Supplementary Information for:

Charge Separation in a Copper(I) Donor-Chromophore-Acceptor Assembly for both Photoanode and Photocathode Sensitization

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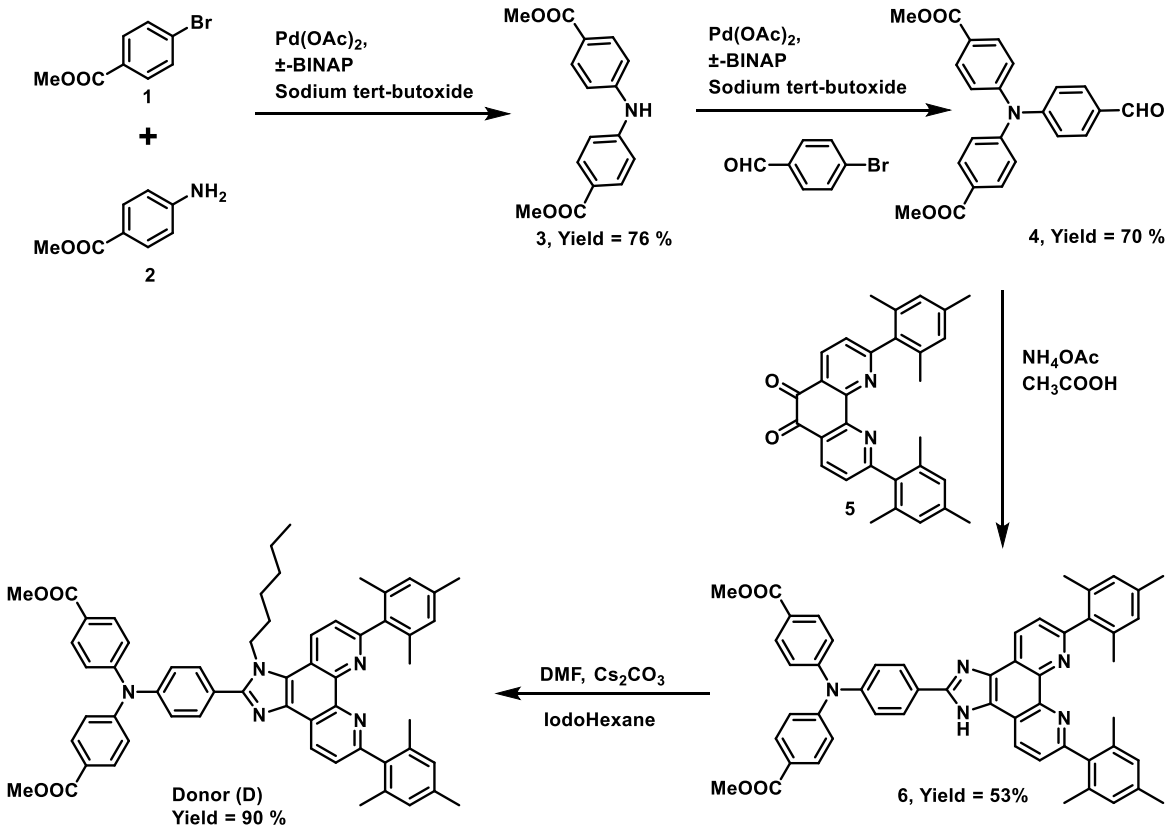
Experimental Methods

General Procedures.

DFT calculations were carried out with Gaussian 16[1] using the B3PW91 functional[2] with LANL2DZ as basis set.[3] The optimizations were conducted without symmetry constraint, and frequency calculations were made to confirm reaching the energy minima. GaussView5[4] and IQmol were used for data analysis, visualization and plots. All calculations were conducted for gas phase complexes.

All photoluminescence data were collected using a Horiba PTI QuantaMaster 8075 Spectrofluorometer. Emission data were collected at excitation wavelengths of 340 and 460 nm with an integration time of 1 s, step size of 1 nm, and slits of 2 nm (for 340 nm) and 5 nm, (for 460 nm) with an automatic 5 s dark background collection and were measured in a 1 cm pathlength quartz cuvette in CH_2Cl_2. Excitation data were collected under identical conditions, unless otherwise stated, with an emission wavelengths of 540 nm and 690 nm and slit widths of 3 nm. All data reported are corrected to account for fluctuations in lamp intensity and detector sensitivity.

Synthesis of Donor (D). Donor (D) was synthesized using reaction Scheme 1. Dimethyl 4,4'-azanediyldibenzoate (3) was synthesized using a Buchwald-Hartwig coupling between methyl-4-bromobenzoate (1) and methyl-4-aminobenzoate (2) in 76 % yield, which after another coupling with 4-bromobenzaldehyde under similar conditions yielded dimethyl 4,4'-(4-formylphenyl)azanediyl)-dibenzoate (4) in fair yields. Separately, the synthesis of 2,9-dimesityl-1,10-phenanthroline-5,6-dione (5) was done using modifications of the previous reported procedures.[5, 6] Synthesis of dimethyl 4,4'-((4-(6,9-dimesityl-1H-imidazo[4,5-f][1,10]phenanthrolin-2-yl)phenyl)azanediyl)-dibenzoate (6) was carried out using a modification of a previously reported procedure through the condensation of 5 with 4.[7] Finally, donor (D) was synthesized by alkylating the imidazole nitrogen in 6 using reported methods in 90 % yield.[7] Identities of all known compounds were confirmed by comparison of basic characterization data to previous reports.



Scheme **S1**: Synthesis steps for the donor (**D**).

*Synthesis of dimethyl 4,4'-azanediyldibenzoate (**3**).* Methyl-4-bromobenzoate (550 mg, 2.33 mmol) and methyl-4-aminobenzoate (354 mg, 2.33 mmol) were dissolved in 40 mL toluene: water (9:1) in a 100 mL three-neck round bottom flask fitted with a condenser under nitrogen atmosphere. Potassium *t*-butoxide (1.1 g, 9.2 mmol) was also added to the flask and the mixture was deaerated by bubbling nitrogen for 15 minutes while stirring. To this mixture palladium acetate (51.6 mg, 0.23 mmol) and ±-BINAP (186.6 mg, 0.3 mmol) were added, and the resulting solution was heated to 100 ℃ for 16 hours. Then, the reaction flask was cooled to room temperature, and the solvents were rotary-evaporated. The resulting crude black solid was dissolved in dichloromethane and washed with water (3×). The organic layers were concentrated and loaded onto a silica column for purification using a 1:1 v/v ethyl acetate:hexane solvent mixture. The final product **3** (465 mg, 1.63 mmol) was obtained in 76 % yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.8 Hz, 4H), 7.13 (d, *J* = 8.8 Hz, 4H), 3.90 (s, 6H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 166.70, 145.80, 131.45, 123.10, 116.89, 51.90 ppm. HR-MS (ESI+): *m/z* = 286.1073, calculated for $[C_{16}H_{16}NO_4]^+$ *m/z* = 286.1074.

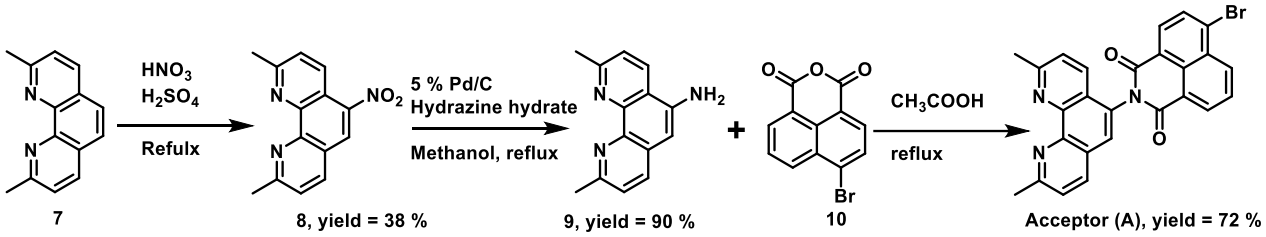
*Synthesis of dimethyl 4,4'-(4-formylphenyl)azanediyl)-dibenzoate (**4**).* As in the procedure described for the synthesis of **3**, a Buchwald-Hartwig coupling of **3** (400 mg, 1.40 mmol) and 4-bromobenzaldehyde (260 mg, 1.40 mmol) yielded the aldehyde product **4** (381 mg, 0.98 mmol) in 70 % yield after purification by silica column chromatography using 1 % v/v methanol in dichloromethane as eluting solvent. ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.91 (s, 1H), 7.98 (d, *J* = 6.9 Hz, 4H), 7.77 (d, 6.7 Hz, 2H), 7.15 (m, 6H), 3.91 (s, 6H) ppm. ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.37, 166.21, 151.61, 149.93, 131.19, 125.94, 123.22, 122.86, 116.73, 51.74 ppm. HR-MS (ESI+): *m/z* = 390.1344, calculated for $[C_{23}H_{20}NO_5]^+$ *m/z* = 390.1336.

*Synthesis of dimethyl 4,4'-((4-(6,9-dimesityl-1H-imidazo[4,5-f][1,10]phenanthrolin-2-yl)phenyl)azanediyl)-dibenzoate (**6**).* Synthesis of donor **6** was carried out using a modification of a previously reported procedure (Scheme S1) through the condensation of 2,9-dimesityl-1,10-phenanthroline-5,6-dione **5** with aldehyde **4**. In a representative procedure, **4** (100 mg, 0.26 mmol), **5** (115 mg, 0.26 mmol), and ammonium acetate (320 mg, 4.2 mmol) were dissolved in 10 mL of acetic acid in a two-neck flask fitted with a condenser under nitrogen. The dark red mixture was refluxed for 24 hours, cooled down to room temperature and the solvent was evaporated using a rotary evaporator. The black slurry obtained was then taken up in dichloromethane and washed twice sequentially with aqueous saturated sodium bicarbonate and brine. The organic layer was collected, concentrated by rotary evaporation and purified using column chromatography on silica with CH_2Cl_2:MeOH (99:2 v/v) as the mobile phase to give **D (**116 mg,0.14 mmol) in 55 % yield as a yellow powder. ^{1}H NMR (300 MHz, DMSO-*d6*) δ 13.84 (s, 1H), 9.01 (d, *J* = 8.3 Hz, 2H), 8.39 – 8.30 (m, 2H), 8.01 – 7.90 (4, 2H), 7.77 (m, 2H), 7.40 (d, *J* = 8.5 Hz, 2H), 7.28 – 7.17 (m, 4H), 6.98 (s, 4H), 3.85 (s, 6H), 2.30 (s, 6H), 2.01 (s, 12H) ppm. ^{13}C NMR (75 MHz, DMSO) δ 166.16, 157.45, 150.77, 147.06, 137.19, 135.78, 131.49, 128.61, 128.46, 127.19, 126.63, 124.55, 123.41, 21.21, 20.53 ppm. HR-MS (ESI+): *m/z* = 816.3536, calculated for $[C_{53}H_{46}N_5O_4]^+$ *m/z* = 816.3544.

*Synthesis of Donor (**D**).* **6** (100 mg, 0.12 mmol) and Cs_2CO_3 (325 mg, 1.00 mmol) were dissolved in 10 mL of dry DMF under nitrogen. The yellow mixture was heated at 100 °C for 30 minutes, where the colour of the mixture turned to green. *N*-Hexyl iodide (0.1 mL) was injected into the flask and the mixture was further stirred at 100 °C for 4 hours and then allowed to cool to room temperature. The solvents were removed by rotary evaporation and the crude product was purified by column chromatography on silica (CH_2Cl_2:CH_3OH 99:1 v/v) to give donor **D** (99 mg, 90%).

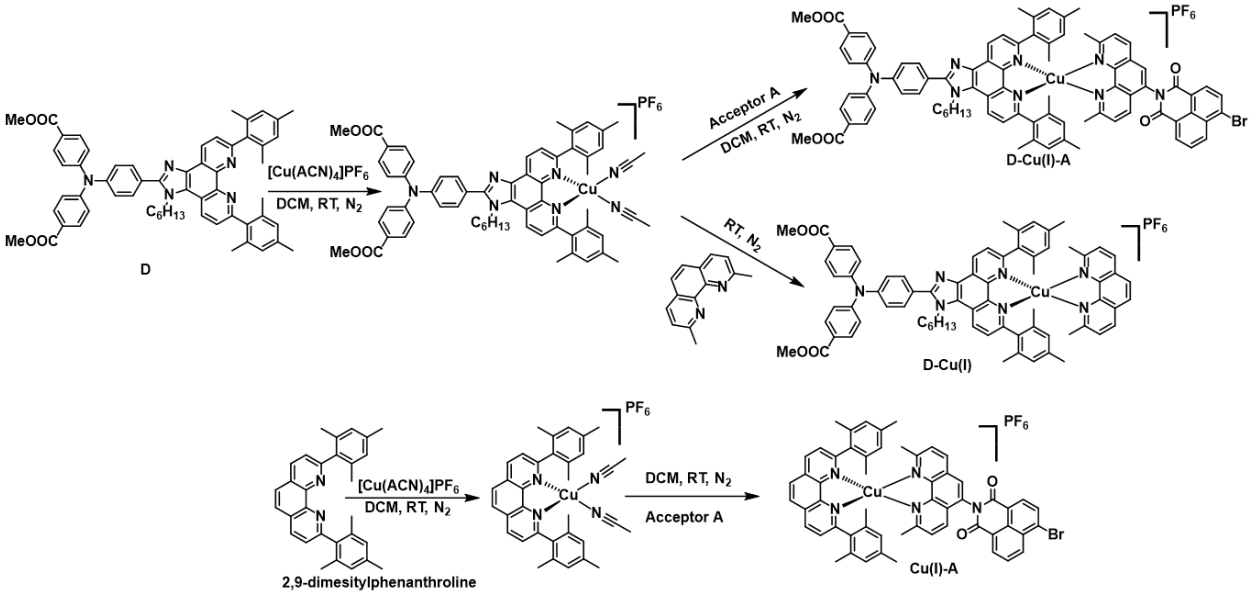
^{1}H NMR (300 MHz, DMSO-*d6*) δ 8.93 (dd, *J* = 19.7, 8.6 Hz, 2H), 7.96 (d, *J* = 8.8 Hz, 4H), 7.90 – 7.67 (m, 2H), 7.39 (d, *J* = 8.6 Hz, 2H), 7.23 (d, *J* = 6.7 Hz, 4H), 6.99 (s, 4H), 4.80 (s, 2H), 3.85 (s, 6H), 2.30 (s, 6H), 2.03 (d, *J* = 9.2 Hz, 12H), 1.12 (m, 10H), 0.75 (m, 3H) ppm. ^{13}C NMR (126 MHz, dmso) δ 166.13, 157.98, 156.90, 153.52, 150.76, 147.17, 138.49, 138.08, 137.31, 136.42, 135.83, 135.74, 131.99, 131.47, 128.68, 128.62, 126.20, 125.33, 124.66, 123.49, 122.28, 118.52, 52.46, 30.59, 29.73, 25.42, 21.20, 20.53, 20.48, 14.12 ppm. HR-MS (ESI+): *m/z* = 900.4480, calculated for $[C_{59}H_{57}N_5O_4]^+$ *m/z* = 900.4483.

Synthesis of Acceptor (A). The detailed synthesis of A is described in our previous work[8] and starts from the nitration of 2,9-dimethylphenantholine (7) to 5-nitro-2,9-dimethylphenanthroline (8) in 38 % yield. Further, this nitro derivative was reduced using 5 % Pd/C in presence of hydrazine monohydrate to form 5-amino-2,9-dimethylphenthroline in 90 % yield. Finally, this amino derivative was coupled with 4-bromonapthalene-1,8-dicarboxyanhydride derivative to form acceptor ligand A in 72 % yield (Scheme S2).



Scheme **S2**: Synthesis of Acceptor **A.**

Synthesis of Copper Complexes.



Scheme **S3**. Synthetic approach for synthesis of **D-Cu(I)-A, D-Cu(I)** and **Cu(I)-A.**

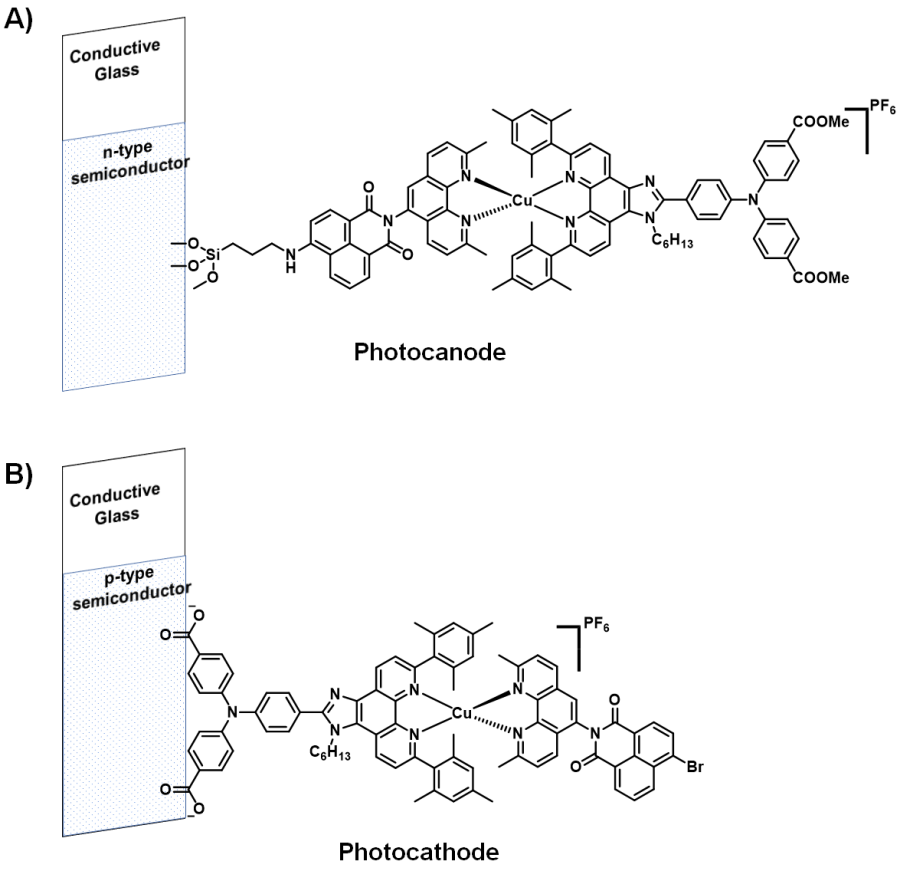


Figure **S1**. A) Mode of anchoring of **D-Cu(I)-A** to construct a photoanode. B) Mode of anchoring of **D-Cu(I)-A** to construct a photocathode.

NMR Analysis

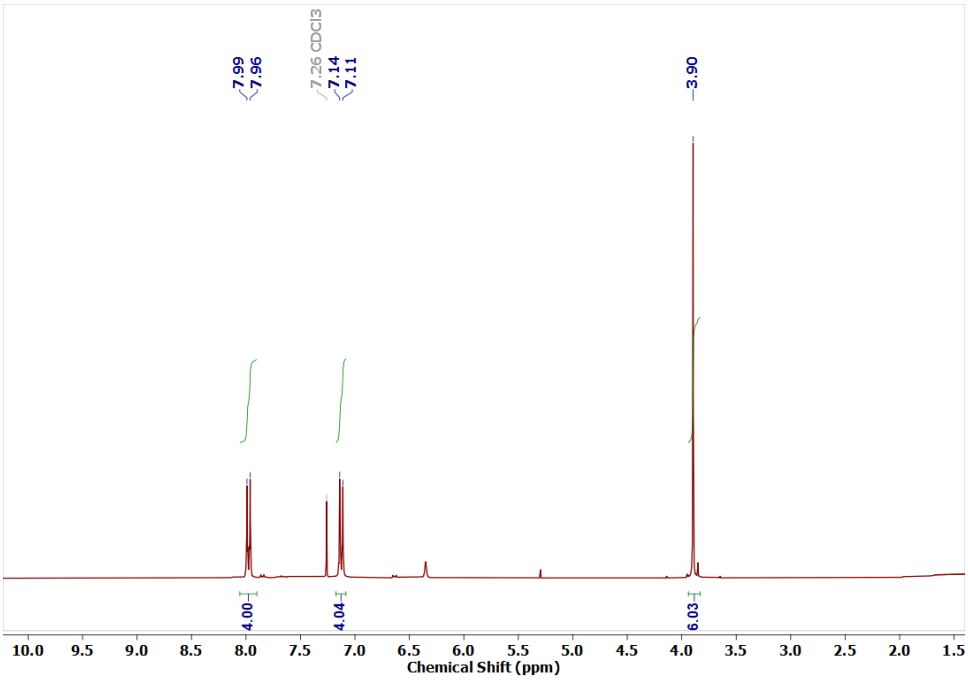


Figure **S2**. ^{1}H NMR of the compound **3** in $CDCl_3$.

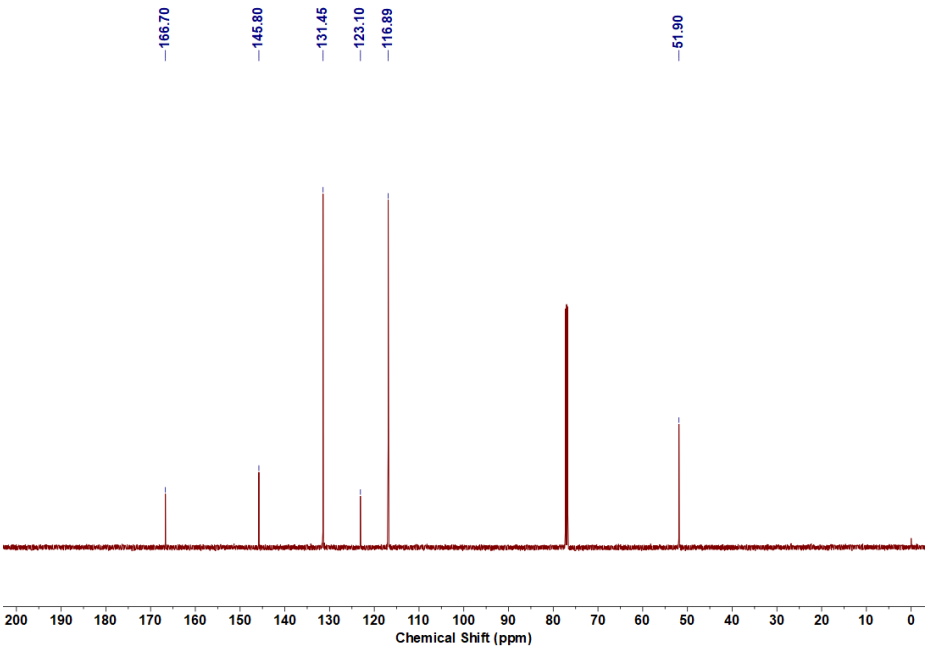


Figure **S3**. ^{13}C NMR of the compound **3** in $CDCl_3$.

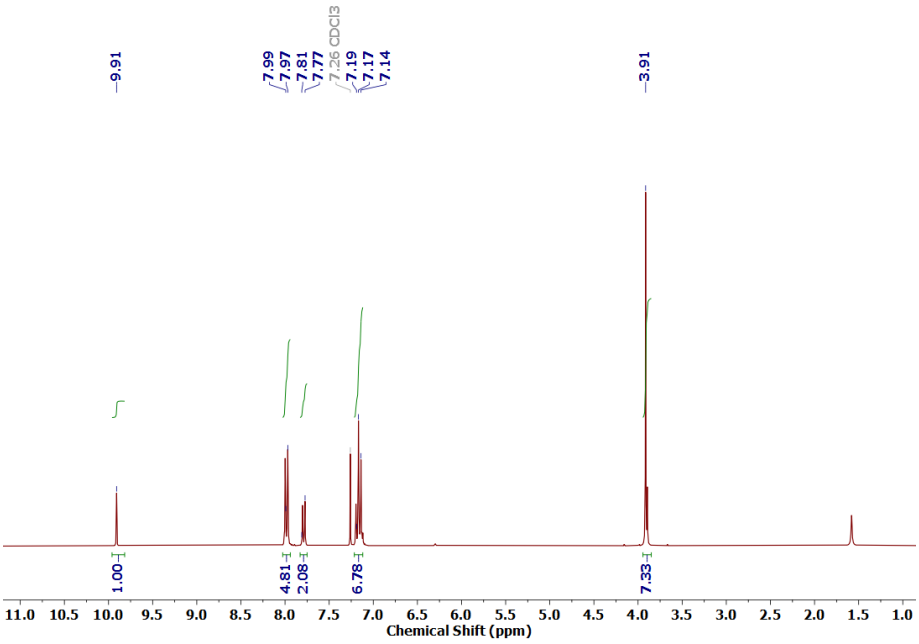


Figure **S4**. ^{1}H NMR of the compound **4** in $CDCl_3$.

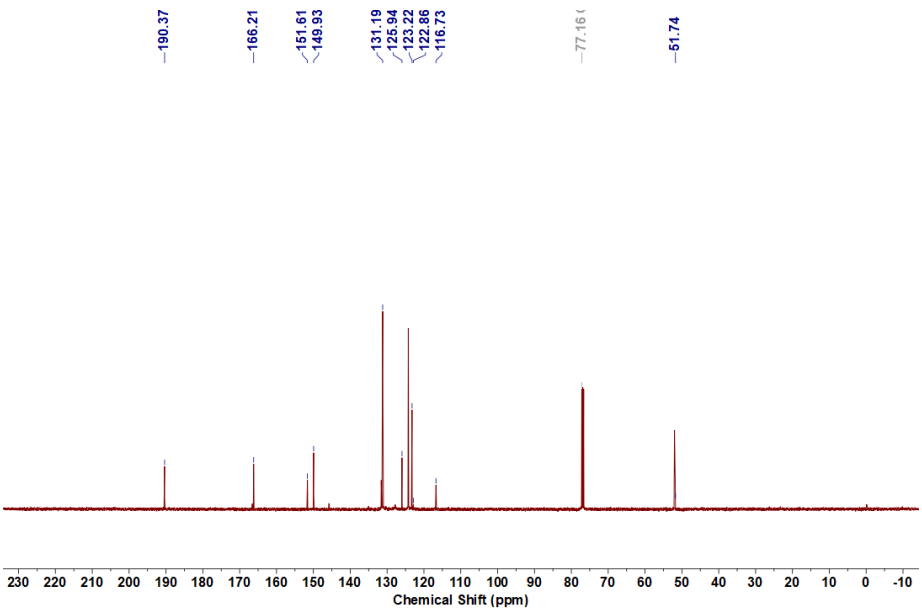


Figure **S5**. ^{13}C NMR of the compound **4** in $CDCl_3$.

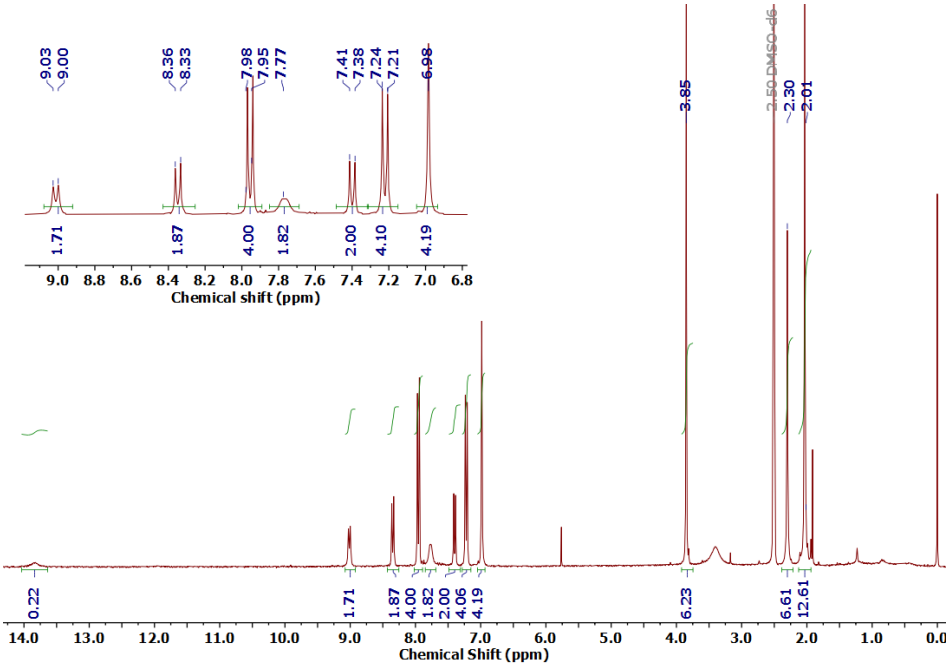


Figure **S6**. ^{1}H NMR of the compound **5** in DMSO-*d6*.

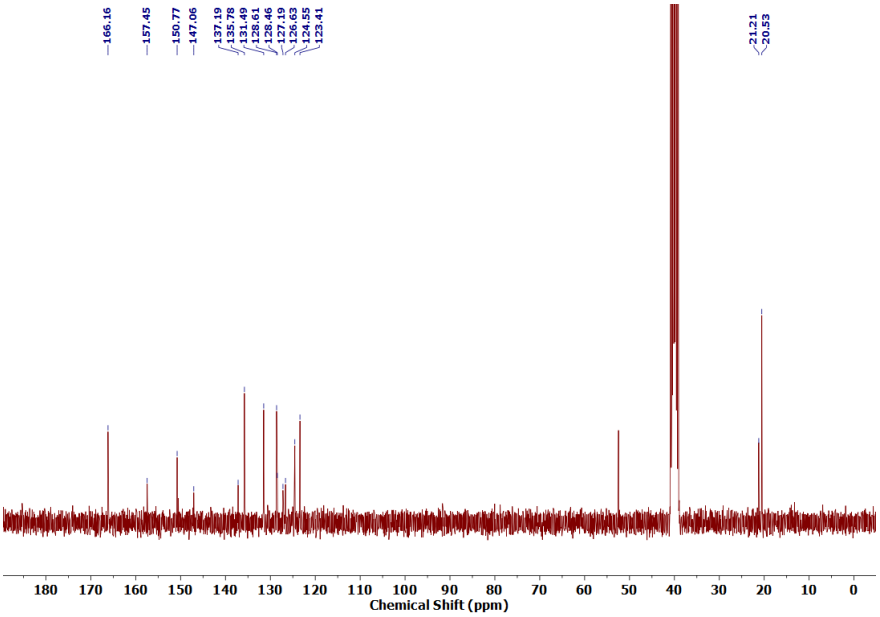


Figure **S7**. ^{13}C NMR of the compound **5** in DMSO-*d6*.

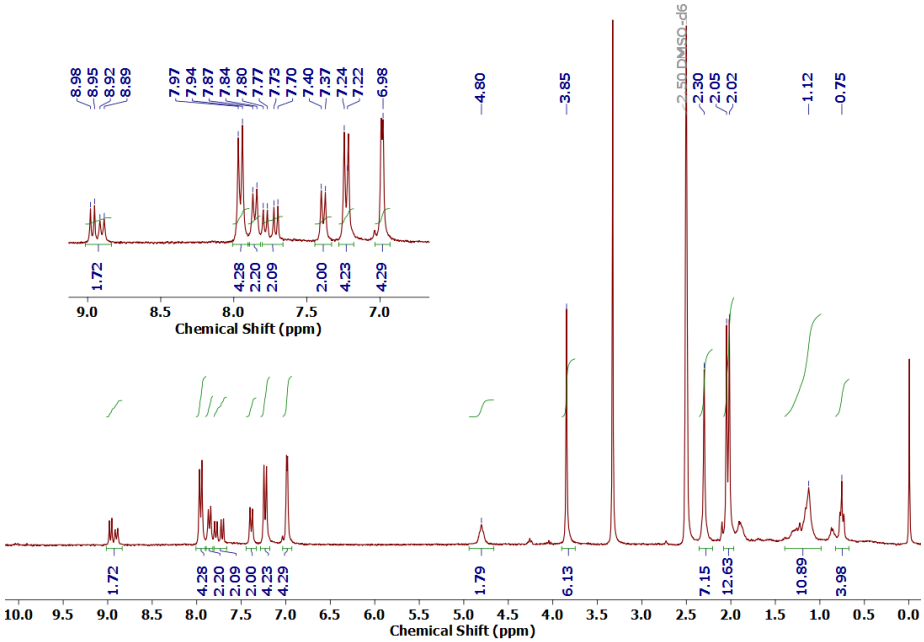


Figure **S8**. [1]H NMR of the donor ligand **D** in DMSO-*d6*.

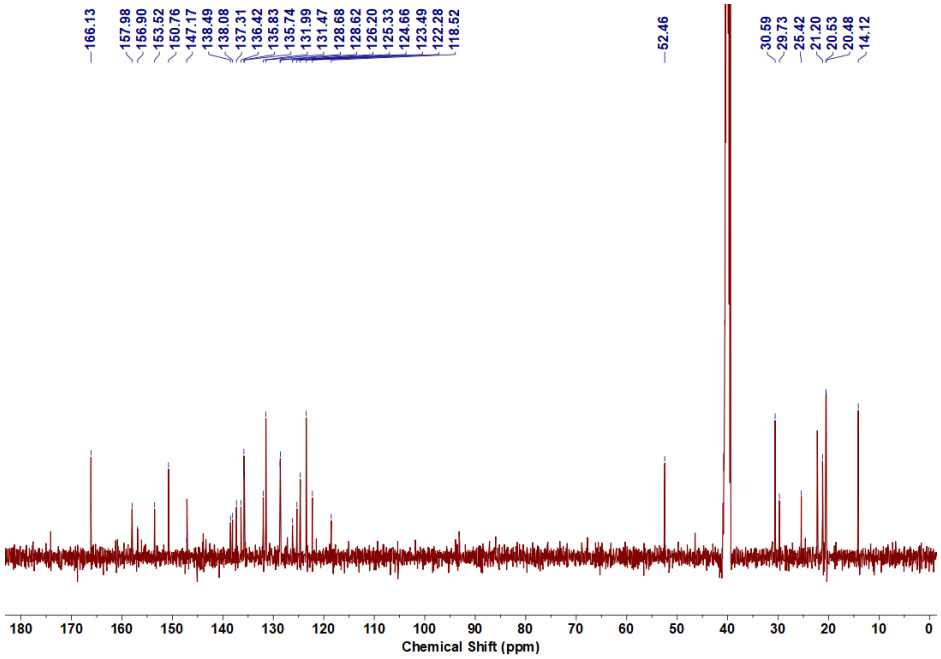


Figure **S9**. [13]C NMR of the donor ligand **D** in DMSO-*d6*.

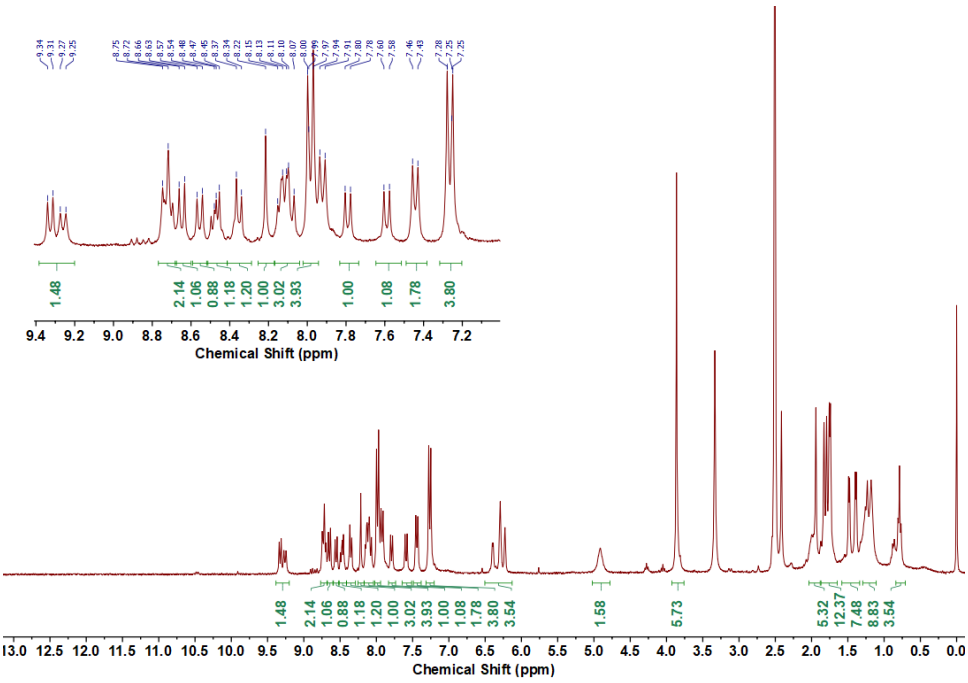


Figure **S10**. ^{1}H NMR of the triad **D-Cu(I)-A** in DMSO-*d6*.

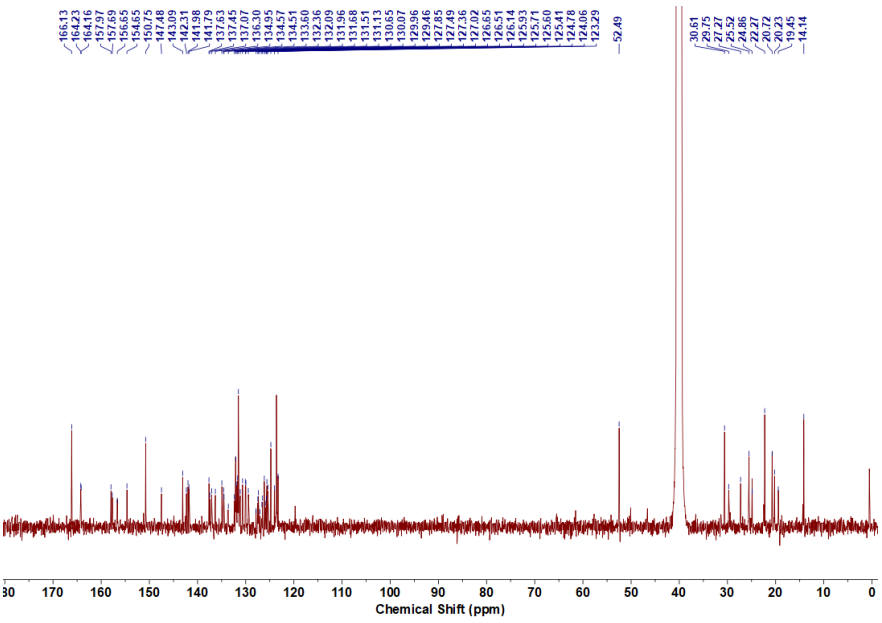


Figure **S11**. ^{13}C NMR of the triad **D-Cu(I)-A** in DMSO-*d6*.

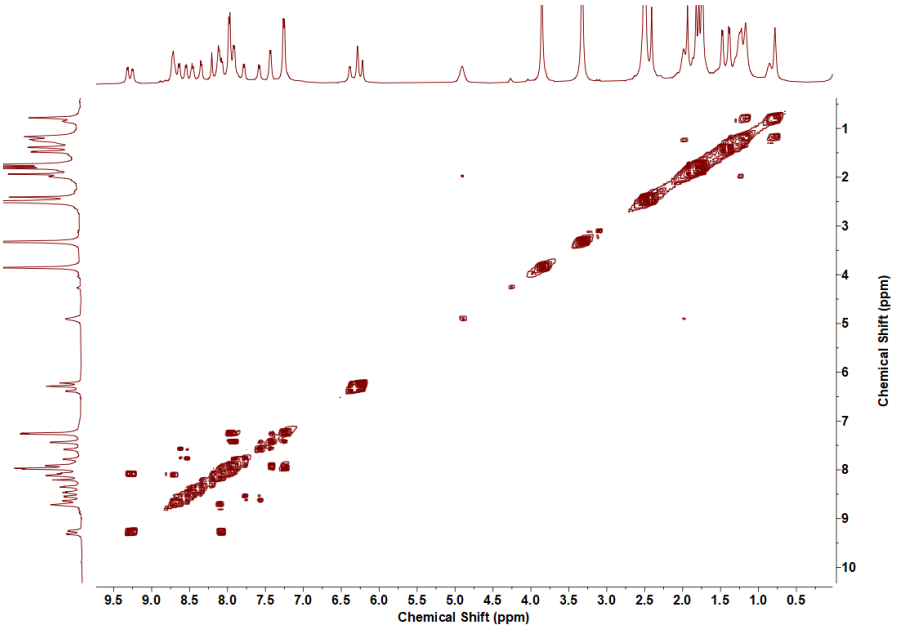


Figure **S12**. Full ^{1}H gCOSY NMR of the triad **D-Cu(I)-A** in DMSO-*d6*.

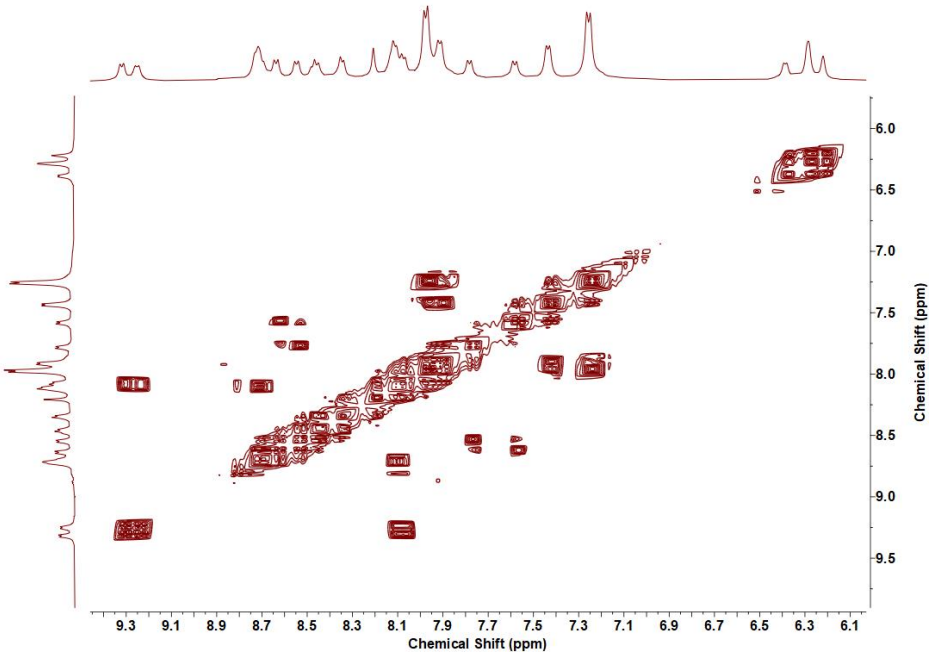


Figure **S13**. ^{1}H gCOSY NMR of the triad **D-Cu(I)-A** in DMSO-*d6* of the aromatic region.

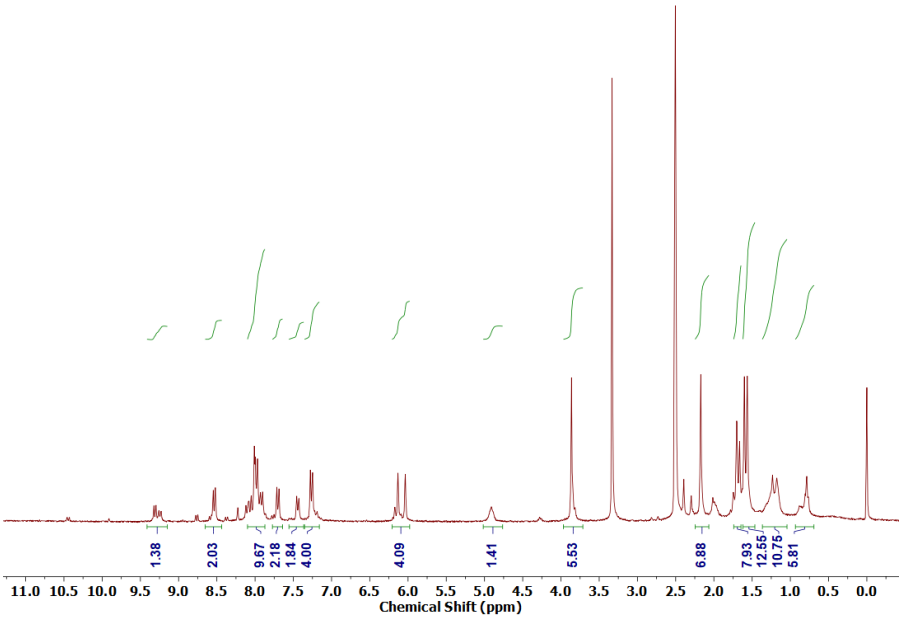


Figure **S14**. ^{1}H NMR of the dyad **D-Cu(I)** in DMSO-*d6*.

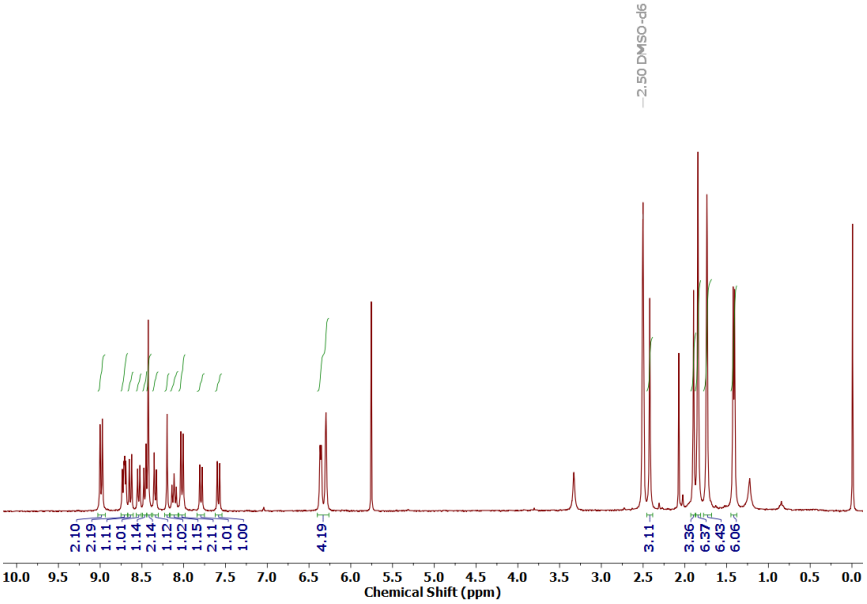


Figure **S15**. ^{1}H NMR of the dyad **Cu(I)-A** in DMSO-*d6*.

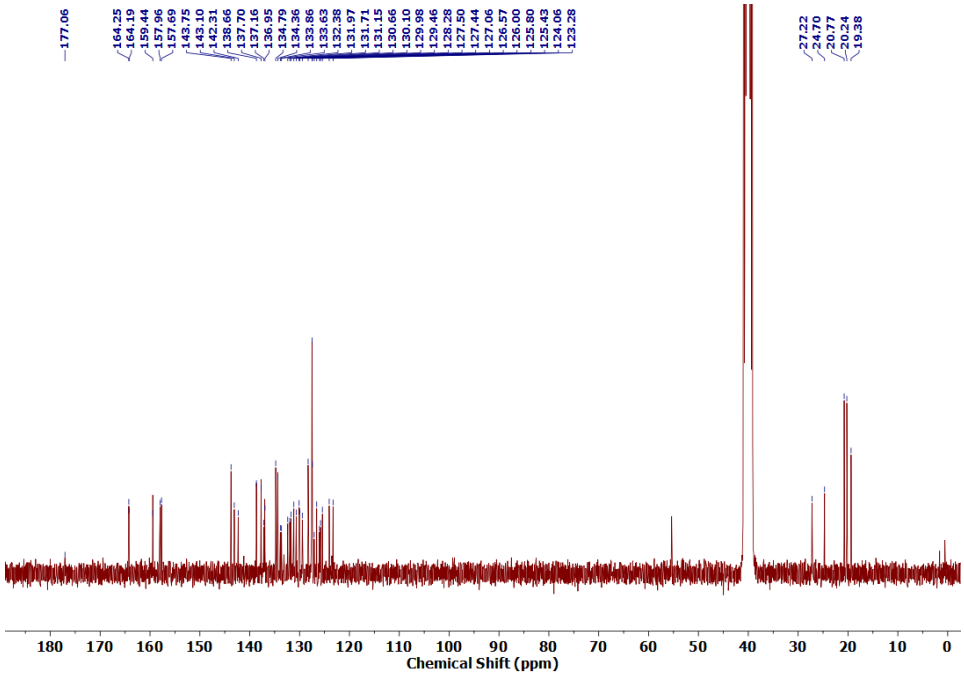


Figure **S16**. ^{13}C NMR of the dyad **Cu(I)-A** in DMSO-*d6*.

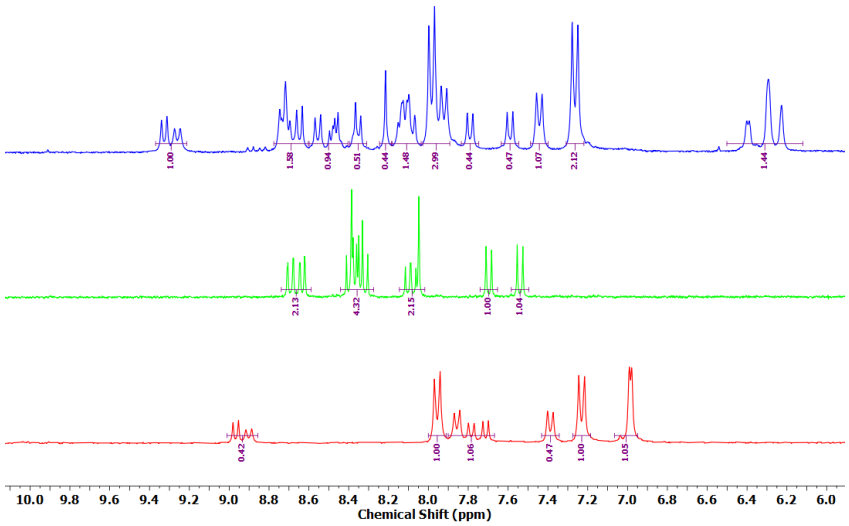


Figure **S17**. Overlaid ^{1}H NMR of the aromatic region for the donor ligand **D** (red), acceptor ligand **A** (green) and triad **D-Cu(I)-A** in DMSO-*d6*.

HR-ESI Mass Spectrum of D-Cu(I)-A

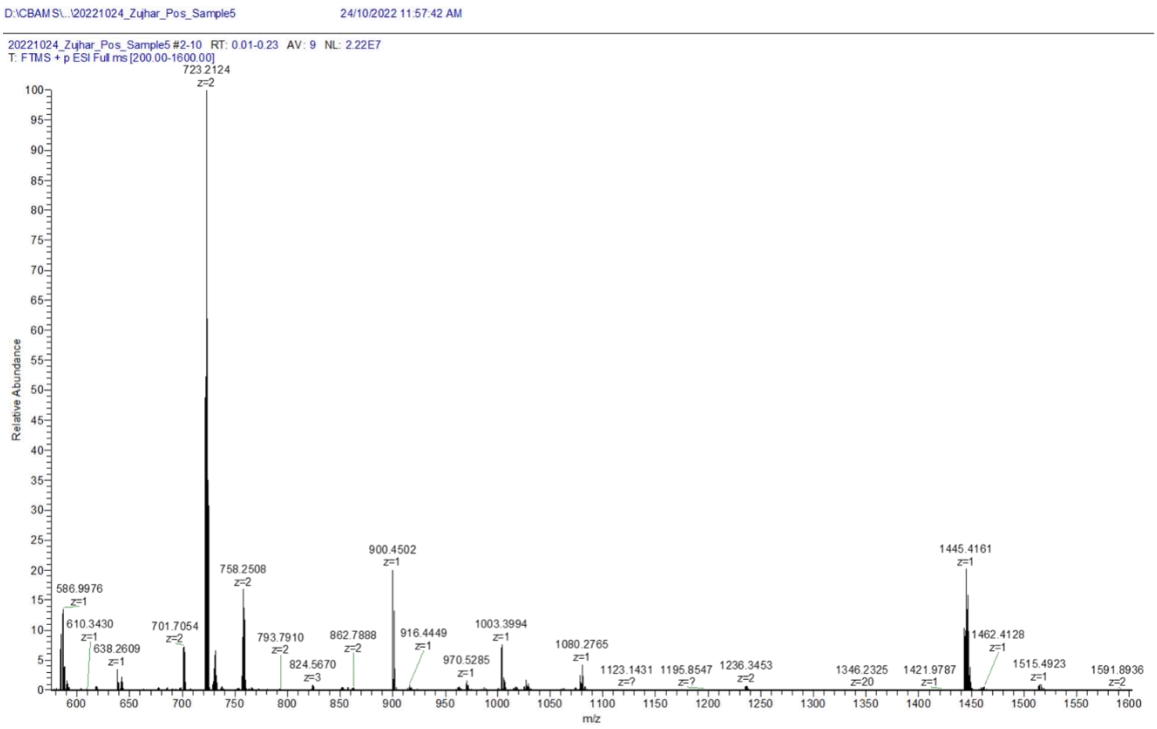


Figure **S18**. HR-ESI mass spectrum of **D-Cu(I)-A**.

Photoluminescence Characterization of the Triad and Dyad Complexes

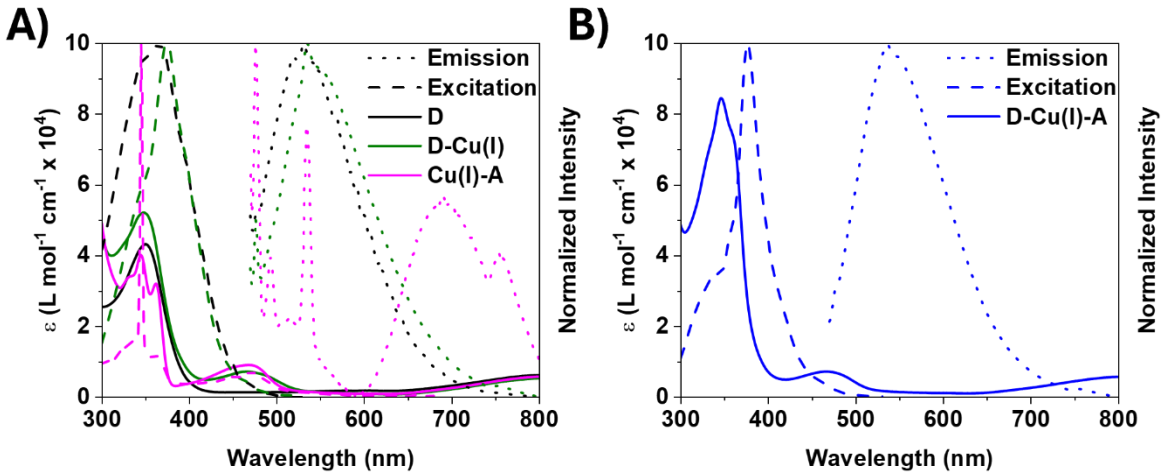


Figure **S19**. Absorbance (solid lines), emission (dotted lines, λ_{ex} = 460 nm) and excitation (dashed lines) for A) **D** (black traces, λ_{em} = 540 nm), and **Cu(I)-A** (pink traces, λ_{em} = 690 nm) and **D-Cu(I)** (green traces, λ_{em} = 540 nm) dyads in CH_2Cl_2 at room temperature, and B) **D-Cu(I)-A** (blue traces, λ_{em} = 540 nm) triad. All data collected in CH_2Cl_2 at room temperature. Emission scans with λ_{ex} = 460 nm were collected with 2 nm slit widths, excitation scans taken with λ_{em} = 540 nm and 690 nm emission were collected with 3 nm slit widths.

DFT Representation of the Triad and Dyad Complexes

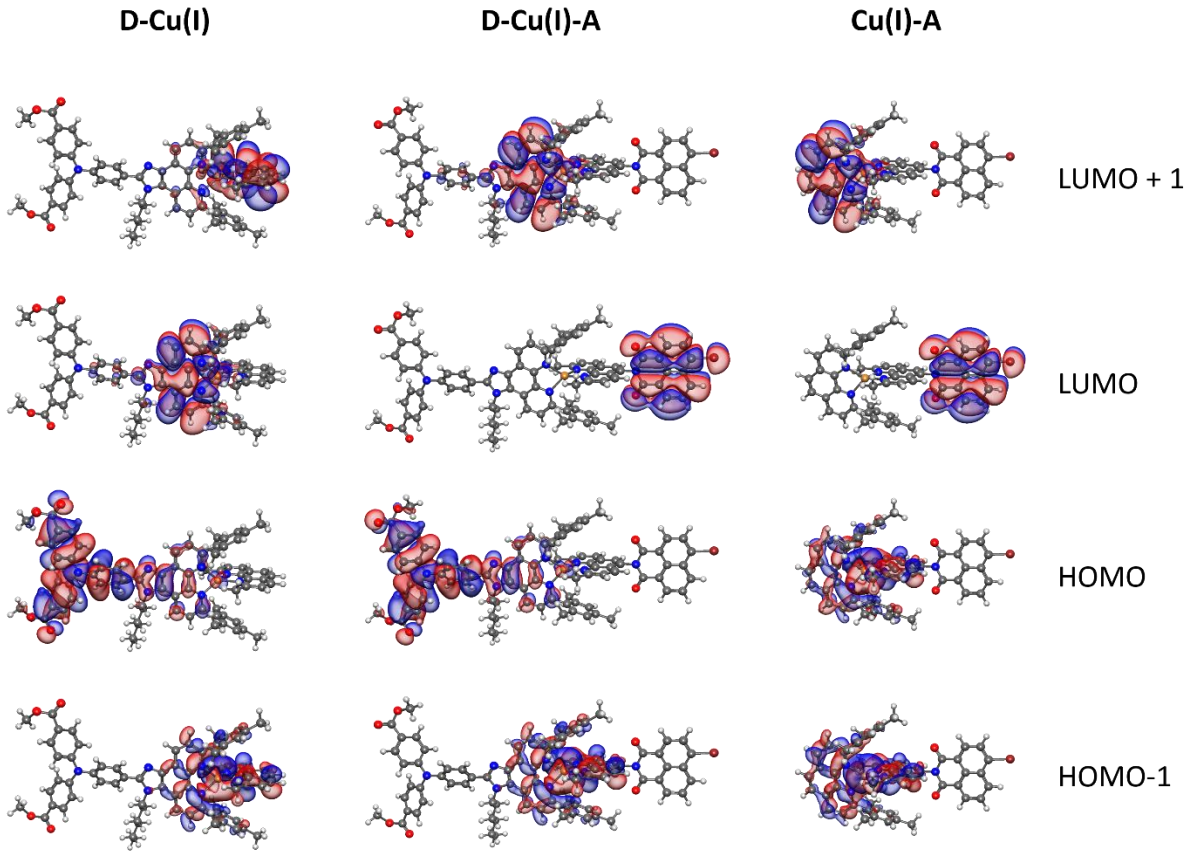


Figure **S20**. Graphical representation of the frontier orbitals of **D-Cu(I)**, **D-C(I)-A** and **Cu(I)-A** drawn at an isovalue of 0.0200 $Å^{-3}$ as calculated using Gaussian 16[1] using the B3PW91 functional[2] with LANL2DZ as the basis set.[3]

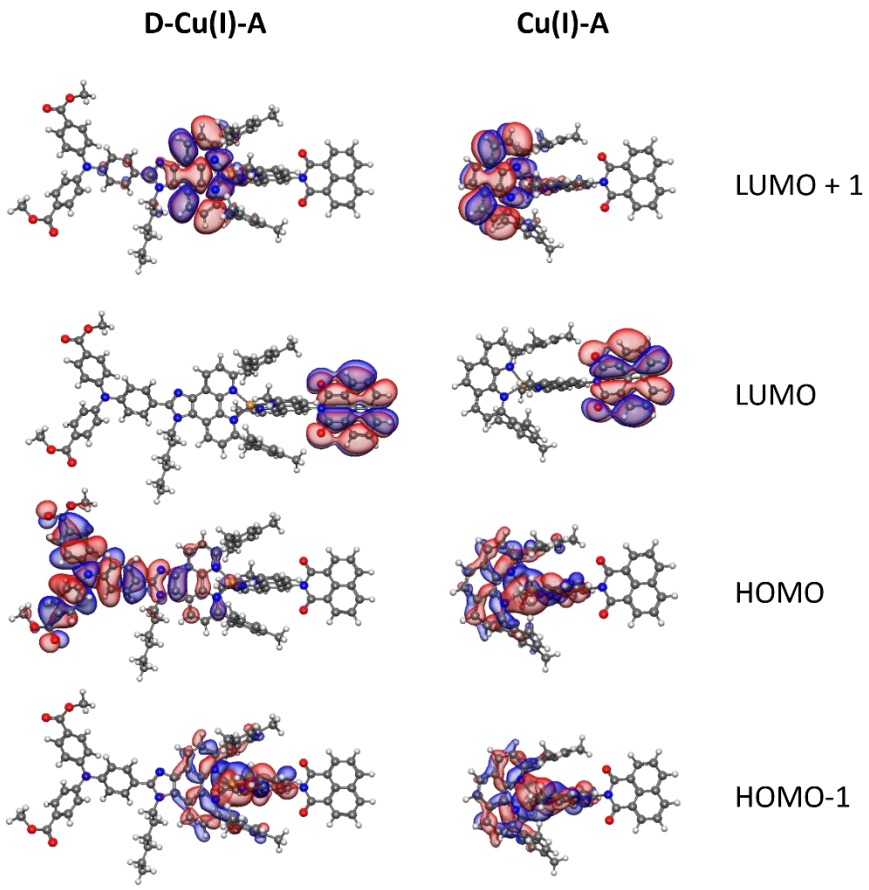


Figure **S21**. Graphical representation of the frontier orbitals of **D-C(I)-A-H** and **Cu(I)-A-H** with a hydrogen replacing the pendant bromine, drawn at an isovalue of 0.0200 $Å^{-3}$ as calculated using Gaussian 16[1] using the B3PW91 functional[2] with LANL2DZ as the basis set.[3]

Spectroelectrochemical Analysis of D-Cu(I)-A

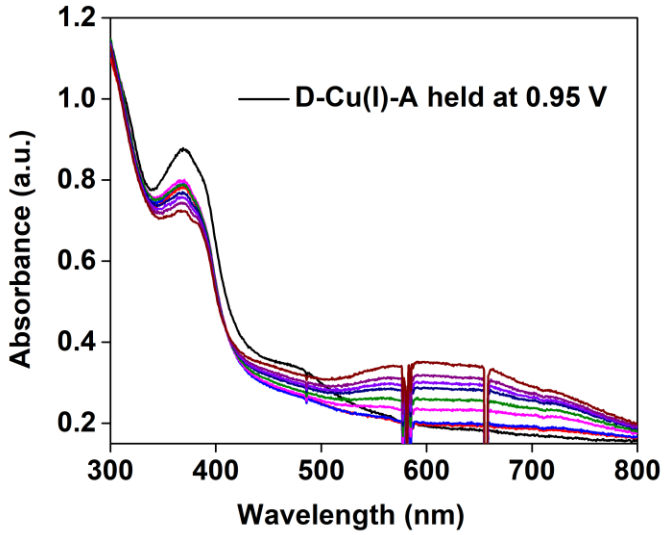


Figure **S22**. Absorbance spectra of the electrochemically oxidized **D-Cu(I)-A** at 0.95 V taken at different intervals of time.

Spectroelectrochemical Analysis of Acceptor

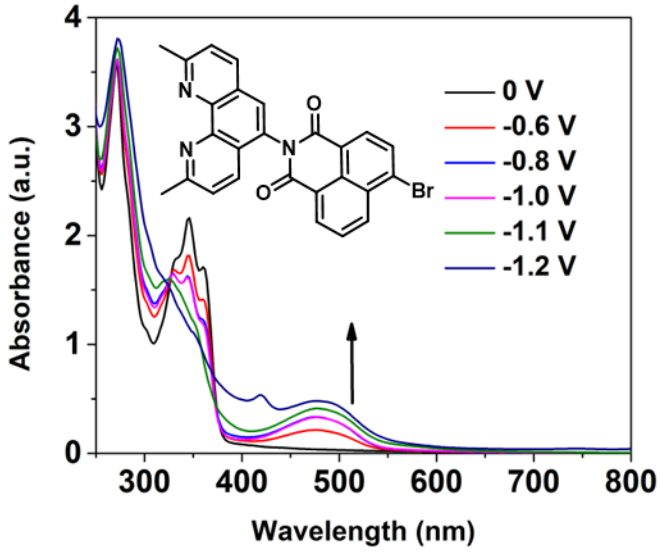


Figure **S23**. Absorbance spectra of the electrochemically reduced acceptor ligand **A**.

Femtosecond Transient Absorption Spectroscopy Analysis of D-Cu(I).

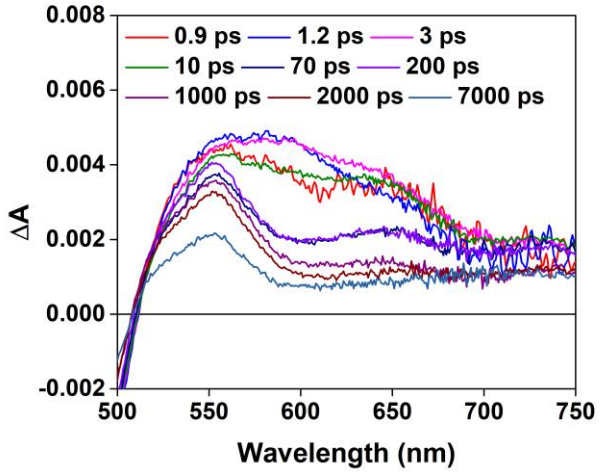


Figure **S24**. Femtosecond transient absorption difference spectra for **D-Cu(I)** at different time delays after 470 nm excitation (2 μJ / pulse).

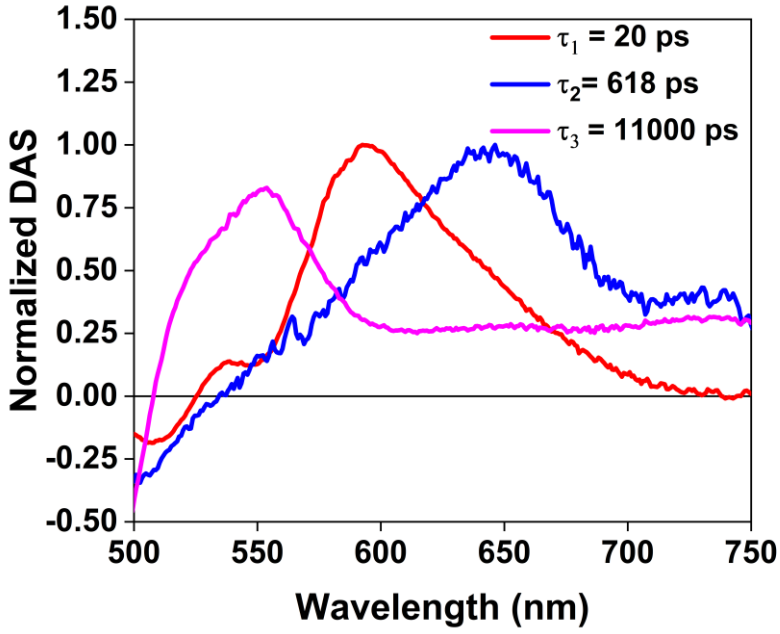


Figure **S25**. Kinetic analysis displaying decay-associated spectra of **D-Cu(I)** collected in acetonitrile solution.

Nanosecond Transient Absorption Spectroscopy Analysis.

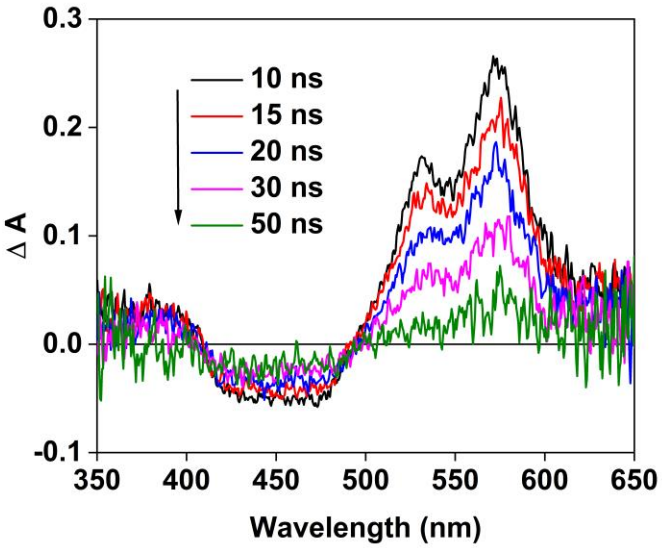


Figure **S26**. Nanosecond transient absorption difference spectra for reference compound [Cu(dmp)(dmesp)]PF6.

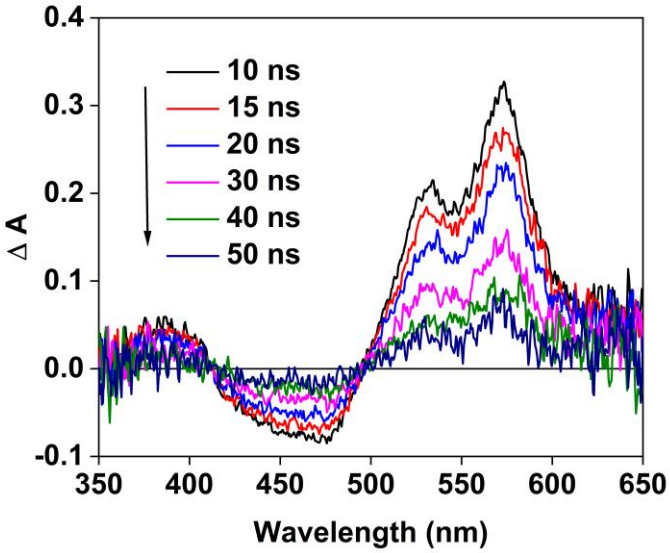


Figure **S27**. Nanosecond transient absorption difference spectra for the dyad **Cu(I)-A.**

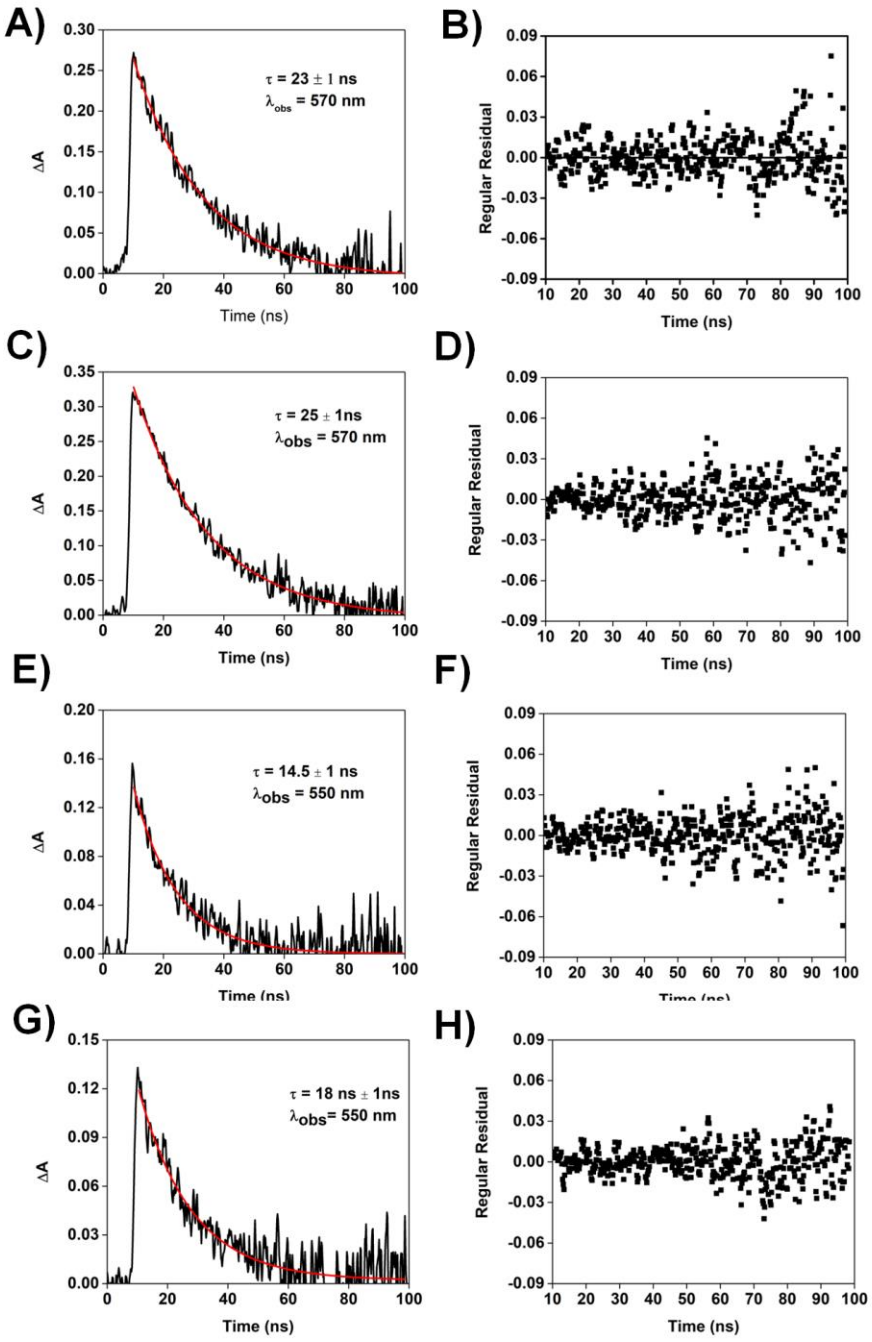


Figure **S28**. Kinetic traces from the corresponding nanosecond transient absorption and the residual plots of the reference compound **[Cu(dmesp)(dmp)[PF$_6$** (**A,B**), dyad **Cu(I)-A** (**C,D**), dyad **D-Cu(I)** (**E, F**) and triad **D-Cu(I)-A** (**G,H**).

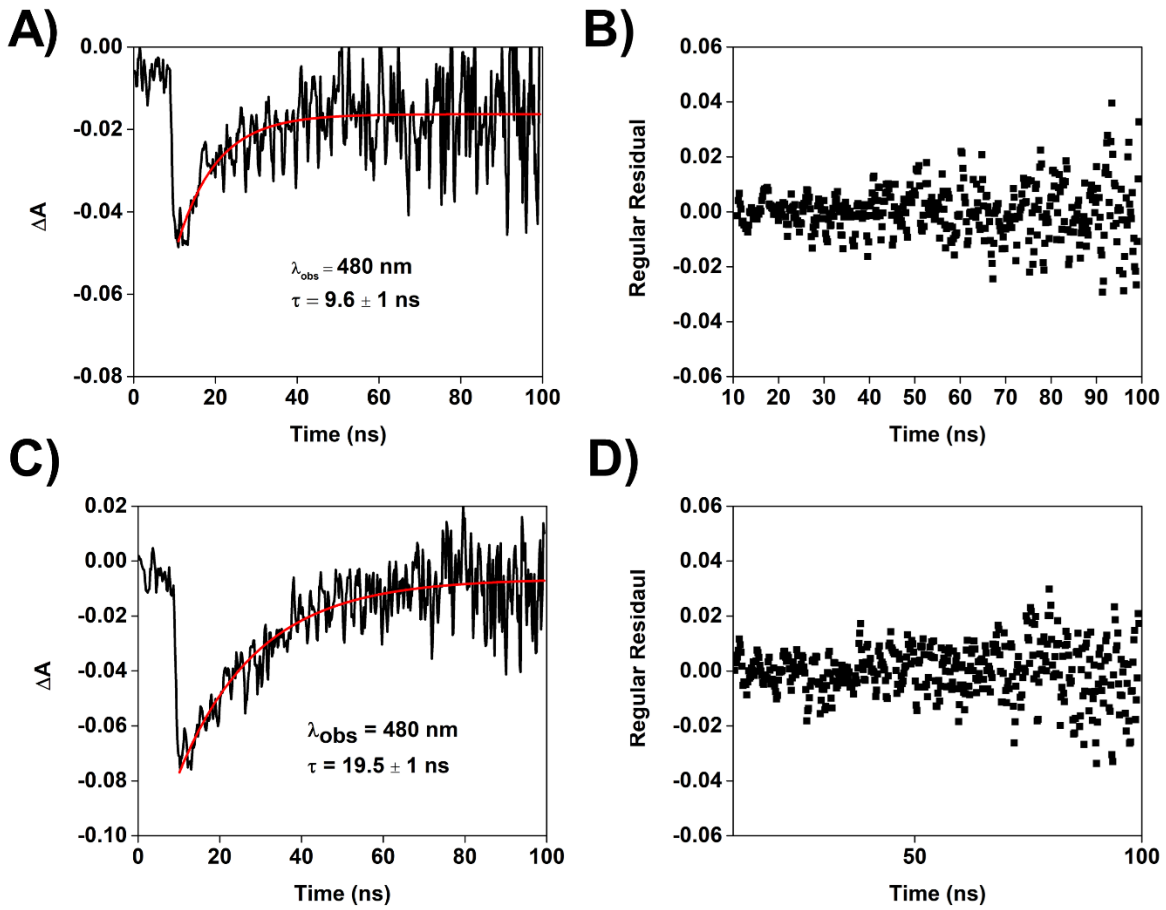


Figure **S29**. Kinetic traces for the recovery of MLCT bleach at 480 nm from the corresponding nanosecond transient absorption and the residual plots of the reference compound **[Cu(dmesp)(dmp)][PF$_6$** (**A,B**), dyad **Cu(I)-A** (**C,D**).

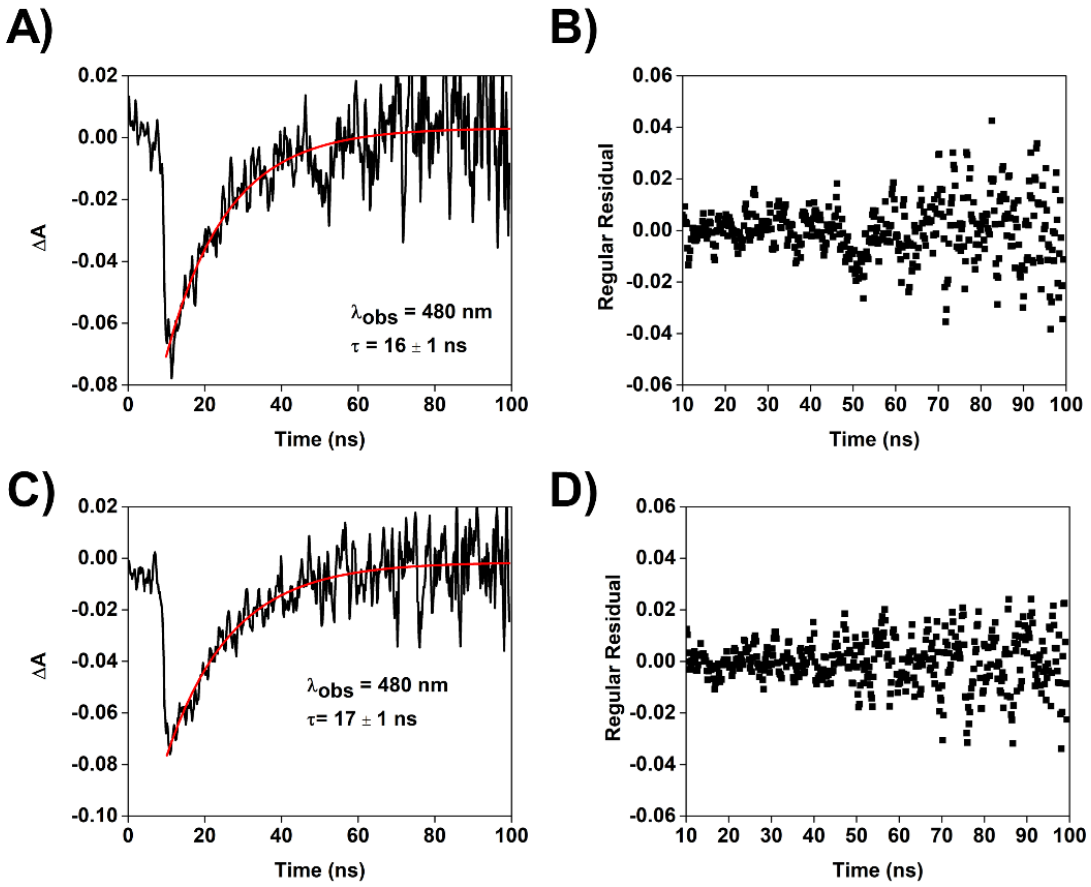


Figure **S30**. Kinetic traces for the recovery of MLCT bleach at 480 nm from the corresponding nanosecond transient absorption and the residual plots of the dyad **D-Cu(I)** (**A,B**) and triad **D-Cu(I)-A** (**C,D**).

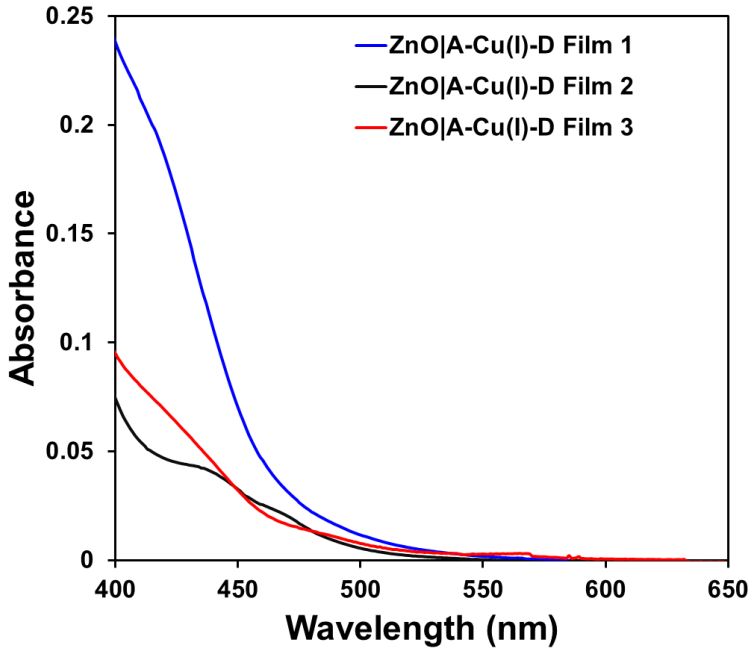


Figure **S31**. Overlaid absorption spectra of the desorbed complex from three different ZnO|A-Cu(I)-D photoanodes. The films were digested using 0.1 M HCl and then extracted with 10 mL of DCM. The organic layers were collected, analyzed by UV-Vis spectroscopy, and the following analysis was performed on each sample:

Loading Calculations:

Molar absorptivity constant (ε) for MLCT transition in A-Cu(I)-D = 6900 L^{-1} mol^{-1} cm^{-1}

Optical pathlength of the cuvette (l) = 1 cm

Average of the MLCT absorbance for three desorbed films = 0.0312

According to the Beer-Lambert Law: $A = \varepsilon C l = (\varepsilon m l) / V$

(Where C = concentration; m = moles; V = volume in Litres)

Therefore, moles of the desorbed A-Cu(I)-D can be calculated as:

$m = 0.0312 * 10/6900 = 4.52 \times 10^{-5}$ mmol

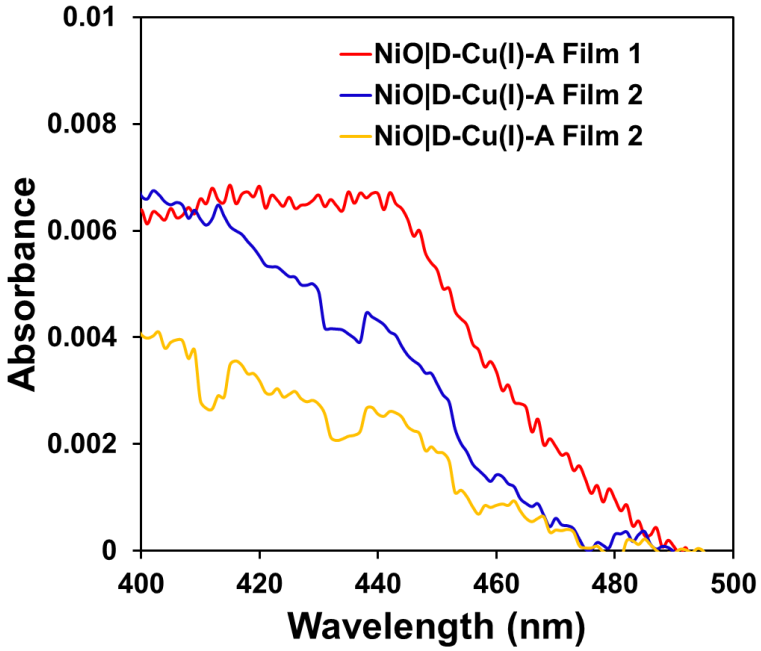


Figure **S32**. Overlaid absorption spectra of the desorbed complex from three different NiO|D-Cu(I)-A photocathodes. The films were digested using 0.1 M HCl and then extracted with 5 mL of DCM. The organic layers were collected, analyzed by UV-Vis spectroscopy, and the following analysis was performed on each sample:

Loading Calculations:

Molar absorptivity constant (ε) for MLCT transition in A-Cu(I)-D = 6900 L^{-1} mol^{-1} cm^{-1}

Optical pathlength of the cuvette (l) = 1 cm

Average of the MLCT absorbance for three desorbed films = 0.00188

According to the Beer-Lambert Law: $A = \varepsilon C l = (\varepsilon m l) / V$

(Where C = concentration; m = moles; V = volume in Litres)

Therefore, moles of the desorbed A-Cu(I)-D can be calculated as:

$m = 0.00188 * 5/6900 = 1.36 \times 10^{-6}$ mmol

DFT Calculations

D-Cu(I)

Standard Orientation					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstrom)		
			X	Y	Z
1	6	0	0.872284	-2.960914	0.017944
2	6	0	0.884583	-1.552046	-0.10588
3	6	0	2.135521	-0.893286	-0.208428
4	7	0	3.322901	-1.585373	-0.189936
5	6	0	3.306208	-2.935956	-0.107073
6	6	0	2.079878	-3.645208	0.008612
7	6	0	-0.301065	-0.752006	-0.140236
8	6	0	-0.252181	0.646986	-0.274667
9	6	0	0.996845	1.345624	-0.41237
10	6	0	2.192022	0.553535	-0.366742
11	6	0	1.173388	2.742395	-0.598038
12	6	0	2.446628	3.272723	-0.75276
13	6	0	3.585893	2.43262	-0.707088
14	7	0	3.442976	1.105283	-0.49262
15	6	0	4.594254	-3.690984	-0.186037
16	6	0	4.94744	3.001035	-0.944314
17	6	0	5.323628	-4.000623	0.985572
18	6	0	6.521066	-4.72881	0.86994
19	6	0	6.999612	-5.177375	-0.373761
20	6	0	6.241208	-4.880758	-1.521196
21	6	0	5.039883	-4.154391	-1.44909
22	6	0	5.429747	3.089859	-2.274288
23	6	0	6.702002	3.642513	-2.500069
24	6	0	7.499141	4.126315	-1.446077
25	6	0	6.986336	4.049311	-0.139339
26	6	0	5.71731	3.505853	0.129245
27	6	0	4.226007	-3.918055	-2.704663
28	6	0	8.27025	-5.991584	-0.471124
29	6	0	4.8114	-3.605905	2.353434
30	6	0	5.180629	3.512856	1.543995
31	6	0	4.5834	2.641097	-3.447671
32	6	0	8.85087	4.747763	-1.716812
33	7	0	-1.603146	-1.200083	-0.059582
34	6	0	-2.371554	-0.100281	-0.134835
35	7	0	-1.591098	1.05711	-0.273856
36	6	0	-3.837817	-0.17126	-0.122674

37	6	0	-4.677683	0.776747	0.501394
38	6	0	-6.065978	0.617371	0.507404
39	6	0	-6.664662	-0.497521	-0.117594
40	6	0	-5.829205	-1.458915	-0.729641
41	6	0	-4.44329	-1.300028	-0.72135
42	7	0	-8.080069	-0.652538	-0.120375
43	6	0	-8.660008	-1.948971	0.026516
44	6	0	-8.920075	0.492682	-0.262872
45	6	0	-10.084501	0.629425	0.522111
46	6	0	-10.899592	1.758023	0.386011
47	6	0	-10.561889	2.782953	-0.520475
48	6	0	-9.388717	2.650441	-1.290808
49	6	0	-8.586304	1.513559	-1.179842
50	6	0	-9.784425	-2.318723	-0.741495
51	6	0	-10.350887	-3.589343	-0.597921
52	6	0	-9.797264	-4.525317	0.298504
53	6	0	-8.660739	-4.159622	1.047794
54	6	0	-8.107762	-2.882958	0.930202
55	6	0	6.228936	-0.746036	-3.139538
56	6	0	3.973193	0.150187	3.230962
57	6	0	5.460996	0.06501	3.023808
58	7	0	5.939282	-0.106264	1.775134
59	6	0	7.296534	-0.188528	1.576455
60	6	0	8.231612	-0.097875	2.64343
61	6	0	7.711808	0.083959	3.952686
62	6	0	6.340969	0.163724	4.138581
63	6	0	7.773419	-0.377441	0.228435
64	6	0	9.170053	-0.470233	-0.011983
65	6	0	10.092416	-0.372722	1.086677
66	6	0	9.639714	-0.192809	2.369591
67	7	0	6.843301	-0.464261	-0.779832
68	6	0	7.256107	-0.647166	-2.048829
69	6	0	8.641546	-0.748382	-2.359943
70	6	0	9.590556	-0.660517	-1.355307
71	29	0	4.934411	-0.289568	-0.069142
72	6	0	-10.286294	-5.933908	0.407222
73	8	0	-9.525047	-6.88253	0.630292
74	8	0	-11.630649	-6.192086	0.194308
75	6	0	-12.69736	-5.26602	0.577275
76	6	0	-11.323576	4.065557	-0.619547
77	8	0	-10.767742	5.146379	-0.850104
78	8	0	-12.688776	4.052717	-0.38996
79	6	0	-13.554808	2.928382	-0.748887

80	6	0	-2.997896	7.979839	2.667232
81	6	0	-3.039719	7.07228	1.427408
82	6	0	-2.51791	5.651806	1.709735
83	6	0	-2.557689	4.73782	0.47204
84	6	0	-2.034277	3.319138	0.760124
85	6	0	-2.098149	2.422261	-0.489045
86	1	0	-0.079354	-3.47421	0.107383
87	1	0	2.111219	-4.726837	0.084842
88	1	0	0.322934	3.409985	-0.63327
89	1	0	2.587165	4.336111	-0.914654
90	1	0	7.084784	-4.960564	1.771864
91	1	0	6.585057	-5.234658	-2.491591
92	1	0	7.074059	3.708157	-3.521016
93	1	0	7.581568	4.429591	0.688913
94	1	0	3.316023	-4.532921	-2.706762
95	1	0	3.905731	-2.874482	-2.79932
96	1	0	4.798468	-4.182648	-3.599525
97	1	0	8.052227	-7.065316	-0.392023
98	1	0	8.778505	-5.8328	-1.428591
99	1	0	8.97139	-5.741596	0.33257
100	1	0	4.422428	-2.583615	2.359335
101	1	0	3.994537	-4.268177	2.67201
102	1	0	5.603089	-3.676761	3.106263
103	1	0	5.988962	3.640046	2.27129
104	1	0	4.47404	4.341596	1.691043
105	1	0	4.650119	2.58602	1.780188
106	1	0	4.159931	1.642522	-3.29288
107	1	0	3.739784	3.325331	-3.610802
108	1	0	5.170317	2.623754	-4.371546
109	1	0	9.521302	4.644114	-0.856837
110	1	0	9.337699	4.290931	-2.5855
111	1	0	8.751595	5.821509	-1.926331
112	1	0	-4.256429	1.619171	1.039894
113	1	0	-6.688597	1.347636	1.014391
114	1	0	-6.269159	-2.324091	-1.21527
115	1	0	-3.807812	-2.045665	-1.188304
116	1	0	-10.335679	-0.137579	1.248013
117	1	0	-11.770351	1.861066	1.026554
118	1	0	-9.119893	3.449834	-1.975009
119	1	0	-7.698688	1.411583	-1.796324
120	1	0	-10.198233	-1.618188	-1.460072
121	1	0	-11.193195	-3.866455	-1.224677
122	1	0	-8.220894	-4.88976	1.720686

123	1	0	-7.246453	-2.607101	1.530436
124	1	0	5.223178	-0.651121	-2.72373
125	1	0	6.37886	0.042381	-3.886429
126	1	0	6.306077	-1.709436	-3.656928
127	1	0	3.446131	0.059842	2.279591
128	1	0	3.625696	-0.646242	3.90076
129	1	0	3.697275	1.104063	3.69767
130	1	0	8.391981	0.157699	4.797009
131	1	0	5.920192	0.30065	5.129679
132	1	0	11.157275	-0.445645	0.881522
133	1	0	10.339069	-0.120734	3.1984
134	1	0	8.936968	-0.895733	-3.393807
135	1	0	10.650334	-0.736877	-1.583049
136	1	0	-13.396559	-5.843993	1.186025
137	1	0	-12.316773	-4.415488	1.151896
138	1	0	-13.204173	-4.912252	-0.325296
139	1	0	-14.367753	3.350846	-1.343825
140	1	0	-13.0223	2.168713	-1.329978
141	1	0	-13.962029	2.485239	0.164541
142	1	0	-3.375362	8.983264	2.437674
143	1	0	-3.613402	7.569564	3.478164
144	1	0	-1.97296	8.086396	3.046215
145	1	0	-2.443736	7.524941	0.620766
146	1	0	-4.071953	7.011774	1.052578
147	1	0	-3.115891	5.200656	2.516304
148	1	0	-1.485336	5.713174	2.087668
149	1	0	-1.963984	5.196055	-0.335106
150	1	0	-3.591158	4.680384	0.097724
151	1	0	-2.62332	2.864457	1.567852
152	1	0	-1.004197	3.37367	1.137862
153	1	0	-1.53895	2.871422	-1.318141
154	1	0	-3.132744	2.336302	-0.832867

D-Cu(I)-A

Standard Orientation					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstrom)		
			X	Y	Z
1	6	0	1.803487	2.919315	0.087663
2	6	0	1.827388	1.510965	-0.040864
3	6	0	0.592261	0.820642	-0.124934
4	7	0	-0.611857	1.481598	-0.08671
5	6	0	-0.630998	2.832743	0.000452
6	6	0	0.578102	3.572506	0.099618
7	6	0	3.031841	0.739683	-0.097162
8	6	0	3.014578	-0.660217	-0.234118
9	6	0	1.781128	-1.390519	-0.351431
10	6	0	0.569368	-0.626877	-0.284478
11	6	0	1.632443	-2.791149	-0.534423
12	6	0	0.368372	-3.352944	-0.657215
13	6	0	-0.788925	-2.540445	-0.585825
14	7	0	-0.668858	-1.208122	-0.386005
15	6	0	-1.947054	3.540125	-0.057421
16	6	0	-2.152491	-3.125518	-0.761633
17	6	0	-2.7158	3.739421	1.114767
18	6	0	-3.959425	4.383968	1.012542
19	6	0	-4.452992	4.855923	-0.217915
20	6	0	-3.649943	4.688026	-1.359517
21	6	0	-2.399332	4.045359	-1.300798
22	6	0	-2.709825	-3.198722	-2.061554
23	6	0	-4.00427	-3.726176	-2.217937
24	6	0	-4.754376	-4.193393	-1.123613
25	6	0	-4.158533	-4.149812	0.150549
26	6	0	-2.866645	-3.634759	0.349467
27	6	0	-1.55009	3.940066	-2.551259
28	6	0	-5.805455	5.527134	-0.298565
29	6	0	-2.194137	3.323555	2.472485
30	6	0	-2.245914	-3.682381	1.729052
31	6	0	-1.920137	-2.76425	-3.278916
32	6	0	-6.158475	-4.724123	-1.300623
33	7	0	4.324624	1.218349	-0.036557
34	6	0	5.117598	0.137067	-0.126613
35	7	0	4.362537	-1.038056	-0.255895
36	6	0	6.581937	0.239546	-0.137338
37	6	0	7.450016	-0.694833	0.46836
38	6	0	8.835087	-0.512841	0.447063

39	6	0	9.403644	0.613006	-0.186783
40	6	0	8.539623	1.563204	-0.776794
41	6	0	7.156783	1.380815	-0.742654
42	7	0	10.815395	0.783856	-0.224486
43	6	0	11.395443	2.079213	-0.076772
44	6	0	11.661572	-0.358205	-0.376996
45	6	0	12.82442	-0.498255	0.408808
46	6	0	13.64511	-1.621383	0.26001
47	6	0	13.313399	-2.636232	-0.659695
48	6	0	12.140392	-2.500861	-1.429737
49	6	0	11.332535	-1.368899	-1.306057
50	6	0	12.533629	2.439723	-0.830933
51	6	0	13.121508	3.694835	-0.662026
52	6	0	12.571031	4.634569	0.232802
53	6	0	11.433938	4.273676	0.983078
54	6	0	10.857274	3.007875	0.839833
55	8	0	-8.66648	-2.393986	0.071822
56	8	0	-8.868845	2.138573	0.950172
57	35	0	-15.616579	1.139811	-0.518065
58	6	0	-11.458301	-2.552867	-0.473323
59	6	0	-12.847193	-2.573012	-0.739684
60	6	0	-13.597478	-1.408065	-0.646666
61	6	0	-12.989633	-0.17181	-0.282623
62	6	0	-13.701444	1.064974	-0.169851
63	6	0	-13.062434	2.245067	0.187727
64	6	0	-11.674347	2.242574	0.450193
65	6	0	-9.381072	-1.37154	0.162083
66	6	0	-10.832972	-1.361972	-0.113713
67	6	0	-11.579358	-0.152272	-0.010513
68	6	0	-10.938557	1.065478	0.354762
69	6	0	-9.490666	1.099565	0.64004
70	7	0	-8.799635	-0.137115	0.54575
71	6	0	-3.341486	0.702562	-3.107975
72	6	0	-1.38107	-0.299553	3.337856
73	6	0	-2.857063	-0.313001	3.04736
74	7	0	-3.277617	-0.129203	1.779871
75	6	0	-4.623757	-0.137299	1.507305
76	6	0	-5.60458	-0.335717	2.514743
77	6	0	-5.147846	-0.528301	3.844995
78	6	0	-3.787206	-0.51579	4.105833
79	6	0	-5.04298	0.069788	0.143022
80	6	0	-6.425378	0.075047	-0.17749
81	6	0	-7.388584	-0.137432	0.870868

82	6	0	-6.994825	-0.334468	2.165576
83	7	0	-4.067133	0.262105	-0.804423
84	6	0	-4.417957	0.475618	-2.086287
85	6	0	-5.786777	0.495704	-2.472647
86	6	0	-6.782004	0.295564	-1.532545
87	29	0	-2.193246	0.151389	0.00673
88	6	0	13.293119	5.928433	0.427548
89	8	0	14.520621	6.026159	0.319834
90	8	0	12.563208	7.047634	0.799403
91	6	0	11.202801	7.308167	0.328217
92	6	0	14.083034	-3.913327	-0.776302
93	8	0	13.53088	-4.994345	-1.016186
94	8	0	15.448526	-3.896272	-0.556376
95	6	0	16.306451	-2.756125	-0.886477
96	6	0	5.95219	-7.942405	2.634667
97	6	0	5.956987	-7.029551	1.398039
98	6	0	5.415374	-5.619539	1.695106
99	6	0	5.417131	-4.700534	0.460496
100	6	0	4.872668	-3.292864	0.763253
101	6	0	4.896147	-2.391114	-0.483823
102	1	0	2.742322	3.45751	0.165138
103	1	0	0.520119	4.652494	0.183136
104	1	0	2.49712	-3.438874	-0.589385
105	1	0	0.249974	-4.420147	-0.811348
106	1	0	-4.554984	4.525575	1.912762
107	1	0	-3.999984	5.071281	-2.316233
108	1	0	-4.433873	-3.77886	-3.216556
109	1	0	-4.712285	-4.529419	1.007542
110	1	0	-0.696883	4.630243	-2.50907
111	1	0	-1.139152	2.933729	-2.690064
112	1	0	-2.130807	4.197721	-3.442947
113	1	0	-6.607052	4.831826	-0.017861
114	1	0	-5.864938	6.383073	0.385216
115	1	0	-6.014485	5.891682	-1.309477
116	1	0	-1.693034	2.352752	2.433246
117	1	0	-1.464304	4.053629	2.849405
118	1	0	-3.005781	3.263131	3.204812
119	1	0	-3.01611	-3.734549	2.505628
120	1	0	-1.610079	-4.571984	1.839771
121	1	0	-1.618203	-2.808567	1.925599
122	1	0	-1.466088	-1.776176	-3.14518
123	1	0	-1.102804	-3.467142	-3.490124
124	1	0	-2.557121	-2.730668	-4.168604

125	1	0	-6.896065	-4.037303	-0.866568
126	1	0	-6.405623	-4.858638	-2.358939
127	1	0	-6.281802	-5.693049	-0.801321
128	1	0	7.053547	-1.545599	1.012379
129	1	0	9.479718	-1.234825	0.938019
130	1	0	8.95692	2.435072	-1.270571
131	1	0	6.499292	2.115405	-1.196713
132	1	0	13.074096	0.262844	1.141377
133	1	0	14.516522	-1.726125	0.899157
134	1	0	11.876443	-3.29342	-2.123678
135	1	0	10.444952	-1.262947	-1.922074
136	1	0	12.95411	1.733728	-1.540034
137	1	0	14.013145	3.964364	-1.220388
138	1	0	11.026374	4.959981	1.719338
139	1	0	10.003454	2.729879	1.449808
140	1	0	-10.86117	-3.457092	-0.541997
141	1	0	-13.327623	-3.505587	-1.017565
142	1	0	-14.662926	-1.431032	-0.852472
143	1	0	-13.624874	3.168782	0.267087
144	1	0	-11.165637	3.159485	0.731423
145	1	0	-2.35477	0.611566	-2.648049
146	1	0	-3.421523	-0.021566	-3.926887
147	1	0	-3.432505	1.704293	-3.543939
148	1	0	-0.808633	-0.160032	2.418708
149	1	0	-1.128089	0.509215	4.034646
150	1	0	-1.067465	-1.238533	3.810323
151	1	0	-5.865838	-0.682122	4.645828
152	1	0	-3.412123	-0.658474	5.114247
153	1	0	-7.738331	-0.489385	2.942082
154	1	0	-6.034321	0.670918	-3.514646
155	1	0	-7.827287	0.308826	-1.823214
156	1	0	11.218039	8.310364	-0.106845
157	1	0	10.881196	6.579933	-0.423333
158	1	0	10.519765	7.290407	1.182628
159	1	0	17.128662	-3.16078	-1.480781
160	1	0	15.771862	-1.99192	-1.459408
161	1	0	16.700901	-2.32482	0.037991
162	1	0	6.342968	-8.938239	2.394544
163	1	0	6.574408	-7.524601	3.436578
164	1	0	4.935897	-8.068122	3.030695
165	1	0	5.355202	-7.489479	0.599851
166	1	0	6.981425	-6.949583	1.005902
167	1	0	6.019486	-5.160841	2.492797

168	1	0	4.390833	-5.700416	2.090824
169	1	0	4.817895	-5.166698	-0.337997
170	1	0	6.442707	-4.622862	0.068556
171	1	0	5.467894	-2.829941	1.561718
172	1	0	3.851008	-3.367989	1.159706
173	1	0	4.332519	-2.850004	-1.304527
174	1	0	5.922554	-2.28184	-0.845059

Cu(I)-A

Standard Orientation					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	7.068141	2.757326	-0.146086
2	6	0	7.061408	1.340205	-0.222678
3	6	0	5.795616	0.692877	-0.233115
4	7	0	4.60817	1.38432	-0.173065
5	6	0	4.629299	2.737618	-0.141034
6	6	0	5.863597	3.445032	-0.115298
7	6	0	8.265445	0.555055	-0.292632
8	6	0	8.208767	-0.812651	-0.384259
9	6	0	6.942984	-1.496366	-0.412781
10	6	0	5.736824	-0.748007	-0.33319
11	6	0	6.827802	-2.907012	-0.521884
12	6	0	5.569024	-3.490683	-0.558045
13	6	0	4.400335	-2.683116	-0.481562
14	7	0	4.497788	-1.339331	-0.359942
15	6	0	3.339319	3.491146	-0.180986
16	6	0	3.043648	-3.303521	-0.560209
17	6	0	2.904311	4.03846	-1.412589
18	6	0	1.683729	4.738372	-1.451083
19	6	0	0.897155	4.9243	-0.301327
20	6	0	1.373589	4.404616	0.917038
21	6	0	2.584858	3.699804	0.999478
22	6	0	2.374632	-3.353025	-1.808085
23	6	0	1.093844	-3.928215	-1.869927
24	6	0	0.462243	-4.463553	-0.732021
25	6	0	1.166143	-4.436997	0.485545
26	6	0	2.450679	-3.875631	0.590395
27	6	0	3.092526	3.225737	2.342992
28	6	0	-0.418754	5.666334	-0.359793
29	6	0	3.734523	3.914513	-2.674552
30	6	0	3.185527	-3.933844	1.91301
31	6	0	3.039098	-2.850718	-3.072531
32	6	0	-0.933402	-5.037643	-0.80961
33	8	0	-3.438102	-2.571802	0.089867
34	8	0	-3.680751	1.948116	1.019467
35	35	0	-10.42782	0.895953	-0.415459
36	6	0	-6.23084	-2.75265	-0.443299
37	6	0	-7.621106	-2.784191	-0.701069
38	6	0	-8.382888	-1.628408	-0.588978

39	6	0	-7.785652	-0.390306	-0.21383
40	6	0	-8.509846	0.837304	-0.081012
41	6	0	-7.880951	2.019671	0.287023
42	6	0	-6.491191	2.028838	0.54002
43	6	0	-4.162103	-1.557459	0.19341
44	6	0	-5.615586	-1.559605	-0.073375
45	6	0	-6.373853	-0.359095	0.049069
46	6	0	-5.743582	0.860923	0.42492
47	6	0	-4.294331	0.907083	0.700223
48	7	0	-3.590415	-0.320877	0.584565
49	6	0	1.82371	0.716347	-3.084784
50	6	0	3.848145	-0.388923	3.327623
51	6	0	2.371934	-0.443254	3.042795
52	7	0	1.939439	-0.237803	1.782634
53	6	0	0.592295	-0.271639	1.51664
54	6	0	-0.377417	-0.515986	2.52456
55	6	0	0.091855	-0.733337	3.846602
56	6	0	1.453317	-0.697127	4.100227
57	6	0	0.159649	-0.041463	0.160004
58	6	0	-1.225186	-0.052781	-0.150318
59	6	0	-2.177117	-0.308025	0.898969
60	6	0	-1.769889	-0.532062	2.185055
61	7	0	1.124746	0.190163	-0.790152
62	6	0	0.760256	0.433475	-2.063033
63	6	0	-0.611758	0.437679	-2.438912
64	6	0	-1.595715	0.194112	-1.497151
65	29	0	3.006973	0.062857	0.005194
66	1	0	8.013792	3.292175	-0.122591
67	1	0	5.838379	4.528448	-0.070235
68	1	0	9.223264	1.068243	-0.275794
69	1	0	9.120801	-1.400893	-0.440775
70	1	0	7.724499	-3.517815	-0.583515
71	1	0	5.45194	-4.564745	-0.653582
72	1	0	1.345788	5.153516	-2.398703
73	1	0	0.790539	4.557148	1.823442
74	1	0	0.580193	-3.966581	-2.828684
75	1	0	0.706242	-4.867775	1.373163
76	1	0	3.940399	3.837918	2.680407
77	1	0	2.310779	3.296698	3.105769
78	1	0	3.43424	2.187978	2.298151
79	1	0	-0.626523	6.039983	-1.3675
80	1	0	-1.251268	5.015805	-0.062711
81	1	0	-0.419741	6.525403	0.322696

82	1	0	4.604446	4.584156	-2.645149
83	1	0	4.11801	2.89869	-2.823077
84	1	0	3.147748	4.1883	-3.557305
85	1	0	2.484567	-4.048962	2.746232
86	1	0	3.871028	-4.792124	1.943985
87	1	0	3.784958	-3.035815	2.090584
88	1	0	3.447674	-1.84221	-2.948314
89	1	0	3.873487	-3.502703	-3.365036
90	1	0	2.331086	-2.833891	-3.907174
91	1	0	-1.176279	-5.362313	-1.827277
92	1	0	-1.047059	-5.900809	-0.143749
93	1	0	-1.68053	-4.291043	-0.511078
94	1	0	-5.6249	-3.649749	-0.526691
95	1	0	-8.093559	-3.718317	-0.987245
96	1	0	-9.44938	-1.66016	-0.788092
97	1	0	-8.452662	2.936218	0.381729
98	1	0	-5.990345	2.947621	0.829161
99	1	0	2.816506	0.615857	-2.640012
100	1	0	1.74223	0.031955	-3.937072
101	1	0	1.718196	1.737019	-3.470823
102	1	0	4.182693	-1.299404	3.83879
103	1	0	4.415445	-0.275205	2.401614
104	1	0	4.085665	0.454458	3.988384
105	1	0	-0.617536	-0.92396	4.647139
106	1	0	1.837512	-0.857178	5.10254
107	1	0	-2.504585	-0.720394	2.962532
108	1	0	-0.870695	0.635792	-3.474
109	1	0	-2.64321	0.194422	-1.779988

D-Cu(I)-A-H

Standard Orientation					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstrom)		
			X	Y	Z
1	6	0	1.109643	2.95631	0.056292
2	6	0	1.111994	1.547181	-0.065654
3	6	0	-0.133397	0.876141	-0.154474
4	7	0	-1.327077	1.556265	-0.127043
5	6	0	-1.32531	2.907942	-0.046127
6	6	0	-0.105277	3.628891	0.057431
7	6	0	2.304369	0.756634	-0.110708
8	6	0	2.265731	-0.643444	-0.241373
9	6	0	1.021597	-1.354637	-0.36318
10	6	0	-0.178258	-0.571563	-0.307475
11	6	0	0.851821	-2.753589	-0.540669
12	6	0	-0.420216	-3.295821	-0.668956
13	6	0	-1.564883	-2.464716	-0.608682
14	7	0	-1.424905	-1.13357	-0.414223
15	6	0	-2.629588	3.635796	-0.115704
16	6	0	-2.936438	-3.028937	-0.790496
17	6	0	-3.402489	3.852777	1.050598
18	6	0	-4.63506	4.516437	0.937423
19	6	0	-5.113271	4.99034	-0.298343
20	6	0	-4.305773	4.804355	-1.433981
21	6	0	-3.065907	4.142248	-1.364273
22	6	0	-3.486519	-3.099682	-2.093648
23	6	0	-4.788158	-3.607279	-2.255879
24	6	0	-5.5526	-4.057156	-1.164206
25	6	0	-4.964332	-4.016748	0.113569
26	6	0	-3.665713	-3.521282	0.318381
27	6	0	-2.210552	4.017598	-2.608773
28	6	0	-6.454368	5.682517	-0.390744
29	6	0	-2.896095	3.435187	2.413557
30	6	0	-3.054683	-3.572037	1.70218
31	6	0	-2.682257	-2.68375	-3.30794
32	6	0	-6.963762	-4.566495	-1.347768
33	7	0	3.604182	1.215009	-0.044003
34	6	0	4.380434	0.120874	-0.124027
35	7	0	3.60763	-1.042712	-0.252778
36	6	0	5.846254	0.200095	-0.125848
37	6	0	6.695578	-0.745155	0.489492

38	6	0	8.083469	-0.585202	0.476208
39	6	0	8.673781	0.528627	-0.158971
40	6	0	7.828669	1.489709	-0.758664
41	6	0	6.442927	1.329383	-0.732529
42	7	0	10.088282	0.676934	-0.188442
43	6	0	10.687848	1.963569	-0.042511
44	6	0	10.917152	-0.479045	-0.330765
45	6	0	12.072749	-0.63407	0.462886
46	6	0	12.876394	-1.770719	0.324046
47	6	0	12.534293	-2.784211	-0.593341
48	6	0	11.368368	-2.633633	-1.37128
49	6	0	10.577849	-1.48847	-1.257516
50	6	0	11.836381	2.302744	-0.790867
51	6	0	12.442986	3.549123	-0.623531
52	6	0	11.901789	4.501343	0.263731
53	6	0	10.754372	4.161754	1.008208
54	6	0	10.158648	2.904619	0.866651
55	8	0	-9.443139	-2.190134	-0.001737
56	8	0	-9.578931	2.349301	0.853605
57	1	0	-16.332247	1.450662	-0.653167
58	6	0	-12.233628	-2.307332	-0.563993
59	6	0	-13.62095	-2.306721	-0.839155
60	6	0	-14.353178	-1.129564	-0.756543
61	6	0	-13.728059	0.098649	-0.394542
62	6	0	-14.420802	1.347119	-0.29227
63	6	0	-13.76538	2.518646	0.063763
64	6	0	-12.379202	2.495394	0.335151
65	6	0	-10.141933	-1.156042	0.079043
66	6	0	-11.591721	-1.124771	-0.206092
67	6	0	-12.319405	0.097119	-0.11348
68	6	0	-11.661642	1.306311	0.250071
69	6	0	-10.215229	1.318797	0.544468
70	7	0	-9.543377	0.070856	0.46053
71	6	0	-4.049512	0.806214	-3.162012
72	6	0	-2.146176	-0.196212	3.300838
73	6	0	-3.620327	-0.18747	3.000977
74	7	0	-4.029872	-0.003094	1.729971
75	6	0	-5.37421	0.008927	1.448834
76	6	0	-6.364439	-0.168971	2.450898
77	6	0	-5.919259	-0.36236	3.784944
78	6	0	-4.560268	-0.370275	4.054424
79	6	0	-5.781434	0.216057	0.080925

80	6	0	-7.161511	0.241806	-0.248456
81	6	0	-8.134602	0.049712	0.794694
82	6	0	-7.752244	-0.147304	2.092818
83	7	0	-4.796661	0.388262	-0.861143
84	6	0	-5.135915	0.601294	-2.146201
85	6	0	-6.501769	0.641376	-2.541401
86	6	0	-7.505992	0.461544	-1.606777
87	29	0	-2.929962	0.251642	-0.037633
88	6	0	12.643043	5.784456	0.4576
89	8	0	13.872611	5.862249	0.357434
90	8	0	11.928624	6.916707	0.819878
91	6	0	10.57551	7.196606	0.338901
92	6	0	13.284237	-4.073858	-0.699637
93	8	0	12.716473	-5.14703	-0.938297
94	8	0	14.648444	-4.077489	-0.471249
95	6	0	15.526386	-2.952558	-0.800937
96	6	0	5.069459	-7.957736	2.679435
97	6	0	5.096498	-7.050878	1.438688
98	6	0	4.575417	-5.631106	1.725828
99	6	0	4.599501	-4.718039	0.487054
100	6	0	4.075504	-3.300536	0.779883
101	6	0	4.121087	-2.405117	-0.471136
102	1	0	2.056387	3.479926	0.137317
103	1	0	-0.146622	4.710039	0.135671
104	1	0	1.706424	-3.415203	-0.587087
105	1	0	-0.554598	-4.361725	-0.818906
106	1	0	-5.233998	4.671703	1.833139
107	1	0	-4.643622	5.188565	-2.394689
108	1	0	-5.212151	-3.658028	-3.256992
109	1	0	-5.529523	-4.383298	0.968777
110	1	0	-1.346775	4.694353	-2.564317
111	1	0	-1.81478	3.004228	-2.740289
112	1	0	-2.781449	4.28021	-3.50534
113	1	0	-7.268633	5.001456	-0.111586
114	1	0	-6.504419	6.54275	0.28839
115	1	0	-6.651351	6.045218	-1.404735
116	1	0	-2.409574	2.456722	2.381947
117	1	0	-2.157717	4.155805	2.792033
118	1	0	-3.713326	3.390433	3.140778
119	1	0	-3.830581	-3.607628	2.474004
120	1	0	-2.434276	-4.471378	1.821432
121	1	0	-2.41398	-2.707645	1.898441

122	1	0	-2.213521	-1.702309	-3.176057
123	1	0	-1.874791	-3.400476	-3.510426
124	1	0	-3.312903	-2.644528	-4.201902
125	1	0	-7.693151	-3.866124	-0.921587
126	1	0	-7.206285	-4.702075	-2.407017
127	1	0	-7.105524	-5.531011	-0.844825
128	1	0	6.282265	-1.58707	1.034739
129	1	0	8.713472	-1.315072	0.974438
130	1	0	8.262845	2.352625	-1.253612
131	1	0	5.800029	2.07222	-1.194004
132	1	0	12.329956	0.126179	1.19373
133	1	0	13.742067	-1.886457	0.969069
134	1	0	11.096155	-3.424947	-2.063445
135	1	0	9.695889	-1.37116	-1.87952
136	1	0	12.250126	1.587105	-1.49424
137	1	0	13.342317	3.802075	-1.17729
138	1	0	10.353051	4.85762	1.738901
139	1	0	9.29667	2.642828	1.472307
140	1	0	-11.650537	-3.22125	-0.624504
141	1	0	-14.114388	-3.2329	-1.115633
142	1	0	-15.41753	-1.136617	-0.969067
143	1	0	-14.313545	3.451552	0.135092
144	1	0	-11.857765	3.405472	0.615258
145	1	0	-3.067306	0.701524	-2.695392
146	1	0	-4.136011	0.079705	-3.978152
147	1	0	-4.121661	1.80726	-3.603055
148	1	0	-1.565778	-0.070542	2.384689
149	1	0	-1.884631	0.611911	3.99521
150	1	0	-1.850701	-1.137699	3.779953
151	1	0	-6.644663	-0.500846	4.581886
152	1	0	-4.193898	-0.514044	5.065882
153	1	0	-8.503034	-0.286618	2.86526
154	1	0	-6.739889	0.815608	-3.585757
155	1	0	-8.54907	0.490061	-1.904191
156	1	0	10.609342	8.19653	-0.100318
157	1	0	10.247204	6.470266	-0.411583
158	1	0	9.88688	7.193351	1.188989
159	1	0	16.345682	-3.372809	-1.388405
160	1	0	15.007525	-2.18249	-1.380436
161	1	0	15.921975	-2.523522	0.1241
162	1	0	5.445928	-8.960735	2.446378
163	1	0	5.693148	-7.546062	3.483371

164	1	0	4.048828	-8.065521	3.069548
165	1	0	4.492545	-7.504975	0.6388
166	1	0	6.124523	-6.98895	1.052724
167	1	0	5.181677	-5.17828	2.525242
168	1	0	3.547251	-5.693927	2.115374
169	1	0	3.997997	-5.178406	-0.313094
170	1	0	5.628626	-4.658425	0.101303
171	1	0	4.672948	-2.843342	1.57999
172	1	0	3.050311	-3.357649	1.170171
173	1	0	3.555356	-2.858841	-1.293262
174	1	0	5.151329	-2.313833	-0.826398

Cu(I)-A-H

Standard Orientation					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.744046	-4.107053	-1.169935
2	6	0	-5.212252	-2.787905	-1.405952
3	6	0	-4.394145	-1.715152	-0.956556
4	7	0	-3.19595	-1.919475	-0.319555
5	6	0	-2.762701	-3.180718	-0.093873
6	6	0	-3.532678	-4.298414	-0.520425
7	6	0	-6.458227	-2.505786	-2.067256
8	6	0	-6.870509	-1.211994	-2.261773
9	6	0	-6.069299	-0.106107	-1.808213
10	6	0	-4.826582	-0.350814	-1.161972
11	6	0	-6.46458	1.246786	-1.97233
12	6	0	-5.656827	2.25742	-1.473541
13	6	0	-4.430903	1.946126	-0.820403
14	7	0	-4.017205	0.662346	-0.699228
15	6	0	-1.466527	-3.379375	0.620637
16	6	0	-3.624235	3.050462	-0.217366
17	6	0	-0.29705	-3.707722	-0.108133
18	6	0	0.915871	-3.856506	0.584624
19	6	0	0.995393	-3.719885	1.982911
20	6	0	-0.188604	-3.436454	2.687116
21	6	0	-1.421111	-3.267117	2.03141
22	6	0	-2.487371	3.570084	-0.884007
23	6	0	-1.773092	4.623367	-0.291157
24	6	0	-2.162219	5.186208	0.938928
25	6	0	-3.30862	4.671188	1.567739
26	6	0	-4.056608	3.619557	1.005841
27	6	0	-2.678446	-3.019576	2.837334
28	6	0	2.317419	-3.890598	2.694901
29	6	0	-0.331189	-3.928277	-1.6061
30	6	0	-5.313404	3.143655	1.707278
31	6	0	-2.061369	3.032934	-2.231735
32	6	0	-1.381074	6.329626	1.545998
33	8	0	4.527478	-1.841636	0.652284
34	8	0	4.24184	2.614842	-0.543895
35	6	0	7.311055	-1.974147	0.006674
36	6	0	8.686668	-1.980344	-0.32975
37	6	0	9.295437	-0.824848	-0.803962

38	6	0	8.55118	0.381047	-0.960206
39	6	0	9.144124	1.583813	-1.444501
40	6	0	8.389941	2.742156	-1.585917
41	6	0	7.014397	2.742347	-1.248833
42	6	0	5.125596	-0.827744	0.227724
43	6	0	6.556713	-0.810832	-0.134146
44	6	0	7.16074	0.384429	-0.619
45	6	0	6.406607	1.582574	-0.771897
46	6	0	4.972368	1.607837	-0.424504
47	7	0	4.420737	0.393876	0.07132
48	6	0	-1.208303	-0.52653	-3.29998
49	6	0	-2.860031	0.737244	3.186524
50	6	0	-1.399716	0.710918	2.837025
51	7	0	-1.037609	0.432221	1.569479
52	6	0	0.293232	0.439149	1.228932
53	6	0	1.318664	0.706419	2.172476
54	6	0	0.924949	0.987187	3.507123
55	6	0	-0.421348	0.994079	3.831283
56	6	0	0.648093	0.170148	-0.142987
57	6	0	2.014527	0.156311	-0.528977
58	6	0	3.026784	0.414703	0.461346
59	6	0	2.691076	0.684406	1.759222
60	7	0	-0.371383	-0.056995	-1.03553
61	6	0	-0.08188	-0.303483	-2.327883
62	6	0	1.266979	-0.338294	-2.778192
63	6	0	2.305448	-0.111745	-1.891053
64	29	0	-2.207704	-0.111455	-0.0181
65	1	0	-5.339341	-4.956095	-1.495063
66	1	0	-3.15624	-5.295383	-0.318619
67	1	0	-7.068683	-3.337848	-2.407896
68	1	0	-7.813647	-1.001394	-2.75897
69	1	0	-7.399353	1.479221	-2.475332
70	1	0	-5.939392	3.300042	-1.571187
71	1	0	1.821003	-4.081171	0.023979
72	1	0	-0.154161	-3.351765	3.771634
73	1	0	-0.897503	5.01809	-0.803148
74	1	0	-3.637185	5.103989	2.510823
75	1	0	-3.233265	-2.149507	2.470477
76	1	0	-3.357638	-3.881362	2.784119
77	1	0	-2.440889	-2.855482	3.89317
78	1	0	2.639854	-4.9403	2.674085
79	1	0	3.101645	-3.297656	2.211029

80	1	0	2.250604	-3.587929	3.74529
81	1	0	-0.661973	-4.948272	-1.846111
82	1	0	-1.017356	-3.240728	-2.110563
83	1	0	0.664882	-3.800209	-2.041928
84	1	0	-6.21596	3.509093	1.199615
85	1	0	-5.38514	2.050543	1.739466
86	1	0	-5.350593	3.515787	2.736203
87	1	0	-1.828894	1.965232	-2.172698
88	1	0	-2.855277	3.157979	-2.980328
89	1	0	-1.17199	3.554559	-2.598234
90	1	0	-0.306836	6.110377	1.570248
91	1	0	-1.510411	7.248462	0.959104
92	1	0	-1.706703	6.542529	2.569255
93	1	0	6.824134	-2.870227	0.379759
94	1	0	9.26303	-2.892694	-0.213942
95	1	0	10.351641	-0.829413	-1.061529
96	1	0	10.200093	1.583786	-1.703065
97	1	0	8.851786	3.652463	-1.954717
98	1	0	6.413632	3.64089	-1.354002
99	1	0	-2.163782	-0.588528	-2.775055
100	1	0	-1.263273	0.295627	-4.024984
101	1	0	-1.056557	-1.449049	-3.872488
102	1	0	-3.460698	0.390165	2.342453
103	1	0	-3.069328	0.108894	4.059828
104	1	0	-3.171875	1.759504	3.432023
105	1	0	1.679344	1.197018	4.260275
106	1	0	-0.749856	1.213493	4.842028
107	1	0	3.46914	0.884526	2.490223
108	1	0	1.465892	-0.539195	-3.826039
109	1	0	3.335967	-0.13388	-2.229983

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