H	0.45632682734734	6.15781174467858	1.16158745101418
H	3.72248271711860	6.86932946233685	-1.41528801418432
C	4.12609094687608	8.93487363985648	0.47014233765454
H	4.68027246502651	8.82909331032179	1.41110529252522
H	3.65859473813179	9.92623842708043	0.42994198996246
H	4.82072462143406	8.82834341678276	-0.37012060960983
N	2.53585942381486	4.32714173357937	-3.03284079122559
C	3.22780596646178	4.16363505082574	-3.95422532906178
C	4.08818242925860	3.95686072665717	-5.10186708674473
H	4.79713122996413	4.79147512775049	-5.19483798820224
H	3.48294326524650	3.89750369481506	-6.01690368107005
H	4.65055662341867	3.02020258242177	-4.98373688765131

[Cu(2,2′-bipyridine)(N-methylimidazole)$_2$]$^+$

Charge: 1 Spin Multiplicity: 1

H	1.40995369409261	0.15591861795685	1.60693378153205
C	0.74073028924516	0.84048566644908	1.08588851801407
C	-0.63819713260484	0.61734083901271	1.03573089069617
H	-1.08171565494559	-0.25376460754170	1.51869479200378
C	-1.44206228665239	1.52702027030583	0.35345380175360
H	-2.51793889988246	1.36408946846906	0.30243575906568
C	-0.85680142957724	2.64171294531654	-0.26567776317738
N	0.48678749705347	2.85536461558247	-0.21463792911205
C	1.25429147492203	1.96687182785151	0.44876112892005
H	2.32556114768917	2.17664011328047	0.46234989688691
C	-1.63852089025005	3.65341622447081	-1.01584284450570
C	-3.03475179346292	3.60156332555248	-1.14308582683585
H	-3.60437542671857	2.79608623232833	-0.68236798458816
C	-3.69745711087654	4.59033002007870	-1.86584980719475
H	-4.78242147323166	4.55953320631601	-1.97322371258970
C	-2.94849553390252	5.61675695307931	-2.44837924483879
H	-3.42279377594898	6.41305090363622	-3.02211576486477
C	-1.56628668524969	5.60640599423816	-2.28233690827243
H	-0.94532413441844	6.38891785786631	-2.72177243932869
N	-0.91249409092829	4.65394532120758	-1.58616311816664
Cu	1.12556078957411	4.52875344097897	-1.25616951059958
N	1.96344587808934	6.01020759602977	-0.17766214595775
C	2.11961087717916	6.06492076842763	1.19758038891708
C	2.70059872717425	7.26109676612389	1.54729206463449
N	2.90118069484681	7.94959225135913	0.36716745152992
C	2.44598596943847	7.16441867891863	-0.64421492738146
H	2.98359140566894	7.67566323362874	2.50815645171865
H	1.80580532132811	5.25045140147576	1.84152618075748
H	2.48092821606804	7.46764113832586	-1.68558556659143
C	3.49500908166089	9.27790488418476	0.22827804715408
H	4.52605757098829	9.27068327403225	0.60215789840589
H	2.90662954545260	10.01329362641360	0.79006247574960
H	3.49707386600564	9.55133948938752	-0.83219814921320
H	5.56532053621982	4.57869844633817	-5.47152818190244
H	5.74007743705202	2.88242740173349	-4.92125863918491
C	5.44087481534233	3.89455816637555	-4.62285608357404
H	3.04946708743369	3.12931679000100	-5.93328899401064
C	2.95319465246133	3.49155092413123	-4.91608688438569
N	4.04893823710808	3.89308333828708	-4.17720651792410

C	1.86016774778322	3.65800793766972	-4.09913273587168
C	3.59602591930965	4.28440631414546	-2.95743154198522
N	2.27001132166358	4.15599457615697	-2.87307651658162
H	0.81705610891943	3.44971761645948	-4.31146581838185
H	4.25239715184899	4.64646936089955	-2.17270241873975
H	6.07441325703095	4.22783678305907	-3.79408155197926

[Cu(2,2′-bipyridine)(acetonitrile)]$^{+}$

Charge: 1 Spin Multiplicity: 1

H	2.24753914063841	0.61750969756404	1.68626541607777
C	1.53770709190117	1.24115008405373	1.14418537992228
C	0.19459631446770	0.88405609344529	1.02354328579065
H	-0.17998462604615	-0.03544753810585	1.47333278726864
C	-0.66991939655735	1.71919443204339	0.31675015908069
H	-1.72028982120945	1.45140927855901	0.21576808525437
C	-0.17282884138835	2.89458062910768	-0.25664868340952
N	1.13687773113561	3.23699836395265	-0.13410525055144
C	1.96634216448567	2.42672732805733	0.55016820609045
H	3.00612236999004	2.74731656570442	0.61843453998865
C	-1.01723466416907	3.84636576143383	-1.02517083469119
C	-2.38187440708685	3.64504728402231	-1.25871442646682
H	-2.88650717980071	2.75898714875519	-0.87840500975719
C	-3.09770503396132	4.59274037296507	-1.98920480071947
H	-4.16112972393228	4.44681207161579	-2.18043721628730
C	-2.43579463576612	5.72284338024494	-2.46949084385465
H	-2.95682565007976	6.48877815883160	-3.04292220845190
C	-1.07515469175002	5.86060876825219	-2.20077993039989
H	-0.51566913816944	6.72627695828471	-2.55635603269240
N	-0.37853732496465	4.94846554803618	-1.49772558767235
N	3.04200239893003	6.08434355280208	-1.33670740473640
C	3.94803499826943	6.78518002289741	-1.53690729839917
C	5.07798392073039	7.65243802389543	-1.78635107338560
H	5.91739984834655	7.37355711953233	-1.13442055671253
H	4.79637435037680	8.69648929224793	-1.58916500056416
H	5.38900358478206	7.55692533128839	-2.83614141678919
Cu	1.59907122082767	4.98636627051291	-1.03709428393234

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