

Supplementary Information

Homo- and Heterogeneous Benzyl Alcohol Catalytic Oxidation Promoted by Mononuclear Copper(II) Complexes: The Influence of the Ligand upon Product Conversion

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Table of contents (order of appearance)

Figure S1. FTIR (ATR) spectra of complexes 1-3 .	3
Figure S2. UV-Vis spectra of complexes 1-3 in acetonitrile. $[C] = 1.0 \times 10^{-4} \text{ mol L}^{-1}$, insets $[C] = 1.0 \times 10^{-2} \text{ mol L}^{-1}$.	4
Figure S3. Cyclic voltammograms of 1-3 in acetonitrile. Conditions: Scan rate 100 mV s^{-1} (1) and 300 mV s^{-1} (2 and 3). The ferrocene/ferrocinium redox pair was used as standard. Supporting electrolyte: $0.1 \text{ mol L}^{-1} n\text{-Bu}_4\text{NPF}_6$; Working electrode: Pt, counter: Pt wire and reference: Ag/Ag^+ . Complexes concentration $5.0 \times 10^{-3} \text{ mol L}^{-1}$.	5
Figure S4. Size distributions from Fe_3O_4 (top), $\text{Fe}_3\text{O}_4@\text{SiO}_2$ (middle) and $\text{Fe}_3\text{O}_4@\text{SiO}_2\text{-3}$ (bottom) obtained by DLS.	6
Figure S5. TEM images from Fe_3O_4 (A-B), $\text{Fe}_3\text{O}_4@\text{SiO}_2$ (C -D) and $\text{Fe}_3\text{O}_4@\text{SiO}_2\text{-3}$ (E-F).	7
Figure S6. XRD patterns for Fe_3O_4 and $\text{Fe}_3\text{O}_4@\text{SiO}_2$ nanoparticles.	8
Figure S7. X-Ray Energy Dispersive Spectroscopy (EDS) of the composite $\text{Fe}_3\text{O}_4@\text{SiO}_2\text{-3}$.	9
Figure S8. Linear correlation between the conversion (%) of benzyl alcohol (BnOH) into benzaldehyde (BA) and reaction volume (mL) reciprocal. Conditions: 1.0 mol% of 3 - $\text{Fe}_3\text{O}_4@\text{SiO}_2$, 20-fold H_2O_2 over BnOH, 24 h, 20°C .	10
Table S1. Selected bond lengths for the calculated complexes within D3-B3LYP/Def2-TZVP(-f) level of theory, and some crystallographic data values for comparison.	11
Table S2. Attributions of IR bands for complexes 1-3 (experimental and calculated within D3-B3LYP/Def2-TZVP(-f) level of theory).	11
Figure S9. Theoretical absorption spectra of 1-3 within D3-B3LYP/Def2-TZVP(-f) level of theory in CH_3CN and convoluted with Gaussians of 25 nm width.	12
Table S3. Data for the TD-DFT excitations within D3-B3LYP/Def2-TZVP(-f) level for complex 1 . For the TD-DFT difference densities between ground and a specified excited state, hydrogens were omitted for clarity, blue indicates decreased and red indicates increased electronic density.	13
Table S4. Data for the TD-DFT excitations within D3-B3LYP/Def2-TZVP(-f) level for complex 2 . For the TD-DFT difference densities between ground and a specified excited	14

state, hydrogens were omitted for clarity, blue indicates decreased and red indicates increased electronic density.

Table S5. Data for the TD-DFT excitations within D3-B3LYP/Def2-TZVP(-f) level for complex **3**. For the TD-DFT difference densities between ground and a specified excited state, hydrogens were omitted for clarity, blue indicates decreased and red indicates increased electronic density. 15

Table S6. Calibration parameters obtained for product quantification extracted from the GC-MS analysis. 16

Table S7. Set of experiments considering the Box-Behnken approach for catalytic assays. (Average values calculated with previously determined upper and lower limits) 16

Figure S10. Residual graph obtained by modeling %conversion as a function of catalyst concentration (**1**, top; **2**, middle; **3** bottom), H₂O₂ concentration and reaction time with a 10-coefficients quadratic regression equation. $R^2 = 0.97$ for **1**, 0.93 for **2** and 0.98 for **3**. 17

Table S8. Cartesian coordinates for the optimized geometry of Cu(II)-OOH specie derived from complex **1**. 18

Table S9. Cartesian coordinates for the optimized geometry of Cu(II)-OOH specie derived from complex **2**. 19

Table S10. Cartesian coordinates for the optimized geometry of Cu(II)-OOH specie derived from complex **3**. 20

Table S11. Cartesian coordinates for the optimized geometry of [Cu(II)-O•]⁺ specie derived from complex **1**. 21

Table S12. Cartesian coordinates for the optimized geometry of [Cu(II)-O•]⁺ specie derived from complex **2**. 22

Table S13. Cartesian coordinates for the optimized geometry of [Cu(II)-O•]⁺ specie derived from complex **3**. 23

Table S14. Cartesian coordinates for the reactants, TS, and products between [Cu(II)-O•]⁺ species derived from complex **1** and BA. 24

Table S15. Cartesian coordinates for the reactants, TS, and products between [Cu(II)-O•]⁺ species derived from complex **2** and BA. 27

Table S16. Cartesian coordinates for the reactants, TS, and products between [Cu(II)-O•]⁺ species derived from complex **3** and BA. 30



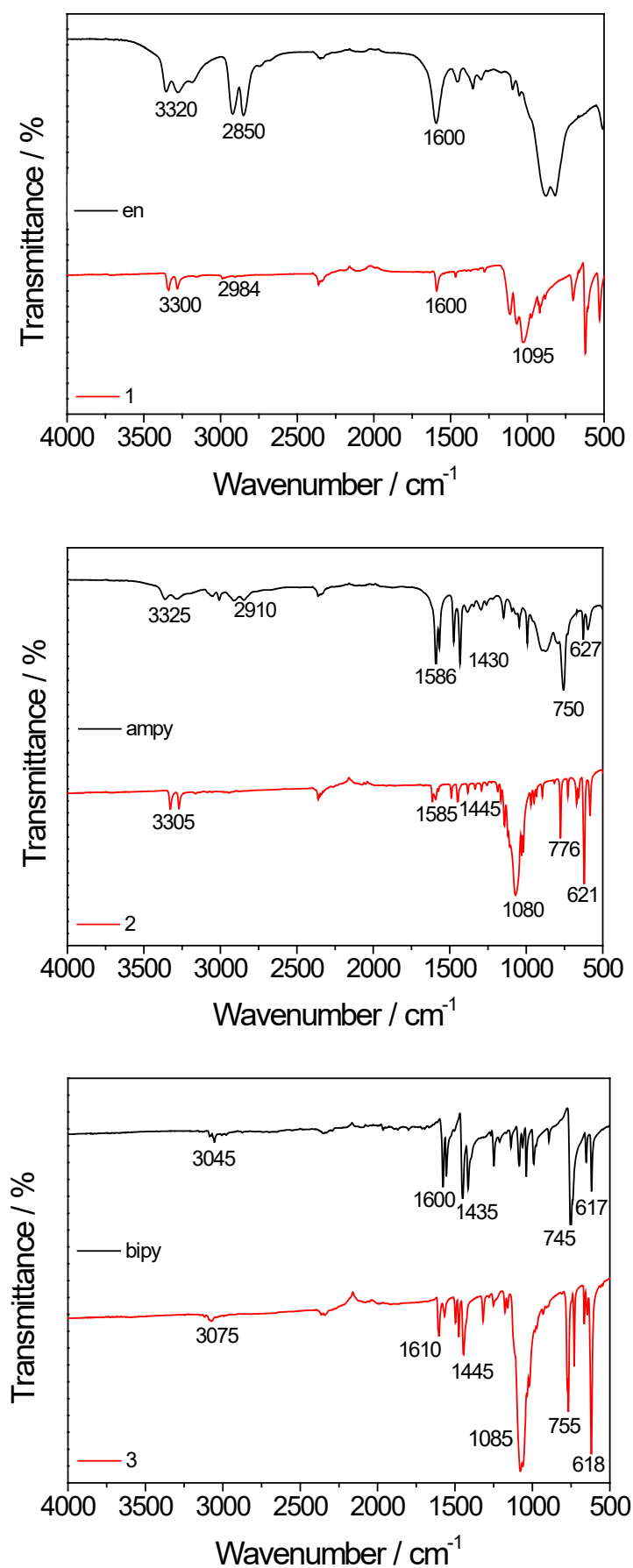


Figure S1. FTIR (ATR) spectra of complexes **1-3**.



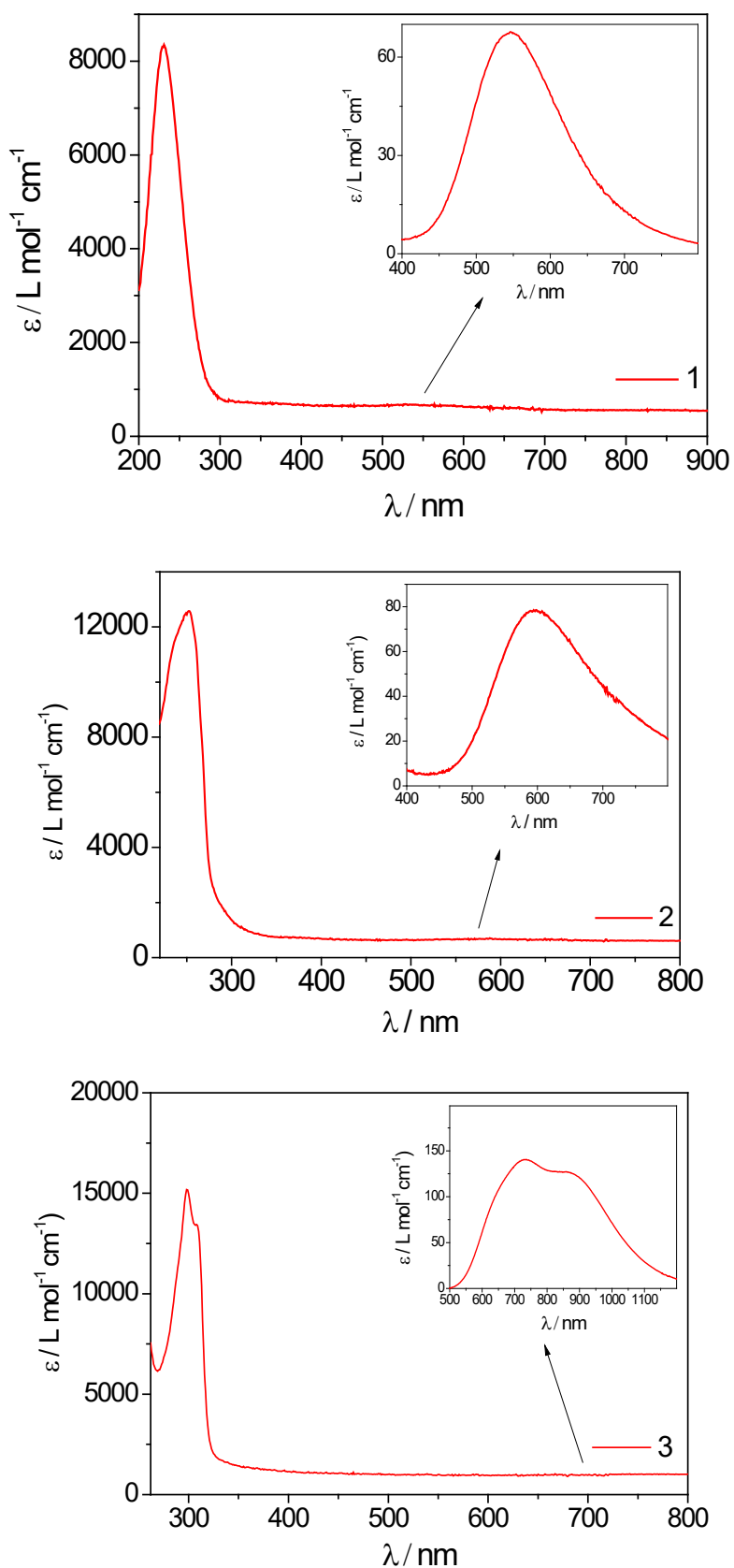


Figure S2. UV-Vis spectra of complexes **1-3** in acetonitrile. $[C] = 1.0 \times 10^{-4} \text{ mol L}^{-1}$, insets $[C] = 1.0 \times 10^{-2} \text{ mol L}^{-1}$.

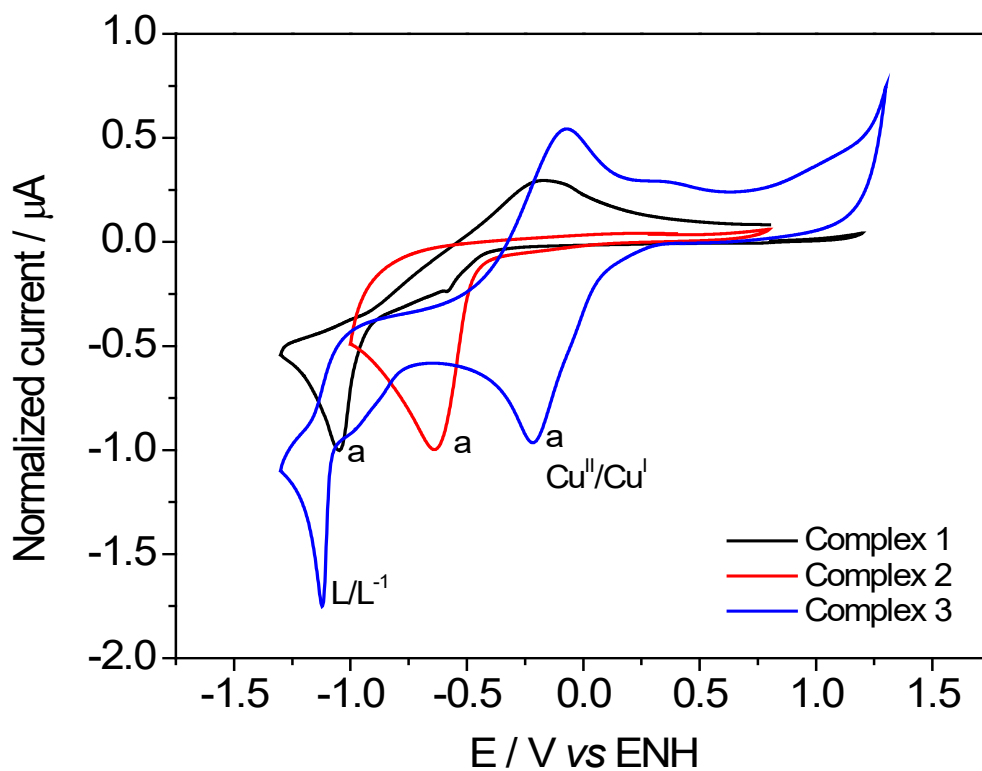


Figure S3. Cyclic voltammograms of **1-3** in acetonitrile. Conditions: Scan rate 100 mV s^{-1} (**1**) and 300 mV s^{-1} (**2** and **3**). The ferrocene/ferrocinium redox pair was used as standard. Supporting electrolyte: $0.1 \text{ mol L}^{-1} n\text{-Bu}_4\text{NPF}_6$; Working electrode: Pt, counter: Pt wire and reference: Ag/Ag^+ . Complexes concentration $5.0 \times 10^{-3} \text{ mol L}^{-1}$.

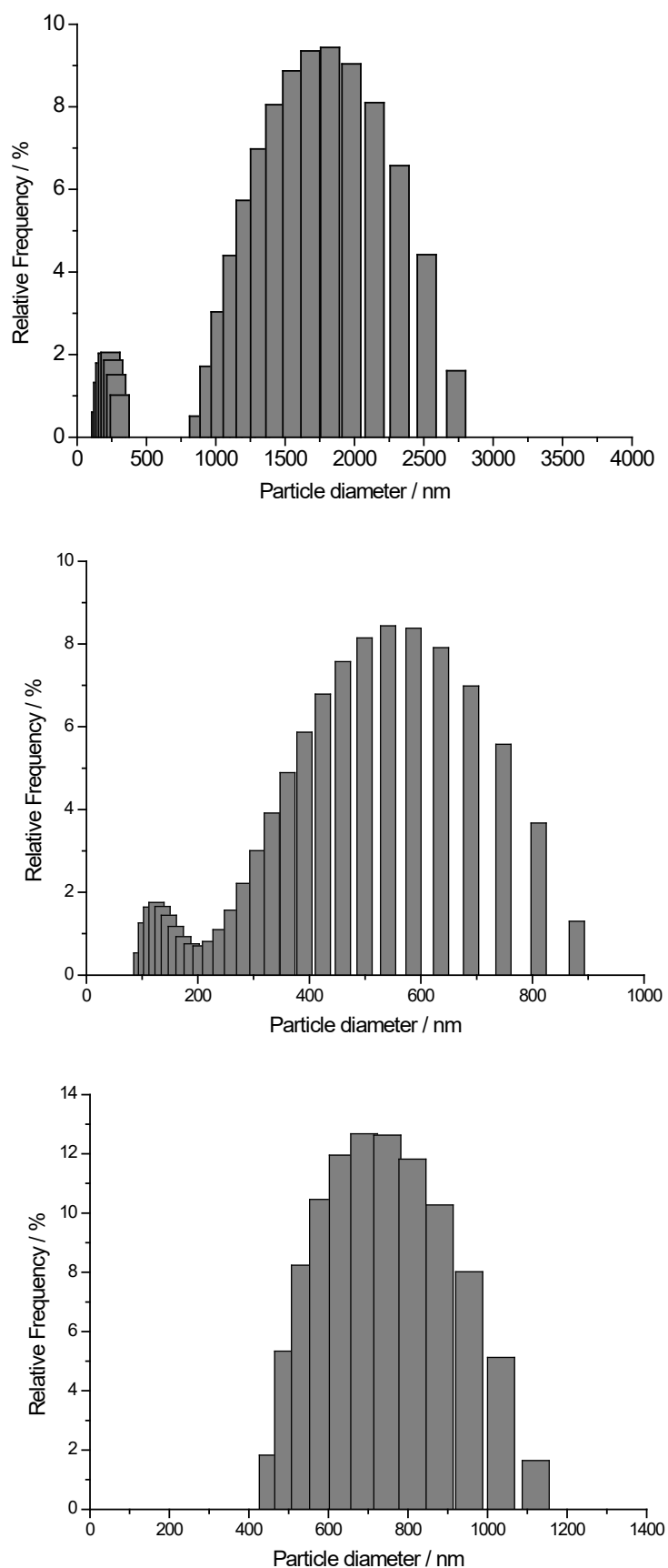


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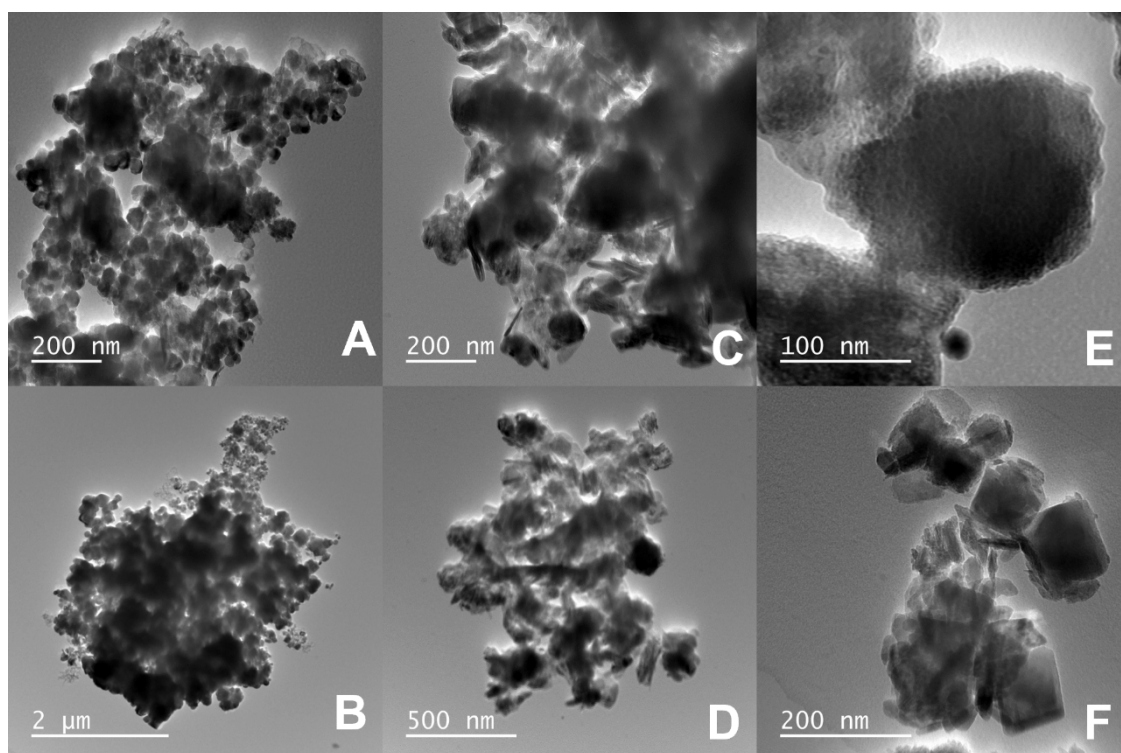


Figure S5. TEM images from Fe_3O_4 (A-B), $\text{Fe}_3\text{O}_4@\text{SiO}_2$ (C -D) and $3\text{-Fe}_3\text{O}_4@\text{SiO}_2$ (E-F).

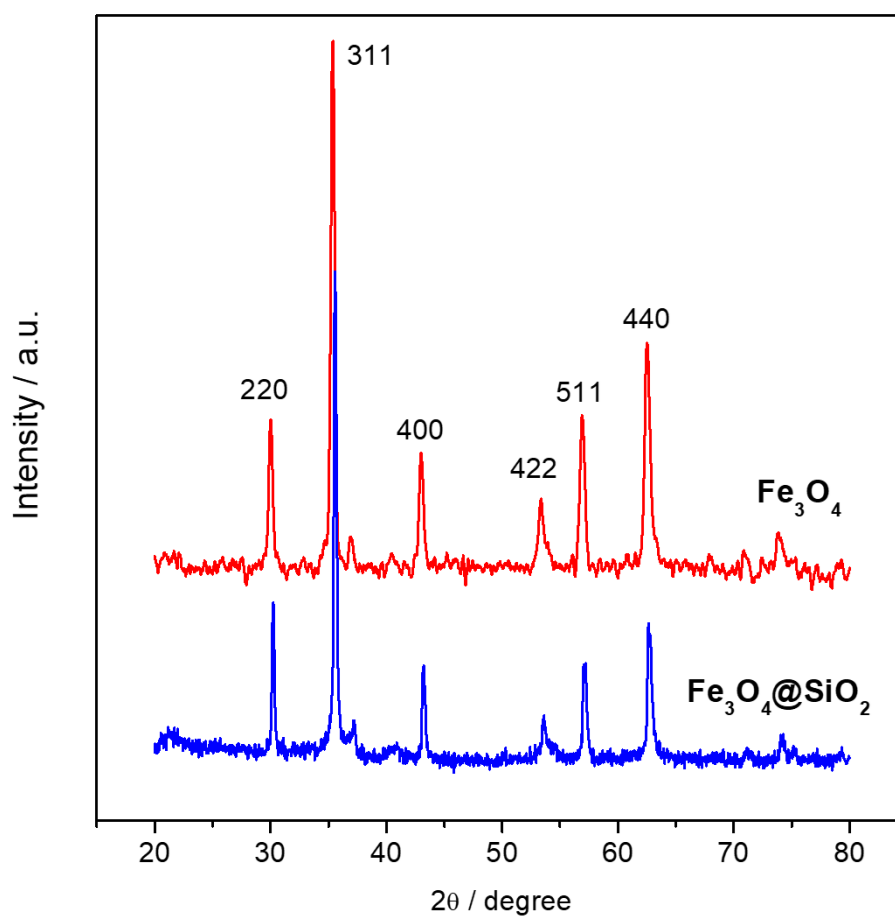


Figure S6. XRD patterns for Fe_3O_4 and $\text{Fe}_3\text{O}_4@\text{SiO}_2$ nanoparticles.

Full scale counts: 1505

Base(3)

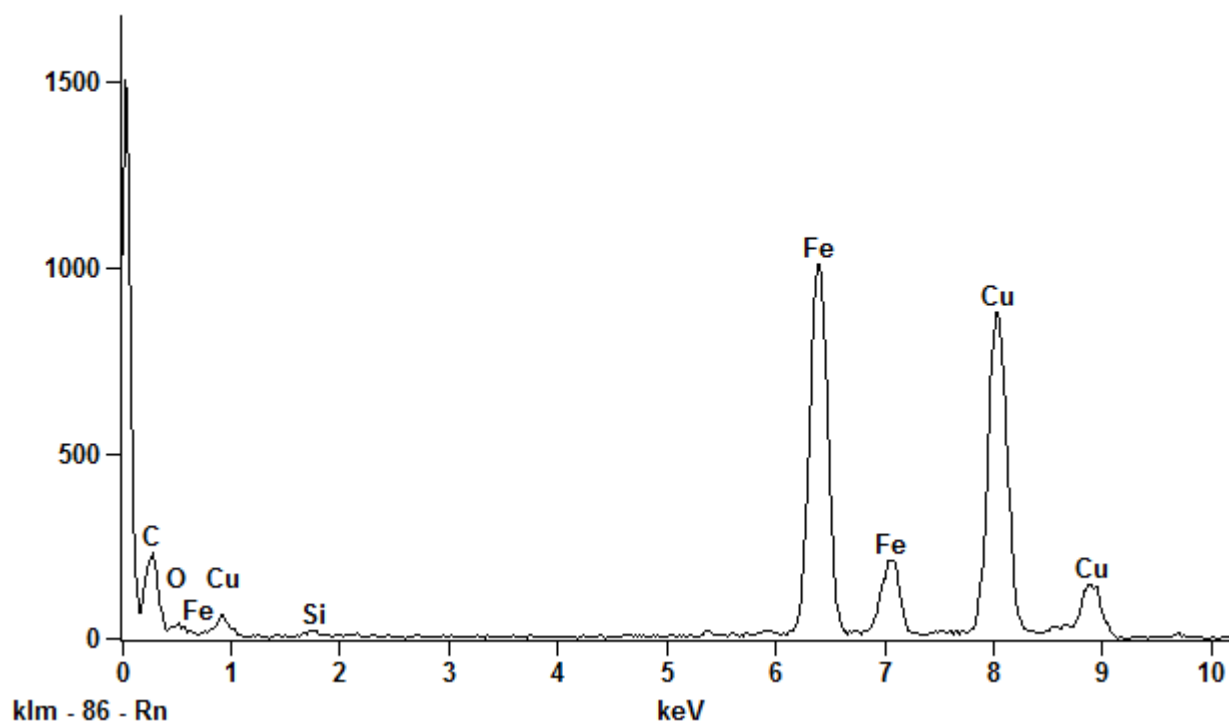


Figure S7. X-Ray Energy Dispersive Spectroscopy (EDS) of the composite **3**-Fe₃O₄@SiO₂.

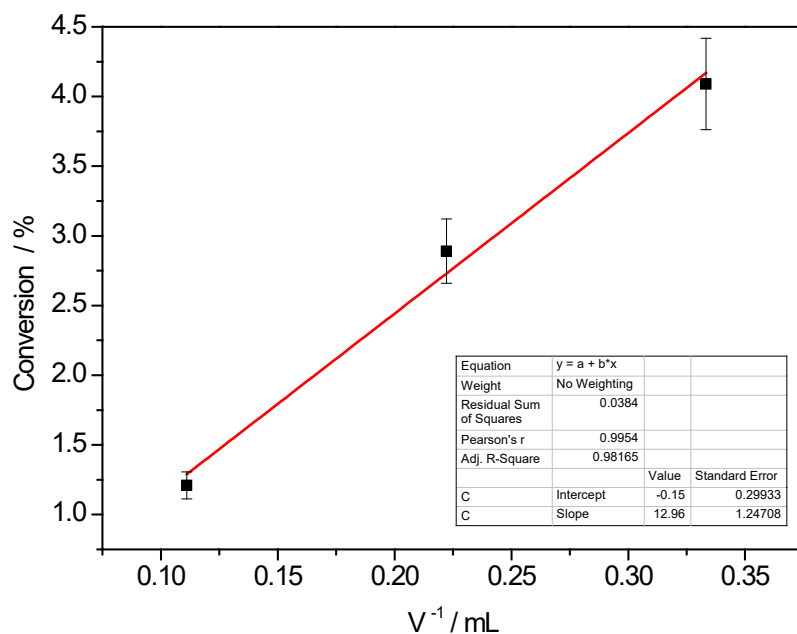


Figure S8. Linear correlation between the conversion (%) of benzyl alcohol (BnOH) into benzaldehyde (BA) and reaction volume (mL) reciprocal. Conditions: 1.0 mol% of **3**-Fe₃O₄@SiO₂, 20-fold H₂O₂ over BnOH, 24 h, 20 °C.

Table S1. Selected bond lengths for the calculated complexes within D3-B3LYP/Def2-TZVP(-f) level of theory, and some crystallographic data values for comparison.

Theoretical	1 ^a	1 Theo	2 Theo	3 ^b	3 Theo
Cu(II)-N₁	2.002	2.037	2.032	2.004	2.006
Cu(II)-N₂	2.003	2.038	2.018	1.986	2.002
Cu(II)-N₃	2.018	2.036	2.030	2.006	2.002
Cu(II)-N₄	2.003	2.038	2.017	1.979	2.003
N₁-Cu(II)-N₂	84.75	84.55	82.00	81.89	81.81
N₁-Cu(II)-N₃	180.00	176.83	169.87	154.95	152.66
N₁-Cu(II)-N₄	95.25	95.49	98.65	101.74	104.51
N₂-Cu(II)-N₃	95.25	95.48	98.46	102.95	104.69
N₂-Cu(II)-N₄	180.00	177.07	172.80	159.03	153.11
N₃-Cu(II)-N₄	84.75	84.63	82.16	82.57	81.82

Experimental DRX data reported by (a) Altahan, A.M.; Beckett, M.A.; Coles, S.J.; Horton, P.N. Synthesis and characterization of polyborates templated by cationic copper(II) complexes: Structural (XRD), spectroscopic, thermal (TGA/DSC) and magnetic properties. *Polyhedron*. **2017**, 135, 247-257. (b) Kamp, K.R.; Wang, Y.; Poeppelmeier, K.R. Targeting Oxide Concentration in Tantalum Oxide-Fluoride Anions. *Sol. State Sci.* **2023**, 146, 107369.

Table S2. Attributions of IR bands for complexes **1-3** (experimental and calculated within D3-B3LYP/Def2-TZVP(-f) level of theory).

Attribution	1 Exp. (Calc.)	2 Exp. (Calc.)	3 Exp. (Calc.)
<i>v</i> (N-H)	3335 - 3280 (3539 - 3464)	3327 - 3270 (3545 - 3474)	- (-)
<i>v</i> (CH_{ar} - CH_{aliph})	2988 - 2901 (3120 - 3063)	- (3225 - 3063)	3118 - 3072 (3236 - 3202)
δ (N-H)	1590 (1629 - 1625)	1613 - 1592 (1654 - 1643)	- (-)
<i>v</i> (C=C and C=N)	- (-)	1490 - 1447 (1526 - 1484)	1602 - 1445 (1648 - 1513)
<i>v</i> (C-C and C-N)	1113 - 1069 (1097 - 1009)	1070 - 1030 (1035)	- (-)
δ (C-H_{ar})	- (-)	776 (775 - 747)	767 (776 - 752)



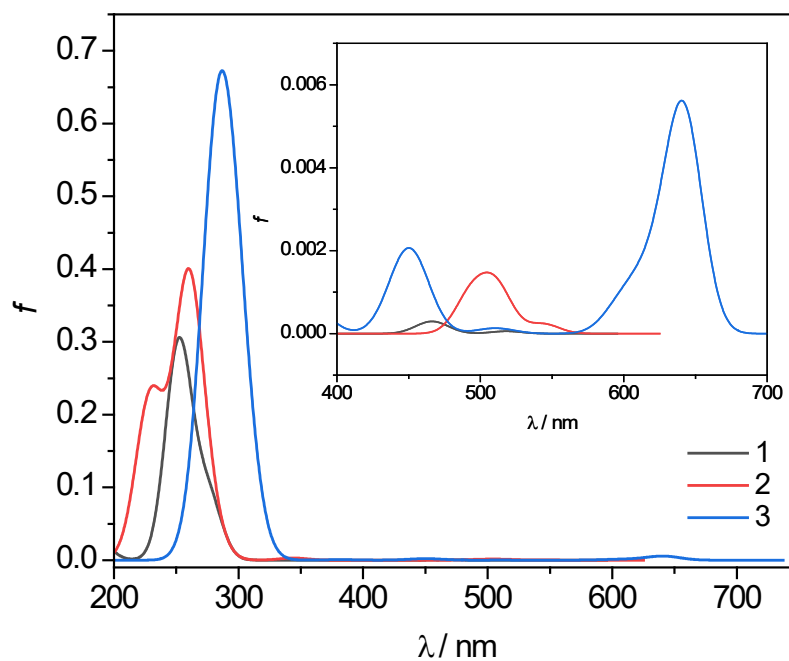
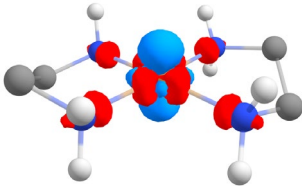
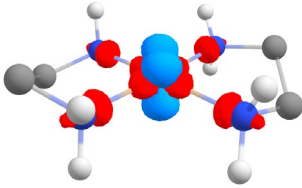
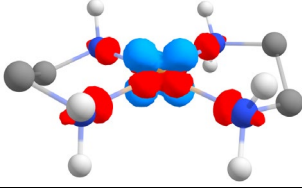
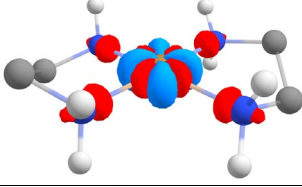
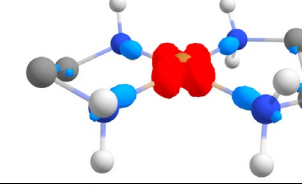
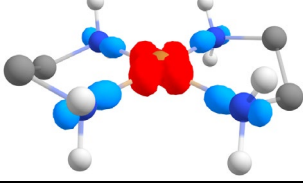


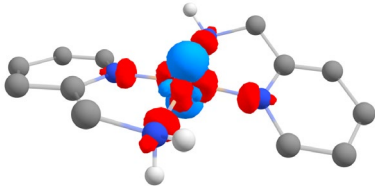
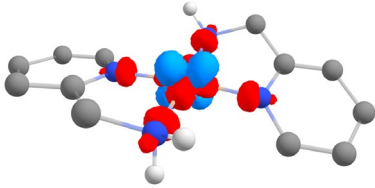
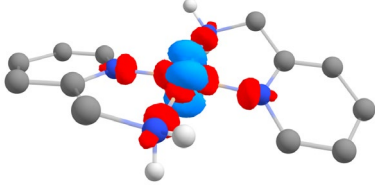
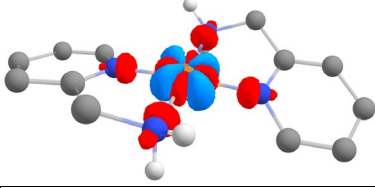
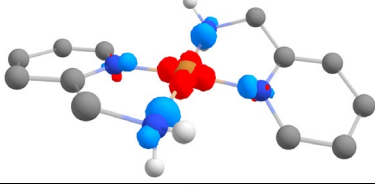
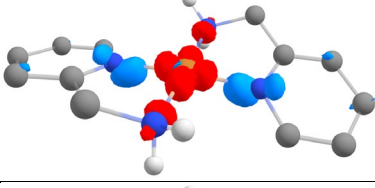
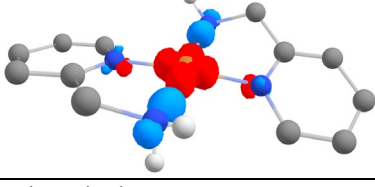
Figure S9. Theoretical absorption spectra of **1-3** within D3-B3LYP/Def2-TZVP(-f) level of theory in CH₃CN and convoluted with Gaussians of 25 nm width.

Table S3. Data for the TD-DFT excitations within D3-B3LYP/Def2-TZVP(-f) level for complex **1**. For the TD-DFT difference densities between ground and a specified excited state, hydrogens were omitted for clarity, blue indicates decreased and red indicates increased electronic density.

State	Energy		f	Attribution ^a	Difference Densities
	eV	nm			
S ₁	2.393	518	6×10^{-5}	$dz^2 \rightarrow dx^2-y^2$	
S ₂	2.637	470	0.0001	$dxz \rightarrow dx^2-y^2$	
S ₃	2.681	462	0.0001	$dyz \rightarrow dx^2-y^2$	
S ₄	2.703	458	1×10^{-6}	$dxy \rightarrow dx^2-y^2$	
S ₅	4.502	275	0.0887	LMCT $n(\text{NH}_2) \rightarrow dx^2-y^2$	
S ₆	4.921	252	0.2977	LMCT $n(\text{NH}_2) \rightarrow dx^2-y^2$	

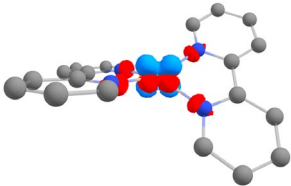
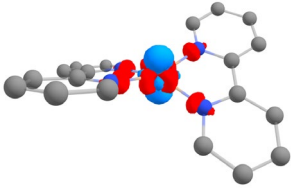
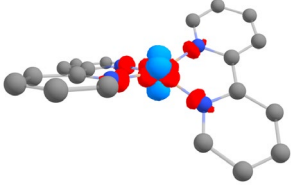
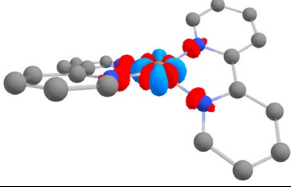
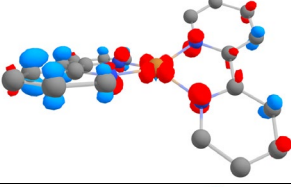
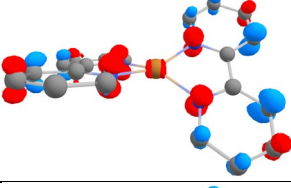
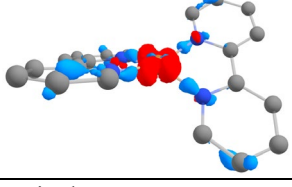
^a Attributions were given based on the most significant contribution transitions for each excited state.

Table S4. Data for the TD-DFT excitations within D3-B3LYP/Def2-TZVP(-f) level for complex **2**. For the TD-DFT difference densities between ground and a specified excited state, hydrogens were omitted for clarity, blue indicates decreased and red indicates increased electronic density.

State	Energy		<i>f</i>	Attribution ^a	Difference Densities
	eV	nm			
S ₁	2.280	544	0.0002	$dz^2 \rightarrow dx^2-y^2$	
S ₂	2.426	511	0.0011	$dxz \rightarrow dx^2-y^2$	
S ₃	2.513	493	0.0009	$dyz \rightarrow dx^2-y^2$	
S ₄	2.650	468	9×10^{-7}	$dxy \rightarrow dx^2-y^2$	
S ₁₂	4.464	277	0.0238	LMCT $n(\text{NH}) \rightarrow dx^2-y^2$ MLCT $dx^2-y^2 \rightarrow \pi^*(\text{pyridine})$	
S ₁₅	4.701	264	0.1480	LMCT $n(\text{NH}) \rightarrow dx^2-y^2$	
S ₁₆	4.821	257	0.2206	LMCT $n(\text{NH}) \rightarrow dx^2-y^2$	

^a Attributions were given based on the most significant contribution transitions for each excited state.

Table S5. Data for the TD-DFT excitations within D3-B3LYP/Def2-TZVP(-f) level for complex **3**. For the TD-DFT difference densities between ground and a specified excited state, hydrogens were omitted for clarity, blue indicates decreased and red indicates increased electronic density.

State	Energy		<i>f</i>	Attribution ^a	Difference Densities
	eV	nm			
S ₁	1.933	641	0.0053	$dxz \rightarrow dx^2-y^2$	
S ₂	2.006	618	0.0011	$dz^2 \rightarrow dx^2-y^2$	
S ₃	2.069	599	0.0007	$dyz \rightarrow dx^2-y^2$	
S ₄	2.429	510	0.0001	$dxy \rightarrow dx^2-y^2$	
S ₁₇	4.176	297	0.1491	LMCT $\pi(\text{pyridine}) \rightarrow dx^2-y^2$	
S ₂₄	4.339	286	0.1132	$\pi(\text{pyridine}) \rightarrow \pi^*(\text{pyridine})$	
S ₂₇	4.437	280	0.1631	LMCT $\pi(\text{pyridine}) \rightarrow dx^2-y^2$	

^a Attributions were given based on the most significant contribution transitions for each excited state.

Table S6. Calibration parameters obtained for product quantification extracted from the GC-MS analysis.

Compound	Benzaldehyde (BA)	Benzoic acid (BzA)
Linear range (%conversion)	0.20 – 60	0.90-60
LOQ (%conversion)	0.20%	0.90%
R ²	0.9976	0.9861

LOQ = Limit of quantification.

Table S7. Set of experiments considering the Box-Behnken approach for catalytic assays. (Average values calculated with previously determined upper and lower limits)

Entry	Catalyst load / mol%	H ₂ O ₂ / (nH ₂ O ₂ /nBnOH)	Time / h
1	0.10	10.5	8
2	3.00	10.5	8
3	1.55	1.0	8
4	1.55	20.0	8
5	3.00	10.5	24
6	1.55	1.0	24
7	0.10	10.5	24
8	1.55	20.0	24
9	0.10	1.0	16
10	3.00	1.0	16
11	0.10	20.0	16
12	3.00	20.0	16
13	1.55	10.5	16
14	1.55	10.5	16
15	1.55	10.5	16



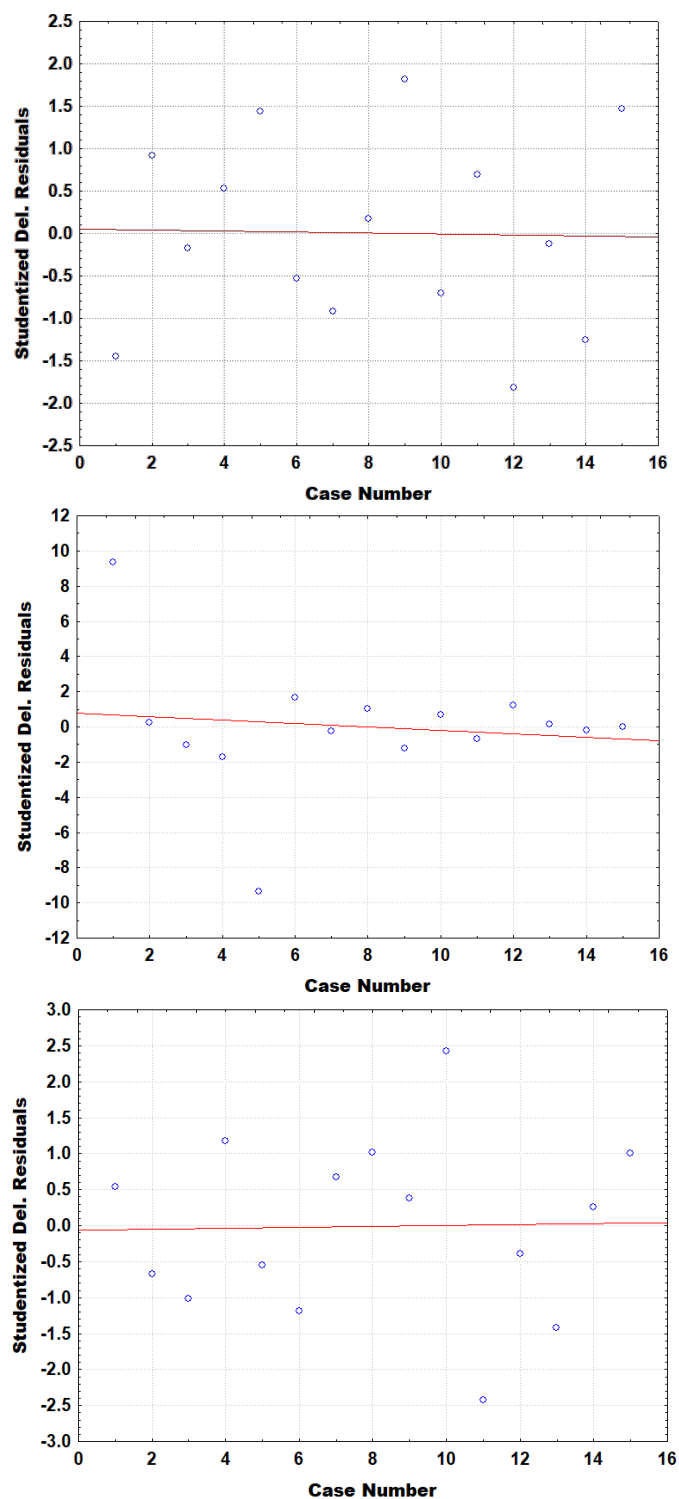


Figure S10. Residual graph obtained by modeling %conversion as a function of catalyst concentration (1, top; 2, middle; 3 bottom), H_2O_2 concentration and reaction time with a 10-coefficients quadratic regression equation. $R^2 = 0.97$ for 1, 0.93 for 2 and 0.98 for 3.

Table S8. Cartesian coordinates for the optimized geometry of Cu(II)-OOH specie derived from complex 1.

Cu	5.03050842574261	9.15505558443390	6.55157821609912
N	4.74819620951170	10.61115769111753	4.78133143016667
C	5.27871071188184	11.88298928900756	5.28715305953078
C	6.52630042570518	11.62684425118119	6.12662711169254
N	3.83020923040801	7.62491379844082	5.92979597926982
C	2.62789755003655	7.56474665697529	6.77439734990520
C	2.15195765758010	8.99053316579563	7.02877160221127
N	6.21295587127866	10.71208485772580	7.24324090466183
O	6.68276715904840	8.16508014310338	6.32795332222065
N	3.27857806015797	9.77471720287180	7.56969235382469
H	1.84981906521495	9.45241008451905	6.07534647607392
H	1.27583588351571	8.99468518320873	7.69814540850740
H	3.40846412771238	9.57841607636852	8.56512382246103
H	3.09848309124714	10.77707994026587	7.49670345451128
H	5.74361593019892	11.21886313413078	7.99689753416162
H	7.29697633929693	11.14457180343206	5.50477403357498
H	6.93986911986972	12.58263397219149	6.48988128034956
H	2.90512939327980	7.08797298901230	7.72800643496284
H	1.82354442890623	6.96416533265544	6.31851396977921
H	3.58654430862581	7.77957496946297	4.94917509555050
H	5.52297927297898	12.60452602034382	4.48675375667174
H	3.78678013791825	10.71736931058050	4.45746772790493
H	5.29200959810769	10.28823205865619	3.97902634382295
H	4.42279927065846	6.79113375938744	5.96941511388676
H	7.06795071278381	10.32184069584047	7.64275980761201
H	4.50493087790740	12.34944711512014	5.91937528760277
O	6.51729022619019	6.79531337520536	5.89378942882705
H	6.70896691423598	6.85379153896477	4.94245369415610

Table S9. Cartesian coordinates for the optimized geometry of Cu(II)-OOH specie derived from complex 2.

Cu	4.16276002992402	10.50743216514085	7.57555043700386
N	3.85982078953139	12.33168922777695	6.67044201296695
C	5.13221587986688	12.81198525129106	6.11173368567553
C	5.93116292754326	11.65108234337114	5.56898000601084
C	6.87120242922570	11.79730149405456	4.54514276608284
H	7.02761078935928	12.77696631495141	4.08904705827486
C	7.58917512276983	10.67848663779939	4.12236338201671
H	8.32999464313959	10.76775852607550	3.32424500231894
C	7.33761476459791	9.44157623338426	4.72368013867998
C	6.37863290682032	9.37662221341712	5.73072854068470
H	6.13830363953872	8.42622082065023	6.21236611857995
H	7.86773851889866	8.53873070806268	4.41577403449760
N	3.01136614957959	8.96536669567386	6.26465012390953
C	2.59457582115450	9.08932618115027	5.00037219521343
C	2.29820201472261	7.98733825330797	4.19668296663911
H	1.95723604086978	8.13089699778345	3.16954030398427
C	2.45886969718845	6.70984641412406	4.74004447368537
H	2.24671701457722	5.82052890874908	4.14142005388052
C	2.90655967897432	6.58344526764362	6.05699792311247
H	3.05666682314626	5.60171256689792	6.51131270053656
H	2.49936811253754	10.10913621132552	4.61343175177083
C	3.16923255159153	7.74307055679671	6.79382530076198
C	3.61263339603066	7.69658902457413	8.24066923557899
N	5.70367784080522	10.45776287423469	6.14591436452523
O	3.15114798924772	11.19712315986608	9.07172723534977
N	4.58982506250013	8.75263399043271	8.55473988516730
H	2.72626999814429	7.87046192045965	8.87278294699263
H	3.99627798238067	6.69542695177809	8.48849169376267
H	5.54780765898966	8.42489990593105	8.42644101779865
H	3.15849605179991	12.22164767175659	5.93434896517769
H	5.70698592879376	13.28239220458185	6.92686776255849
H	4.99070313645232	13.57522738896362	5.33070312960466
H	4.47068572051963	9.04610675606757	9.52939332485876
H	3.47757212502472	12.99512879501096	7.34563909659917
O	3.11364840295412	10.36129829170409	10.24535741758219
H	2.22479236079938	9.96919107521020	10.19783294815628

Table S10. Cartesian coordinates for the optimized geometry of Cu(II)-OOH specie derived from complex 3.

Cu	6.19368374834488	5.54398555052999	6.21638119198634
N	7.81646953168238	4.89533720529459	7.28197126874464
C	7.92904018385209	3.66516009636598	7.79348717460878
C	9.03191172227003	3.28419703899059	8.55850051821775
H	9.09309264416283	2.27162931128341	8.96069191488687
C	10.03737839033663	4.22433552124488	8.79071846924864
H	10.91559703441779	3.96494587929638	9.38620398932115
C	9.91163852036257	5.50753480091095	8.25534627144076
H	10.68749703541583	6.25237732098349	8.43006060217838
H	7.10112644322055	2.98813277900163	7.56926317117549
C	8.77756535782272	5.81814044542752	7.49740516362717
C	8.52721395848522	7.14776069980660	6.88956319862095
C	9.39601029822478	8.23684648451746	7.02236258359447
H	10.32263833724148	8.14524429991408	7.58829263230133
C	9.05693854868431	9.45006960386344	6.42201834416311
H	9.72218044070596	10.31129754416942	6.51530847822282
C	7.86115728512750	9.54728641404157	5.70827344671758
C	7.04724975267225	8.41799545912244	5.61930301211883
H	6.10177001133985	8.44328353833448	5.07421584390874
H	7.55671843617120	10.47782330244860	5.22638897929112
N	4.60849229320266	6.44803780405857	7.49033616907835
C	4.61329311359104	6.55907863636213	8.81893587082406
C	3.52313224849638	7.06577166022251	9.52975105858034
H	3.56128502735571	7.14144986130301	10.61797792810750
C	2.39697624447770	7.46668568241804	8.80824540970431
H	1.52102116239298	7.86957231280869	9.32176809836055
C	2.39829041447711	7.35171152492462	7.41710122173330
H	1.52691062703165	7.66904196169481	6.84535865885250
H	5.52168434004580	6.22836898085944	9.33218117100956
C	3.53318763097077	6.83035022352436	6.78000388007507
C	3.63536670277165	6.67902297187545	5.30038477403019
C	2.57836591766732	6.97957848499735	4.43153475777150
H	1.62227361603877	7.33093030607446	4.81748955474863
C	2.75639549461310	6.81658934044809	3.05750664222410
C	3.98598553911153	6.36347043499468	2.57671541629422
C	4.99195134903555	6.08500480468865	3.50182165547936
H	5.97281518338625	5.72415138908640	3.18059209015118
H	4.16824390884948	6.22402585492817	1.50993130692763
H	1.93823409081921	7.04230389126797	2.36989061087054
N	7.37726395764707	7.25606051664557	6.19120017964920
O	5.51220154138029	3.74753856395904	6.13831657366223
N	4.81461675507405	6.23951091225987	4.81717231941420
O	4.08542120487994	3.70294037012287	6.06116025582453
H	3.82178395614242	3.74648021492706	6.99630814225133

Table S11. Cartesian coordinates for the optimized geometry of $[\text{Cu(II)}-\text{O}\cdot]^+$ specie derived from complex 1.

Cu	0.62444401588621	-1.79448609154173	-1.76471079899248
N	-1.08555368920136	-1.28072063080065	-2.84421542983213
N	2.22940345842625	-2.38840962523898	-0.57230321687943
N	-0.37245641226695	-0.82189942702790	-0.21531697600230
N	2.06132121795438	0.05064494635619	-2.11390525975398
C	-1.38929749352310	0.05862239323038	-0.82935010020119
C	-2.09785155977063	-0.72225712424032	-1.92069674163474
H	-2.63884572123460	-1.55923354323539	-1.48073738508155
H	-2.81449148264479	-0.08670692995336	-2.44349519110982
O	1.20264915794747	-2.94522113459511	-3.13444327019897
C	3.43630298612368	-1.63395828541663	-0.97218924705238
H	2.02331691811414	-2.22720140285524	0.40908301653725
C	3.12013795450082	-0.15184437972970	-1.11135967206450
H	2.44343411773504	-0.03455646516689	-3.05021110761949
H	3.76847854500727	-2.03267028852921	-1.93178880975297
H	4.24456830161499	-1.77214559592483	-0.25022186535977
H	2.75699381237441	0.23297236147780	-0.15562973721321
H	4.04226924477855	0.38542659520917	-1.35263266573056
H	1.67198899452916	0.98340387143161	-2.03842087612114
H	2.37487993799037	-3.38876158549923	-0.68657020878614
H	-0.82258610345022	-1.51483349158063	0.37756554833107
H	-2.10988547541634	0.42447191238275	-0.09539845960982
H	-0.86934542317774	0.91725340892096	-1.25619637084649
H	0.25284897132951	-0.28931688929279	0.38028293711555
H	-0.80421636822086	-0.58555264397729	-3.52939552984818
H	-1.45777405191969	-2.07110433804059	-3.35911603804063

Table S12. Cartesian coordinates for the optimized geometry of $[\text{Cu(II)}-\text{O}\cdot]^+$ specie derived from complex 2.

Cu	0.66299865985112	-1.70282422273955	-2.05510948803398
N	-0.82920990730398	-1.05465630103781	-3.33042531644373
N	2.13759342825709	-2.44507842657460	-0.76737954721176
N	-0.69745228694976	-0.97674000028474	-0.66315924853430
N	2.03938344241365	0.17346587781729	-1.65552520014427
C	-1.91452713392605	-0.72594671838175	-1.16496410592269
C	-2.12085402690394	-1.03461758824063	-2.62225792023830
H	-2.56897957620254	-2.02521741898718	-2.70950413377735
H	-2.81646665087133	-0.31873963456534	-3.06207982401497
O	1.50743750114934	-2.61164273513537	-3.46616649584013
C	3.40148540836742	-1.71208664089299	-0.98150510021422
H	1.86883222905795	-2.39479311176241	0.21002070187750
C	3.16777335385446	-0.22217264902160	-1.05909995539621
H	3.81651362182634	-2.05230312101788	-1.93207392516308
H	4.12915910444742	-1.93378157256870	-0.19986050703836
C	-2.93977506494079	-0.22702980524291	-0.37140541579825
H	-0.56696695546772	-0.11814690861437	-3.62491457567847
H	-0.88626211306746	-1.62660050357413	-4.16546786312481
C	-0.45843679473060	-0.72462064031494	0.62892928439149
C	-1.42853078771266	-0.23315734906748	1.48188670357184
C	-2.69716048167033	0.01486790909036	0.97096103531873
H	0.54371985770216	-0.91420197196616	0.98517097595858
H	-3.48229029405288	0.39964883268277	1.60851152047796
H	-1.19074615349834	-0.04856833526044	2.51993551576856
H	-3.90915475923138	-0.03207302847771	-0.81011964046377
C	1.78671309909536	1.47801148240742	-1.77417999358572
C	2.65780650378324	2.45387765775598	-1.31233275133821
C	3.83440368351816	2.04694340053455	-0.69431296593883
H	0.85075990886427	1.74410191943013	-2.25246073071418
C	4.09223083230805	0.68942088228938	-0.55999406352751
H	2.41530955477104	3.50123027688198	-1.42911750251503
H	4.53685983714889	2.77697237517679	-0.31325602331111
H	4.99090277701861	0.33686880346285	-0.07118770455101

Table S13. Cartesian coordinates for the optimized geometry of $[\text{Cu(II)}-\text{O}\cdot]^+$ specie derived from complex 3.

Cu	1.05232594362391	-1.68011267967389	-1.58649278569744
N	-0.38608329048589	-1.08911565994853	-2.88595352262312
N	2.50755579038978	-2.10839775631191	-0.18196698031404
N	-0.32005073460221	-0.88645975395365	-0.26667947335218
N	2.29739897594666	0.27046273927237	-1.42831268905825
C	-1.38212248968211	-0.31331139202968	-0.86230648280326
C	-1.42824328288724	-0.44255596277700	-2.33266804105241
C	-2.47163526901677	0.02814917349700	-3.12121711019939
O	1.89848544977903	-2.78994804920950	-2.83015342146564
C	3.38133663276751	-1.14729457242028	0.17361252247381
C	3.19472854598855	0.19425475347462	-0.43593366660147
C	4.41088738262032	-1.42674879689455	1.06954541975893
C	-2.36548819216146	0.32494239116763	-0.11548980794633
C	-0.33897353677319	-1.28967003808896	-4.20299836128101
C	-0.21337173291878	-0.86521376172291	1.06120322001897
C	-1.16342468131993	-0.26173939395156	1.86984055532872
C	-2.25318247020252	0.34957067566250	1.26654205116014
H	0.65592643630734	-1.34823815192925	1.48390819947715
H	-3.01308716774566	0.83625450393257	1.86315915662799
H	-1.04338296126607	-0.27363575786019	2.94380909008409
H	-3.21198578178575	0.78831906349226	-0.59890809193893
C	2.06862415467695	1.43840214236839	-2.02227334723118
C	2.73020390519828	2.60404902997902	-1.65921192335910
C	3.65759950028442	2.53696459670388	-0.62826762670103
H	1.32678597454790	1.43727142328183	-2.81235013855597
C	3.89453290829608	1.32041439718589	-0.00436046784049
H	2.51764158537585	3.53389264862029	-2.16828473339395
H	4.18913442630574	3.42268632540494	-0.30612204343655
H	4.60257291703736	1.26157126617401	0.80842055078274
C	-2.42933335044706	-0.18244109852139	-4.49200483761599
C	-1.34762083538027	-0.85247000655020	-5.04647871710476
H	-3.31040771240240	0.54288787302875	-2.67753309590247
H	0.53074831959719	-1.81590530448637	-4.57217436838629
H	-3.23658180131274	0.17279806356177	-5.11845215878780
H	-1.28087347218747	-1.03752008720050	-6.10913746089216
C	2.62269335084750	-3.33814909513935	0.32559811354667
C	3.61558269814877	-3.67898139772351	1.22831238210710
C	4.52661259393997	-2.70125967244210	1.60272010189127
H	1.89135640707436	-4.06106201982774	-0.00645155469332
H	3.66936047003695	-4.68536535117052	1.61859460717201
H	5.32349471859724	-2.92678774176078	2.29896400861760
H	5.12323642288745	-0.66320729581289	1.34214995199004

Table S14. Cartesian coordinates for the reactants, TS, and products between [Cu(II)-O•]⁺ species derived from complex **1** and BA.

Cu	0.62444401588621	-1.79448609154173	-1.76471079899248
N	-1.08555368920136	-1.28072063080065	-2.84421542983213
N	2.22940345842625	-2.38840962523898	-0.57230321687943
N	-0.37245641226695	-0.82189942702790	-0.21531697600230
N	2.06132121795438	0.05064494635619	-2.11390525975398
C	-1.38929749352310	0.05862239323038	-0.82935010020119
C	-2.09785155977063	-0.72225712424032	-1.92069674163474
H	-2.63884572123460	-1.55923354323539	-1.48073738508155
H	-2.81449148264479	-0.08670692995336	-2.44349519110982
O	1.20264915794747	-2.94522113459511	-3.13444327019897
C	3.43630298612368	-1.63395828541663	-0.97218924705238
H	2.02331691811414	-2.22720140285524	0.40908301653725
C	3.12013795450082	-0.15184437972970	-1.11135967206450
H	2.44343411773504	-0.03455646516689	-3.05021110761949
H	3.76847854500727	-2.03267028852921	-1.93178880975297
H	4.24456830161499	-1.77214559592483	-0.25022186535977
H	2.75699381237441	0.23297236147780	-0.15562973721321
H	4.04226924477855	0.38542659520917	-1.35263266573056
H	1.67198899452916	0.98340387143161	-2.03842087612114
H	2.37487993799037	-3.38876158549923	-0.68657020878614
H	-0.82258610345022	-1.51483349158063	0.37756554833107
H	-2.10988547541634	0.42447191238275	-0.09539845960982
H	-0.86934542317774	0.91725340892096	-1.25619637084649
H	0.25284897132951	-0.28931688929279	0.38028293711555
H	-0.80421636822086	-0.58555264397729	-3.52939552984818
H	-1.45777405191969	-2.07110433804059	-3.35911603804063
H	-3.61501252875775	-3.67399103011122	0.64654183788227
H	-3.67512167491793	-4.27209642724543	-1.75300049629348
C	-2.71401718646527	-4.01457306594770	0.15230034624174
C	-2.74990763353380	-4.35246731719387	-1.19741186492538
C	-1.52313747458344	-4.11263402812680	0.87156001743167
C	-1.59275835839595	-4.78599022511765	-1.82947892806956
H	-1.50316981117719	-3.85280809374604	1.92220529391034
H	-1.60489982127240	-5.04358633026517	-2.88195129659130
C	-0.36664998643115	-4.54236650246726	0.24012359442214
C	-0.39640182574707	-4.87775784075921	-1.11624846704143
H	0.56476819244336	-4.62144932037851	0.78498745276990
C	0.81960761068143	-5.32512008526560	-1.81673268706161
O	1.92615418438750	-5.38978119753880	-1.30465133669435
H	0.66397246028367	-5.64725415219891	-2.85761001023281

Cu	5.30783903700000	5.47729484500000	3.80649395800000
N	3.49033319500000	5.94380378500000	2.79788928800000
N	4.24731861200000	6.30355607000000	5.47308057500000
N	6.64481039400000	7.24364940300000	3.62194679100000
N	6.87361461100000	4.79166281400000	5.10184621800000
C	2.52163890200000	6.46423417600000	3.75229211500000
C	3.24494840800000	7.20085016600000	4.90822907300000
C	7.66266428700000	7.04713256500000	4.67072739100000
C	8.08549732500000	5.58236624400000	4.76144228800000
C	5.47480776100000	1.72776474100000	3.92367148000000
C	4.28927272600000	2.30791919800000	4.62331679600000
C	3.05086753800000	2.38512940900000	3.91823169400000
C	1.90394398800000	2.85639538200000	4.54035335700000
C	1.95695783100000	3.17548098900000	5.90463524000000
C	3.13315541800000	3.03520559200000	6.63350097000000
C	4.31741103000000	2.61551317400000	6.00991944200000
H	3.27452713100000	5.08750228200000	2.32177557900000
H	3.82674033100000	6.63349204400000	2.17235811100000
H	1.98745236700000	5.63153871500000	4.19980672300000
H	1.80810983400000	7.13770088400000	3.26840270200000
H	2.53306524800000	7.50394181100000	5.65606718300000
H	3.82803773200000	8.05991338700000	4.54139671300000
H	3.81886759000000	5.59431675800000	6.02271569400000
H	4.95366116600000	6.76352837700000	6.03107947800000
H	7.11198508200000	7.21977501400000	2.72100410600000
H	6.29015748000000	8.21199908400000	3.65826048100000
H	8.56868858500000	7.68521654400000	4.52598215000000
H	7.28601783700000	7.40892231500000	5.64846572900000
H	8.39802621600000	5.27160759000000	3.78172263200000
H	8.93463869000000	5.46777786500000	5.47510583600000
H	7.06993984000000	3.80709227300000	4.91391183100000
H	6.54757881100000	4.91865817200000	6.04993135600000
H	3.09175911400000	2.18619035300000	2.85945647500000
H	0.92251298200000	2.96111724000000	4.00340218800000
H	1.05643519300000	3.47444578400000	6.38958174100000
H	3.15650173600000	3.27766439500000	7.67274135500000
H	5.28026214200000	2.47722453700000	6.55686926000000
H	6.27566168500000	3.28835273400000	2.53868137000000
O	5.82225285200000	4.14301463200000	2.43917318900000
O	6.64244972900000	1.73188470800000	4.33547951300000

Cu	0.65300606818443	-1.76401114153500	-1.85662587496684
N	-1.04754575809336	-1.19619040656484	-2.91767572464785
N	2.24303653030489	-2.35156499394233	-0.63240841958028
N	-0.38018341904549	-0.88233969354444	-0.27230920713268
N	2.05982199048945	0.14025445343435	-2.08240133411129
C	-1.39541795613080	0.02746128631319	-0.84501992182665
C	-2.08228814878982	-0.68858646025571	-1.99404796342101
H	-2.63418224416705	-1.54680349267935	-1.61242041126594
H	-2.78730182471330	-0.02224837077495	-2.49401756822416
O	1.18561509109304	-2.84677534285356	-3.35337771871155
C	3.43933896928713	-1.53575970349938	-0.94090635317464
H	1.99273465504377	-2.23971314128684	0.34587219341892
C	3.07139772370092	-0.06296038337629	-1.03306137792496
H	2.49282825151975	0.10119173701298	-2.99942837541349
H	3.83262218821019	-1.87896787566851	-1.89911894140698
H	4.21719117117226	-1.67711428993497	-0.18706104841742
H	2.64222022063732	0.26439269727844	-0.08329413164810
H	3.98253801892558	0.51976854235461	-1.19924492160590
H	1.63581020264247	1.05679487081559	-1.99578649318187
H	2.44820108960361	-3.33750099949694	-0.76499166586422
H	-0.83032231207908	-1.61599736107857	0.26936548780500
H	-2.12759461096637	0.34297971833207	-0.09925633586759
H	-0.87488767079759	0.91336367441723	-1.21087454147221
H	0.22763917796848	-0.38132930414922	0.36714851098096
H	-0.75858903953051	-0.47299913364246	-3.56941143647617
H	-1.38792095938333	-1.97517576771822	-3.47004130167404
H	-3.55168213698338	-3.63376289061521	0.71694801762467
H	-3.64096236716345	-4.13739186161696	-1.70267235891580
C	-2.66427935863307	-3.98516318535227	0.20616207930953
C	-2.71684755611770	-4.26952505102892	-1.15573945002776
C	-1.47653196554838	-4.14920842636918	0.91762138058136
C	-1.58155092658880	-4.72358543771887	-1.81051284420925
H	-1.44376430659461	-3.92862561447836	1.97685064827356
H	-1.60341906383283	-4.94893159884169	-2.86856553625874
C	-0.33601256864507	-4.59300073873849	0.26686716388836
C	-0.38902606712612	-4.88025612438578	-1.10297085571807
H	0.59448389649377	-4.71970553612488	0.80443868374116
C	0.80296248806865	-5.37532444773167	-1.80223326091419
O	1.92719338101280	-5.45710302972062	-1.41501567475225
H	2.04373914657154	-3.24845517523376	-3.18140311681147

Table S15. Cartesian coordinates for the reactants, TS, and products between [Cu(II)-O•]⁺ species derived from complex **2** and BA.

Cu	0.66299865985112	-1.70282422273955	-2.05510948803398
N	-0.82920990730398	-1.05465630103781	-3.33042531644373
N	2.13759342825709	-2.44507842657460	-0.76737954721176
N	-0.69745228694976	-0.97674000028474	-0.66315924853430
N	2.03938344241365	0.17346587781729	-1.65552520014427
C	-1.91452713392605	-0.72594671838175	-1.16496410592269
C	-2.12085402690394	-1.03461758824063	-2.62225792023830
H	-2.56897957620254	-2.02521741898718	-2.70950413377735
H	-2.81646665087133	-0.31873963456534	-3.06207982401497
O	1.50743750114934	-2.61164273513537	-3.46616649584013
C	3.40148540836742	-1.71208664089299	-0.98150510021422
H	1.86883222905795	-2.39479311176241	0.21002070187750
C	3.16777335385446	-0.22217264902160	-1.05909995539621
H	3.81651362182634	-2.05230312101788	-1.93207392516308
H	4.12915910444742	-1.93378157256870	-0.19986050703836
H	2.26700731057387	-3.43170822592822	-0.97856509110000
C	-2.93977506494079	-0.22702980524291	-0.37140541579825
H	-0.56696695546772	-0.11814690861437	-3.62491457567847
H	-0.88626211306746	-1.62660050357413	-4.16546786312481
H	-3.51989415926437	-3.34568238808922	1.08136473409840
H	-3.87363306838920	-3.93415684617539	-1.29270158330763
C	-2.70357330824194	-3.75352478458449	0.49950951502521
C	-2.90379405407769	-4.08398039823361	-0.83669523410172
C	-1.45570935304470	-3.94121655074183	1.09382483607309
C	-1.85219636609585	-4.59438908219613	-1.58504359168218
H	-1.30814053302232	-3.68027896650488	2.13333556654646
H	-1.99250780658733	-4.84706798627500	-2.62929519753256
C	-0.40592154202136	-4.45161329805085	0.35064265021921
C	-0.59789189890502	-4.77518924575809	-0.99706569199554
H	0.56744060099924	-4.60140295472397	0.79881012799795
C	0.49978166244026	-5.29948009187079	-1.81888291818258
O	1.65109654834366	-5.43529184060958	-1.43738251039452
H	0.21829615038800	-5.57692807405859	-2.84886135050788
C	-0.45843679473060	-0.72462064031494	0.62892928439149
C	-1.42853078771266	-0.23315734906748	1.48188670357184
C	-2.69716048167033	0.01486790909036	0.97096103531873
H	0.54371985770216	-0.91420197196616	0.98517097595858
H	-3.48229029405288	0.39964883268277	1.60851152047796
H	-1.19074615349834	-0.04856833526044	2.51993551576856
H	-3.90915475923138	-0.03207302847771	-0.81011964046377
C	1.78671309909536	1.47801148240742	-1.77417999358572
C	2.65780650378324	2.45387765775598	-1.31233275133821
C	3.83440368351816	2.04694340053455	-0.69431296593883
H	0.85075990886427	1.74410191943013	-2.25246073071418
C	4.09223083230805	0.68942088228938	-0.55999406352751
H	2.41530955477104	3.50123027688198	-1.42911750251503
H	4.53685983714889	2.77697237517679	-0.31325602331111
H	4.99090277701861	0.33686880346285	-0.07118770455101



Cu	5.84990662500000	5.09817771000000	4.52891078000000
N	4.22229983000000	5.72252977100000	3.21467641900000
N	4.49403841800000	5.78623952200000	5.88203497100000
N	7.16069375900000	6.89096257900000	4.82708414600000
N	7.34585553800000	4.23904041200000	5.78777626200000
C	2.96795671800000	5.74172935200000	3.99301719900000
C	3.26663715700000	6.12205604800000	5.40732166000000
C	2.29643860500000	6.70430360900000	6.22699954400000
C	2.60464554200000	6.93373470900000	7.57217156600000
C	3.90710021300000	6.64910581000000	8.03484644800000
C	4.79468534400000	6.02397933000000	7.18952742200000
C	6.92120302000000	8.25611861300000	4.80777826500000
C	7.81901873100000	9.19120947000000	5.33107417700000
C	9.00622824700000	8.76431262700000	5.91001127800000
C	9.21635552300000	7.38617519000000	6.00346027900000
C	8.29231208400000	6.48568691300000	5.47329801000000
C	8.57645194100000	4.99760126300000	5.53957091400000
C	5.37073966900000	1.32728228300000	4.90641883500000
C	4.46755796500000	2.09038483000000	5.81829555200000
C	3.17702520100000	2.35079298300000	5.36659811200000
C	2.27016284200000	2.97138633200000	6.19128786600000
C	2.62864485200000	3.27135020000000	7.52233336500000
C	3.91401223700000	2.96756169800000	8.01946992500000
C	4.82513876300000	2.36933982000000	7.15474720600000
H	4.18611940100000	5.09867371000000	2.44750356100000
H	4.55976694800000	6.61115353200000	2.90723297600000
H	2.53423852600000	4.73005289200000	3.96226192700000
H	2.34575906600000	6.55345912200000	3.59174892900000
H	1.34111661800000	6.92659136600000	5.83001953700000
H	1.86507919700000	7.45897532200000	8.19312967700000
H	4.18521691300000	6.85505844200000	9.09954979900000
H	5.83669552600000	5.82006345600000	7.47926363900000
H	6.00433739900000	8.56328682200000	4.32886757200000
H	7.61266521800000	10.22833538700000	5.26776538800000
H	9.67010340000000	9.48203777900000	6.37598662100000
H	10.08416730800000	7.08002510900000	6.56013299100000
H	8.92787027800000	4.71633616800000	4.52050886500000
H	9.30338669100000	4.75124677600000	6.34662399000000
H	7.39305460800000	3.27129838000000	5.46356089100000
H	7.09706062700000	4.32038690300000	6.75956056300000
H	2.91266381800000	2.08881006000000	4.36197343300000
H	1.27206342800000	3.18401864100000	5.82795627300000
H	1.89098172600000	3.70194024300000	8.17718094100000
H	4.17611711300000	3.15777766900000	9.09537435700000
H	5.83097990000000	2.09347296900000	7.46677748200000
H	6.19150388400000	3.58410087200000	2.55185286100000
O	6.81154638700000	4.09483628200000	3.12504081000000
O	6.53772471400000	1.19235989600000	5.18428365300000

Cu	0.77296190929346	-1.81988313901905	-2.26745842839417
N	-0.76626007403428	-1.15693914026038	-3.47606937290818
N	2.24436025957804	-2.59353058000414	-0.99577600511311
N	-0.51049264292981	-1.05112523614670	-0.82004799925131
N	2.17695549919256	0.05150874254067	-1.86472482822307
C	-1.72914631032838	-0.72914855494806	-1.27677196630066
C	-2.02138868266924	-1.08209993523785	-2.70786577517042
H	-2.49361536685072	-2.06556871521399	-2.73862155740569
H	-2.72368761282852	-0.36624540270908	-3.13639797334624
O	1.68981509720069	-2.74680999604403	-3.67162364768605
C	3.50916963881008	-1.85764885803879	-1.20316983751470
H	2.00623455210941	-2.60856442352935	-0.00932801436985
C	3.28100473380326	-0.36572512641273	-1.23664579826837
H	3.90338043735789	-2.17014785121422	-2.17081721511724
H	4.24700268535054	-2.10532483256418	-0.43913098187288
C	4.18334722323956	0.52742068872586	-0.66879989915169
H	2.36965396925547	-3.56098587797715	-1.27638525066863
C	-2.67506022108223	-0.11947046614556	-0.46343247899134
H	-0.49796243624506	-0.23546352513707	-3.81068786588813
H	-0.88418200029636	-1.74790687332274	-4.29171165501936
H	-3.03209411016232	-3.04661466633301	1.63690823318842
H	-3.76182982188541	-3.54855114686545	-0.66936402007640
C	-2.35768962933458	-3.54882241394687	0.95578969023394
C	-2.77004763826806	-3.83048425875809	-0.34195648624374
C	-1.07794458618001	-3.89907515004206	1.38473193797077
C	-1.90356101061851	-4.46748465057312	-1.21873611288592
H	-0.76440305365511	-3.67093397922274	2.39500884100298
H	-2.20661128037354	-4.69627816258504	-2.23216168032981
C	-0.20484632717893	-4.52810392862758	0.51468121134320
C	-0.61884863897373	-4.81086574996127	-0.79474297827476
H	0.79276115623960	-4.80250100636371	0.83179832954140
C	0.28778467432862	-5.47752099710509	-1.73311211379284
O	1.43968649341728	-5.75377746483163	-1.61089749152089
H	1.34249059186331	-2.45730550161348	-4.52255148544734
C	-0.19447276937523	-0.76705587702685	0.44839915315767
C	-1.08354603671596	-0.16539297116178	1.31953807968234
C	-2.35104543131970	0.16165627220816	0.85424210765936
H	-3.64583470076059	0.13186620029943	-0.86902509239556
H	-3.07263546077044	0.63599020877591	1.50629953957622
H	-0.78322897054897	0.04235902973667	2.33678149758630
H	0.80347087454956	-1.02129332662590	0.77355512236150
C	1.92889771766740	1.35923566342457	-1.94705503399239
C	2.77993359338514	2.31826301703157	-1.41642825012695
H	1.01261224233898	1.64327070374764	-2.45251322206706
C	3.93036642099326	1.88939533341824	-0.76550822272567
H	2.54157925299457	3.36925008336422	-1.50637082219347
H	4.61580148419274	2.60513314515810	-0.33012104837478
H	5.06156430622421	0.15751069713802	-0.15616313219524

Table S16. Cartesian coordinates for the reactants, TS, and products between [Cu(II)-O•]⁺ species derived from complex **3** and BA.

Cu	1.05232594362391	-1.68011267967389	-1.58649278569744
N	-0.38608329048589	-1.08911565994853	-2.88595352262312
N	2.50755579038978	-2.10839775631191	-0.18196698031404
N	-0.32005073460221	-0.88645975395365	-0.26667947335218
N	2.29739897594666	0.27046273927237	-1.42831268905825
C	-1.38212248968211	-0.31331139202968	-0.86230648280326
C	-1.42824328288724	-0.44255596277700	-2.33266804105241
C	-2.47163526901677	0.02814917349700	-3.12121711019939
O	1.89848544977903	-2.78994804920950	-2.83015342146564
C	3.38133663276751	-1.14729457242028	0.17361252247381
C	3.19472854598855	0.19425475347462	-0.43593366660147
C	4.41088738262032	-1.42674879689455	1.06954541975893
C	-2.36548819216146	0.32494239116763	-0.11548980794633
C	-0.33897353677319	-1.28967003808896	-4.20299836128101
H	-2.96477816525833	-3.06214099980646	1.39214502516425
H	-3.88289130800630	-2.43495722069415	-0.81553290183756
C	-2.51546609364557	-3.45538616905686	0.48950200293379
C	-3.03294295053220	-3.10103532291033	-0.75156732646786
C	-1.41211707926969	-4.30482625921846	0.57763278738948
C	-2.44106416708925	-3.58807044724525	-1.90910773285211
H	-1.00883679059999	-4.56849212880283	1.54675174866948
H	-2.82232419768321	-3.30243840921638	-2.88236033560103
C	-0.83291986056445	-4.80706049050464	-0.57494499454881
C	-1.34388516038291	-4.44643612590014	-1.82609684673861
H	0.01684894979596	-5.47490729155136	-0.52435460416523
C	-0.75614565468140	-4.96558872691532	-3.06918996498639
O	0.11814716606470	-5.81005339317470	-3.12935809104558
H	-1.18004143584508	-4.53330728440316	-3.99410578871617
C	-0.21337173291878	-0.86521376172291	1.06120322001897
C	-1.16342468131993	-0.26173939395156	1.86984055532872
C	-2.25318247020252	0.34957067566250	1.26654205116014
H	0.65592643630734	-1.34823815192925	1.48390819947715
H	-3.01308716774566	0.83625450393257	1.86315915662799
H	-1.04338296126607	-0.27363575786019	2.94380909008409
H	-3.21198578178575	0.78831906349226	-0.59890809193893
C	2.06862415467695	1.43840214236839	-2.02227334723118
C	2.73020390519828	2.60404902997902	-1.65921192335910
C	3.65759950028442	2.53696459670388	-0.62826762670103
H	1.32678597454790	1.43727142328183	-2.81235013855597
C	3.89453290829608	1.32041439718589	-0.00436046784049
H	2.51764158537585	3.53389264862029	-2.16828473339395
H	4.18913442630574	3.42268632540494	-0.30612204343655
H	4.60257291703736	1.26157126617401	0.80842055078274
C	-2.42933335044706	-0.18244109852139	-4.49200483761599
C	-1.34762083538027	-0.85247000655020	-5.04647871710476
H	-3.31040771240240	0.54288787302875	-2.67753309590247
H	0.53074831959719	-1.81590530448637	-4.57217436838629
H	-3.23658180131274	0.17279806356177	-5.11845215878780
H	-1.28087347218747	-1.03752008720050	-6.10913746089216



C	2.62269335084750	-3.33814909513935	0.32559811354667
C	3.61558269814877	-3.67898139772351	1.22831238210710
C	4.52661259393997	-2.70125967244210	1.60272010189127
H	1.89135640707436	-4.06106201982774	-0.00645155469332
H	3.66936047003695	-4.68536535117052	1.61859460717201
H	5.32349471859724	-2.92678774176078	2.29896400861760
H	5.12323642288745	-0.66320729581289	1.34214995199004
Cu	6.26486846100000	5.22218132800000	5.80199628100000
N	4.79900686700000	5.75392185000000	4.65430112200000
N	4.94750523700000	6.06006068700000	7.16054596800000
N	7.43649183400000	7.16862796300000	5.93562798100000
N	7.68173777800000	4.83219945400000	7.24664843900000
C	4.80656210400000	5.53787818600000	3.23866209000000
C	3.76531789600000	5.98918058000000	2.44095258400000
C	2.67711472300000	6.66968858200000	3.01046845400000
C	2.64498520200000	6.90116755500000	4.34157072600000
C	3.68696299100000	6.47205729700000	5.15366263400000
C	3.76540770900000	6.64818658400000	6.55361916100000
C	2.83222820700000	7.28810031000000	7.35701340900000
C	2.96532766200000	7.38467812700000	8.72006670900000
C	4.12766357400000	6.74459969600000	9.32152854700000
C	5.00577905400000	6.13242688500000	8.53931299200000
C	7.20878403900000	8.37327251200000	5.36311706500000
C	7.88285657400000	9.54001749100000	5.65196748700000
C	8.84674333000000	9.48172873800000	6.70981024600000
C	9.09945141200000	8.30292285400000	7.35133600300000
C	8.39044076200000	7.14019723500000	7.00415608700000
C	8.58317159400000	5.86831909100000	7.57687827900000
C	9.62987771400000	5.56182961200000	8.49494093900000
C	9.74565358900000	4.32190043500000	9.03726976600000
C	8.80530122900000	3.27291694700000	8.66648195300000
C	7.80209554900000	3.58990421400000	7.75014726900000
C	4.16104700500000	2.20600225900000	4.34990450600000
C	3.64355734500000	2.59987752500000	5.66050190400000
C	2.52842522700000	3.40143153500000	5.72344134300000
C	2.07658171100000	3.88722598000000	6.90132655400000
C	2.72251755900000	3.53443796800000	8.10655480400000
C	3.84741942100000	2.67773186600000	8.02577169000000
C	4.31175690300000	2.20178454000000	6.82465873800000
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