Supporting Information for

Photochemical charge accumulation in a heteroleptic copper(I)-anthraquinone molecular dyad via proton-coupled electron transfer

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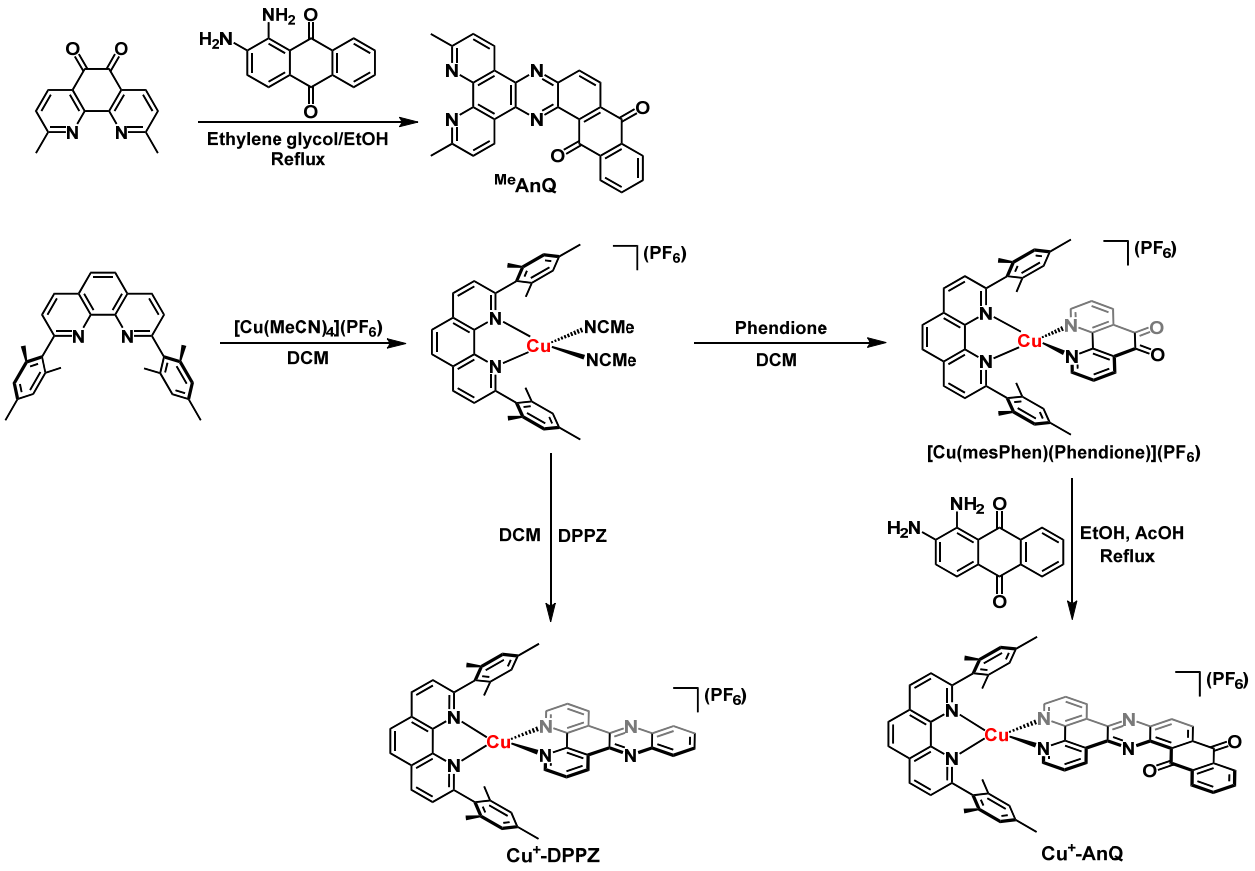
Contents

1. Synthetic procedures



Scheme S1. Synthesis of ^{Me}**AnQ**, **Cu$^+$-AnQ** and **Cu$^+$-DPPZ**

General considerations. All reagents were purchased from commercial sources and were used without further purification. Several chemicals were synthesized according to published procedures: 2,9-dimesityl-1,10-phenanthroline (mesPhen)[1], 1,10-phenanthroline-5,6-dione (Phendione)[2], 2,9-dimethyl-1,10-phenanthroline-5,6-dione[3], dipyridophenazine (DPPZ)[4]. ^{1}H NMR was collected on a Bruker DMX 500 and referenced to TMS or residual solvent peak. ESI-MS was performed on a ThermoFisher LCQ Fleet from dilute CH_3CN solutions in positive ionization mode. UV-Vis absorption measurements were performed on a Beckman-Coulter DU800 spectrophotometer.

[Cu(mesPhen)(Phendione)](PF$_6$). Under N_2 atmosphere, $[Cu(MeCN)_4](PF_6)$ (100 mg, 0.27 mmol) and mesPhen (112 mg, 0.27 mmol) were added to a round bottom flask and dissolved in deaerated dichloromethane (20 mL) with stirring. The solution turned bright yellow, and was allowed to stir at room temperature for five minutes. Phendione (56 mg, 0.27 mmol) was then added followed by the addition of dichloromethane (20 mL). The resulting red solution was stirred at room temperature for three hours. The mixture was filtered and concentrated by rotary evaporation and the dark red solid was precipitated with diethyl ether. The analytically pure product was isolated by filtration and allowed to dry in air as a dark red powder (216 mg, 96% yield)

^{1}H NMR (500 MHz, acetone-*d*$_6$) δ 8.98 (d, J = 8.2 Hz, 2H), 8.84 (s, 2H), 8.62 (s, 2H), 8.41 (s, 2H), 8.03 (d, J = 8.2 Hz, 2H), 7.93 (dd, J = 5.1, 7.7 Hz, 2H), 6.40 (s, 4H), 1.86 (s, 6H), 1.83 (s, 12H).

MS (ESI$^+$): m/z calcd. for $[M–PF_6^-]^+$ 689.20, obsd. 689.00; $[M+MeOH–PF_6^-]^+$ 721.22, obsd. 721.08.

Cu^+-AnQ. [Cu(mesPhen)(Phendione)](PF_6) (200 mg, 0.24 mmol) and 1,2-diaminoanthroquinone (57 mg, 0.24 mmol) were mixed in 80 mL absolute ethanol. Then, 80 μL of acetic acid was added to the mixture. The reaction was refluxed for 7 days, after which large amount of dark brown solid precipitated. After cooling down, the brown precipitate was isolated by filtration, washed with copious diethyl ether and dried in vacuum. The solvent of the filtrate was removed. The residue was dissolved in dichloromethane (2 mL), precipitated by adding diethyl ether. The resultant solid was combined with the previous precipitate and recrystallized via diffusion of diethyl ether into the concentrated acetonitrile solution to give analytically pure product as a dark brown solid (140 mg, 56% yield)

^{1}H NMR (500 MHz, acetone-d_6) δ 9.93 (dd, J = 1.4, 8.0 Hz, 1H), 9.79 (dd, J = 1.2, 8.0 Hz, 1H), 9.06 (m, 2H), 9.00 (dd, J = 8.2 Hz, 2H), 8.93 (dd, J = 13.3, 8.8 Hz, 2H), 8.45 (d, J = 7.8 Hz, 1H), 8.44 (s, 2H), 8.36 (d, J = 7.3 Hz, 1H), 8.27 (d, J = 8.1 Hz, 1H), 8.26 (d, J = 8.0, 4.8 Hz, 1H), 8.19 (dd, J = 4.8, 8.1 Hz, 1H), 8.04 (m,4H), 6.14 (d, J = 6.9 Hz, 4H), 1.86 (d, J = 7.8 Hz, 12H), 1.34 (s, 6H).

MS (ESI$^+$): m/z calcd. for [M–PF_6^-]$^+$ 891.25, obsd. 891.19.

Anal. calcd. for $C_{56}H_{40}CuF_6N_6O_2P$: C, 64.83; H, 3.89; N, 8.10. Found: C, 64.67; H, 3.87; N, 8.05.

Cu^+-DPPZ. Under N_2 atmosphere, [Cu(CH_3CN)$_4$]PF_6 (33 mg, 0.0885mmol) and mesPhen (37 mg, 0.0885 mmol) were added to a Schlenk flask and dissolved in deoxygenated dichloromethane (20 mL). Upon addition of dichloromethane the solution turned bright yellow, and was allowed to stir at room temperature for five minutes. Dipyridophenazine (DPPZ) (25 mg, 0.0885 mmol) was then added followed by dichloromethane (5 mL). The dark red solution was allowed to stir under N_2 at room temperature for two hours. The mixture was filtered and concentrated by rotary evaporation and the product was precipitated with diethyl ether. The resulting solid was isolated by filtration, washed with small amount of dichloromethane/diethyl ether (v:v=1:1), and dried in vacuo to give analytically pure product as a dark red powder (79 mg, 98% yield).

^{1}H NMR (500 MHz, acetone-d_6) δ 9.71 (dd, J = 1.5, 8.1 Hz, 2H), 8.98 (m, 4H), 8.48 (dd, J = 3.4, 6.5 Hz, 2H), 8.43 (s, 2H), 8.17 (dd, J = 3.4, 6.5 Hz, 2H), 8.13 (dd, J = 4.8, 8.1 Hz, 2H), 8.03 (d, J = 8.2 Hz, 2H), 6.12 (s, 4H), 1.84 (s, 12H), 1.30 (s, 6H)

MS (ESI$^+$): m/z calcd. for [M–PF_6^-]$^+$ 761.25, obsd. 761.33.

Anal. calcd. for $C_{48}H_{38}CuF_6N_6P$: C, 63.54; H, 4.22; N, 9.26. Found: C, 63.45; H, 4.37; N, 9.14.

^{Me}AnQ. 2,9-dimethyl-1,10-phenanthroline-5,6-dione (200 mg, 0.84 mmol) and 1,2-diaminoanthroquinone (200 mg, 0.84 mmol) were mixed in 20 mL of ethylene glycol and 4 mL of absolute ethanol. The mixture was refluxed for 24 hours. After cooling down, the volatile was removed. The resulting solid was isolated by filtration and washed by ethanol, water and ethanol. Further purification of the solid was achieved by dissolving the solid in hot chloroform (300 mL) and filtration to remove the undissolved residue. The filtrate was reduced to 2 mL and the black solid was precipitated by diethyl ether, isolated by filtration and dried in vacuo to give the analytically pure product as a black powder (197 mg, 53% yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 9.87 (d, J = 8.3 Hz, 1H), 9.60 (d, J = 8.3 Hz, 1H), 8.84 (d, J = 8.9 Hz, 1H), 8.71 (d, J = 8.8 Hz, 1H), 8.44 (dd, J = 0.9, 7.7 Hz, 1H), 8.35 (dd, J = 1.1, 7.6 Hz, 1H), 7.91 (dt, J = 1.3, 11.2 Hz, 1H), 7.86 (dt, J = 1.3, 7.5 Hz, 1H), 7.85 (d, J = 8.4 Hz, 1H), 7.78 (d, J = 8.2 Hz, 1H), 3.17 (s, 1H), 3.13 (s, 6H).

MS (ESI$^+$): m/z calcd. for $[M+H]^{1+}$ 441.13, obsd. 441.08.

2. NMR spectra

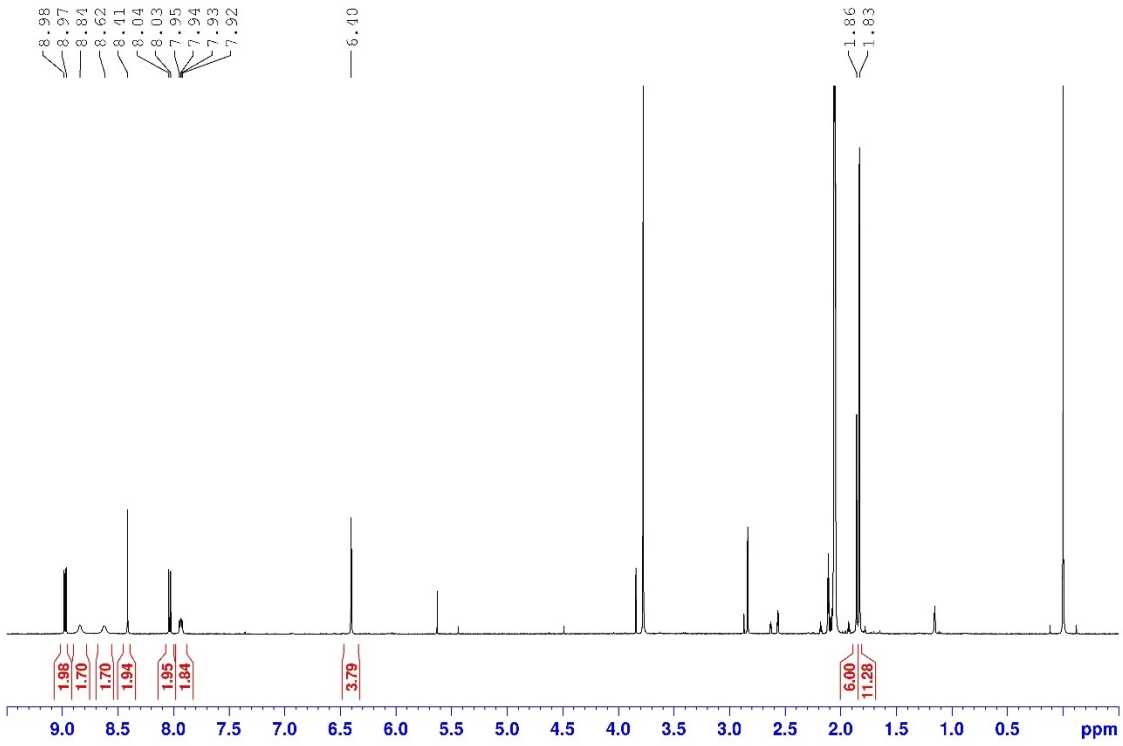


Figure S1. ^{1}H NMR spectrum of [Cu(mesPhen)(Phendione)](PF_6) in acetone-d_6.

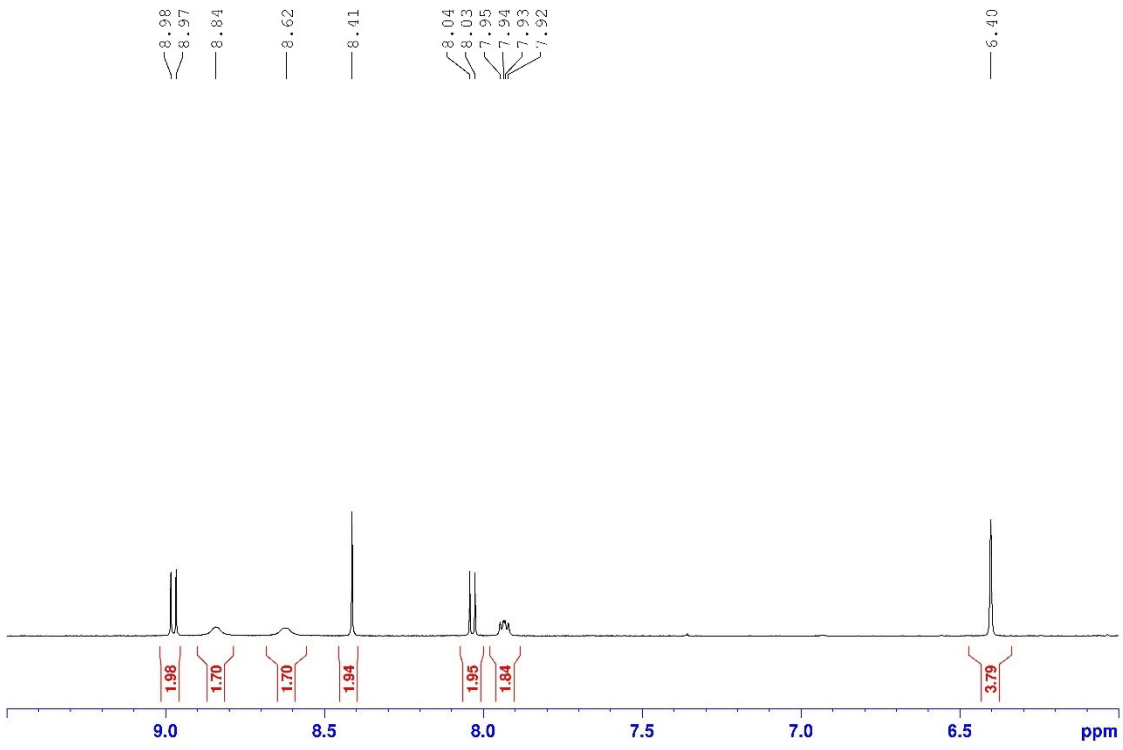


Figure S2. Aromatic region of ^{1}H NMR spectrum of [Cu(mesPhen)(Phendione)](PF_6) in acetone-d_6.

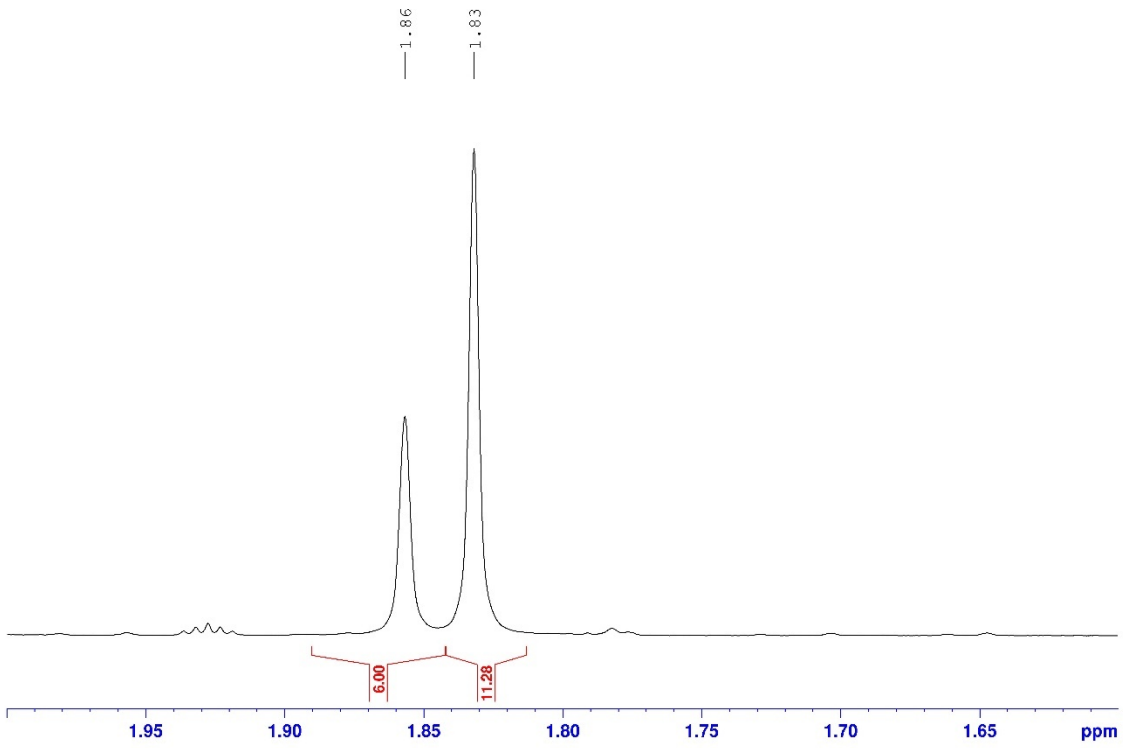


Figure S3. Aliphatic region of ^{1}H NMR spectrum of [Cu(mesPhen)(Phendione)](PF_6) in acetone-d_6.

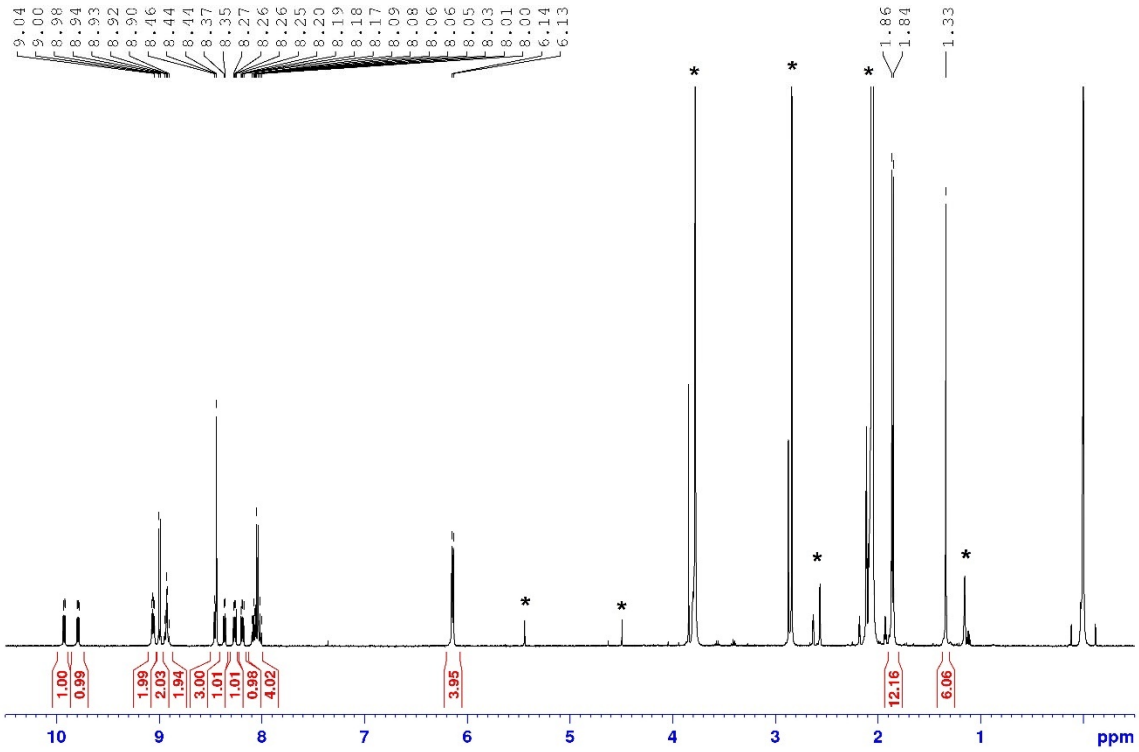


Figure S4. ^{1}H NMR spectrum of **Cu^{+}-AnQ** in acetone-d_6 (* indicates residual solvent).

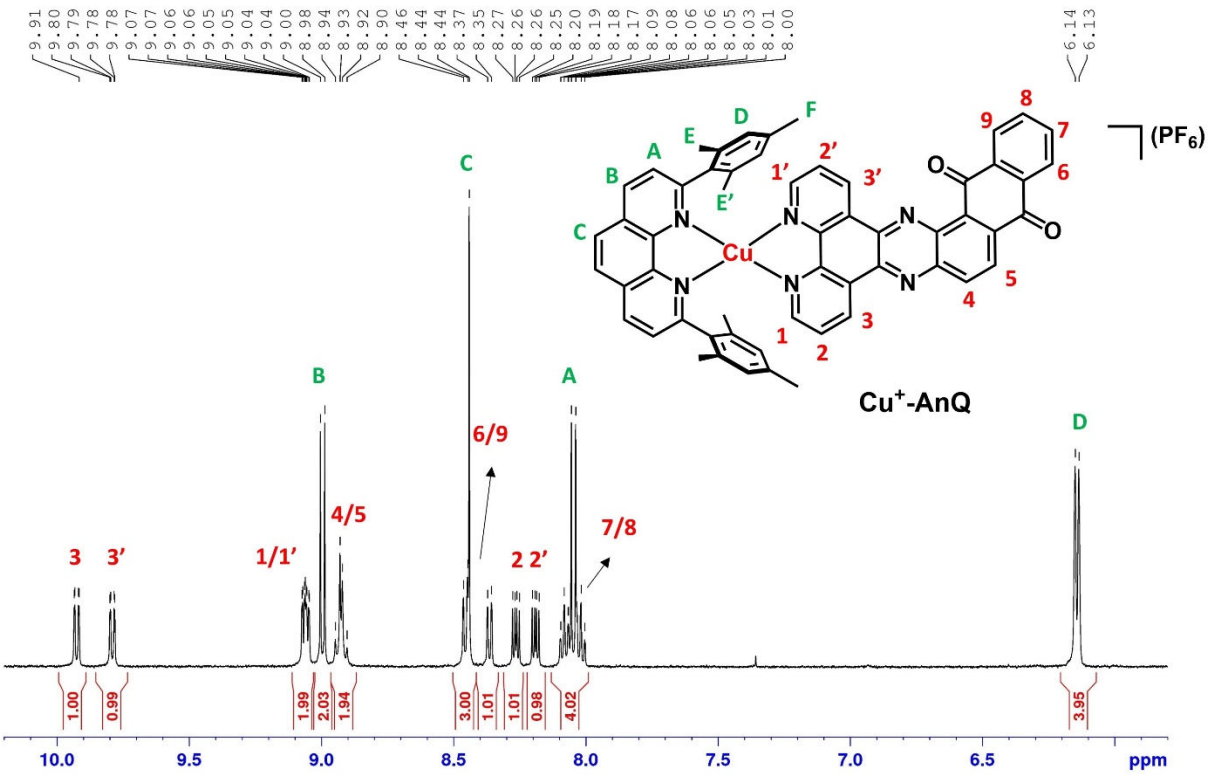


Figure S5. Aromatic region of ^{1}H NMR spectrum of **Cu^{+}-AnQ** in acetone-d_6 (peak assignment included).

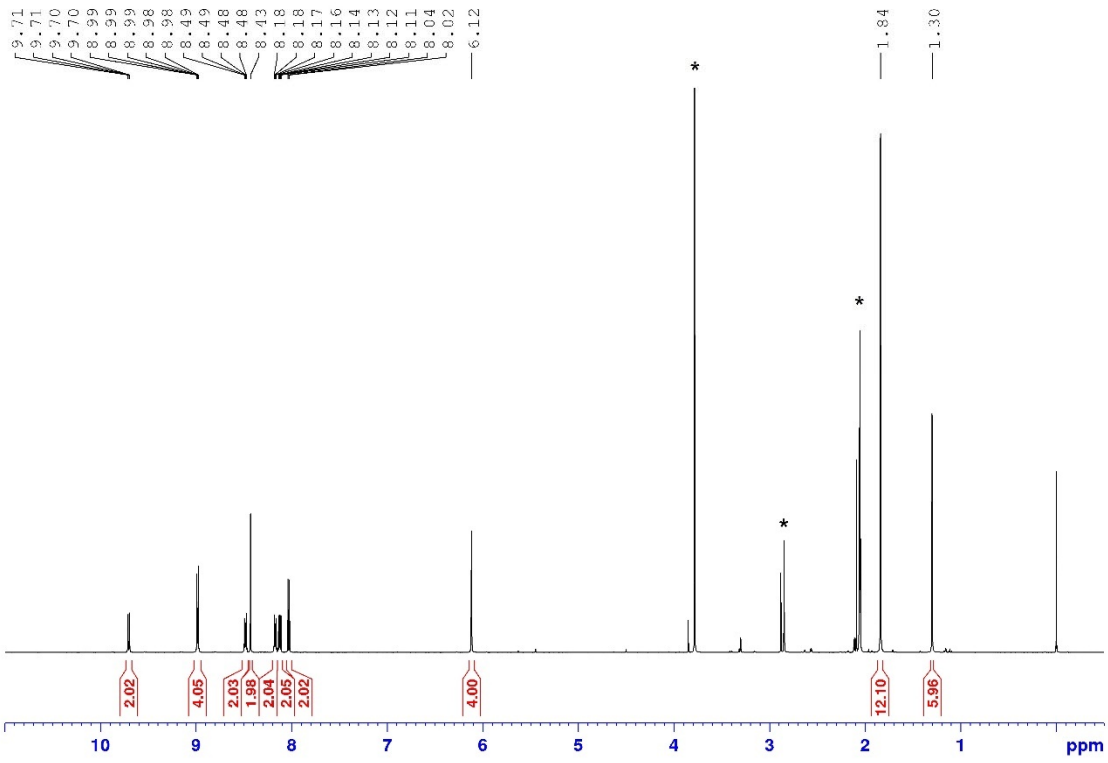


Figure S6. ^{1}H NMR spectrum of **Cu^{+}-DPPZ** in acetone-d_6(* indicates residual solvent).

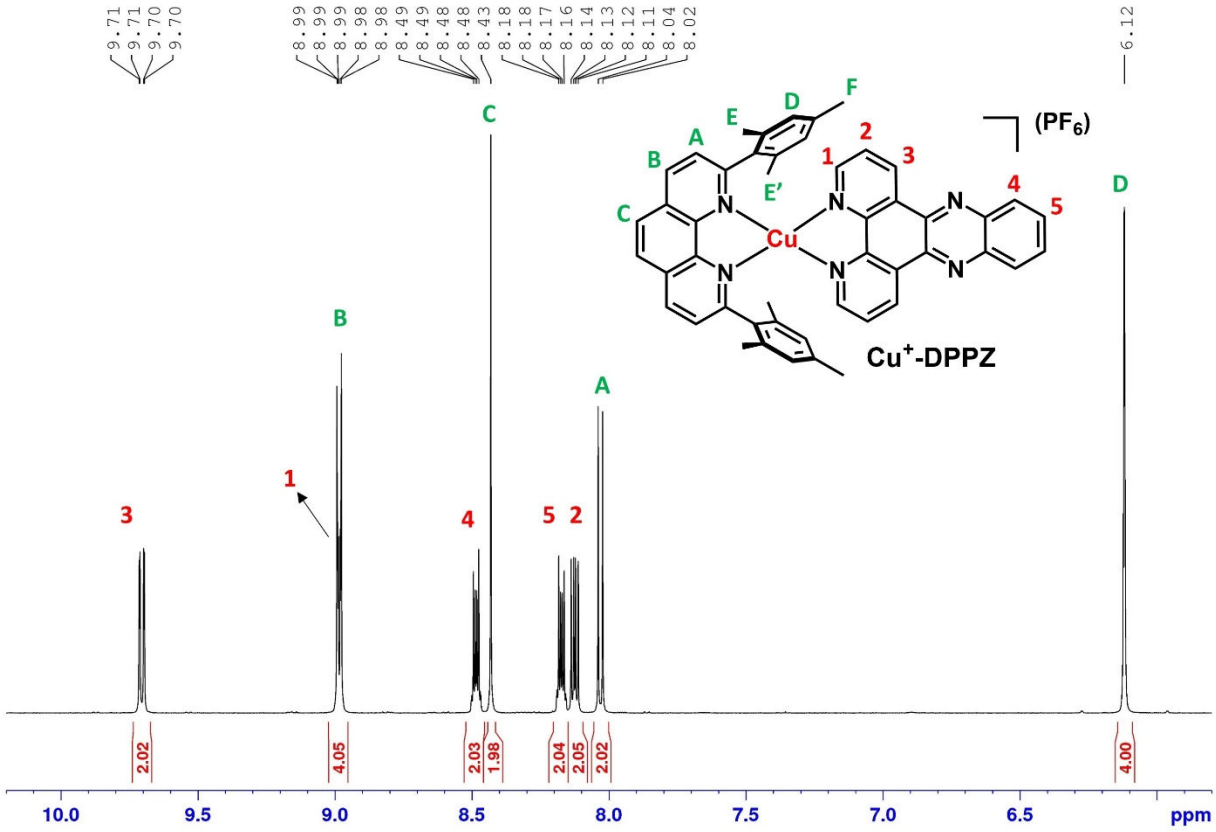


Figure S7. Aromatic region of ^{1}H NMR spectrum of **Cu^{+}-DPPZ** in acetone-d_6 (peak assignment included).

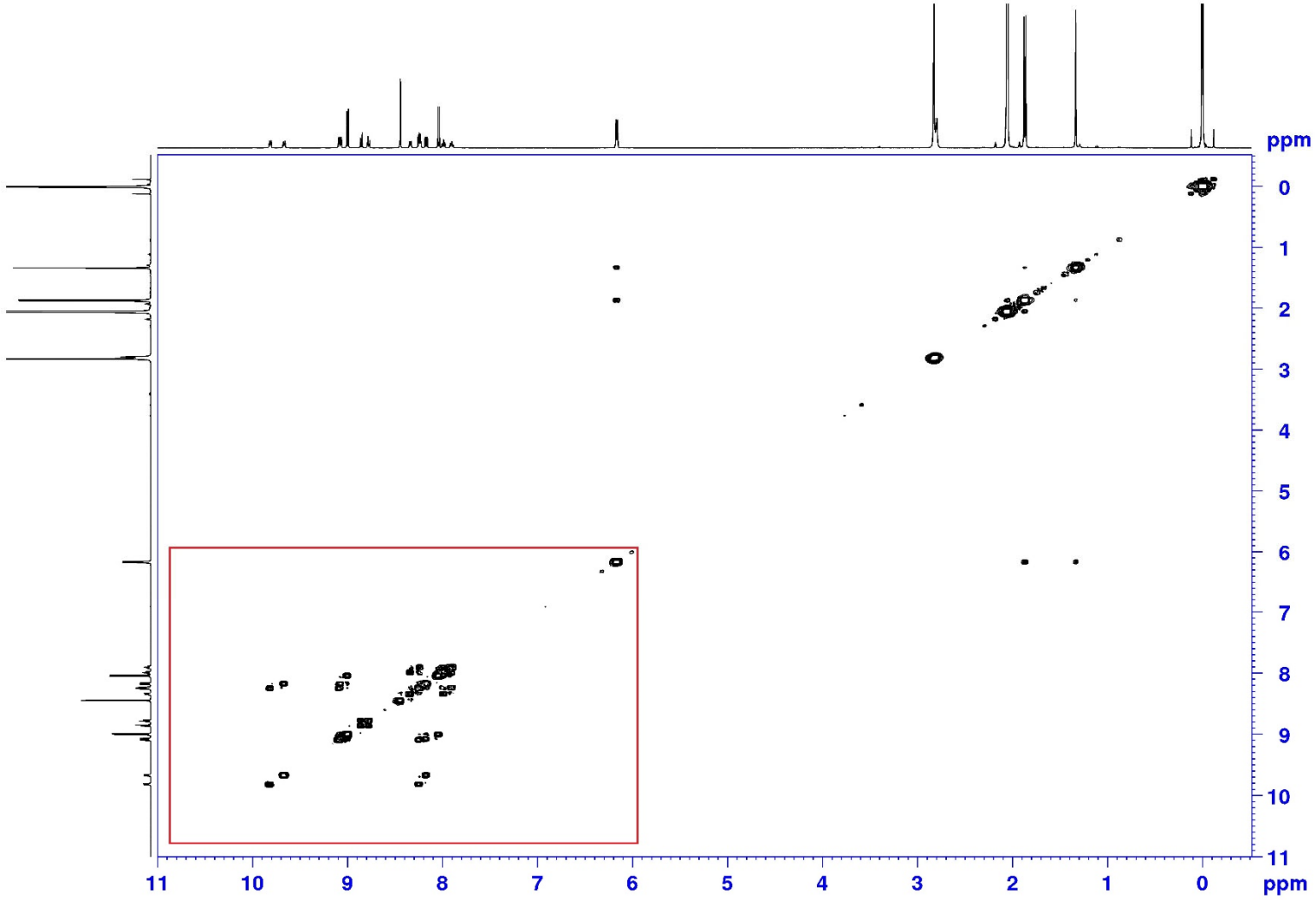


Figure S8. COSY spectrum of **Cu^{+}-AnQ** in acetone-d_6 (an enlarged image of the red box is shown in **Figure S9**).

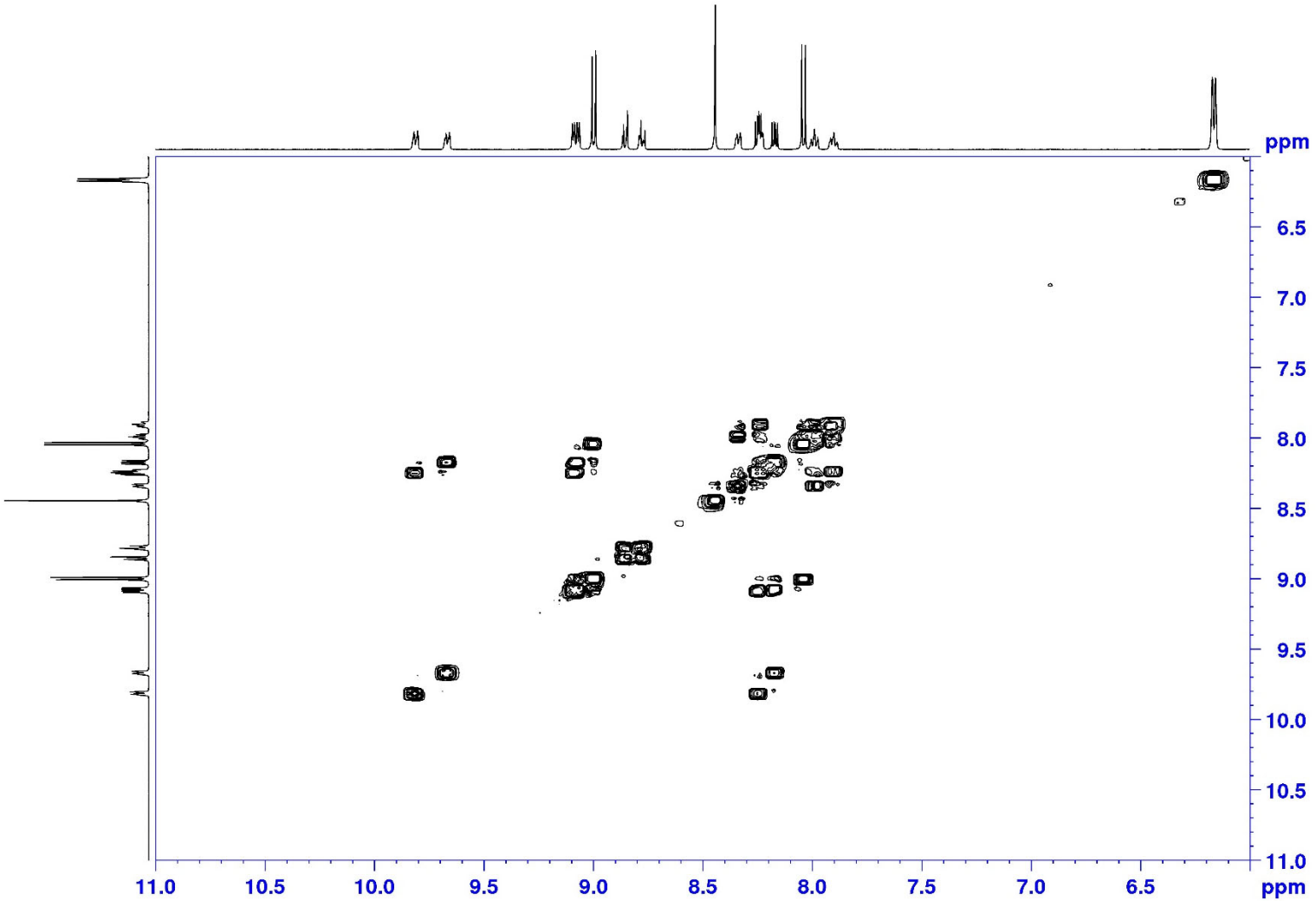


Figure S9. The aromatic region of the COSY spectrum of **Cu^{+}-AnQ** in acetone-d_6.

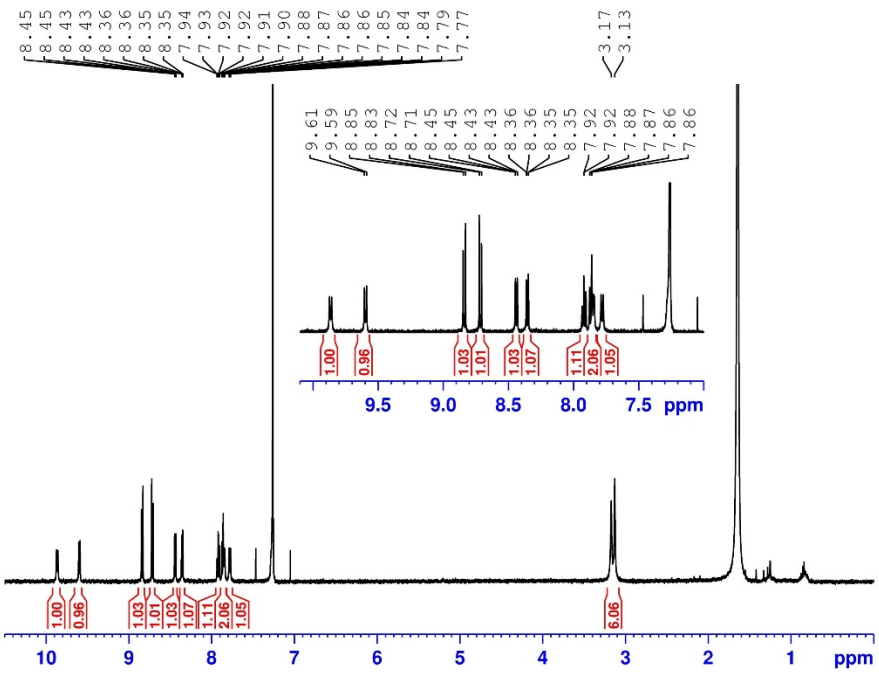


Figure S10. ^{1}H NMR spectrum of **^{Me}AnQ** in $CDCl_3$ (Inset: aromatic region of ^{1}H NMR spectrum of **^{Me}AnQ**)

3. Self-association of Cu^+-AnQ and Cu^+-DPPZ

The self-association of **Cu^+-AnQ** and **Cu^+-DPPZ** complexes were monitored through concentration-dependent NMR spectroscopy (**Figure S11** and **S12**). Upon increasing the concentration of the complexes in CD_3CN, the chemical shifts of the protons attached to the π-conjugated ligands (AnQ and DPPZ) were shifted upfield as a result of the dimerization of individual molecules in solution state via π-π interactions between two conjugated ligands. Similar dimerization effect has been reported in the literature where Ru(II)/Os(II) complexes with extended π-conjugated ligand were studied.[5–8] To determine the scale of dimerization and association constant, a monomer-dimer model was applied to data fitting.[9,10] In a typical monomer-dimerization equilibrium (Eq. 1), a dimerization constant K_D is given by Eq. 2:

$$2M \rightleftharpoons D \quad \text{Eq. 1}$$

$$K_D = \frac{c_D}{(c_M)^2} \quad \text{Eq. 2}$$

where c_D is the concentration of dimer in solution and c_M is the concentration of monomer. The chemical shift of a species in a monomer-dimer equilibrium is determined by the mole fraction weighted-average of the chemical shift of monomer and dimer as follows,

$$P = \alpha P_M + \lambda P_D \quad \text{Eq. 3}$$

where P, P_M and P_D are the chemical shifts of the mixture, pure monomer and pure dimer, respectively. The mole fractions of monomer and dimer are represented by α and λ, respectively. Rearrangement of Eq. 3 yields:

$$P - P_M = (P_D - P_M)(1 + (1 - \sqrt{8L + 1})/4L \quad \text{Eq. 4}$$

Variable $L = K_D C_T$, *where* C_T is the total concentration of the species in solution, which has a formula of $c_T = 2c_D + c_M$. Based on Eq. 4, we performed non-linear least-squares analysis of the concentration-dependent chemical shifts to obtained the association constant K_D and the change of Gibbs free energy of dimerization $\Delta_D G°$ at 295 K. The fitting for each proton signal is shown in **Figure S11B, S11C, S12B** and **S11C**). The thermodynamics constants are tabulated in **Table S1**. Importantly, the mole fraction of monomer α at various c_T can be calculated with known K_D. Based on the thermodynamics of the dimerization, there is about 95% of **Cu^+-AnQ** exists in the monomer form when c_T = 0.5 mM, whereas for **Cu^+-DPPZ**, around 98% of the complex is monomer at 2.5 mM.

Table S1. Thermodynamics of dimerization of **Cu^+-AnQ** and **Cu^+-DPPZ**.

		K_D	Standard deviation	$\Delta_D G°$ kJ/mol	Standard deviation
Cu^+-AnQ	H_2	60.2	6.1	-10.1	2.2
	H_3	62.3	5.5	-10.1	2.2
	Average	61.3	5.8	-10.1	2.2
Cu^+-DPPZ	H_3	3.7	1.2	-3.2	0.8
	H_4	3.8	1.2	-3.2	0.8
	Average	3.7	1.2	-3.2	0.8

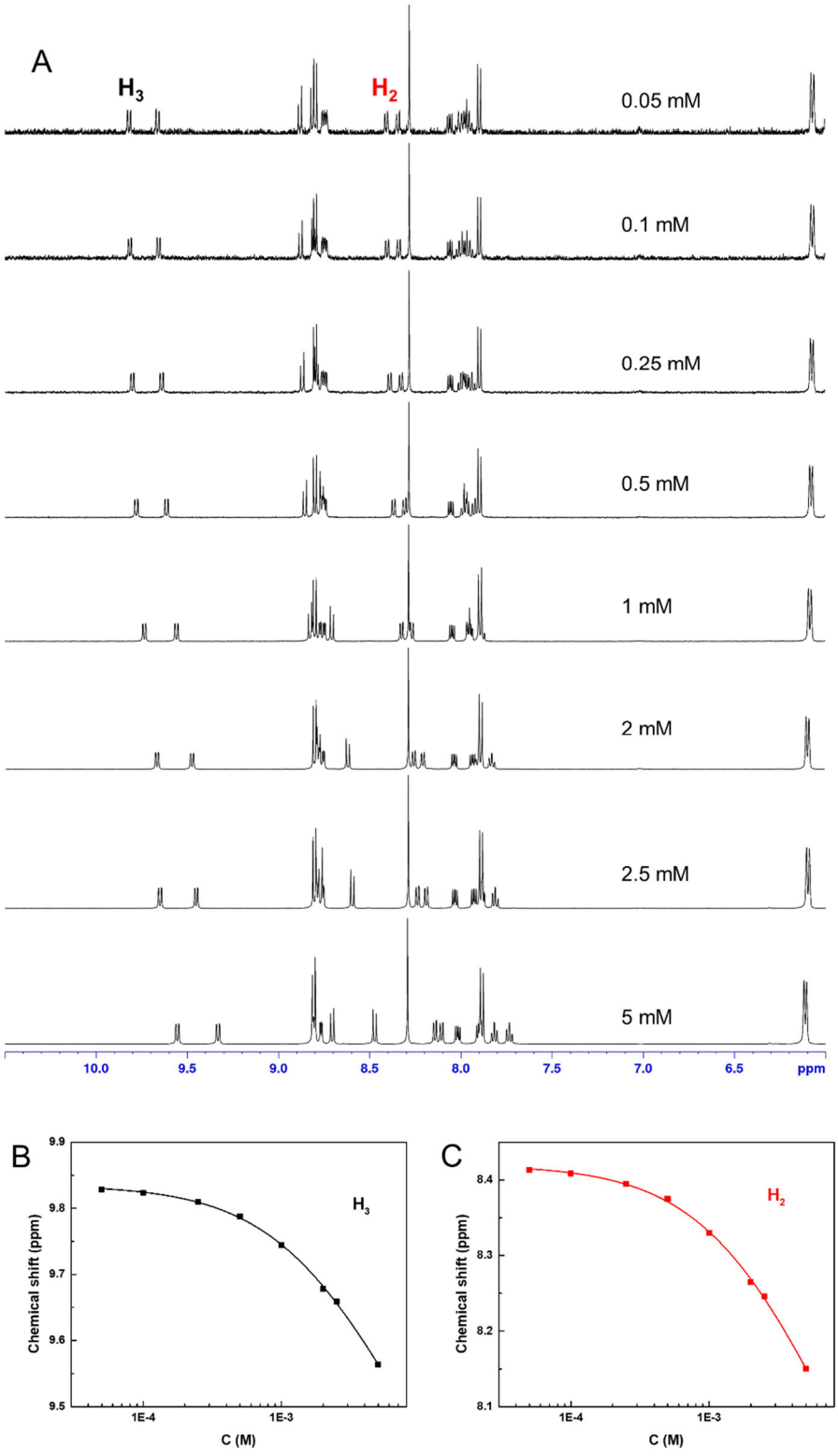


Figure S11. (A) Comparison of ^{1}H NMR of **Cu^{+}-AnQ** in CD_3CN over the range of concentrations from 0.05 mM to 5 mM at 295 K. Change of chemical shifts of H_3 (B) and H_2 (C) as a response to concentration.

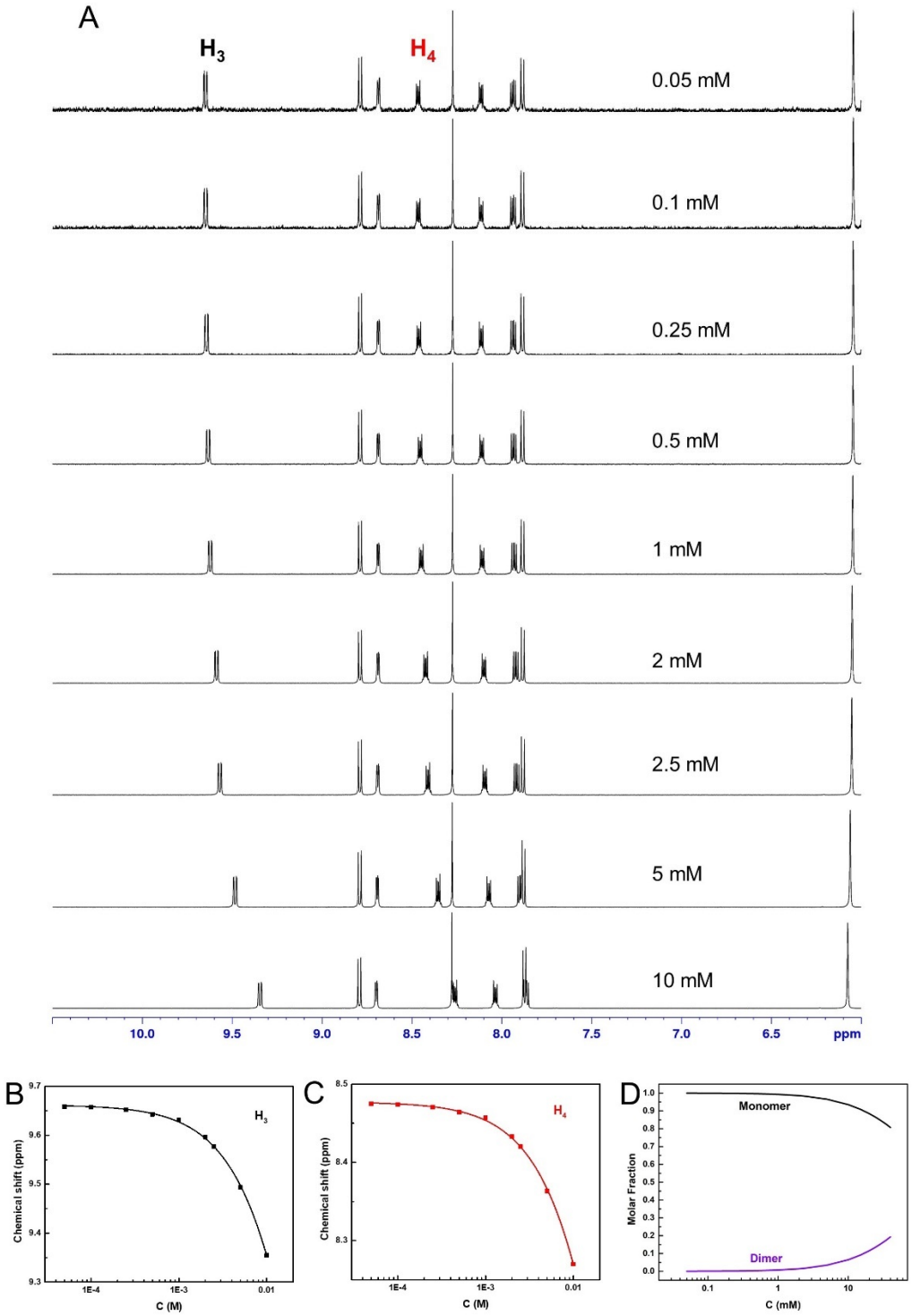


Figure S12. (A) Comparison of ^{1}H NMR of **Cu^{+}-DPPZ** in CD_3CN over the range of concentrations from 0.05 mM to 10 mM at 295 K. Change of chemical shifts of H_3 (B) and H_4 (C) as a response to concentration. (D) Calculated molar fractions of monomer and dimer **Cu^{+}-DPPZ** as functions of the total concentration of **Cu^{+}-DPPZ** in acetonitrile (calculation was based on the K_D constant).

4. X-ray Diffraction

X-ray diffraction of **Cu^{+}-AnQ** and **Cu^{+}-AnQH^{-}** was collected on a Rigaku Oxford Diffraction SuperNova Dual Source diffractometer using a μ-focus Cu Kα radiation source (λ = 1.5418 Å) with collimating mirror monochromators. The data were collected at 100 K using an Oxford Cryostream low temperature device. Details of crystal data, data collection and structure refinement are listed in **Table S2**. Data collection, unit cell refinement and data reduction were performed using Agilent Technologies CrysAlisPro V 1.171.41.70a.[11] The structure was solved by direct methods using SHELXT[12] and refined by full-matrix least-squares on F^2 with anisotropic displacement parameters for the non-H atoms using SHELXL-2016/6.[13] Structure analysis was aided by use of the programs PLATON[14] and OLEX2[15]. The hydrogen atoms were calculated in ideal positions with isotropic displacement parameters set to 1.2xUeq of the attached atom (1.5xUeq for methyl hydrogen atoms).

For **Cu^{+}-AnQ**, the hexafluorophosphate anion was disordered. The disorder was modeled by fitting two groups to the region of the anion. The geometry of the two anions was restrained to be equivalent while the sum of their site occupancy factors was set to equal one. Two molecules of acetonitrile were disordered. The disorder could not be modeled satisfactorily. As a consequence, the program, SQUEEZE[16], was used to remove the contributions to the calculated scattering factors due to these molecules in the final refinement model. For **Cu^{+}-AnQH^{-}**, a hydrogen atom was disordered at two different atoms, O1 and N5. The bond lengths from H to these atoms was restrained to be approximately 0.84Å.

The function, $\Sigma w(|F_o|^2 - |F_c|^2)^2$, was minimized, where $w = 1/[(\sigma(F_o))^2 + (0.0647*P)^2 + (1.2395*P)]$ and $P = (|F_o|^2 + 2|F_c|^2)/3$. $R_w(F^2)$ refined to 0.122, with R(F) equal to 0.0438 and a goodness of fit, S, = 1.08. Definitions used for calculating R(F), $R_w(F^2)$ and S are $R_w(F^2) = \{\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w(|F_o|)^4\}^{1/2}$ where w is the weight given each reflection, $R(F) = \Sigma(|F_o| - |F_c|)/\Sigma|F_o|\}$ for reflections with $F_o > 4(\sigma(F_o))$ and $S = [\Sigma w(|F_o|^2 - |F_c|^2)^2/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters. The data were checked for secondary extinction effects but no correction was necessary. Neutral atom scattering factors and values used to calculate the linear absorption coefficient are from the International Tables for X-ray Crystallography (1992).[17] All figures were generated using SHELXTL/PC.[18] Tables of positional and thermal parameters, bond lengths and angles, torsion angles and figures are found in **Table S3**.

Table S2. Parameters of X-ray crystallography.

Compound	**Cu^+-AnQ**	**Cu^+-AnQH^-**
CCDC number	2278030	2278029
Formula	$C_{56}H_{40}CuF_6N_6O_2P$	$C_{56}H_{41}CuN_6O_2$
FW	1037.45	893.49
T (K)	100(2)	100(2)
size (mm)	0.25 × 0.14 × 0.088	0.21 x 0.085 x 0.071
System	triclinic	monoclinic
space group	*P-1*	*P 1 2_1/n 1*
Z	2	4
λ (Å)	1.54184	1.54184
a (Å)	10.8051(3)	16.4587(2)
b (Å)	13.6401(3)	13.34870(17)
c (Å)	20.0438(5)	20.0214(2)
α (°)	82.066(2)	90
β (°)	88.421(2)	102.2042(13)
γ (°)	72.642(2)	90
V (Å^3)	2792.31(13)	4299.35(10)
d_{calc} (g/cm^3)	1.234	1.380
m (mm^{-1})	1.364	1.133
R(int)	0.0243	0.0212
Completeness to theta = 67.684°	99.5 %	99.0 %
GOF on F^2	1.029	1.041
*R*1/w*R*2 [*I*>2σ(*I*)]	0.0438	0.0481
	0.1170	0.1250
*R*1/w*R*2 (all data)	0.0491	0.0549
	0.1223	0.1299

Table S3. Selected bond length (Å) and angle (°) for **Cu^{+}-AnQ** and **Cu^{+}-AnQH^{-}**.

Bond Length (Å)	**Cu^{+}-AnQ**	**Cu^{+}-AnQH^{-}**
Cu1-N1	1.9967(15)	2.0027(16)
Cu1-N2	2.0910(15)	2.0734(18)
Cu1-N3	2.0065(15)	2.0619(17)
Cu1-N4	2.0755(15)	2.0046(18)
C=O anthraquinone	1.223(2)	1.300(3)
	1.217(2)	1.255(3)
Bond Angle (°)		
N1-Cu1-N2	82.30(6)	82.09(7)
N1-Cu1-N3	145.63(6)	131.44(7)
N1-Cu1-N4	120.50(6)	131.94(7)
N3-Cu1-N2	119.23(6)	108.87(7)
N3-Cu1-N4	82.03(6)	82.33(7)
N4-Cu1-N2	104.50(6)	123.16(8)
s_4 value	0.67	0.69

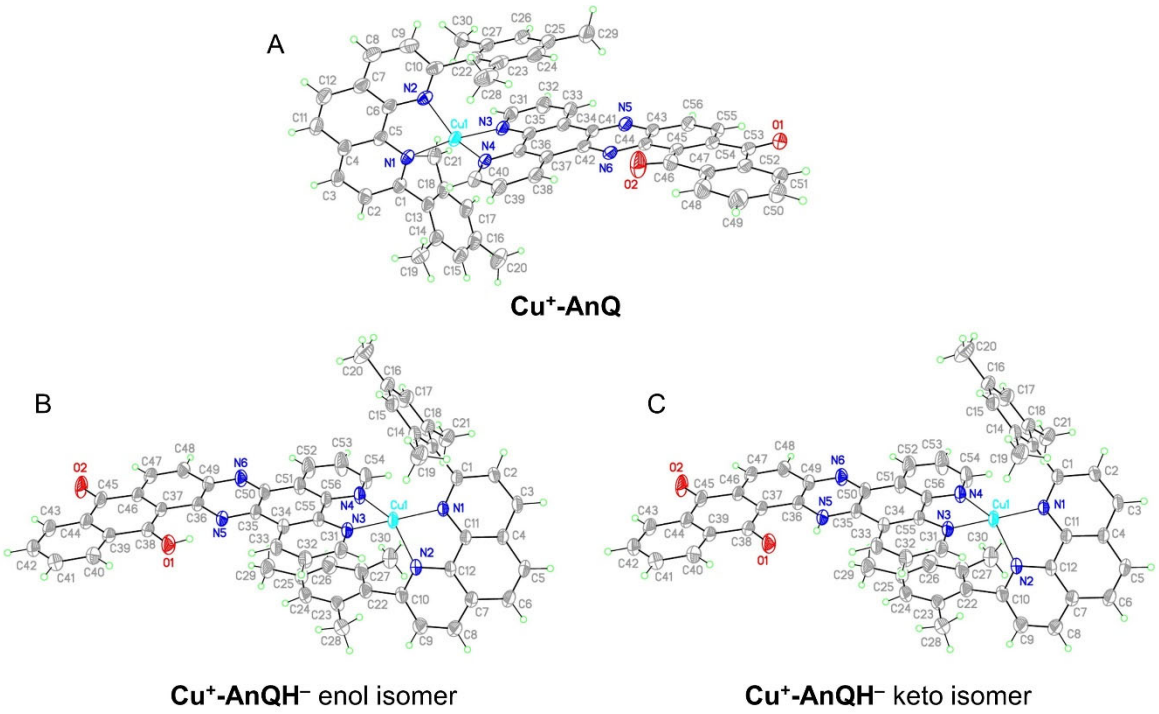


Figure S13. ORTEP diagrams for **Cu⁺-AnQ** (A), **Cu⁺-AnQH⁻** enol isomer (B) and **Cu⁺-AnQH⁻** keto isomer (C). 50% thermal ellipsoids; the counterion PF_6^- are omitted for clarity.

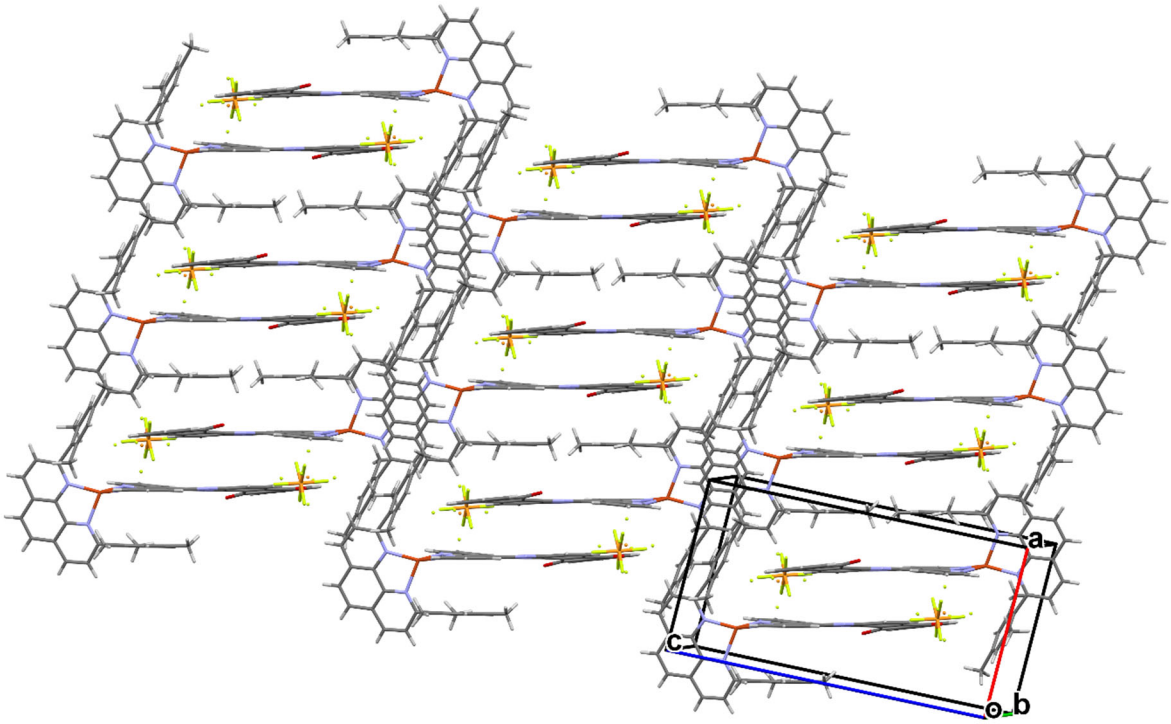


Figure S14. Crystal packing diagram of **Cu⁺-AnQ**

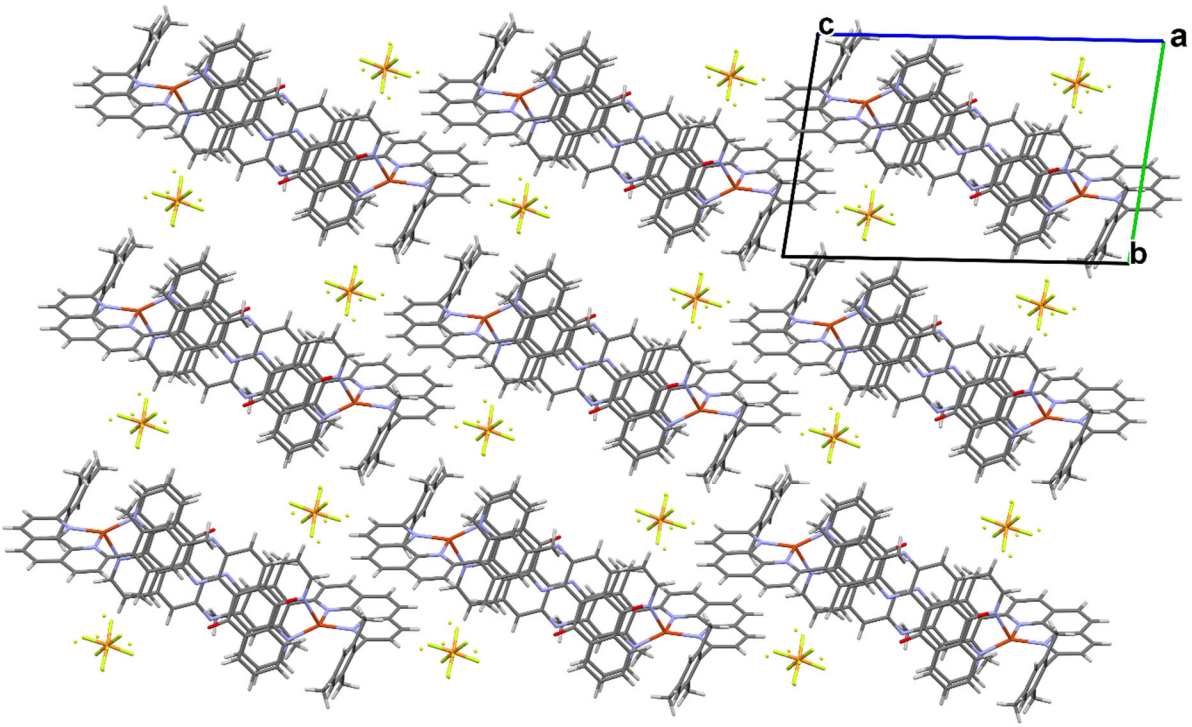


Figure S15. Crystal packing diagram of **Cu^{+}-AnQ**

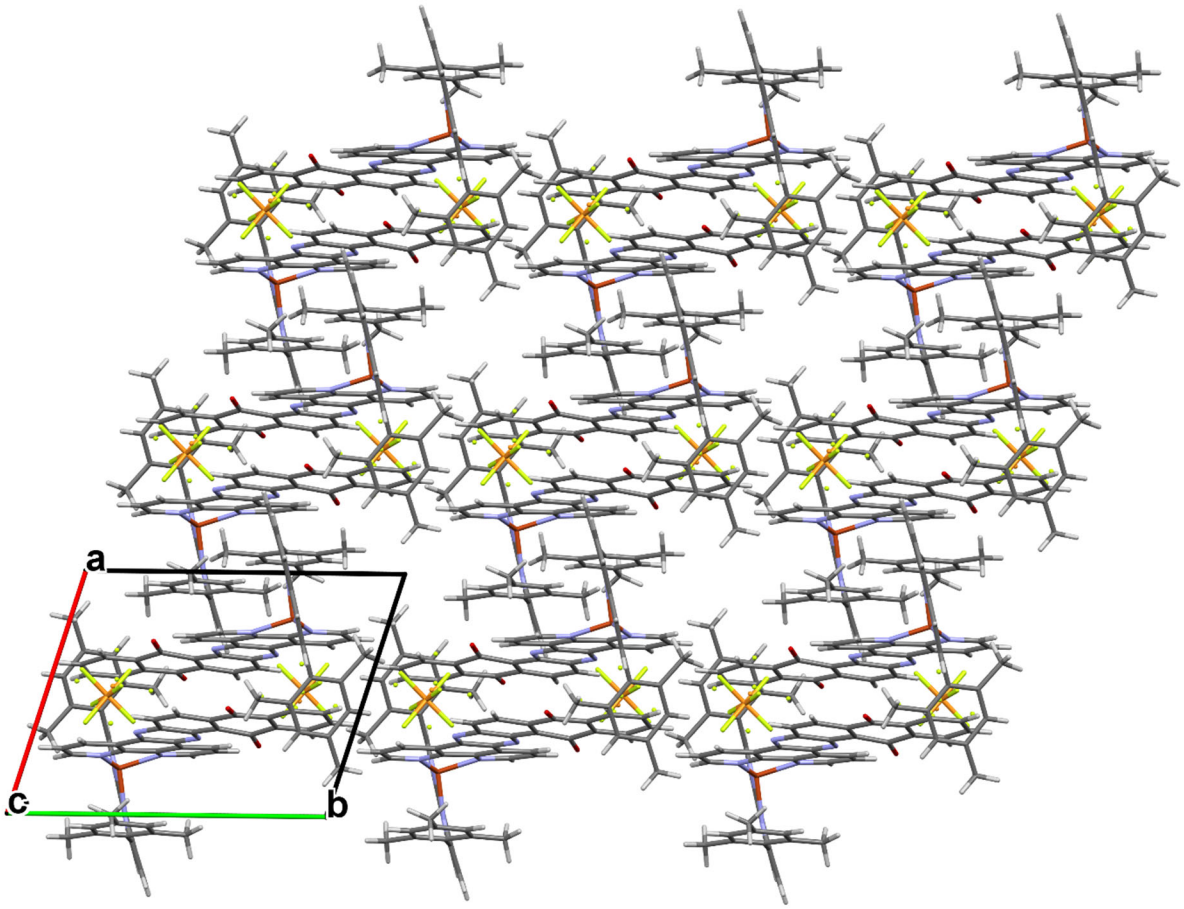


Figure S16. Crystal packing diagram of **Cu^{+}-AnQ**

5. Electrochemistry

Cyclic voltammetry was conducted using a standard three-electrode cell on a Pine Research WaveNow potentiostat (AFTP1) with a 1.6 mm-diameter Pt working electrode, a Pt wire auxiliary electrode, and a non-aqueous Ag^+/Ag reference electrode (0.01 M $AgNO_3$, 0.1 M tetrabutylammonium hexafluorophosphate ($TBAPF_6$) in CH_3CN). Each sample was prepared as solutions (0.2 mM for **Cu^+-AnQ**, 1 mM for **Cu^+-DPPZ**, 1 mM for anthraquinone, ~0.1 mM for **^{Me}AnQ** and 1 mM for triethylamine TEA) in anhydrous acetonitrile, purged with N_2 prior to measurement and subsequently maintained under a blanket of N_2. $TBAPF_6$ (0.1 M) was used as the supporting electrolyte. Ferrocene (purified by sublimation) was added as an internal standard and redox potentials were referenced to the ferrocene/ferrocenium couple (0.40V vs. SCE (CH_3CN)). All scans were performed at 100 mV/s.

UV-Vis spectroelectrochemical (SEC) measurements of all samples, except for **^{Me}AnQ**, were conducted in a UV-Vis spectroelectrochemical cell (BASi) with a Pt mesh working electrode, Pt wire counter electrode and a Ag^+/Ag pseudoreference electrode. The UV-Vis spectrum was collected using a Beckman-Coulter DU800 spectrophotometer. Each complex was prepared as a 0.2 mM solutions in anhydrous acetonitrile, purged with N_2 prior to measurement and subsequently maintained under a blanket of N_2. The SEC study of **^{Me}AnQ** was performed in a honeycomb UV-Vis spectroelectrochemical cell designed by Pine Research with a patterned "honeycomb" Pt electrode and a Pt counter electrode mounted on a plate and a Ag^+/Ag reference electrode (0.01 M $AgNO_3$, 0.1 M $TBAPF_6$ in CH_3CN). The UV-Vis spectrum was collected using an AvaSpec-ULS2048-EVO Fiber-optic Spectrometer interfaced with the potentiostat.

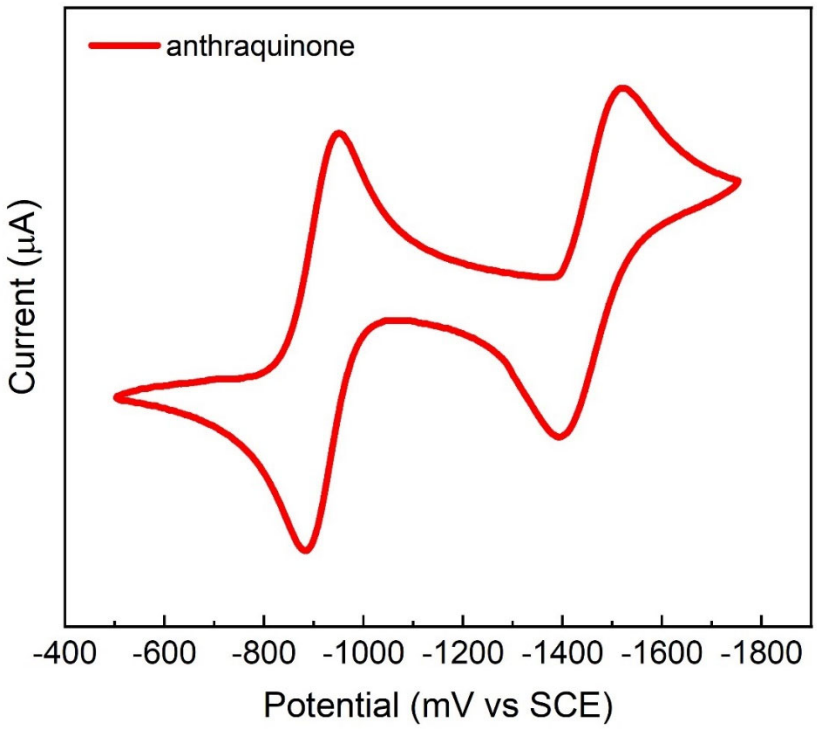


Figure S17. Cyclic voltammogram of anthraquinone in acetonitrile (1 mM for anthraquinone, 0.1 M $TBAPF_6$; working: Pt disc, counter: Pt wire, Reference: Ag/Ag^+ non-aqueous).

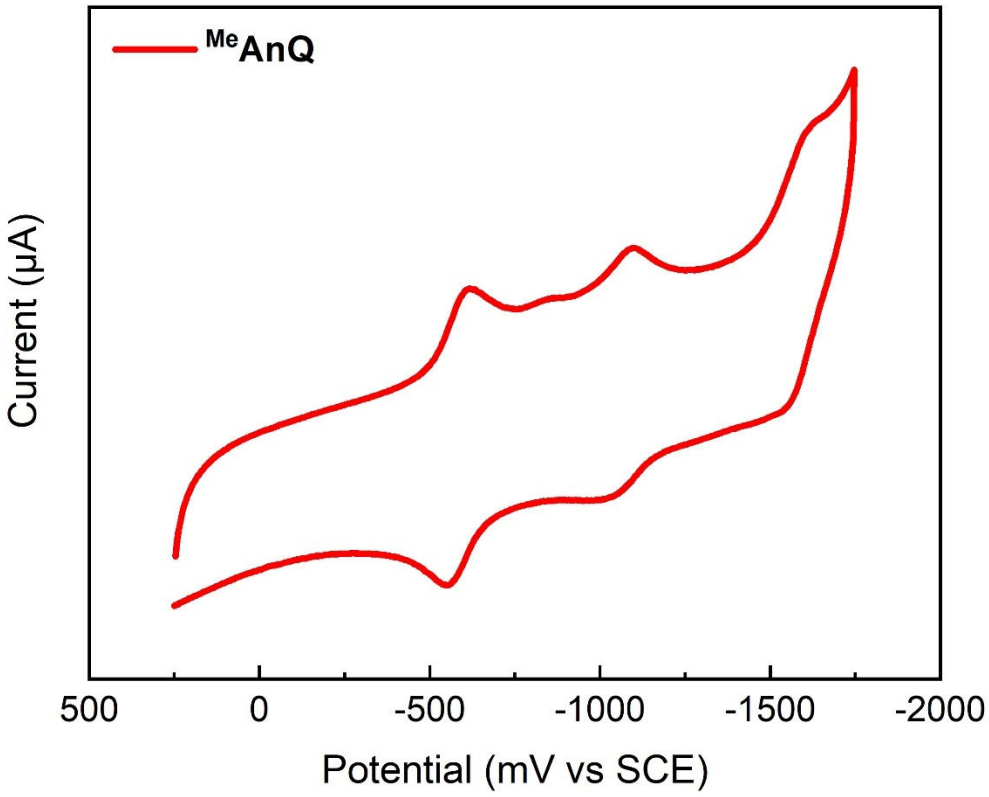


Figure S18. Cyclic voltammogram of ^{Me}**AnQ** in acetonitrile (~0.1 mM for ^{Me}**AnQ**, 0.1 M $TBAPF_6$; working: Pt disc, counter: Pt wire, Reference: Ag/Ag^+ non-aqueous).

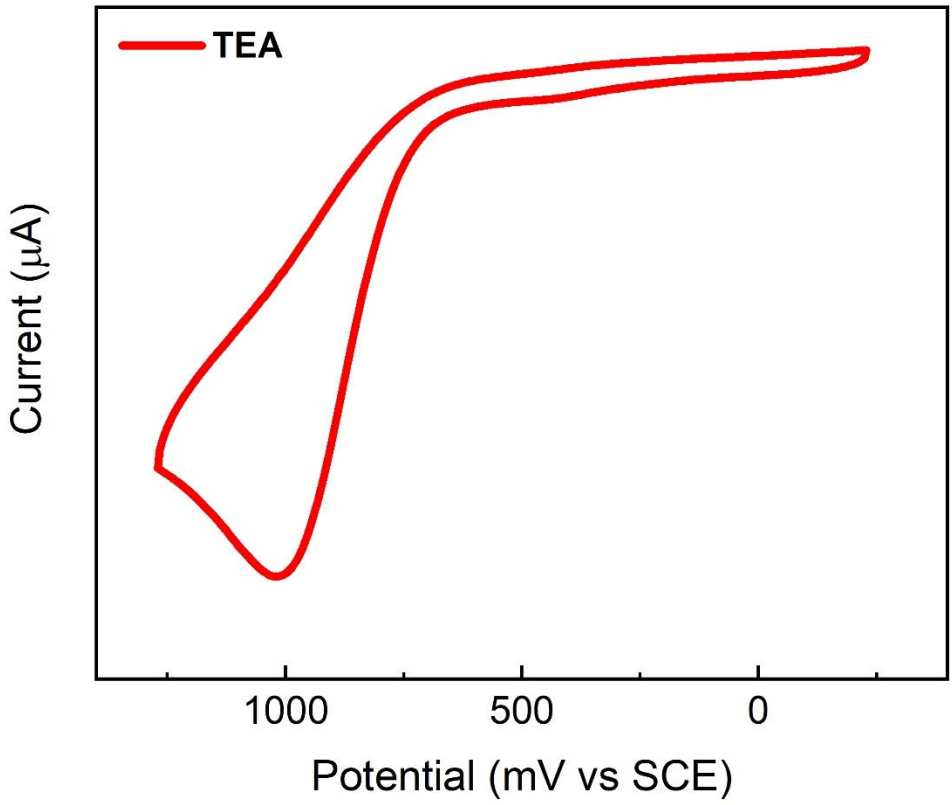


Figure S19. Cyclic voltammogram of TEA in acetonitrile (1 mM for TEA, 0.1 M $TBAPF_6$; working: Pt disc, counter: Pt wire, Reference: Ag/Ag^+ non-aqueous).

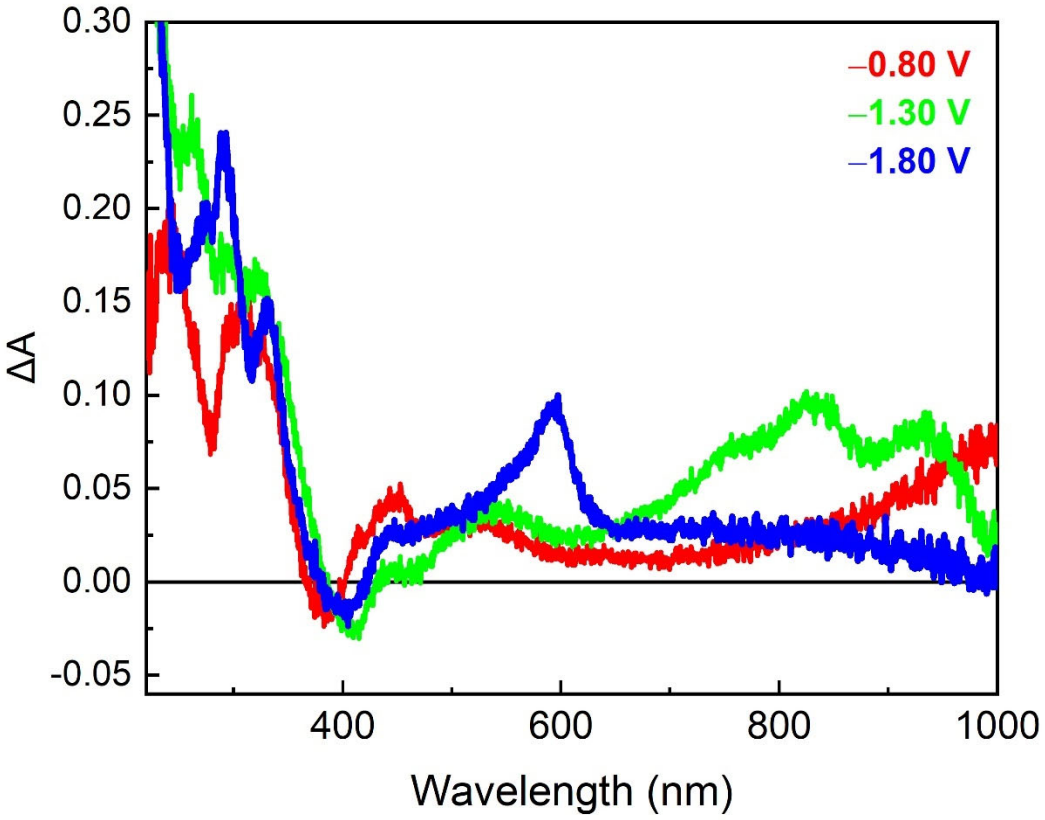


Figure S20. SEC study of ^{Me}**AnQ** (~0.1 mM) in 0.1 M $TBAPF_6$/anhydrous acetonitrile. The potential steps shown in the figure are referenced to SCE.

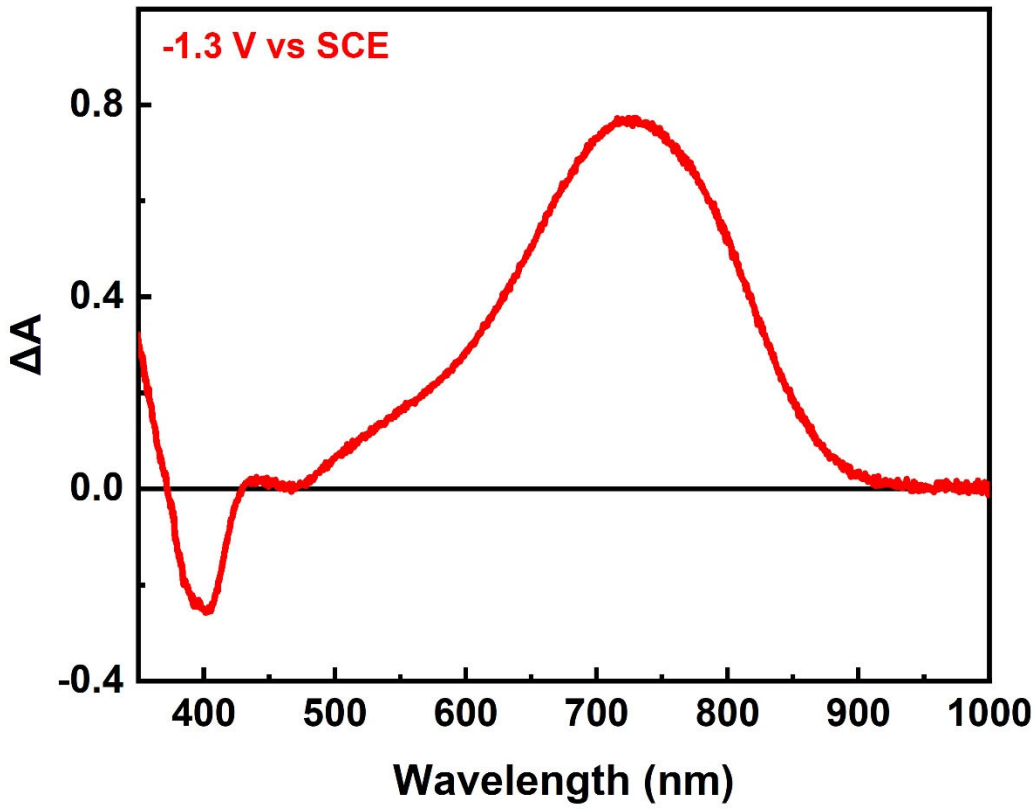


Figure S21. SEC study of **Cu^{+}-AnQ** (0.2 mM) in acetonitrile with 0.1 M $TBAPF_6$ and 8.3 M H_2O. The potential steps shown in the figure are referenced to SCE.

6. Chemical reduction of Cu^{+}-AnQ

General procedures for chemical reduction of Cu^{+}-AnQ generating Cu^{+}-AnQ^{-} and Cu^{+}-AnQ^{2-}. To a solution of **Cu^{+}-AnQ** in anhydrous acetonitrile, aliquots of 4 mM $CoCp_2$ solution in anhydrous acetonitrile was titrated. The process of reduction was monitored by UV-Vis spectrum. The NMR of the reduced species was obtained by repeating the titration in CD_3CN.

^{1}H NMR of **Cu^{+}-AnQ^{-}** (500 MHz, CD_3CN) δ 8.76 (d, J = 7.8 Hz), 8.24 (s), 7.86 (d, J = 8.3 Hz), 5.94 (s), 1.58 (s), 1.27 (s).

^{1}H NMR of **Cu^{+}-AnQ^{2-}** (500 MHz, CD_3CN) δ 9.43 (d, J = 7.9 Hz, 1H), 9.04 (d, J = 8.0 Hz, 1H), 8.77 (d, J = 8.2 Hz, 2H), 8.62 (d, J = 7.8 Hz, 1H), 8.56 (d, J = 3.8 Hz, 1H), 8.52 (d, J = 4.9 Hz, 1H), 8.50 (d, J = 8.6 Hz, 1H), 8.41 (d, J = 8.8 Hz, 1H), 8.26 (s, 2H), 7.90 (q, J = 4.0 Hz, 1H), 7.87 (d, J = 8.3 Hz, 2H), 7.81 (q, J = 4.2 Hz, 1H), 7.68 (t, J = 7.6 Hz, 1H), 7.53 (t, J = 7.2 Hz, 1H), 6.79 (d, J = 8.7 Hz, 1H), 6.07 (d, J = 12.7 Hz, 4H), 1.74 (d, J = 9.3 Hz, 12H), 1.45 (s, 6H).

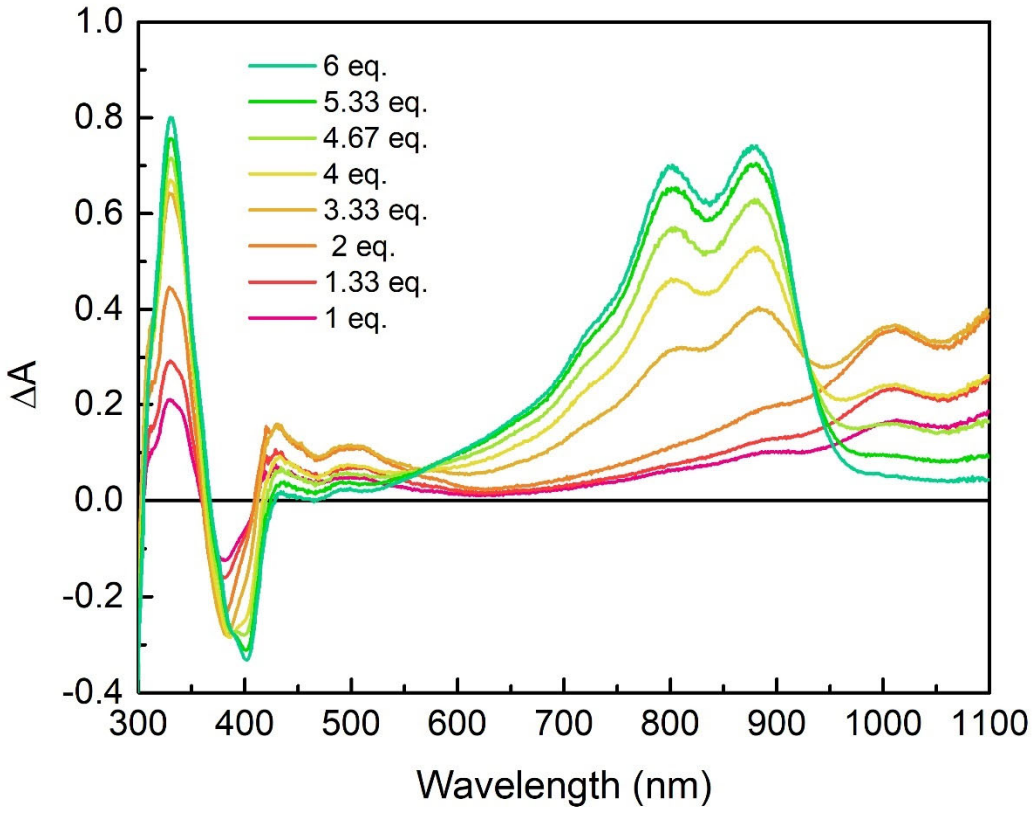


Figure S22. Difference absorption spectra of **Cu^{+}-AnQ** titrated with $CoCp_2$ in CH_3CN.

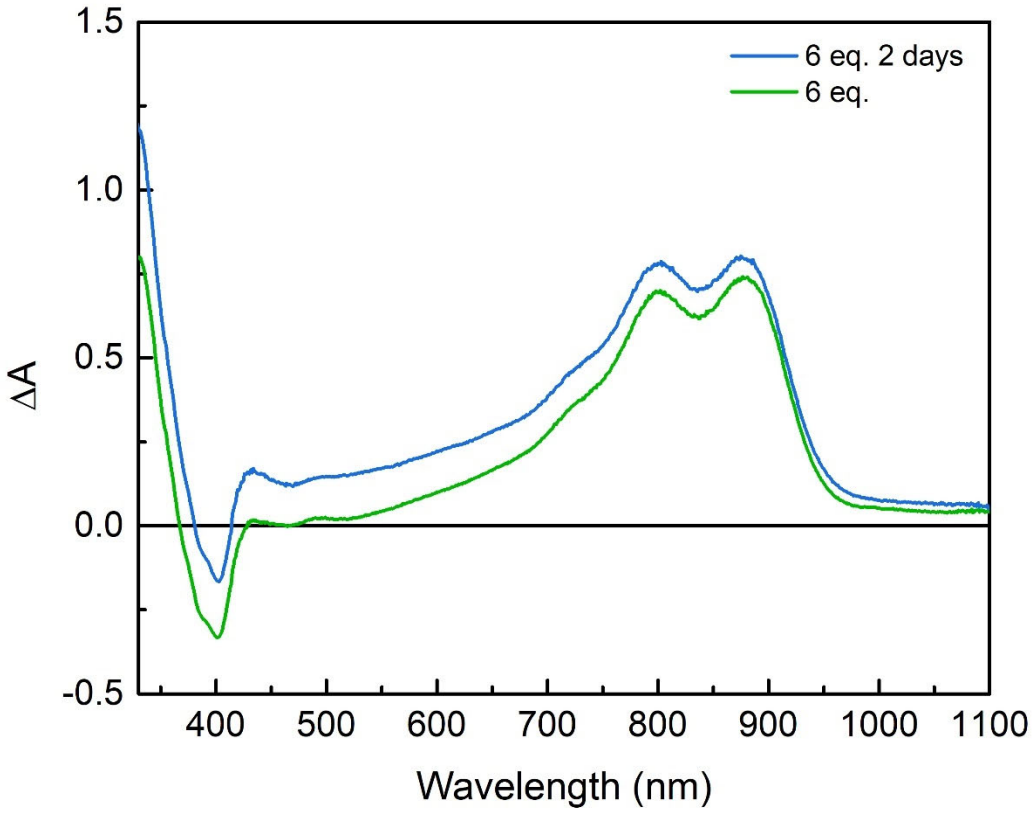


Figure S23. Comparison of the difference absorption spectra of newly generated **Cu^{+}-AnQ^{2-}** and the same solution stored in N_2 atmosphere for 2 days.

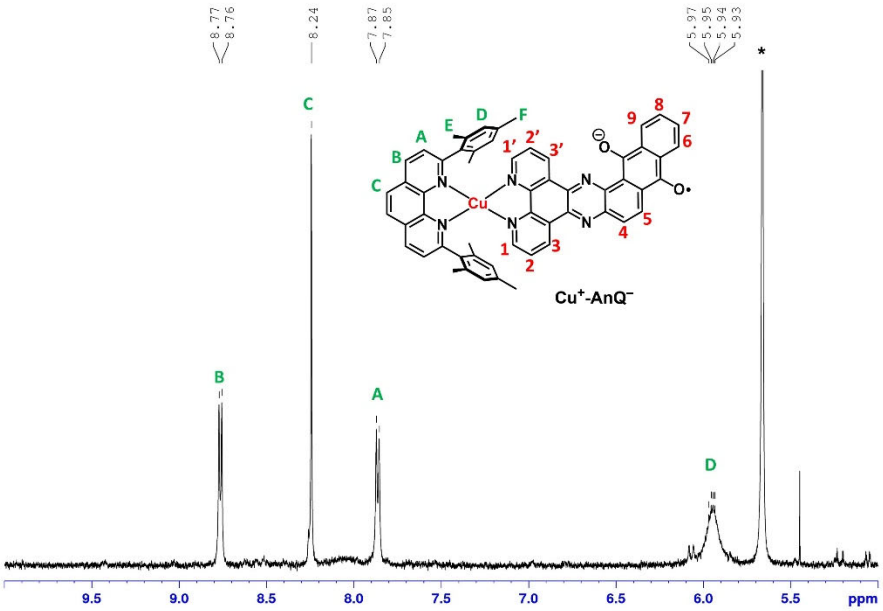


Figure S24. Aromatic region of the ^{1}H NMR of **Cu^{+}-AnQ^{-}** in CD_3CN (0.5 mM concentration). The complex was generated by treating with 1 equivalent of $CoCp_2$ (* indicates solvent impurity).

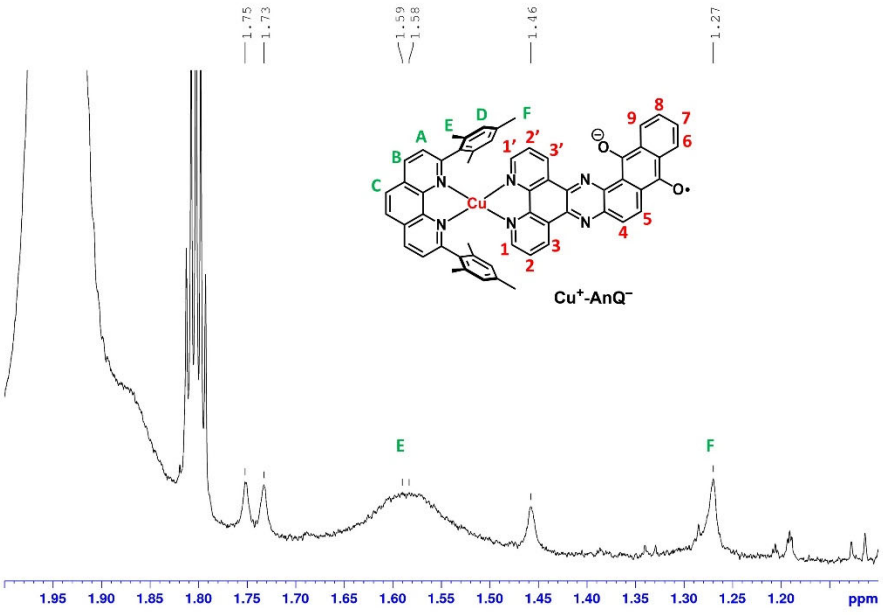


Figure S25. Aliphatic region of the ^{1}H NMR of **Cu^{+}-AnQ^{-}** in CD_3CN (0.5 mM concentration). The complex was generated by treating with 1 equivalent of $CoCp_2$.

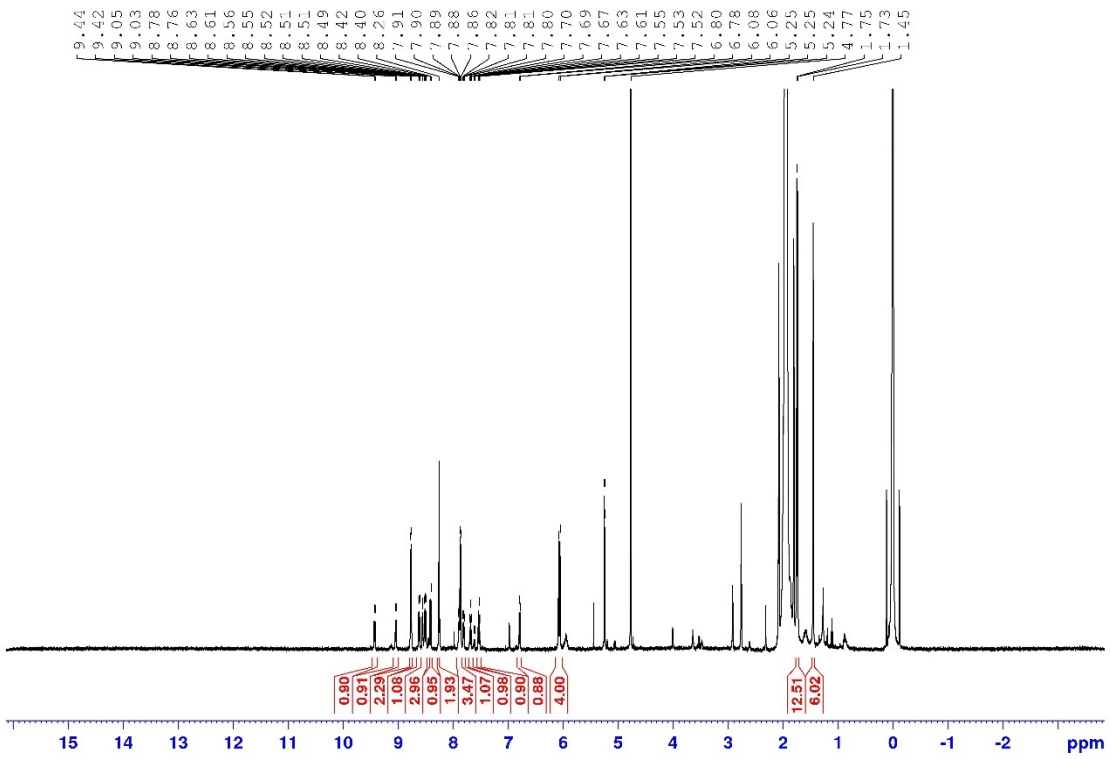


Figure S26. The ^{1}H NMR of **Cu^{+}-AnQ^{2-}** in CD_3CN (0.5 mM concentration). The complex was generated by treating with 6 equivalents of $CoCp_2$.

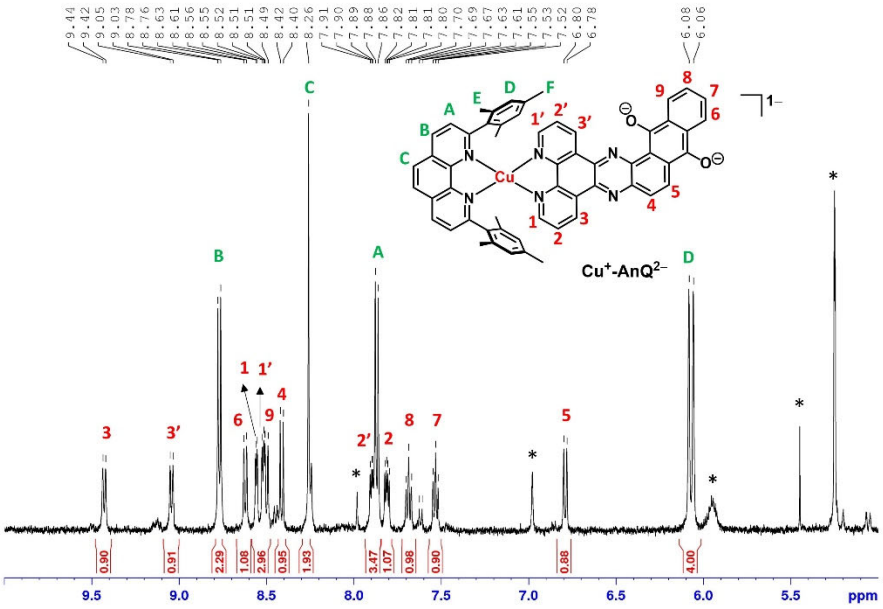


Figure S27. Aromatic region of the ^{1}H NMR of **Cu^{+}-AnQ^{2-}** in CD_3CN (0.5 mM concentration). The complex was generated by treating with 6 equivalents of $CoCp_2$ (* indicates impurity).

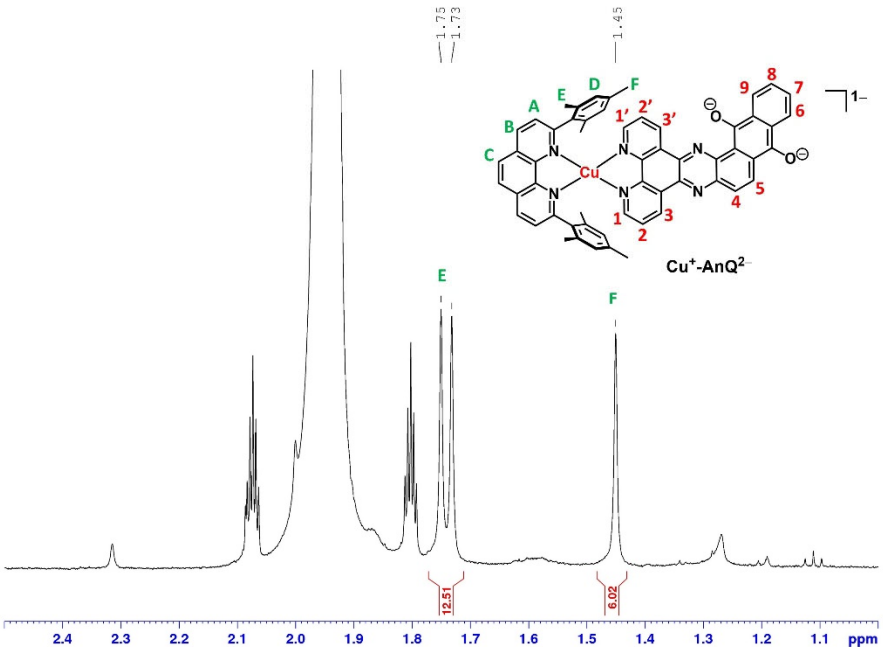


Figure S28. Aliphatic region of the ^{1}H NMR of **Cu^{+}-AnQ^{2-}** in CD_3CN (0.5 mM concentration). The complex was generated by treating with 6 equivalents of $CoCp_2$.

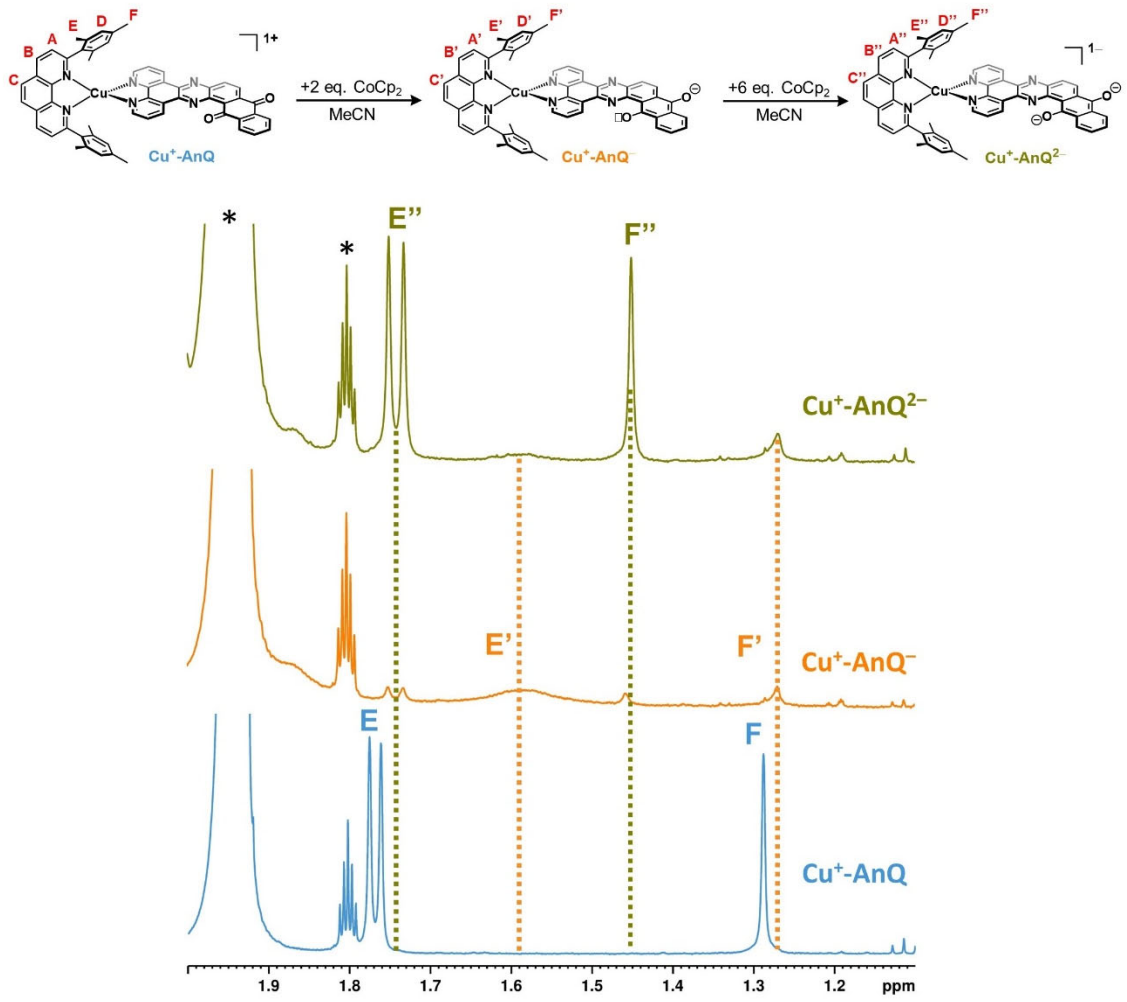


Figure S29. Comparison of the aliphatic region of the ^{1}H NMR of **Cu^{+}-AnQ^{2-}**, **Cu^{+}-AnQ^{-}** and **Cu^{+}-AnQ** (0.5 mM concentration) in CD_3CN. Peaks corresponding to the solvent are denoted by asterisk.

7. EPR spectroscopy and magnetic resonance parameters

Cu^{+}-AnQ^{-} and **Cu^{+}-AnQ^{2-}** were prepared using chemical reductant $CoCp_2$ in air-free solvent mixture of MeCN and DCM (v:v = 1:1; concentration of the complex = 1.2 mM), working under anaerobic conditions in a N_2 glove box. The solutions of the parent **Cu^{+}-AnQ** and the reduced complexes were loaded into 4 mm o.d. quartz EPR tubes, sealed under N_2 atmosphere, and then quickly frozen in liquid nitrogen. Continuous wave (CW) X-band (9.7 GHz) EPR experiments were performed using field modulation with phase sensitive lock-in detection on a Bruker ELEXSYS E580 EPR spectrometer (Bruker Biospin, Ettlingen, Germany), equipped with a dielectric EPR resonator (Bruker ER4118-MD5-W1). This type of detection results in first derivative-type EPR spectra. A CF935 helium gas-flow cryostat and an ITC503 (both from Oxford Instrument, UK), were used for measurements at cryogenic temperatures (50-100 K).

The calculated (DFT) principal components of the g-tensor are 2.0066 (g_x), 2.0048 (g_y), 2.0025 (g_z), which is in the typical range for semiquinone anion radicals (Table S4). The largest calculated hyperfine couplings are from the two phenazine nitrogen atoms (magnetically almost equivalent, $A_{||}$ = 18-19 MHz, $A_{\perp}$ = -0 to -1 MHz), and one of the alpha protons (A_x = -4 MHz, A_y = -12 MHz, A_z = -9 MHz,) of the anthraquinone ring connected to the phenazine moiety.

Table S4. Comparison of g values of **Cu^{+}-AnQ^{-}** with the DFT calculation and literature values.

	g_x	g_y	g_z	g_{iso}
Cu^{+}-AnQ^{-}				2.004-2.005
Cu^{+}-AnQ^{-} (DFT)	2.0066	2.0048	2.0025	2.0046
AnQ anion radical[ref 19]	2.0058	2.0049	2.0022	2.0043
AnQ anion radical[ref 21]	2.0059	2.0048	2.0022	2.0043
AnQ anion radical[ref 20]				2.0040

ref [19–21]

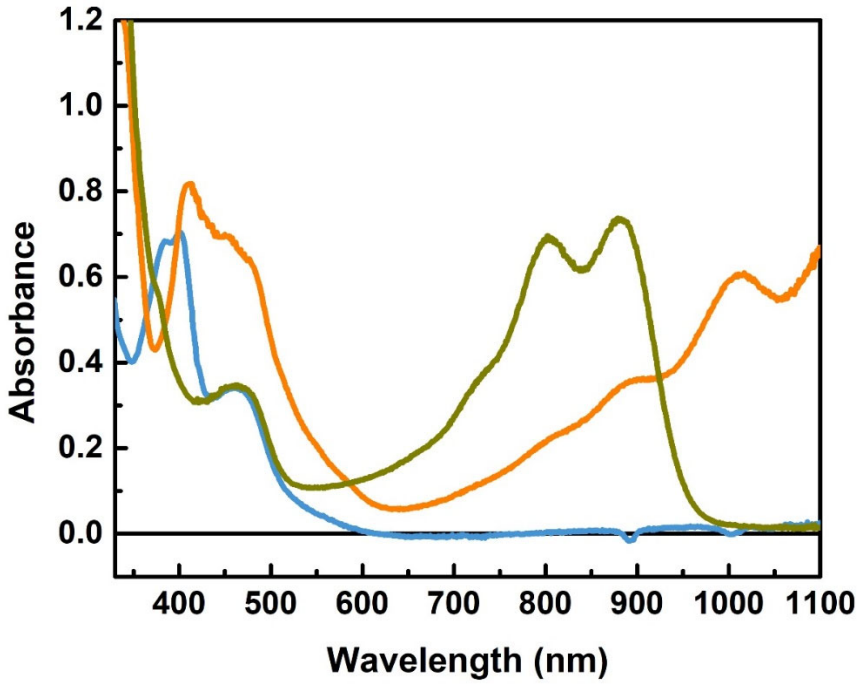


Figure S30. Absorption spectra of **Cu^{+}-AnQ** (blue trace), **Cu^{+}-AnQ^{-}** (orange trace) and **Cu^{+}-AnQ^{2-}** (green trace) in MeCN/DCM mixture (v:v = 1:1).

8. Charge accumulation through photochemical reduction with sacrificial electron donor

General procedures of photolysis. All photolysis experiments were conducted in sealed cuvette (0.2 cm pathlength) under N_2 atmosphere. The complex was dissolved in dry solvent (0.2 mM, MeCN or DMSO) in N_2 box. Sacrificial electron donor BIH was added into the solution in dark. The sample was irradiated with a blue LED (455 nm) while being constantly stirred with a 0.2 mm stir bar. Output from the LED was focused using a Thorlab Aspheric Condenser Lens to a radius of about 0.5 cm approximately 10 cm away from the light source at the position of the sample flask. The light intensity was adjusted using a Thorlab DC2100 power source and most of the experiments were performed at full light power. Full light power for our photocatalytic set-up is the 1600 mA setting on the power supply, which corresponds to a flux of approximately 120 mW/cm^2 measured with a Newport Powermeter Model 1918C at the sample position without considering the loss in power from the cuvette. The reaction was monitored periodically by a Beckman-Coulter DU800 spectrophotometer. Samples for NMR spectroscopy were photolyzed under N_2 atmosphere in deuterated solvents which were degassed by three cycles of freeze-pump-thaw and dried by 4 Å molecular sieves overnight prior to photolysis. Single crystals of **Cu^{+}-AnQH^{-}** suitable for X-ray diffraction were obtained in acetonitrile at room temperature.

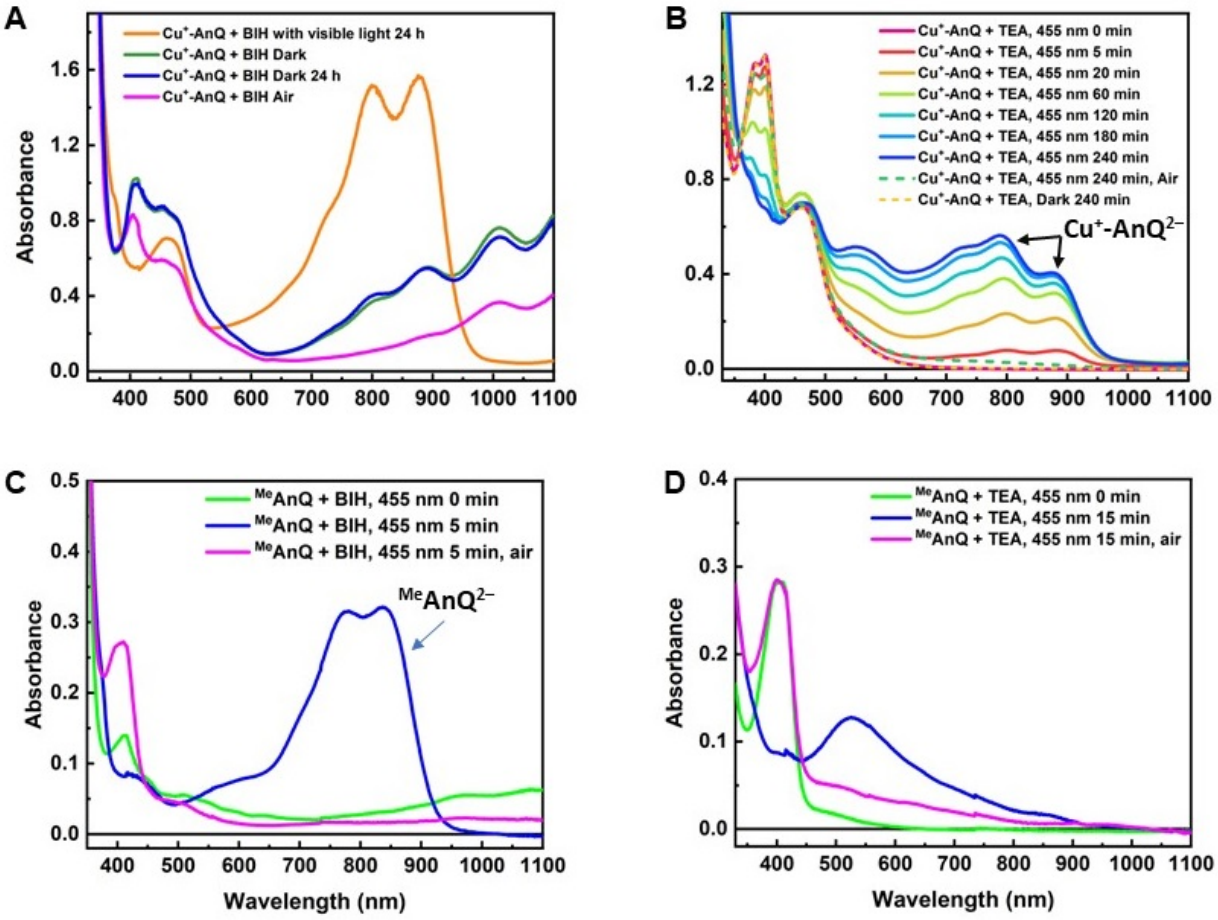


Figure S31. (A) Comparison of the UV-Vis spectra of **Cu$^+$-AnQ** + BIH under visible light after 24 h, **Cu$^+$-AnQ** + BIH under dark conditions for 0 min and 24 h, and **Cu$^+$-AnQ** + BIH in air; (B) Comparison of the UV-Vis spectra of **Cu$^+$-AnQ** + TEA irradiated by 455 nm light from 0 min to 240 min. (C) Comparison of the UV-Vis spectra of **^{Me}AnQ** + BIH irradiated by 455 nm light for 0 min and 5 min; (D) Comparison of the UV-Vis spectra of **^{Me}AnQ** + TEA irradiated by 455 nm light for 0 min and 15 min. The concentration of **Cu$^+$-AnQ**, **^{Me}AnQ** and the sacrificial electron donors were kept at 0.2 mM, 0.2 mM and 0.1 M, respectively, in acetonitrile.

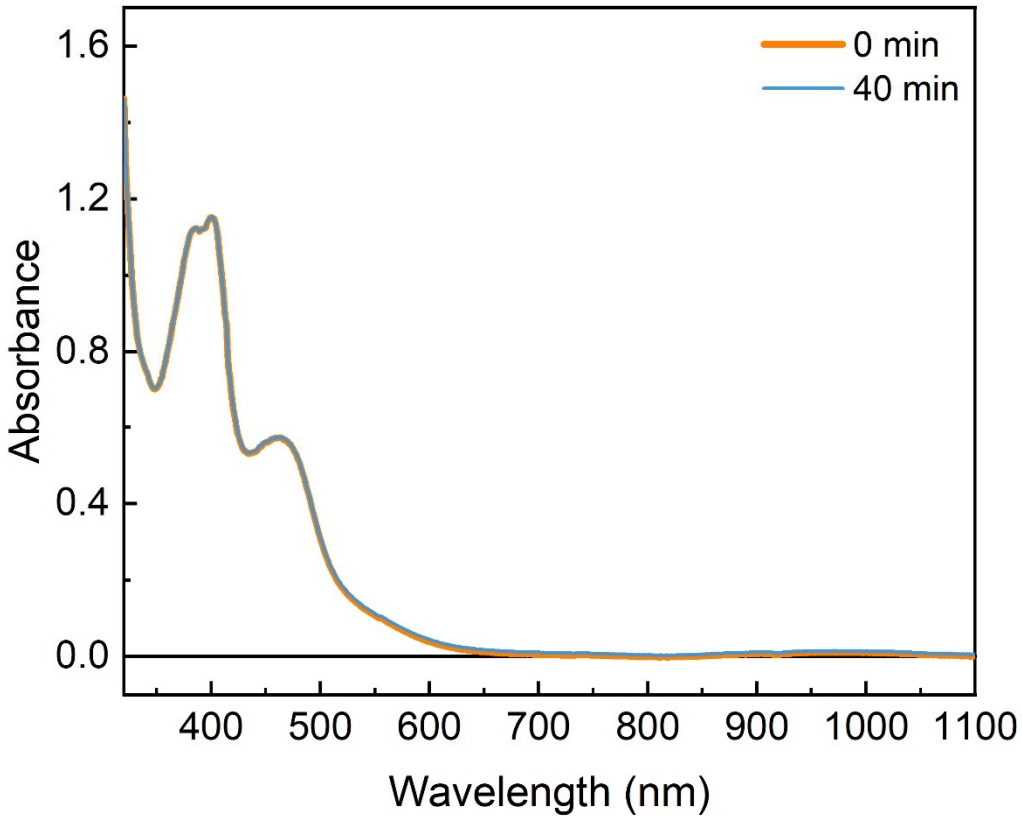


Figure S32. Photolysis experiment of **Cu^{+}-AnQ** in the absence of BIH. The concentration of **Cu^{+}-AnQ** was kept at 0.2 mM.

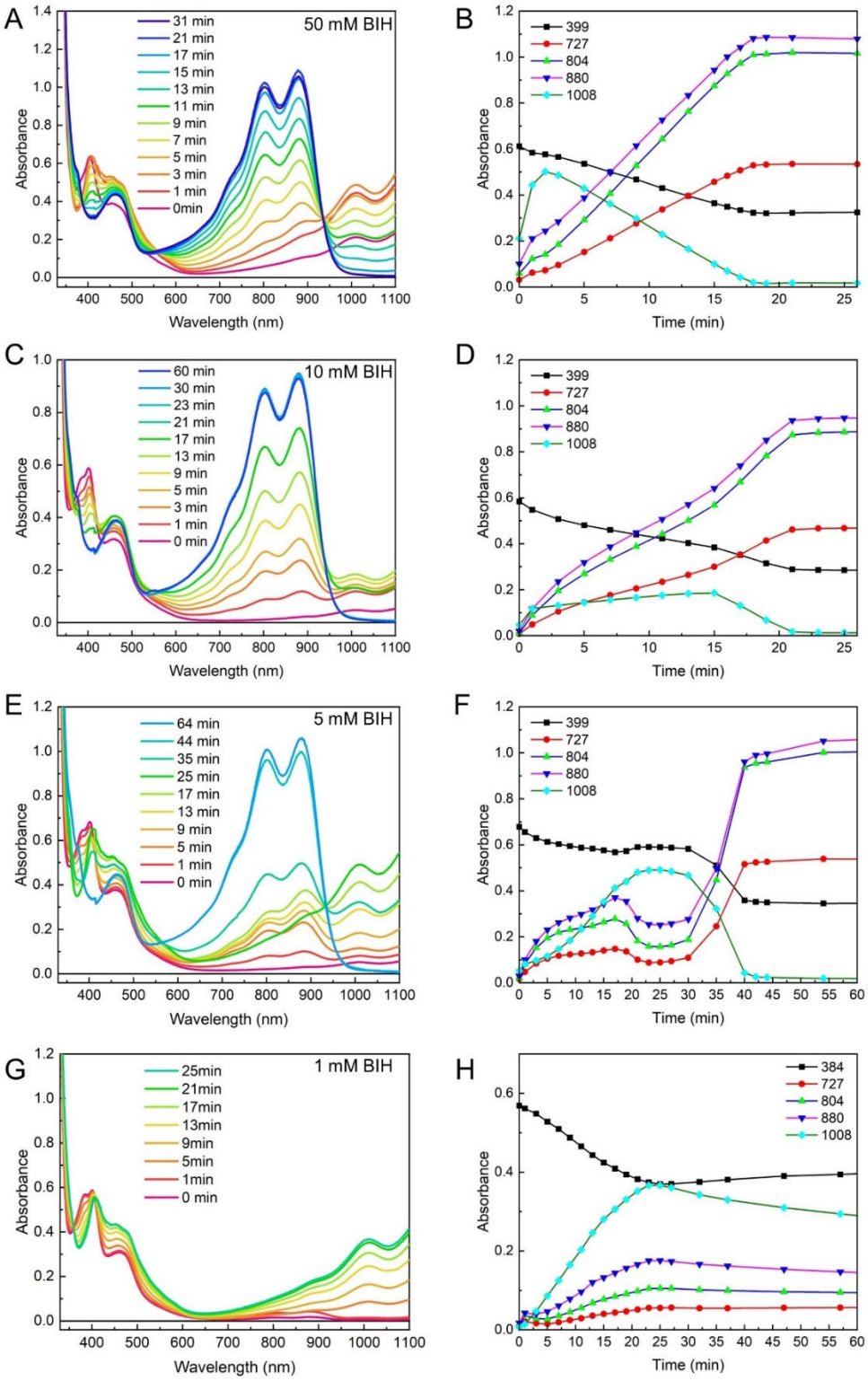


Figure S33. UV/vis monitoring of the photolysis experiments of **Cu^{+}-AnQ** with BIH at (A) 50 mM, (C) 10 mM, (E) 5 mM and (G) 1 mM concentration in acetonitrile under 455 nm light. The concentration of **Cu-AnQ^{PF6}** was kept at 0.2 mM. The kinetics of selected wavelengths from the photolysis experiments are presented alongside the UV/vis spectra of the corresponding experiment.

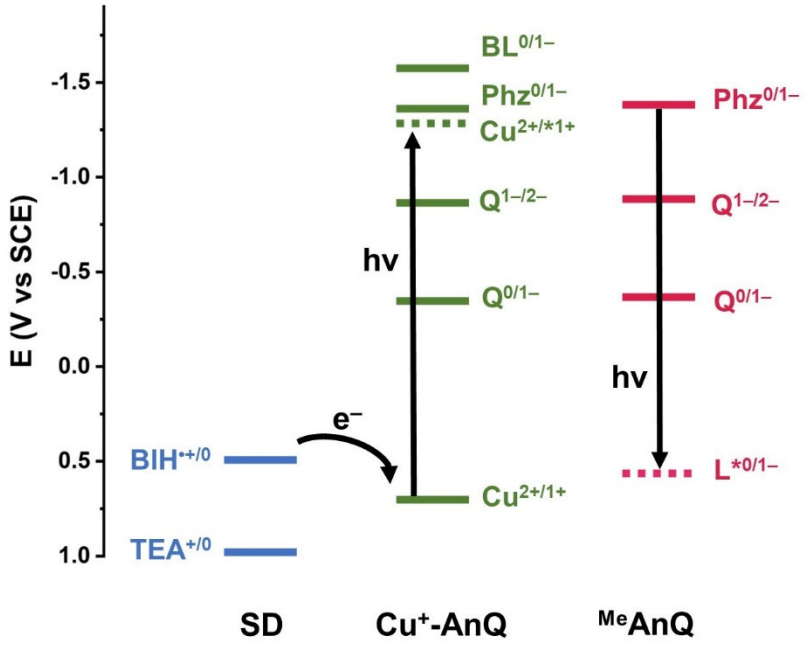


Figure S34. The energy of the redox states of the sacrificial electron donors, **Cu^{+}-AnQ** and **^{Me}AnQ**. The dash lines are estimated excited state potentials calculated by assuming the energy of the zero-zero transition between excited state and ground state (E^{00}) is 2.0 eV.[22–24]

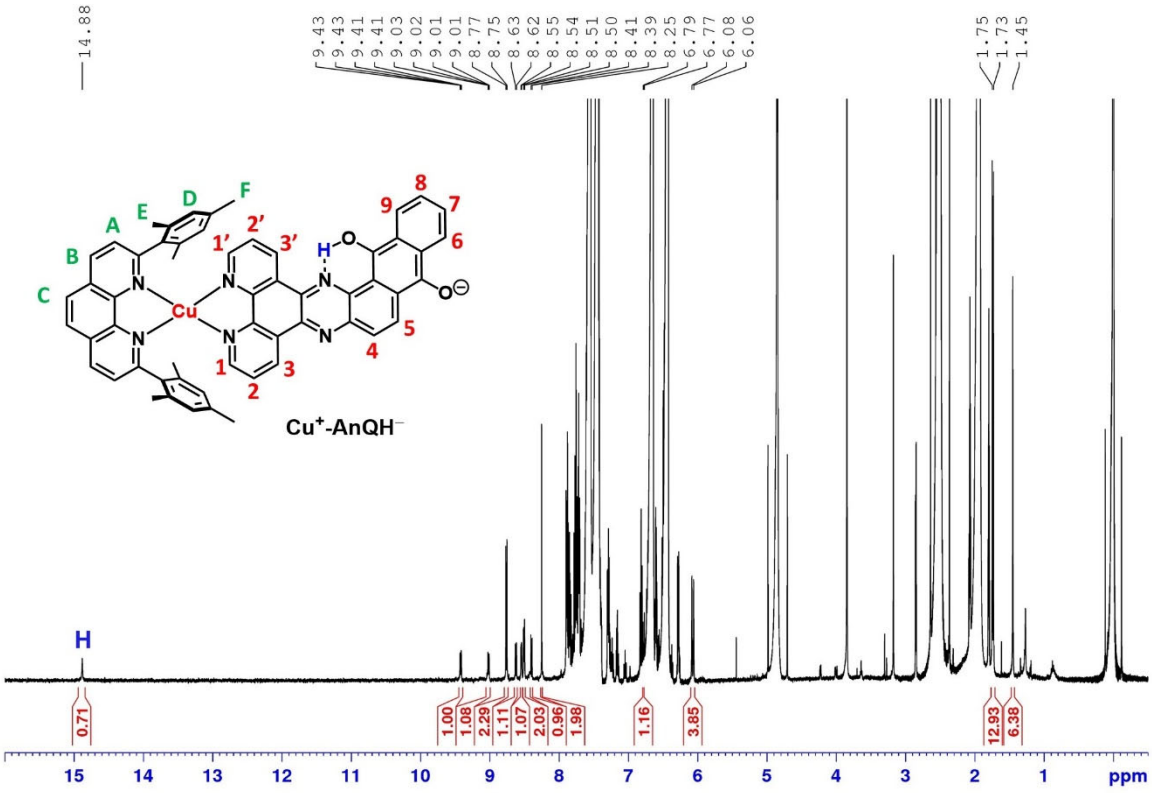


Figure S35. ^{1}H NMR spectrum of the mixture of **Cu^{+}-AnQ** and BIH after illumination for 30 min with 455 nm light in CD_3CN. The concentration of **Cu^{+}-AnQ** and BIH was 0.2 mM and 0.1 M, respectively.

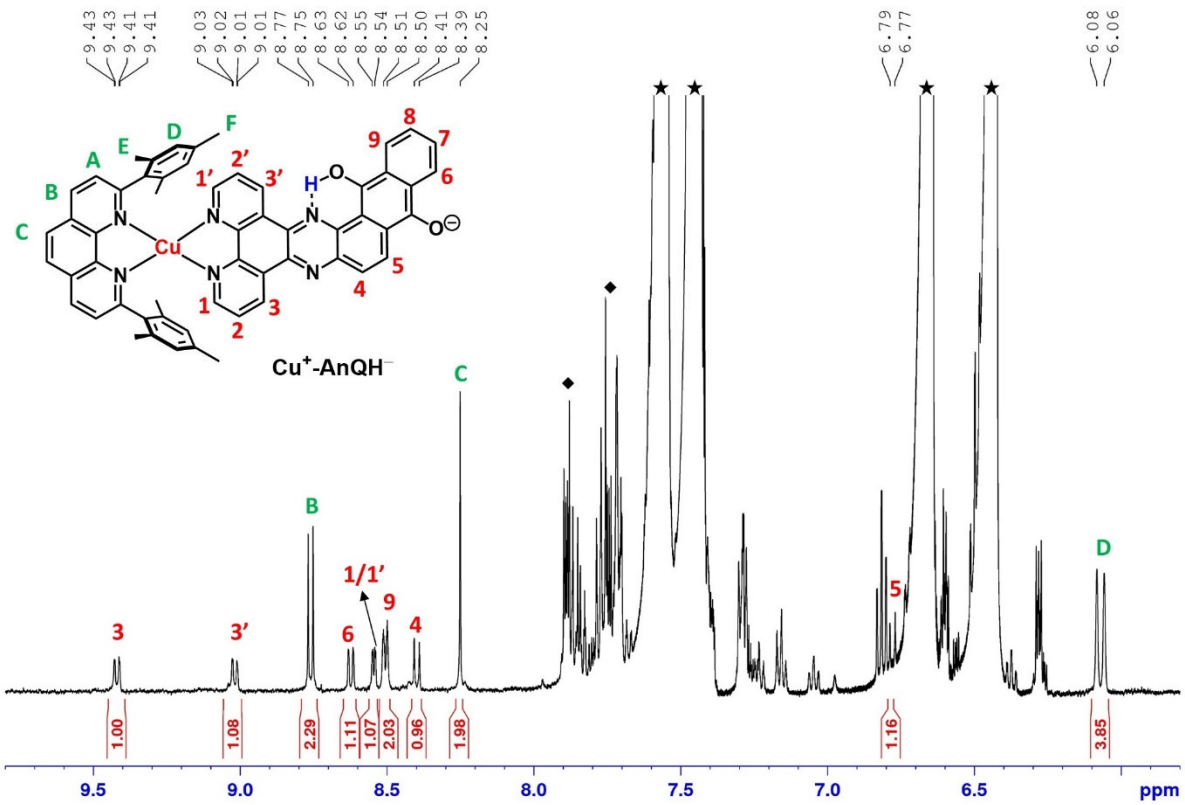


Figure S36. The aromatic region of the ^{1}H NMR spectrum of the mixture of **Cu^{+}-AnQ** and BIH after illumination for 30 min with 455 nm light in CD_3CN. The concentration of **Cu^{+}-AnQ** and BIH was 0.2 mM and 0.1 M, respectively. Signals from BIH (★) and BI^{+} (◆) are indicated in the spectrum.

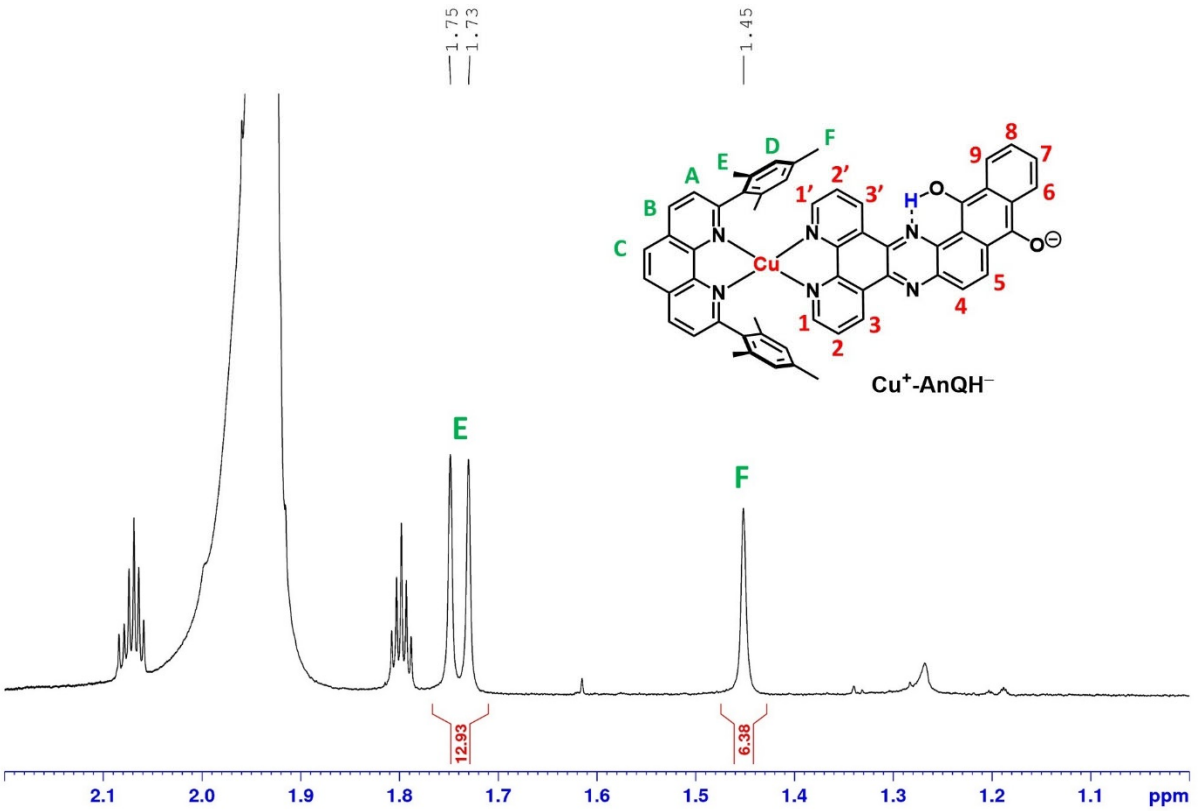


Figure S37. The aliphatic region of the ^{1}H NMR spectrum of the mixture of **Cu^{+}-AnQ** and BIH after illumination for 30 min with 455 nm light in CD_3CN. The concentration of **Cu^{+}-AnQ** and BIH was 0.2 mM and 0.1 M, respectively.

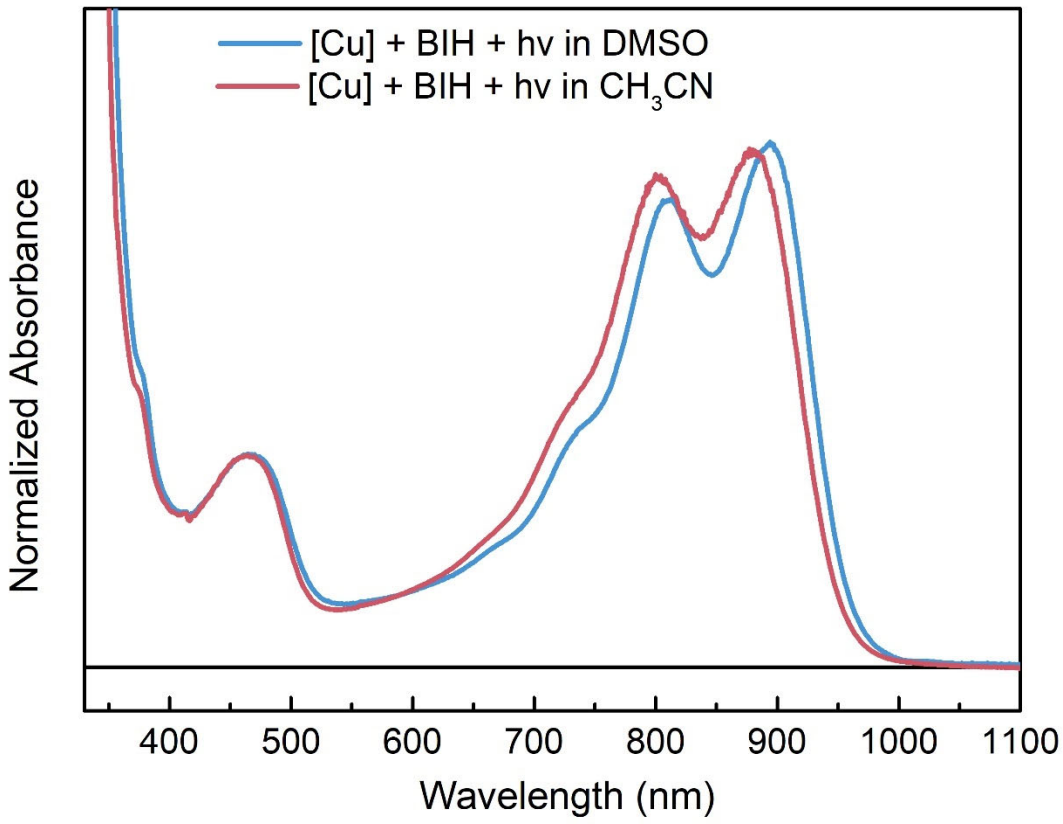


Figure S38. The comparison of the UV-Vis spectra of the CH_3CN and DMSO solution of **Cu^+-AnQ** and BIH after illumination for 30 min with 455 nm light. The concentration of **Cu^+-AnQ** and BIH was 0.2 mM and 0.1 M, respectively. [Cu] = **Cu^+-AnQ**.

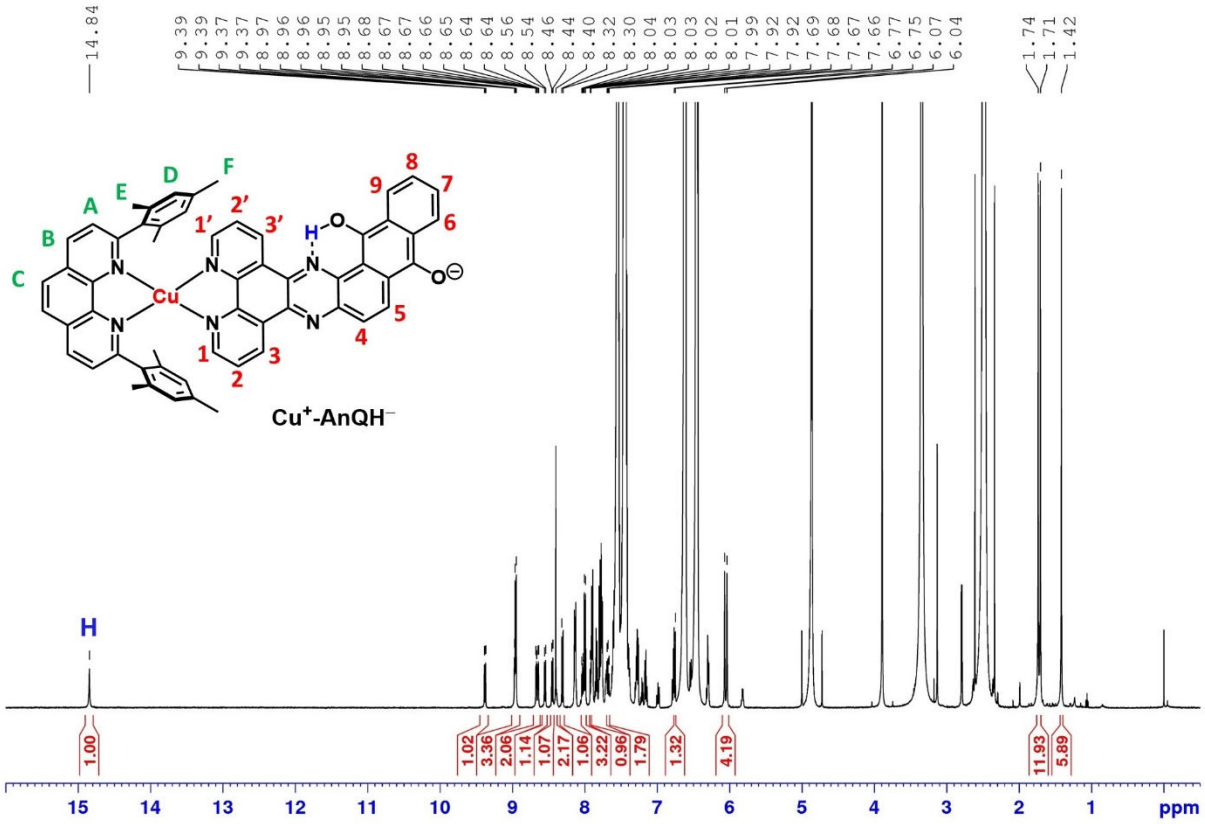


Figure S39. ^{1}H NMR spectrum of the mixture of **Cu^{+}-AnQ** and BIH after illumination for 4 h with 455 nm light in DMSO-d_6. The concentration of **Cu^{+}-AnQ** and BIH was 0.5 mM and 0.1 M, respectively.

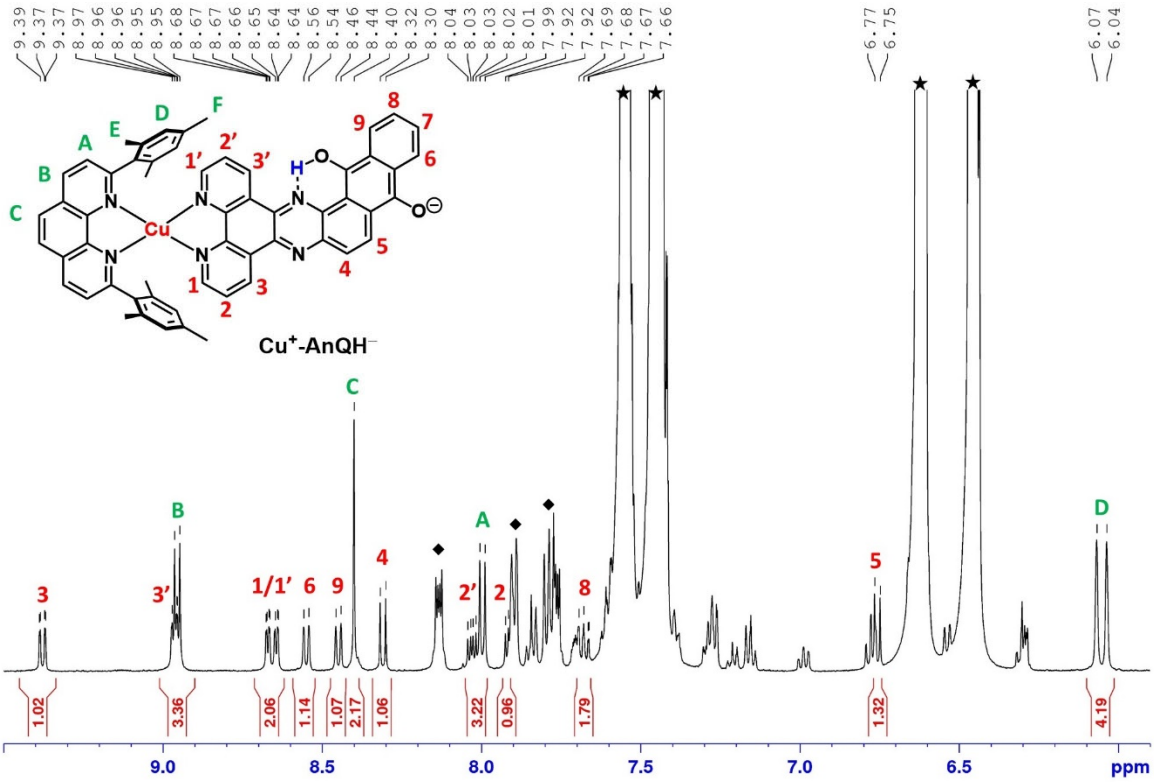


Figure S40. The aromatic region of the ^{1}H NMR spectrum of the mixture of **Cu^{+}-AnQ** and BIH after illumination for 4 h with 455 nm light in DMSO-d_6. The concentration of **Cu^{+}-AnQ** and BIH was 0.5 mM and 0.1 M, respectively. Signals from BIH (★) and BI^{+} (◆) are indicated in the spectrum.

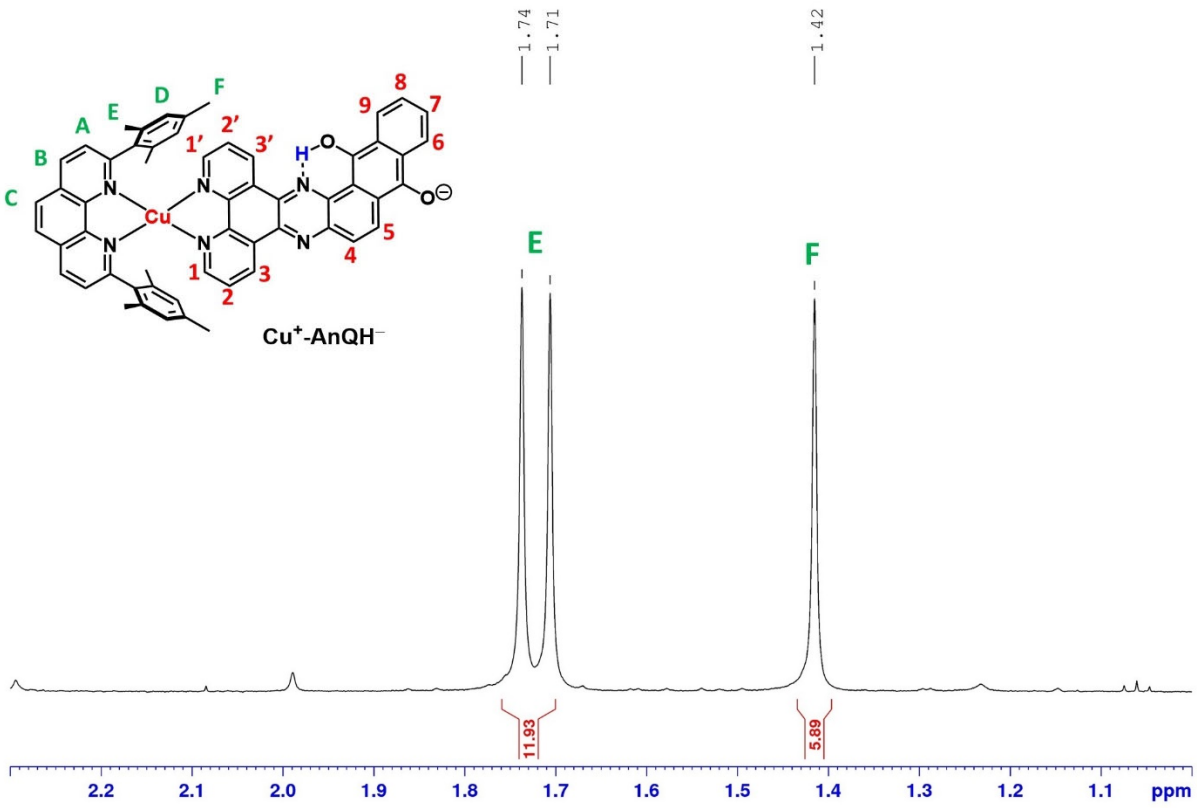


Figure S41. The aliphatic region of the ^{1}H NMR spectrum of the mixture of **Cu^{+}-AnQ** and BIH after illumination for 4 h with 455 nm light in DMSO-d_6. The concentration of **Cu^{+}-AnQ** and BIH was 0.5 mM and 0.1 M, respectively.

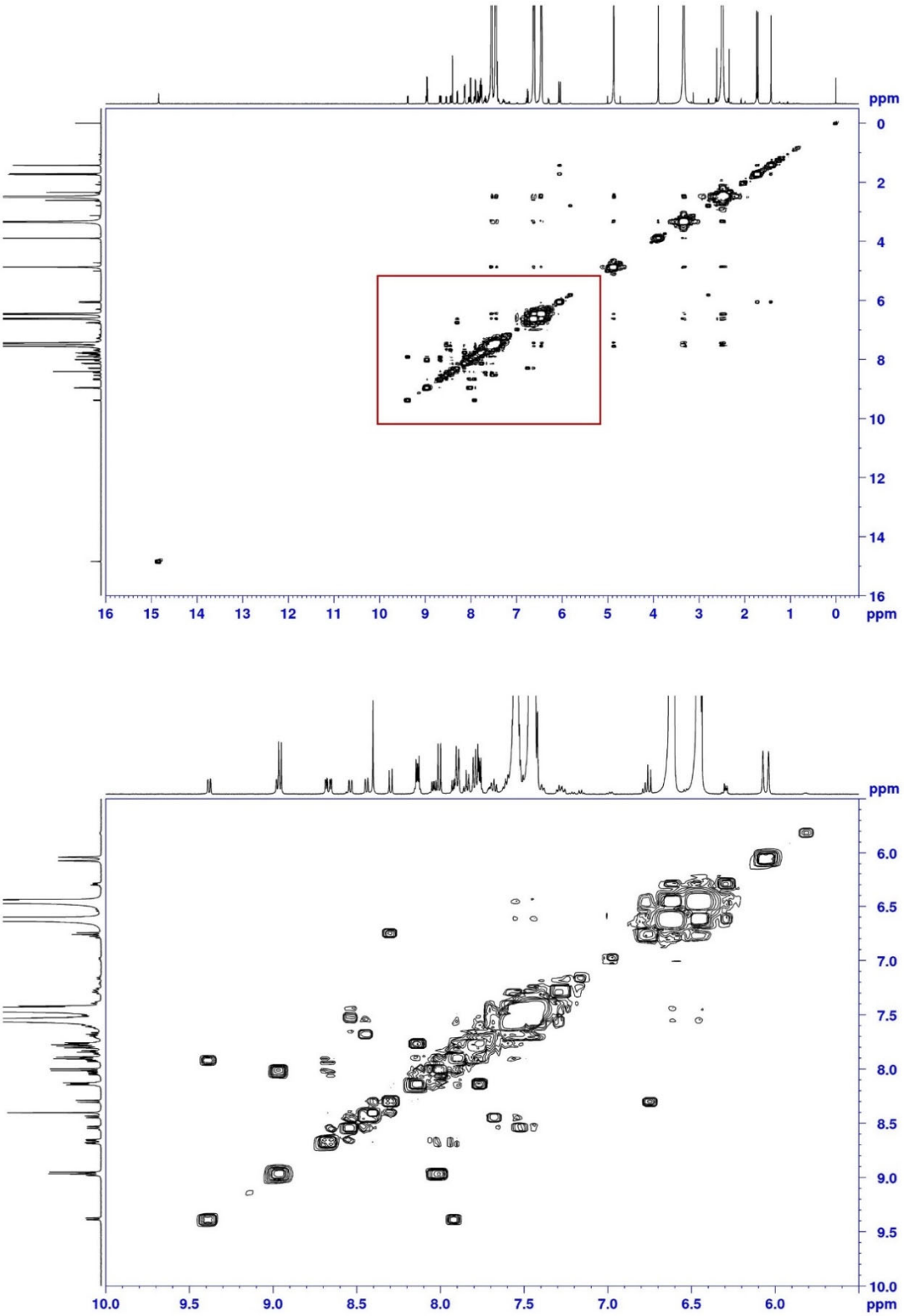


Figure S42. COSY spectrum of **Cu^{+}-AnQ** and BIH after illumination for 4 h with 455 nm light in DMSO-d_6. The concentration of **Cu^{+}-AnQ** and BIH was 0.5 mM and 0.1 M, respectively. The lower spectrum shows the zoomed-in area of the red box in the upper spectrum.

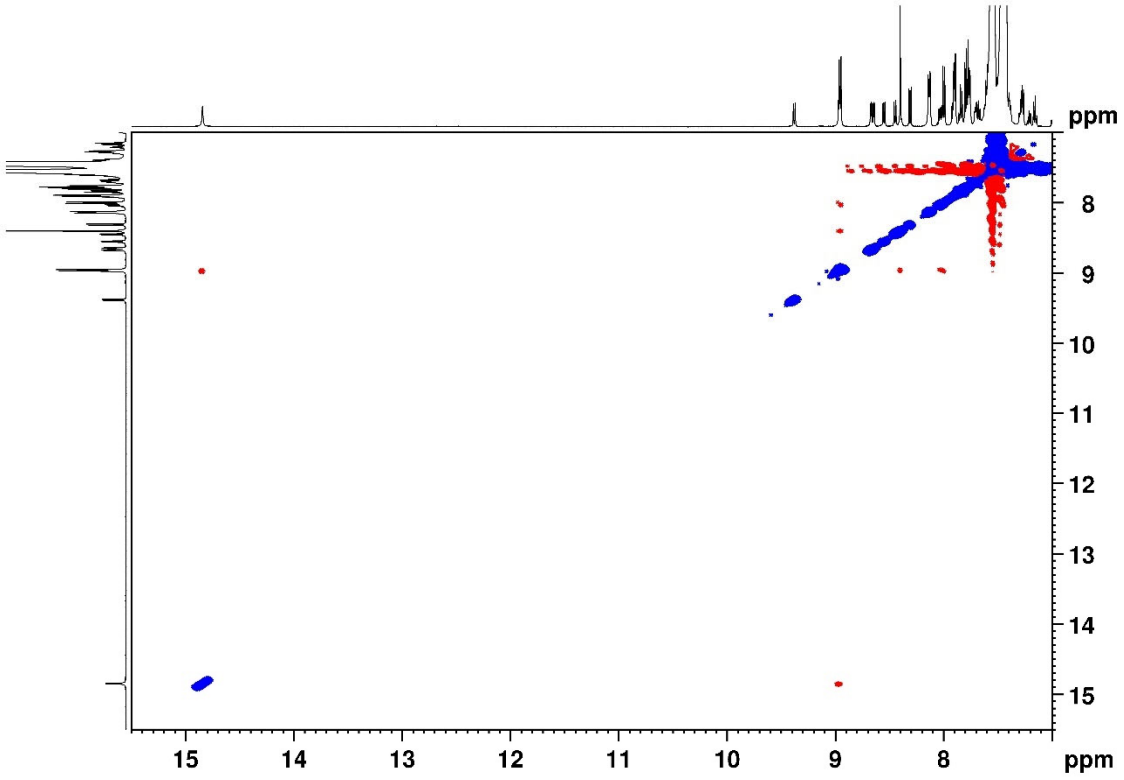


Figure S43. 2D-ROESY spectrum of **Cu^{+}-AnQ** and BIH after illumination for 4 h with 455 nm light in DMSO-d_6. The concentration of **Cu^{+}-AnQ** and BIH was 0.5 mM and 0.1 M, respectively.

9. DFT calculations

All DFT calculations (beside magnetic resonance parameter calculations) were carried out using Gaussian 16, revision C.01,[25] software installed on the Bebop, a high-performance computing cluster operated by the Laboratory Computing Resource Center at Argonne National Laboratory. Geometry optimization of all molecules were carried out using the B3LYP functional[26–28] (spin unrestricted for paramagnetic states), except for the doubly reduced monoprotonated species **Cu^{+}-$AnQH^{-}_{O1}$**, **Cu^{+}-$AnQH^{-}_{N5}$**, **Cu^{+}-$AnQH^{-}_{N6}$** and **Cu^{+}-$AnQH^{-}_{O2}$** which were carried out using the ωB97XD functional.[29] A hybrid basis set (LANL2DZ with effective core potential (ECP)[30] for Cu and 6-31+G(d,p)[31–34] for C, H, O and N) was used for all the calculations. Frequency calculations at the same level of theory were carried out to ensure structures representing energetic minima. Solvent corrections (acetonitrile) were included as needed through polarizable continuum model using the integral equation formalism variant (IEFPCM).[35] Single-point calculations were done on the optimized geometries with LANL2DZ with effective core potential (ECP) for Cu and 6-31+G(d,p) for C, H, O and N. Structure visualization and the generation of spin density plots were performed in GaussView program (version 5.0.9).[36]

Calculations of magnetic resonance parameters (g-tensor and hyperfine tensors) for **Cu^{+}-AnQ^{-}** *in vacuo* were performed with ORCA program (v. 4.2.1)[37,38] using DFT. The B3LYP functional[26–28] with the def2-TZVP basis[39] for cobalt and the EPR-II basis[40] for all other atoms (H,C,N,O) were used. The principal electronic g-values were calculated employing the coupled-perturbed Kohn-Sham equations and the spin-orbit mean-field operator SOMF(1X).[41] Hyperfine couplings were calculated for ^{63}Cu, ^{14}N, and ^{1}H.

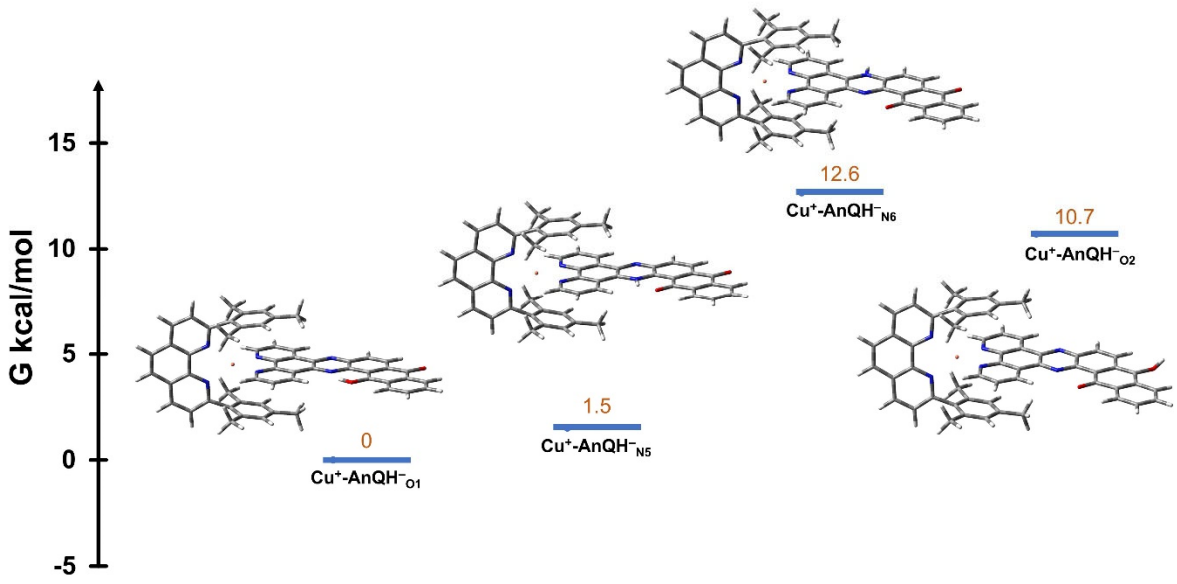
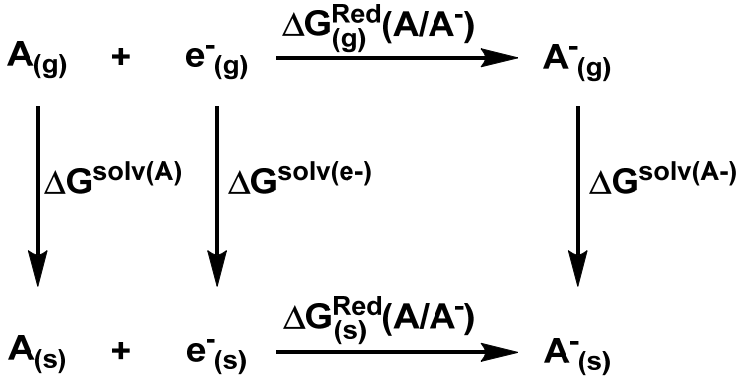


Figure S44. Free energy diagram of the **Cu^{+}-$AnQH^{-}$** protonated at different positions (the energy of **Cu^{+}-$AnQH^{-}_{O1}$** is set to 0 kcal/mol).

Simulation of reduction potential. The reduction potentials (E_{calc} vs. SCE) were calculated according to the literature method.[42–44] For a given redox couple, the Born-Haber cycle was constructed (**Scheme S2**) and the reduction potential $E_{calc}(A/A^-)$ was calculated using eq. 5 and eq. 6.



Scheme S2. Born-Haber cycle for a redox reaction, with (g) and (s) standing for gas phase and solution phase, respectively.

$$\Delta G^{\mathrm{Red}}_{(s)}(A/A^-) = \Delta G^{\mathrm{Red}}_{(g)}(A/A^-) - \Delta G^{\mathrm{solv(A)}} - \Delta G^{\mathrm{solv(e-)}} + \Delta G^{\mathrm{solv(A-)}} \quad \text{eq. 5}$$

$$E_{calc}(A/A^-) = \frac{-\Delta G^{\mathrm{Red}}_{(s)}(A/A^-)}{F} \quad \text{eq.6}$$

$\Delta G^{\mathrm{Red}}_{(g)}(A/A^-)$ and $\Delta G^{\mathrm{Red}}_{(s)}(A/A^-)$ are the change of free energy of the reduction of A in gas phase and solution phase, respectively. $\Delta G^{\mathrm{solv(A)}}$, $\Delta G^{\mathrm{solv(e-)}}$ and $\Delta G^{\mathrm{solv(A-)}}$ refer to the solvation energy when transferring A, e^- and A^- from gas phase to solution phase, respectively. F is Faraday constant (96485 C mol^{-1}). With a given redox couple, the geometry optimized structure of the oxidized species A and the reduced species A^- were obtained in gas phase, and the thermodynamics in gas phase was generated by frequency calculation. The free energy of the solution phase structure and the solubilization energy were obtained by single-point calculation of the optimized structure with solvent correction.

The calculated reduction potential cannot be directly compared with the experimental values because it is not referenced to any standard reference potential. To reference the calculated reduction potential, we chose $FeCp_2^+/FeCp_2$ redox couple and calculated the oxidation potential $E_{calc}(Fc^{1+/0})$ at the same theory level.[43] Calibration curve (**Figure S45**) between the calculated potential and experimental potential of **Cu^+-$AnQ^{0/1-}$**, **Cu^+-$AnQ^{1-/2-}$** and $Fc^{1+/0}$ were generated (the experimental $E_{exp}(Fc^{1+/0})$ vs SCE is +0.40 V based on the literature[45]). A linear relationship between the DFT and experimental reduction potentials was exhibited with a trendline of y = 0.6565x – 3.165. This equation was used for referencing the calculated potential of all the redox couples to SCE. The calculated potentials vs SCE for all the redox couples studied in this paper are tabulated in **Table S5**. Importantly, since $\Delta G^{\mathrm{solv(e-)}}$ is hard to calculate and it is already accounted for in the calibration curve, the calculation of this value is not required.

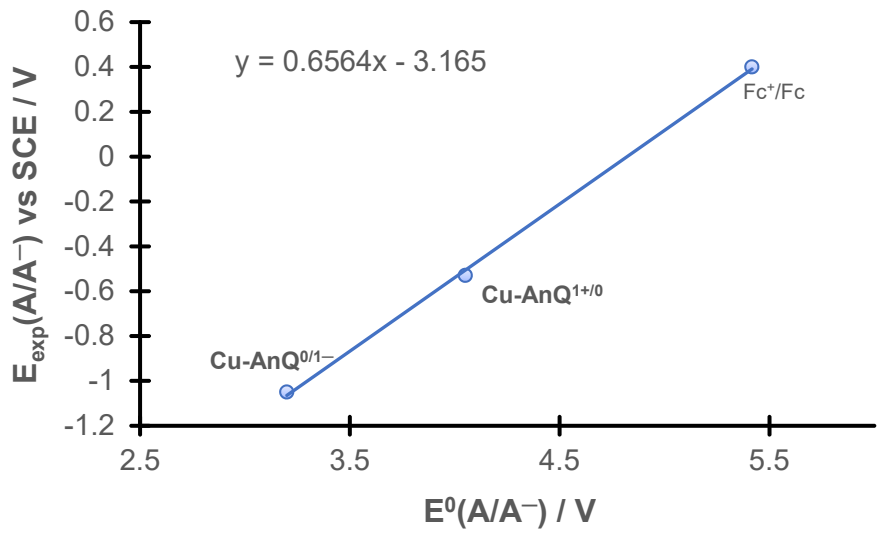


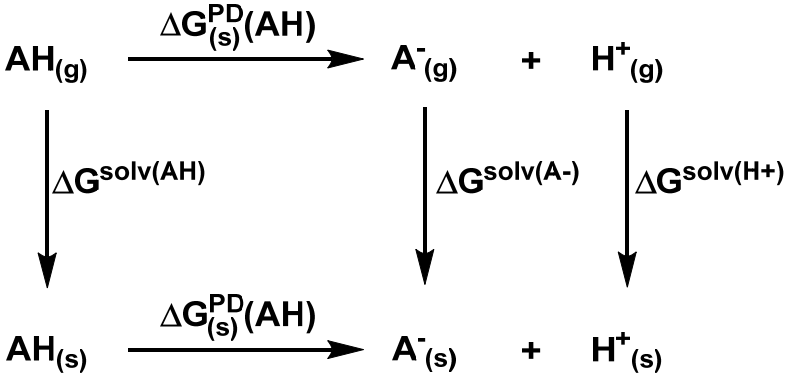
Figure S45. Calibration curve of the calculated potentials and the experimental potentials of **Cu^{+}-$AnQ^{0/1-}$**, **Cu^{+}-$AnQ^{1-/2-}$** and $Fc^{1+/0}$.

Table S5. Calculated reduction potential of the intermediates of the Cu complex.

Redox Couple	E_{exp} vs SCE /V	E_{calc} /V	E_{calc} vs SCE /V
Cu^{+}-$AnQ^{0/1-}$	–0.53	4.05	–0.51
Cu^{+}-$AnQ^{1-/2-}$	–1.05	3.20	–1.06
Cu^{+}-$AnQH^{1+/0}$		5.19	0.24
Cu^{+}-$AnQH^{0/1-}$		4.11	–0.47
$Fc^{1+/0}$	0.40[a]	5.42	0.39

[a] ref [45]

Simulation of pK_a. The pK_a values were calculated according to the literature method.[42] Thermodynamic cycle for proton dissociation was constructed as in **Scheme S3**.



Scheme S3. Thermodynamic cycle for proton dissociation, with (g) and (s) standing for gas phase and solution phase, respectively.

The procedure of calculating the free energy values in the above cycle were similar to the calculation of reduction potentials. However, standard state conversion of the free energy from gas phase at 1 atm to 1 M is required for the simulation of pK_a values. We used eq. 7 to acquire the converted free energy.[42]

$$\Delta G^{PD}_{(g)}(AH, 1\ M) = G_{(g)}(A^-) + G_{(g)}(H^+) - G_{(g)}(AH) + RTln(22.47) \qquad \text{eq. 7}$$

where, $\Delta G^{PD}_{(g)}(AH, 1\ M)$ is the change of free energy of proton dissociation of AH in 1 M standard state in gas phase. $G_{(g)}(A^-)$, $G_{(g)}(H^+)$ and $G_{(g)}(AH)$ are the gas phase free energy of A^-, H^+ and AH, respectively. $RTln(22.47)$ is the factor of converting the standard state from 1 atm to 1 M. The solution phase change of free energy of proton dissociation $\Delta G^{PD}_{(s)}(AH)$ was obtained by eq. 8.

$$\Delta G^{PD}_{(s)}(AH) = \Delta G^{PD}_{(g)}(AH, 1\ M) - \Delta G^{solv(AH)} + \Delta G^{solv(A-)} + \Delta G^{solv(H+)} \qquad \text{eq. 8}$$

where, $\Delta G^{solv(AH)}$, $\Delta G^{solv(A-)}$ and $\Delta G^{solv(H+)}$ refer to the solvation energy of AH, A^- and H^+, respectively. The pK_a calculation were achieved by eq. 9.[46]

$$\Delta G^{PD}_{(s)}(AH) = 2.303RT(pK_a) \qquad \text{eq. 9}$$

The gas phase free energy of proton $G_{(g)}(H^+)$ was calculated by Sackur-Tetrode equation where $G_{(g)}(H^+) = 2.5RT - T\Delta S^0 = 1.48 - 7.76 = -6.28\ kcal/mol$.[47] The solvation energy of proton $\Delta G^{solv(H+)}$ in acetonitrile was acquired from the literature[42], where 252 kcal/mol was estimated from the calculation with a series of carbonyl hydride complexes in acetonitrile.

Lastly, to test the robustness of the method and obtain a calibration curve between the calculated and experimental pK_a values, we calculated the pK_a values of $[Co(dppe)_2H_2]^+$, $[Co(dppe)_2H]$ and $[Co(dppe)_2H]^+$, whose pK_a's were experimentally determined,[48] using the same procedure and the theory level that were applied in the calculation of the pK_a of the Cu complexes. Calibration curve between the calculated and experimental pK_a values of the Co complexes were generated in **Figure S46**, with a trendline of y = 0.9811x – 5.3472. The calculated pK_a values for all Cu complexes studied in this paper are calibrated based on the curve and tabulated in **Table S6**.

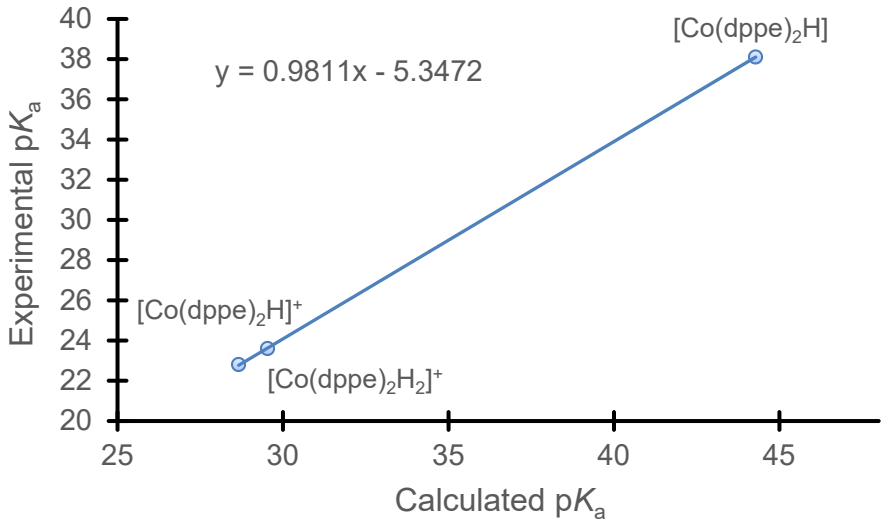


Figure S46. Calibration curve of the calculated and the experimental pK_a of $[Co(dppe)_2H_2]^+$, $[Co(dppe)_2H]$ and $[Co(dppe)_2H]^+$.

Table S6. Calculated pK_a of complexes.

Complex	Experimental pK_a	DFT pK_a	DFT pK_a after calibration
$[Co(dppe)_2H_2]^+$	22.8	28.7	
$[Co(dppe)_2H]^+$	23.6	29.5	
$[Co(dppe)_2H]$	38.1	44.3	
Cu^+-AnQH^{1+}		0.6	–4.7
Cu^+-AnQH		19.8	14.1
Cu^+-AnQH$^-$		35.3	29.2
Cu^+-AnQH$_2$		20.4	14.7

1 kJ/mol = 0.0103641 eV
F = 96485 C/mol
R = 8.31451 J/K/mol
T = 298 K

Cu^+-AnQ + e^- ⟶ Cu^+-AnQ^- (a) $G_{(a)} = -0.0103641FE_a/1000 = -0.0103641F(-0.53)/1000 = 0.53$ eV

$BIH^{\bullet+}$ + e^- ⟶ BIH (b) $G_{(b)} = -0.0103641FE_b/1000 = -0.0103641F(0.32)/1000 = -0.32$ eV

Cu^+-AnQ + BIH $\xrightarrow{h\nu}$ Cu^+-AnQ^- + $BIH^{\bullet+}$ (a) – (b) $\Delta G_{(1)} = 0.85$ eV

Cu^+-AnQ + e^- ⟶ Cu^+-AnQ^- (a) $G_{(a)} = -0.0103641FE_a/1000 = -0.0103641F(-0.53)/1000 = 0.53$ eV

Cu^+-AnQ^- + e^- ⟶ Cu^+-AnQ^{2-} (b) $G_{(b)} = -0.0103641FE_b/1000 = -0.0103641F(-1.05)/1000 = 1.05$ eV

$BIH^{\bullet+}$ + e^- ⟶ BIH (c) $G_{(c)} = -0.0103641FE_c/1000 = -0.0103641F(0.32)/1000 = -0.32$ eV

Cu^+-AnQ + 2BIH $\xrightarrow{h\nu}$ Cu^+-AnQ^{2-} + $2BIH^{\bullet+}$ (a) + (b) – 2*(c) $\Delta G_{(2)} = 2.22$ eV

Cu^+-AnQ + e^- ⟶ Cu^+-AnQ^- (a) $G_{(a)} = -0.0103641FE_a/1000 = -0.0103641F(-0.53)/1000 = 0.53$ eV

Cu^+-AnQ^- + e^- ⟶ Cu^+-AnQ^{2-} (b) $G_{(b)} = -0.0103641FE_b/1000 = -0.0103641F(-1.05)/1000 = 1.05$ eV

Cu^+-$AnQH^-$ ⟶ Cu^+-AnQ^{2-} + H^+ (c) $G_{(c)} = 0.0103641*2.3RT*pK_a/1000 = 0.0103641*2.3RT*29.2/1000 = 1.73$ eV

$BIH^{\bullet+}$ + e^- ⟶ BIH (d) $G_{(d)} = -0.0103641FE_c/1000 = -0.0103641F(0.32)/1000 = -0.32$ eV

$BIH^{\bullet+}$ ⟶ $BI^\bullet$ + H^+ (e) $G_{(e)} = 0.0103641*2.3RT*pK_a/1000 = 0.0103641*2.3RT*14.4/1000 = 0.85$ eV

Cu^+-AnQ + 2BIH $\xrightarrow{h\nu}$ Cu^+-$AnQH^-$ + $BIH^{\bullet+}$ + $BI^\bullet$ (a) + (b) – (c) – 2*(d) + (e) $\Delta G_{(3)} = 1.34$ eV

Cu^+-AnQ^- + e^- ⟶ Cu^+-AnQ^{2-} (a) $G_{(a)} = -0.0103641FE_b/1000 = -0.0103641F(-1.05)/1000 = 1.05$ eV

Cu^+-$AnQH^-$ ⟶ Cu^+-AnQ^{2-} + H^+ (b) $G_{(b)} = 0.0103641*2.3RT*pK_a/1000 = 0.0103641*2.3RT*29.2/1000 = 1.73$ eV

BI^+ + e^- ⟶ $BI^\bullet$ (c) $G_{(c)} = -0.0103641FE_c/1000 = -0.0103641F(-1.67)/1000 = 1.67$ eV

$BIH^{\bullet+}$ ⟶ $BI^\bullet$ + H^+ (d) $G_{(d)} = 0.0103641*2.3RT*pK_a/1000 = 0.0103641*2.3RT*14.4/1000 = 0.85$ eV

Cu^+-AnQ^- + $BIH^{\bullet+}$ ⟶ Cu^+-$AnQH^-$ + BI^+ (a) – (b) – (c) + (d) $\Delta G_{(4)} = -1.50$ eV

Scheme S4. Calculation of the ΔG of the photoinduced single ET, double ET, PCET and HAT processes between **Cu^+-AnQ** and BIH.

Coordinates for the optimized structures

Cu^{+}-AnQ with solvent correction (MeCN)

Cu	-2.84026300	0.01515300	-0.04508900
C	-5.58457000	0.78486500	-0.64150400
C	-4.35201600	2.74816500	-0.39944400
C	-5.61194700	-0.66344700	-0.62346900
C	-6.78024400	1.49674000	-0.91650800
C	-5.50264300	3.52798500	-0.66684200
C	-6.83410400	-1.33604500	-0.88042900
C	-7.99844300	0.78172700	-1.17253300
C	-6.70760200	2.90808400	-0.92382500
H	-5.41981700	4.60944700	-0.66482500
C	-6.81531900	-2.74888000	-0.85162500
C	-8.02433200	-0.58185100	-1.15505600
C	-4.45407800	-2.66553800	-0.33441600
H	-8.89948400	1.35117600	-1.38019400
H	-7.60029000	3.49130900	-1.13059600
C	-5.63417800	-3.40740300	-0.58054900
H	-7.72983800	-3.30307200	-1.04248800
H	-8.94645900	-1.12163800	-1.34869300
H	-5.59247000	-4.49084300	-0.55167800
C	0.08250300	-0.03189700	-0.23189000
C	-0.76054800	-0.05781400	-2.38591900
C	-0.19317400	-0.00111000	1.20719000
C	1.41001600	-0.06358400	-0.70404000
C	0.52501700	-0.09207400	-2.94236400
H	-1.63910900	-0.05320200	-3.02307600
C	0.86620900	0.00802900	2.13741900
C	2.52059000	-0.06670500	0.24958000
C	1.62132700	-0.09613700	-2.09380400
H	0.64590100	-0.11530400	-4.01962800
C	0.54836600	0.04051800	3.50661600
C	2.24921400	-0.01365600	1.66018800

C	-1.77244300	0.05024600	2.89698600
H	2.63585200	-0.12416200	-2.47457200
C	-0.78380000	0.06106900	3.88962200
H	1.34778600	0.04842600	4.23855100
H	-2.82401700	0.06652400	3.16457900
H	-1.06929300	0.08530100	4.93533500
N	-0.98206300	-0.02971700	-1.06837400
N	-1.49160100	0.02048700	1.59071800
N	-4.45273100	-1.32798300	-0.35774500
N	-4.40130800	1.41141200	-0.39041200
C	-3.17006100	-3.37702300	-0.03817300
C	-2.83277800	-3.68442900	1.29668900
C	-2.33018500	-3.77584300	-1.09925700
C	-1.63675800	-4.36893600	1.54956000
C	-1.14371400	-4.45833600	-0.80019000
C	-0.77456500	-4.75901500	0.51703400
H	-1.37586000	-4.60557600	2.57889300
H	-0.49490800	-4.76471300	-1.61798900
C	-3.04294500	3.41741300	-0.11452700
C	-2.70293800	3.74925400	1.21375500
C	-2.18097000	3.75281200	-1.17980000
C	-1.48283700	4.39372900	1.45668500
C	-0.97087900	4.39701900	-0.89073900
C	-0.59932200	4.72080000	0.42038400
H	-1.21993900	4.64924100	2.48098600
H	-0.30500500	4.65454700	-1.71168300
C	-2.70019700	-3.50046300	-2.54059500
H	-3.59707200	-4.05766700	-2.83670300
H	-2.91454700	-2.44016700	-2.70911100
H	-1.88920000	-3.79353100	-3.21227600
C	-3.74757900	-3.31302100	2.44349100
H	-3.99103300	-2.24571100	2.43899500
H	-4.69833400	-3.85673700	2.38810200

H	-3.28292800	-3.55138200	3.40371300
C	0.52618200	-5.46850800	0.81686900
H	1.34369300	-4.74865700	0.95079800
H	0.45664100	-6.05727700	1.73665300
H	0.81296200	-6.13806800	0.00016800
C	-3.63903300	3.44601600	2.36343300
H	-4.56723700	4.02484700	2.28601600
H	-3.92442700	2.38935200	2.38655700
H	-3.17145300	3.69251900	3.32015600
C	-2.55207000	3.45121300	-2.61557700
H	-2.81260100	2.39700400	-2.75440200
H	-3.42069100	4.03903700	-2.93584000
H	-1.72379200	3.68766200	-3.28850700
C	0.72592900	5.38802300	0.71000700
H	0.67619800	5.99659300	1.61808400
H	1.51650400	4.64167800	0.85975000
H	1.03846500	6.03085700	-0.11867100
N	3.76040800	-0.11196300	-0.21585100
C	4.50758100	0.00531200	2.07417000
C	4.78222800	-0.10449600	0.66618300
C	5.57741700	0.10007500	3.00533500
C	6.15266000	-0.15612300	0.22177400
C	6.87212200	0.11346300	2.55691400
H	5.33684400	0.17597000	4.06073200
C	6.51947900	-0.42605300	-1.20587100
C	7.16540500	-0.00212500	1.16982200
H	7.70241000	0.20910400	3.24666600
C	7.92616500	-0.14299600	-1.62345700
C	8.61020800	0.07422600	0.77454100
C	8.24887000	-0.14827600	-2.98643700
C	8.93782100	0.08094200	-0.67020500
C	9.56231500	0.08432100	-3.39639700
H	7.46418800	-0.33068100	-3.71234600

C	10.25875000	0.29561300	-1.08724400
C	10.56892600	0.30404100	-2.44666600
H	9.80372500	0.09196400	-4.45482500
H	11.02706800	0.45599700	-0.33877800
H	11.59092400	0.47913900	-2.76793900
N	3.23891600	0.03602100	2.54026000
O	9.48507100	0.16253300	1.63593100
O	5.72527300	-0.90203900	-2.01241600

Cu^{+}-AnQ^{-} S=2 with solvent correction (MeCN)

Cu	2.84801700	0.00286500	-0.04100500
C	5.60385200	-0.74750500	-0.63631000
C	4.38501500	-2.72003000	-0.40344100
C	5.62139200	0.70096300	-0.61276100
C	6.80496300	-1.45008300	-0.91252600
C	5.54148900	-3.49087200	-0.67192900
C	6.83938200	1.38263100	-0.86655800
C	8.01854700	-0.72595700	-1.16474600
C	6.74245000	-2.86180300	-0.92514500
H	5.46611500	-4.57291100	-0.67402700
C	6.81141300	2.79512600	-0.83355600
C	8.03504900	0.63766000	-1.14262700
C	4.45036600	2.69426000	-0.31831600
H	8.92366300	-1.28854500	-1.37353200
H	7.63946200	-3.43801000	-1.13300000
C	5.62562200	3.44477200	-0.56151600
H	7.72244000	3.35583200	-1.02212200
H	8.95357900	1.18456100	-1.33359600
H	5.57648100	4.52783900	-0.52954900
C	-0.06565200	0.01882400	-0.23651900
C	0.77938900	0.07910000	-2.39126700
C	0.20328600	-0.02100100	1.19703600
C	-1.39729200	0.03542100	-0.70692300

C	-0.50902800	0.10220000	-2.94688900
H	1.65752200	0.09328600	-3.02927100
C	-0.86872400	-0.04869600	2.11822600
C	-2.50768800	0.00609100	0.24008800
C	-1.60472400	0.08060100	-2.09949000
H	-0.62960200	0.13630600	-4.02427200
C	-0.55425300	-0.08600600	3.49088500
C	-2.24367500	-0.03869200	1.63244200
C	1.77313100	-0.06416000	2.89883700
H	-2.62148800	0.09803500	-2.47545700
C	0.77414500	-0.09321000	3.88355600
H	-1.35904500	-0.10801700	4.21677300
H	2.82270500	-0.06956200	3.17544800
H	1.05194100	-0.12079900	4.93162100
N	1.00039300	0.03980800	-1.07560100
N	1.50115300	-0.02934400	1.59257400
N	4.45742500	1.35665200	-0.34545800
N	4.42443200	-1.38290800	-0.38935800
C	3.16205600	3.39774800	-0.02126400
C	2.82062600	3.69775500	1.31417100
C	2.32216300	3.79706000	-1.08217700
C	1.62077500	4.37531800	1.56770800
C	1.13158800	4.47191900	-0.78245300
C	0.75833200	4.76501700	0.53532200
H	1.35650000	4.60569700	2.59759400
H	0.48228100	4.77762400	-1.60010700
C	3.08083600	-3.40092200	-0.12336100
C	2.74393900	-3.74620400	1.20222700
C	2.22072500	-3.73401400	-1.19088600
C	1.52871900	-4.40156600	1.44047700
C	1.01547900	-4.38918300	-0.90653000
C	0.64681200	-4.72613700	0.40208700
H	1.26787700	-4.66659100	2.46288400

H	0.35058700	-4.64394900	-1.72911300
C	2.69568900	3.52888900	-2.52397600
H	3.59198400	4.08915100	-2.81609200
H	2.91198400	2.46963800	-2.69643200
H	1.88521500	3.82300400	-3.19584200
C	3.73414900	3.32410100	2.46126700
H	3.97155700	2.25538300	2.45834600
H	4.68766200	3.86284000	2.40492200
H	3.27064700	3.56601100	3.42117200
C	-0.54730000	5.46530800	0.83542600
H	-1.36247100	4.74027700	0.95452900
H	-0.48643200	6.04266000	1.76302200
H	-0.83164300	6.14387300	0.02526300
C	3.67733300	-3.44348800	2.35426900
H	4.61395500	-4.00745500	2.26899100
H	3.94643700	-2.38286700	2.38979900
H	3.21449800	-3.70807200	3.30849600
C	2.58821900	-3.41656700	-2.62414200
H	2.82641300	-2.35614800	-2.75572600
H	3.46942600	-3.98416800	-2.94645700
H	1.76593700	-3.66565800	-3.29985800
C	-0.67425300	-5.40354700	0.68692500
H	-0.62190400	-6.01536500	1.59268700
H	-1.46987000	-4.66295100	0.83816000
H	-0.98132900	-6.04503400	-0.14487200
N	-3.75748700	0.02108600	-0.24352900
C	-4.51087500	-0.06360900	2.04342900
C	-4.79126400	-0.00641100	0.61855400
C	-5.58633100	-0.11200500	2.97784500
C	-6.16794700	0.01346000	0.15975300
C	-6.88003900	-0.10745900	2.53053800
H	-5.34504400	-0.15490600	4.03549000
C	-6.52236600	0.09844600	-1.26094900

C	-7.20382100	-0.04779600	1.14667100
H	-7.70713500	-0.14824000	3.23088500
C	-7.97297500	0.08318100	-1.60356100
C	-8.62539400	-0.05236300	0.80980800
C	-8.35005600	0.14455100	-2.95997900
C	-8.98208400	0.01093100	-0.61672900
C	-9.68969000	0.13309500	-3.33049300
H	-7.56626600	0.20051500	-3.70749300
C	-10.33766700	0.00162600	-1.00356700
C	-10.69219600	0.06124400	-2.34519600
H	-9.96285000	0.17970500	-4.38101600
H	-11.09377300	-0.05322900	-0.22747100
H	-11.73959200	0.05277300	-2.63346400
N	-3.25201900	-0.07568500	2.51669800
O	-9.51959700	-0.11008800	1.69525800
O	-5.69140700	0.18621800	-2.19476400

Cu^{+}-AnQ^{2-} S=3 with solvent correction (MeCN)

Cu	-2.84259900	0.01258200	-0.04682200
C	-5.62089500	0.72912300	-0.61729700
C	-4.42259400	2.71542400	-0.39921300
C	-5.62223300	-0.71960300	-0.59445300
C	-6.83323100	1.41826600	-0.87983600
C	-5.59059200	3.47294000	-0.65527000
C	-6.83644900	-1.41411900	-0.83296400
C	-8.04190700	0.68113600	-1.11737600
C	-6.78738600	2.83045000	-0.89382900
H	-5.52727900	4.55579000	-0.65910600
C	-6.79408400	-2.82607900	-0.79989200
C	-8.04350200	-0.68246100	-1.09435700
C	-4.42796400	-2.70033600	-0.31382100
H	-8.95546900	1.23395200	-1.31539400
H	-7.69334100	3.39627400	-1.09131600

C	-5.59849500	-3.46308600	-0.54159400
H	-7.70167300	-3.39591200	-0.97739700
H	-8.95832800	-1.23956300	-1.27360200
H	-5.53762900	-4.54560300	-0.50952000
C	0.05771800	0.00595000	-0.23018000
C	-0.77963900	0.00937800	-2.39526400
C	-0.21198100	0.00861400	1.18754800
C	1.40731100	-0.00258800	-0.68960500
C	0.51938800	0.00621900	-2.94402200
H	-1.65416200	0.01164900	-3.03883800
C	0.87120000	0.00893100	2.10998700
C	2.51644600	-0.01643300	0.24321900
C	1.60713000	-0.00094900	-2.09195500
H	0.64673400	0.00791100	-4.02175100
C	0.54959800	0.01506000	3.48442400
C	2.25134900	0.00962900	1.64222600
C	-1.78075000	0.02028500	2.89869300
H	2.62348300	-0.00572900	-2.46832600
C	-0.77554500	0.01957000	3.88390400
H	1.35763700	0.01641900	4.20744100
H	-2.82991100	0.02577800	3.17906300
H	-1.05014600	0.02346000	4.93356200
N	-1.00330300	0.00961500	-1.08252400
N	-1.51226600	0.01504300	1.59441500
N	-4.44781200	-1.36268900	-0.34225700
N	-4.44577500	1.37761300	-0.38296400
C	-3.13069900	-3.39371400	-0.03162500
C	-2.78636200	-3.71851000	1.29712800
C	-2.28542900	-3.76009300	-1.10013500
C	-1.57840200	-4.38663900	1.53709300
C	-1.08709800	-4.42687000	-0.81407300
C	-0.71063200	-4.74325400	0.49744300
H	-1.31119200	-4.63436400	2.56218200

H	-0.43335800	-4.70645900	-1.63750900
C	-3.12402800	3.41385500	-0.13636100
C	-2.76898900	3.75544100	1.18543300
C	-2.28809900	3.76769000	-1.21633000
C	-1.55971600	4.42739800	1.40698400
C	-1.08759300	4.43823700	-0.94846100
C	-0.70054500	4.77109900	0.35578100
H	-1.28461500	4.68884300	2.42656100
H	-0.44062900	4.70751300	-1.78064400
C	-2.66093300	-3.46326200	-2.53568300
H	-3.56758400	-4.00377500	-2.83290300
H	-2.85923000	-2.39750600	-2.68883400
H	-1.85780700	-3.75893100	-3.21565500
C	-3.70295100	-3.37763300	2.45203100
H	-3.94779100	-2.31072500	2.47249500
H	-4.65229800	-3.92240300	2.38467700
H	-3.23686700	-3.63628000	3.40634800
C	0.60446800	-5.43162600	0.78331200
H	1.41219600	-4.69835300	0.90225200
H	0.55632500	-6.01687300	1.70670000
H	0.89096600	-6.10053300	-0.03418200
C	-3.67680200	3.42970400	2.35153300
H	-4.63144600	3.96423600	2.27750200
H	-3.91157700	2.36122000	2.39466400
H	-3.20855900	3.71184500	3.29809800
C	-2.67534800	3.45408700	-2.64524800
H	-2.89336900	2.38985300	-2.78086400
H	-3.57361400	4.00586800	-2.94730900
H	-1.87049200	3.72491500	-3.33349100
C	0.61660000	5.46330100	0.62230300
H	0.57163200	6.07087800	1.53134900
H	1.42292300	4.73132400	0.75775900
H	0.90284100	6.11154400	-0.21172000

N	3.77844800	-0.05180400	-0.25072200
C	4.53388800	0.04015200	2.04891800
C	4.80984200	-0.06079100	0.64591300
C	5.60125200	0.15831900	2.97204600
C	6.19193300	-0.11835800	0.19697700
C	6.90899400	0.20249400	2.54131400
H	5.35325900	0.24034400	4.02783600
C	6.56401200	-0.40157600	-1.20229100
C	7.23068200	0.07917300	1.16274300
H	7.72712200	0.33230700	3.24055200
C	7.96917600	-0.18402500	-1.58017800
C	8.64817200	0.17522900	0.79672000
C	8.34332400	-0.28535700	-2.94199600
C	8.98032100	0.09491000	-0.61210000
C	9.65563500	-0.10116700	-3.34786000
H	7.56654900	-0.50668100	-3.66696400
C	10.32047400	0.26870200	-1.04670300
C	10.65773600	0.17897100	-2.38551600
H	9.91658400	-0.17022300	-4.40073100
H	11.07557900	0.47759800	-0.29526100
H	11.68845900	0.32172000	-2.70022800
N	3.24591200	0.05230000	2.54450700
O	9.54740200	0.34356400	1.68751300
O	5.75889400	-0.85031800	-2.06775700

Cu^{+}-AnQ^{2-} S=1 with solvent correction (MeCN)

Cu	-2.84476900	-0.00341200	-0.03205900
C	-5.56300600	0.81441800	-0.73380300
C	-4.31776500	2.75893000	-0.42310100
C	-5.61462100	-0.63338800	-0.71414400
C	-6.73115600	1.54401300	-1.07498800
C	-5.43990400	3.55566000	-0.75501100
C	-6.83241700	-1.28678700	-1.03568900

C	-7.94453400	0.84799600	-1.39711800
C	-6.63756400	2.95395500	-1.07967200
H	-5.34131800	4.63585500	-0.74699500
C	-6.83994500	-2.69943500	-1.00164800
C	-7.99326200	-0.51480800	-1.37806000
C	-4.51007700	-2.65316500	-0.35323600
H	-8.82321800	1.43139100	-1.65592000
H	-7.50875700	3.54990300	-1.33611000
C	-5.68721600	-3.37609900	-0.66219100
H	-7.75189200	-3.23879700	-1.24128000
H	-8.91171100	-1.04063000	-1.62149000
H	-5.66576000	-4.45997300	-0.62608100
C	0.05843000	-0.04571100	-0.24775200
C	-0.79448000	-0.10648800	-2.40275100
C	-0.20021400	-0.00552300	1.17838400
C	1.39601700	-0.06593500	-0.71923100
C	0.49596900	-0.13619000	-2.96120800
H	-1.67446400	-0.11807900	-3.03899100
C	0.88971900	0.01893200	2.08865700
C	2.51046600	-0.03422500	0.21325600
C	1.59242200	-0.11588600	-2.11728700
H	0.61367400	-0.17379000	-4.03922800
C	0.58041700	0.05362400	3.46729800
C	2.25493700	0.01075800	1.59817300
C	-1.75541500	0.03734800	2.89793000
H	2.60886100	-0.13753300	-2.49339600
C	-0.74220200	0.06112900	3.87295000
H	1.39262800	0.07323300	4.18511400
H	-2.80196900	0.04428300	3.18624800
H	-1.00939900	0.08576900	4.92429800
N	-1.01004700	-0.06425700	-1.08796300
N	-1.49569900	0.00601800	1.59063200
N	-4.48255300	-1.31571600	-0.38297300

N	-4.38555900	1.42280800	-0.41853700
C	-3.26090000	-3.38887100	0.02265800
C	-2.99942300	-3.67377900	1.37932700
C	-2.38001500	-3.83472200	-0.98513900
C	-1.83741800	-4.38445500	1.70749200
C	-1.22895600	-4.54034600	-0.61127300
C	-0.93498300	-4.82026800	0.72919600
H	-1.63486700	-4.60341000	2.75372300
H	-0.54736200	-4.88053200	-1.38799100
C	-3.02150100	3.41372800	-0.05705100
C	-2.74802300	3.71039000	1.29469400
C	-2.10627500	3.77442900	-1.06835400
C	-1.54119400	4.34593600	1.61518300
C	-0.91118100	4.40703900	-0.70221000
C	-0.60566500	4.69626100	0.63378400
H	-1.32961400	4.57385500	2.65770000
H	-0.20335400	4.68149500	-1.48149500
C	-2.66745000	-3.58025400	-2.44895000
H	-3.57194800	-4.10607000	-2.77737500
H	-2.82556400	-2.51592900	-2.65071500
H	-1.83750100	-3.92279100	-3.07233500
C	-3.95665300	-3.24555800	2.47038400
H	-4.13153200	-2.16479800	2.45295600
H	-4.93448500	-3.72902600	2.35835400
H	-3.56437300	-3.50916000	3.45598700
C	0.33049000	-5.55421200	1.10986200
H	1.16260500	-4.85269100	1.25040300
H	0.20600500	-6.10472500	2.04736800
H	0.63075000	-6.26256800	0.33149700
C	-3.73926800	3.37626800	2.38827800
H	-4.67813000	3.92825700	2.26031800
H	-3.99336500	2.31128800	2.39174600
H	-3.33339500	3.63073700	3.37079400

C	-2.40167500	3.50489600	-2.52783700
H	-2.62361000	2.44771200	-2.70613200
H	-3.27031400	4.07753100	-2.87415500
H	-1.54893400	3.78124400	-3.15331900
C	0.70540200	5.34994300	1.00656000
H	0.61843000	5.91537100	1.93937700
H	1.49080500	4.59743700	1.15185600
H	1.04950600	6.03073200	0.22170200
N	3.76759700	-0.04750100	-0.28879400
C	4.53475300	0.04456700	2.00253300
C	4.81332000	-0.01520300	0.56472900
C	5.61843100	0.10145800	2.92433300
C	6.18650800	-0.03263100	0.09846300
C	6.91730400	0.10241500	2.47104200
H	5.38472300	0.14832000	3.98461100
C	6.52668500	-0.11942900	-1.30336300
C	7.25709200	0.03993600	1.10098300
H	7.74110200	0.15160300	3.17707500
C	7.97480100	-0.10811800	-1.63750000
C	8.65678500	0.04828900	0.77639700
C	8.35850900	-0.17891700	-2.99654500
C	8.99347500	-0.02700400	-0.65001600
C	9.69379600	-0.17043500	-3.37636100
H	7.56950400	-0.24017800	-3.73895600
C	10.34924500	-0.02079200	-1.05344500
C	10.70264900	-0.09052400	-2.39295300
H	9.96198500	-0.22513200	-4.42855200
H	11.10601500	0.04049600	-0.27778600
H	11.74998600	-0.08398200	-2.68445200
N	3.27934300	0.05117000	2.48614800
O	9.58951900	0.11734400	1.65471500
O	5.69765800	-0.20664300	-2.26673700

Cu^{+}-$AnQH^{-}_{o1}$ with solvent correction (MeCN)

Cu	-2.90777400	-0.03910600	-0.03773200
C	-5.69806400	0.34716100	-0.73838300
C	-4.53167100	2.30841300	-1.15684000
C	-5.63235300	-1.01633500	-0.26716900
C	-6.92048600	0.88663300	-1.16549100
C	-5.71167300	2.93677500	-1.60149500
C	-6.78913900	-1.80932600	-0.24330200
C	-8.09538000	0.05312300	-1.12798100
C	-6.89777900	2.22853200	-1.60672000
H	-5.67625800	3.96776700	-1.93520900
C	-6.63641800	-3.13367100	0.22420300
C	-8.03241800	-1.23346400	-0.68935100
C	-4.28801900	-2.71378500	0.56504000
H	-9.03991800	0.47275100	-1.46006700
H	-7.81524100	2.69815300	-1.94870400
C	-5.39370100	-3.58513900	0.62407400
H	-7.49883000	-3.79218000	0.26548400
H	-8.92603000	-1.84955500	-0.66878200
H	-5.25747000	-4.59935500	0.98238600
C	-0.03963000	-0.08876700	-0.22927200
C	-0.88530800	-1.04893100	-2.14506400
C	-0.31577500	0.55080600	1.05313500
C	1.28539000	-0.30028100	-0.64065600
C	0.39755300	-1.31763500	-2.63109300
H	-1.76552200	-1.32568800	-2.71589500
C	0.73971900	0.99615700	1.85885500
C	2.37814800	0.14669300	0.20921500
C	1.48840000	-0.93818800	-1.87567000
H	0.52098500	-1.81154100	-3.58760000
C	0.42249000	1.62253200	3.07397000
C	2.11797500	0.79274800	1.42596400
C	-1.88924500	1.27358900	2.57130000

H	2.49288600	-1.12834400	-2.23264100
C	-0.90290900	1.76550000	3.43217600
H	1.22363300	1.98023000	3.71052300
H	-2.94054800	1.36053200	2.82555400
H	-1.18790000	2.24330100	4.36208400
N	-1.09851000	-0.45233700	-0.97978200
N	-1.60783500	0.68390500	1.41677400
N	-4.42610100	-1.46602800	0.13205300
N	-4.54618000	1.04671000	-0.74266200
C	-2.87994500	-3.05128300	0.93891500
C	-2.36588800	-2.57588500	2.15712800
C	-2.03234700	-3.61473800	-0.02597600
C	-0.98999300	-2.63811900	2.37373500
C	-0.66029000	-3.66221000	0.23100100
C	-0.11835600	-3.15431600	1.41190100
H	-0.58330400	-2.23409900	3.29875400
H	0.00482500	-4.06104000	-0.53189900
C	-3.17523300	2.93300600	-1.07583900
C	-2.80368600	3.61347100	0.09243000
C	-2.22032800	2.61394200	-2.05635100
C	-1.45772700	3.93578000	0.28255000
C	-0.88700000	2.94968900	-1.82718200
C	-0.48244200	3.58659800	-0.65137100
H	-1.15920600	4.42628200	1.20648800
H	-0.13799700	2.66768000	-2.56457200
C	-2.57763800	-4.08760200	-1.35075600
H	-3.27891700	-4.91881400	-1.22297200
H	-3.12075600	-3.28461200	-1.86138900
H	-1.77126600	-4.42168000	-2.00782600
C	-3.27508100	-1.95298000	3.18681100
H	-3.77128500	-1.06405300	2.78290900
H	-4.06130200	-2.64873200	3.49814200
H	-2.71231600	-1.65281300	4.07372700

C	1.37177900	-3.14815600	1.64415300
H	1.68104300	-2.24310300	2.17669200
H	1.68128200	-4.00735000	2.24943000
H	1.91927300	-3.19012000	0.69837400
C	-3.82130100	3.92069200	1.16287500
H	-4.59592300	4.60245900	0.79657200
H	-4.32806400	3.00836800	1.49664600
H	-3.34667200	4.38178300	2.03218400
C	-2.61712500	1.86460000	-3.30359900
H	-3.02052200	0.87741500	-3.05405400
H	-3.39332700	2.39921700	-3.86103300
H	-1.75809600	1.72204600	-3.96327000
C	0.97694900	3.86984900	-0.39782500
H	1.16684500	4.04764900	0.66422800
H	1.59873300	3.02725600	-0.71793200
H	1.31161100	4.75307200	-0.95292000
N	3.64895000	-0.06068000	-0.18821300
C	4.37016000	1.02785000	1.82667200
C	4.65291600	0.35740800	0.58122800
C	5.45177300	1.47677400	2.64332000
C	6.03155400	0.13650500	0.16008700
C	6.74098500	1.26523500	2.23888900
H	5.21615400	1.97894400	3.57554600
C	6.33477800	-0.50610400	-1.03032200
C	7.08798900	0.61206900	1.02781600
H	7.56466600	1.60515200	2.86002600
C	7.69888800	-0.70449400	-1.41077600
C	8.47064900	0.44171600	0.69864000
C	8.02794200	-1.35942000	-2.62536000
C	8.74614300	-0.24443600	-0.57014100
C	9.34321100	-1.55038400	-2.98924900
H	7.22504200	-1.70872300	-3.26532500
C	10.08312100	-0.45523300	-0.96999300

C	10.38539900	-1.09474000	-2.15427000
H	9.57837300	-2.05382100	-3.92244300
H	10.86802400	-0.09654100	-0.31211800
H	11.42013500	-1.24823600	-2.44554900
N	3.10860900	1.22732500	2.21809400
O	9.42099200	0.84686800	1.43561300
O	5.38565600	-0.97354600	-1.88350100
H	4.51549900	-0.75375400	-1.47158000

Cu^{+}-$AnQH^{-}_{N5}$ with solvent correction (MeCN)

Cu	2.91063200	0.01093100	-0.05499900
C	5.73623400	-0.29042500	-0.65472400
C	4.66977800	-2.32968300	-0.94602900
C	5.59579100	1.10164500	-0.29842700
C	6.99320500	-0.80542800	-1.00482800
C	5.88833900	-2.93641200	-1.30889700
C	6.71584900	1.94606600	-0.30777400
C	8.12916100	0.08106000	-1.00225800
C	7.04220600	-2.17733600	-1.33849200
H	5.90725900	-3.99068300	-1.56131200
C	6.49161400	3.29523700	0.04581300
C	7.99650400	1.39413200	-0.67071800
C	4.15466500	2.79517800	0.35813300
H	9.10094300	-0.32021400	-1.27268900
H	7.98917100	-2.62950200	-1.61783200
C	5.21895000	3.71877900	0.37513100
H	7.32260400	3.99416400	0.05583100
H	8.86137600	2.05028100	-0.67474100
H	5.02696800	4.75078500	0.64667700
C	0.05057500	-0.02801500	-0.26562200
C	0.88547000	0.65837400	-2.30190400
C	0.32265300	-0.47549100	1.08523600
C	-1.28438800	0.11619200	-0.69670200

C	-0.40412600	0.83854100	-2.81961500
H	1.76072300	0.86316700	-2.90929000
C	-0.74164600	-0.78809500	1.94756500
C	-2.34674500	-0.19158100	0.21571500
C	-1.49147300	0.56729700	-2.01863900
H	-0.53224100	1.18594400	-3.83807300
C	-0.42392700	-1.22836500	3.24584400
C	-2.11498100	-0.64099600	1.50263600
C	1.89184700	-0.97879200	2.69631700
H	-2.49168600	0.70274300	-2.41693400
C	0.89839800	-1.32763700	3.62152200
H	-1.22935400	-1.47790500	3.92697100
H	2.94192300	-1.03606900	2.96417300
H	1.18031200	-1.66253300	4.61303200
N	1.10460200	0.23875700	-1.06509000
N	1.61654300	-0.56542800	1.46905900
N	4.35877000	1.52497600	0.03012000
N	4.61693300	-1.04058500	-0.63195700
C	2.72637700	3.10185900	0.67716500
C	2.22288100	2.76788300	1.94496300
C	1.86404400	3.49634000	-0.35634800
C	0.84413500	2.80835800	2.15065400
C	0.49011800	3.52616300	-0.10962600
C	-0.03971700	3.16501300	1.12971000
H	0.44689100	2.51331000	3.11984800
H	-0.18475400	3.79443000	-0.91966900
C	3.33736800	-3.00227000	-0.85749900
C	2.93250900	-3.55975700	0.36366200
C	2.42380600	-2.84129900	-1.91254600
C	1.59302200	-3.92084400	0.52540500
C	1.09586000	-3.21486200	-1.71195600
C	0.65551800	-3.72797600	-0.48948700
H	1.26742600	-4.32164900	1.48294600

H	0.37755500	-3.06199800	-2.51495300
C	2.40169900	3.81039000	-1.73021400
H	3.07333900	4.67513200	-1.71040200
H	2.97528500	2.96624400	-2.12860000
H	1.58901200	4.02661100	-2.42764300
C	3.14896800	2.31230100	3.04455000
H	3.68796000	1.40598100	2.74847400
H	3.90017700	3.07465600	3.27636000
H	2.59197700	2.09127500	3.95800900
C	-1.52972500	3.14957900	1.36199300
H	-1.81344900	2.33362300	2.03371900
H	-1.86700000	4.08688400	1.81843600
H	-2.07420800	3.02079300	0.42216000
C	3.90609500	-3.69809500	1.50746300
H	4.72899700	-4.37502200	1.25505300
H	4.35228600	-2.72997600	1.76067800
H	3.40855700	-4.08524600	2.39974200
C	2.85454300	-2.21286000	-3.21401800
H	3.20189600	-1.18650700	-3.05260200
H	3.68115700	-2.76524400	-3.67289800
H	2.02638400	-2.18145300	-3.92579400
C	-0.80842200	-4.00683900	-0.26072900
H	-1.34564000	-3.07130400	-0.06116800
H	-1.27056200	-4.46716000	-1.13887800
H	-0.96207900	-4.66574000	0.59786400
N	-3.66387700	-0.03509400	-0.17554700
C	-4.38402700	-0.78786400	1.97578700
C	-4.70873800	-0.31033700	0.64456500
C	-5.46883100	-1.08431200	2.83583000
C	-6.03785200	-0.13710100	0.21719600
C	-6.77683200	-0.91746300	2.41664300
H	-5.24150800	-1.44417000	3.83396800
C	-6.30427500	0.34388100	-1.10834000

C	-7.11327300	-0.45390100	1.13969800
H	-7.59076800	-1.15133400	3.09683600
C	-7.72208400	0.50733500	-1.49847400
C	-8.49271800	-0.30295700	0.77363800
C	-8.02860000	0.97807500	-2.78433300
C	-8.76502800	0.19913100	-0.60348100
C	-9.34704800	1.14218700	-3.18043200
H	-7.21192300	1.21009300	-3.45945300
C	-10.09359900	0.36968100	-1.01852200
C	-10.38584700	0.83576200	-2.29170600
H	-9.57352100	1.50728400	-4.17739600
H	-10.88557400	0.12772800	-0.31775700
H	-11.41919500	0.96315900	-2.59947900
N	-3.11699400	-0.94109700	2.37950500
O	-9.45098900	-0.56628700	1.53745600
O	-5.39299300	0.62777000	-1.93782700
H	-3.96069400	0.30317100	-1.10087900

Cu^{+}-$AnQH^{-}_{N6}$ with solvent correction (MeCN)

Cu	2.92211300	0.03393700	-0.06578400
C	5.73016500	-0.34722900	-0.72047500
C	4.59814700	-2.34734500	-1.03036200
C	5.64009100	1.04006700	-0.33063900
C	6.96410500	-0.89172000	-1.10662300
C	5.79083600	-2.98213800	-1.43002200
C	6.78532100	1.85026700	-0.34389000
C	8.12627100	-0.03996300	-1.10909300
C	6.96591600	-2.25718900	-1.46877100
H	5.77306500	-4.03135600	-1.70288200
C	6.61036500	3.19681700	0.04558500
C	8.04069600	1.26863200	-0.74612900
C	4.26608400	2.76090600	0.39532200
H	9.07955800	-0.46397200	-1.40907900

H	7.89330600	-2.73121700	-1.77616600
C	5.35847400	3.65089900	0.41176600
H	7.46270900	3.86957800	0.05407800
H	8.92498200	1.89832200	-0.75397800
H	5.20413800	4.68145600	0.71145300
C	0.06059900	0.02387300	-0.23315600
C	0.86616700	0.79562200	-2.24962800
C	0.34608700	-0.47634800	1.09182300
C	-1.27391900	0.18337200	-0.64311900
C	-0.43166800	1.00301800	-2.74097000
H	1.73250700	1.02314600	-2.86264700
C	-0.72111600	-0.83117000	1.94909000
C	-2.36719100	-0.16768700	0.23909500
C	-1.50572500	0.69525700	-1.93508400
H	-0.57006700	1.39808900	-3.74093800
C	-0.37444900	-1.32580700	3.22731900
C	-2.06737700	-0.66783300	1.48860700
C	1.93628800	-1.03604500	2.66692300
H	-2.53085200	0.83322900	-2.26035100
C	0.95131900	-1.42953400	3.58369600
H	-1.13233000	-1.62659300	3.94259000
H	2.98897300	-1.09809900	2.92187800
H	1.24053400	-1.80492800	4.55836800
N	1.10787500	0.32399500	-1.03725100
N	1.64120300	-0.57506200	1.46220500
N	4.42376700	1.49314100	0.03329400
N	4.58893300	-1.06370900	-0.69053300
C	2.85372400	3.09994600	0.74942600
C	2.36307500	2.74140000	2.01658100
C	1.98491200	3.54356600	-0.25707400
C	0.98975500	2.80333200	2.24481100
C	0.61499900	3.59386000	0.01235200
C	0.09710600	3.20342500	1.24668000

H	0.60096300	2.48969100	3.21175000
H	-0.06613400	3.89948700	-0.77881700
C	3.25193100	-2.98878800	-0.92529500
C	2.86671700	-3.57421700	0.28871100
C	2.31567500	-2.77949200	-1.95210800
C	1.52500500	-3.91709400	0.47285800
C	0.98686300	-3.13573400	-1.72964500
C	0.56724000	-3.67917100	-0.51262600
H	1.21561300	-4.34010100	1.42623200
H	0.25165700	-2.94557100	-2.50907200
C	2.50649900	3.88438100	-1.63077100
H	3.20841400	4.72423600	-1.59775700
H	3.04181300	3.03403900	-2.06765200
H	1.68834600	4.15068400	-2.30405400
C	3.29684900	2.23549100	3.08728700
H	3.79912900	1.31788000	2.76266200
H	4.07755600	2.96824300	3.31700600
H	2.75221700	2.01478000	4.00825700
C	-1.38923400	3.18552900	1.50003300
H	-1.69447000	2.23018500	1.93999700
H	-1.68267500	3.97835300	2.19664300
H	-1.95144300	3.32249400	0.57250000
C	3.86472900	-3.76380400	1.40384800
H	4.66668300	-4.45057200	1.11328800
H	4.33726300	-2.81240000	1.67208600
H	3.38062500	-4.16487900	2.29739100
C	2.72660200	-2.12225200	-3.24569000
H	3.09796100	-1.10782900	-3.06432000
H	3.53033500	-2.67740100	-3.74060400
H	1.88176100	-2.05456600	-3.93496600
C	-0.89498900	-3.94719000	-0.26148800
H	-1.43313000	-3.00335500	-0.11081200
H	-1.36032000	-4.45581500	-1.11116400

H	-1.04194400	-4.56022200	0.63161900
N	-3.64010200	0.02123700	-0.22662300
C	-4.45448400	-0.83808900	1.89361100
C	-4.67859200	-0.29068400	0.56168400
C	-5.49492800	-1.18544500	2.73123000
C	-6.04161700	-0.10996500	0.15107500
C	-6.81877600	-1.00838400	2.30372400
H	-5.28397200	-1.59316100	3.71576700
C	-6.36992300	0.44310600	-1.14401800
C	-7.11072000	-0.48975300	1.06053400
H	-7.63910800	-1.28151100	2.95867100
C	-7.82826100	0.58791700	-1.48819700
C	-8.52896100	-0.34740500	0.72374900
C	-8.16946200	1.11720700	-2.73993500
C	-8.85457400	0.21413600	-0.60915800
C	-9.49925500	1.27048700	-3.10841100
H	-7.36827000	1.40342500	-3.41247500
C	-10.19546900	0.37054800	-0.98524500
C	-10.52030200	0.89545100	-2.22752900
H	-9.74682400	1.68209000	-4.08225200
H	-10.96874700	0.07255200	-0.28509900
H	-11.56035000	1.01463300	-2.51468800
N	-3.15036800	-1.00059800	2.29488900
O	-9.44024700	-0.67370600	1.50040100
O	-5.54597400	0.81236800	-2.00133000
H	-2.99586800	-1.37577300	3.21720700

Cu^{+}-AnQ$H^{-}$$_{O2}$ with solvent correction (MeCN)

Cu	-2.93108400	0.04238300	-0.04581600
C	-5.65008500	1.04599400	-0.26022900
C	-4.28069900	2.73746800	0.54192700
C	-5.73509100	-0.32249800	-0.71326200
C	-6.79796600	1.85192800	-0.23615800

C	-5.37626300	3.62171100	0.59970200
C	-6.96714900	-0.85376700	-1.12272900
C	-8.05129500	1.28458200	-0.66465400
C	-6.62698400	3.17984000	0.21453900
H	-5.22589300	4.63822900	0.94566700
C	-6.96345200	-2.20175800	-1.54561900
C	-8.13227200	-0.00664100	-1.08639600
C	-4.59484300	-2.30257500	-1.11351200
H	-8.93783900	1.91084400	-0.64430600
H	-7.48165800	3.84843100	0.25486800
C	-5.78553700	-2.92347500	-1.53987100
H	-7.88906800	-2.66538700	-1.87358300
H	-9.08419800	-0.41981800	-1.40520300
H	-5.76453800	-3.95939500	-1.85929600
C	-0.06886400	0.06609600	-0.25742900
C	-0.90893400	0.98539000	-2.19420700
C	-0.33896700	-0.54337500	1.04183400
C	1.25168900	0.26193100	-0.68004900
C	0.37478900	1.23053000	-2.69265100
H	-1.78800700	1.25595900	-2.77019300
C	0.72364400	-0.97131900	1.85099500
C	2.36033300	-0.16010000	0.17091100
C	1.46550500	0.86261600	-1.92967600
H	0.49549200	1.69748000	-3.66321600
C	0.41024000	-1.56885600	3.08192800
C	2.09534200	-0.77591200	1.40208700
C	-1.90533200	-1.22821400	2.58518000
H	2.48562700	1.01933500	-2.26419600
C	-0.91382300	-1.70137500	3.45055800
H	1.21327600	-1.91359800	3.72365400
H	-2.95520800	-1.30765600	2.84755500
H	-1.19374200	-2.15722900	4.39313700
N	-1.12824100	0.41965800	-1.01387400

N	-1.62872100	-0.66558400	1.41579300
N	-4.59122100	-1.03506000	-0.71731100
N	-4.43552700	1.48670000	0.12364100
C	-3.24505000	-2.94133000	-1.03359700
C	-2.87029100	-3.60300600	0.14418100
C	-2.29562000	-2.65096500	-2.02837600
C	-1.52596200	-3.93538100	0.32894800
C	-0.96405000	-2.99620800	-1.80445700
C	-0.55556100	-3.61401500	-0.61968000
H	-1.22436100	-4.41085400	1.25972800
H	-0.21858000	-2.73582200	-2.55330300
C	-2.86689000	3.06364800	0.90385200
C	-2.35571800	2.60998000	2.13140200
C	-2.01468700	3.59255700	-0.07636300
C	-0.97864300	2.65998300	2.34331800
C	-0.64151200	3.62852100	0.17609000
C	-0.10302200	3.14209800	1.36750400
H	-0.57452200	2.27170400	3.27618600
H	0.02667900	3.99963600	-0.59800200
C	-2.69585900	-1.91979600	-3.28522900
H	-3.48366700	-2.45499900	-3.82559900
H	-3.08508100	-0.92357500	-3.04926300
H	-1.84165100	-1.79900000	-3.95542500
C	-3.88146700	-3.87876200	1.22921800
H	-4.37259600	-2.95415000	1.55240300
H	-4.66865200	-4.55614300	0.88196700
H	-3.40444900	-4.33137900	2.10168600
C	0.90360700	-3.90408600	-0.37309000
H	1.52535800	-3.05503900	-0.67590600
H	1.09447700	-4.10371600	0.68481800
H	1.23732800	-4.77523700	-0.94747000
C	-3.26972300	2.01983000	3.17594600
H	-4.05152300	2.72820000	3.46945200

H	-3.77122400	1.12416200	2.79406100
H	-2.70938400	1.73789000	4.07037400
C	-2.55773900	4.03978500	-1.41083800
H	-3.10932800	3.22999200	-1.90123100
H	-3.25070700	4.88058400	-1.30151200
H	-1.74935000	4.35025300	-2.07694800
C	1.38750900	3.12018700	1.59577000
H	1.70865000	3.97883000	2.19580200
H	1.68733100	2.21394700	2.13178600
H	1.93274500	3.14977300	0.64832500
N	3.60421900	0.05693200	-0.26640100
C	4.34758500	-0.97668900	1.75881800
C	4.63561600	-0.33289100	0.49470600
C	5.43131900	-1.41717300	2.60020100
C	6.00538000	-0.12302300	0.08234100
C	6.70953500	-1.21694900	2.22358800
H	5.17807700	-1.90695000	3.53531200
C	6.34872500	0.49333400	-1.17926200
C	7.05624500	-0.56387200	0.97585200
H	7.52451200	-1.54598000	2.85808900
C	7.79083900	0.66884300	-1.44719700
C	8.39188400	-0.38140800	0.67787000
C	8.18695100	1.28069400	-2.65503300
C	8.79054800	0.25732900	-0.52867600
C	9.51731800	1.49102700	-2.95553000
H	7.40507600	1.58491000	-3.34305300
C	10.15520700	0.49232300	-0.84766300
C	10.50961700	1.09481200	-2.03498100
H	9.80103900	1.96394000	-3.89085300
H	10.92679900	0.20709800	-0.13951200
H	11.55801200	1.26875000	-2.25973900
N	3.10739100	-1.18248300	2.18466000
O	9.35390400	-0.77080300	1.59933900

O	5.52108800	0.88547700	-2.04576300
H	9.96046900	-1.39737900	1.19037400

Cu^{+}-AnQ no solvent correction

Cu	-2.84005200	0.00013300	-0.04971100
C	-5.60820100	0.72410900	-0.61620200
C	-4.40582700	2.70624800	-0.36108500
C	-5.60803300	-0.72448000	-0.61638000
C	-6.81961500	1.41685800	-0.87026000
C	-5.57491700	3.46731300	-0.60638000
C	-6.81931000	-1.41744700	-0.87052300
C	-8.02575100	0.68143800	-1.12393100
C	-6.77117400	2.82946700	-0.85900700
H	-5.50944200	4.55013400	-0.59106900
C	-6.77056100	-2.83004600	-0.85951700
C	-8.02560800	-0.68224100	-1.12404100
C	-4.40519900	-2.70640500	-0.36178400
H	-8.94065500	1.23442000	-1.31598300
H	-7.67625400	3.40009300	-1.04885300
C	-5.57414800	-3.46768000	-0.60708200
H	-7.67552600	-3.40083700	-1.04941100
H	-8.94039700	-1.23538400	-1.31617700
H	-5.50844100	-4.55049000	-0.59197700
C	0.07484300	0.00025500	-0.22805100
C	-0.75164300	0.00110900	-2.38602800
C	-0.20282500	-0.00030800	1.21106100
C	1.40412400	0.00038400	-0.69429800
C	0.53775700	0.00125100	-2.93567200
H	-1.62635400	0.00140200	-3.02953200
C	0.85686600	-0.00073200	2.14320800
C	2.51099600	-0.00002700	0.26230900
C	1.63063200	0.00087200	-2.08233100
H	0.66500700	0.00163900	-4.01303500

C	0.53871200	-0.00129100	3.51224000
C	2.24154900	-0.00057100	1.66842400
C	-1.78141700	-0.00096300	2.90097700
H	2.65337500	0.00092600	-2.44658900
C	-0.79399200	-0.00141100	3.89474200
H	1.34301900	-0.00161200	4.23965400
H	-2.83398700	-0.00104300	3.16770300
H	-1.08016100	-0.00184100	4.94111900
N	-0.98545800	0.00061400	-1.07095200
N	-1.50166100	-0.00041600	1.59513800
N	-4.43320900	-1.36866400	-0.36932400
N	-4.43353900	1.36850100	-0.36889100
C	-3.10583100	-3.39627600	-0.08586700
C	-2.75822900	-3.72785500	1.24018600
C	-2.25851300	-3.74712300	-1.15753600
C	-1.54845600	-4.39290600	1.47294300
C	-1.05857000	-4.41148500	-0.87739700
C	-0.68477800	-4.74662000	0.42949900
H	-1.27894900	-4.64803200	2.49556600
H	-0.40314100	-4.68020900	-1.70300500
C	-3.10667000	3.39637100	-0.08481600
C	-2.75908200	3.72719000	1.24142800
C	-2.25954900	3.74821400	-1.15631900
C	-1.54950900	4.39248500	1.47453700
C	-1.05980300	4.41277700	-0.87582700
C	-0.68601900	4.74715900	0.43126800
H	-1.28002900	4.64705000	2.49730600
H	-0.40452000	4.68226300	-1.70130300
C	-2.63468800	-3.44063600	-2.59109200
H	-3.50788100	-4.02212300	-2.91071000
H	-2.88799900	-2.38422700	-2.72920600
H	-1.81283200	-3.68407500	-3.26935200
C	-3.67549800	-3.40191600	2.39910300

H	-3.95778400	-2.34384100	2.41104400
H	-4.60667700	-3.97912000	2.34927300
H	-3.19563400	-3.63637200	3.35283600
C	0.59369000	-5.50488500	0.70140200
H	1.36426500	-5.27147400	-0.03967700
H	0.99282500	-5.27627800	1.69428900
H	0.42072100	-6.58755800	0.66121900
C	-3.67615700	3.40012600	2.40018000
H	-4.60817700	3.97593200	2.35003500
H	-3.95688000	2.34163100	2.41220500
H	-3.19685300	3.63541100	3.35398900
C	-2.63572100	3.44257500	-2.59005700
H	-2.88930600	2.38631000	-2.72876200
H	-3.50873900	4.02446600	-2.90942500
H	-1.81376500	3.68616900	-3.26814100
C	0.59224100	5.50563600	0.70355900
H	0.99083500	5.27748300	1.69676300
H	1.36325100	5.27195800	-0.03698900
H	0.41922300	6.58827900	0.66278700
N	3.74816100	0.00009100	-0.20928800
C	4.50048700	-0.00077500	2.07880000
C	4.77482500	-0.00035000	0.66241600
C	5.57235500	-0.00102400	3.01315600
C	6.14564100	-0.00027100	0.20515400
C	6.86444900	-0.00081400	2.56170300
H	5.33119800	-0.00134900	4.07126000
C	6.50469900	-0.00015900	-1.25879200
C	7.15501900	-0.00041900	1.16690800
H	7.70520800	-0.00094700	3.24642900
C	7.95800800	0.00049300	-1.61754800
C	8.61408300	-0.00011300	0.79793700
C	8.31335200	0.00102000	-2.97324200
C	8.96879800	0.00048800	-0.63815600

C	9.65717300	0.00157600	-3.34524000
H	7.52429600	0.00098200	-3.71719400
C	10.31851300	0.00101000	-1.01705800
C	10.66129000	0.00156800	-2.36759800
H	9.92536900	0.00200700	-4.39753300
H	11.07692900	0.00096700	-0.24137200
H	11.70655400	0.00198800	-2.66134500
N	3.23340900	-0.00089400	2.54928600
O	9.46647800	-0.00030400	1.67980700
O	5.66065200	-0.00066600	-2.14619900

Cu^{+}-AnQ^{-} no solvent correction

Cu	2.82873500	0.00004600	-0.05659600
C	5.64859900	-0.72517800	-0.41448800
C	4.41980700	-2.70317200	-0.30533200
C	5.64908100	0.72334300	-0.41443500
C	6.87962600	-1.41961100	-0.53642000
C	5.60764700	-3.46652300	-0.42152600
C	6.88057500	1.41696100	-0.53627400
C	8.10630000	-0.68373800	-0.65522500
C	6.82704600	-2.83186500	-0.53488600
H	5.53645400	-4.54920600	-0.42215500
C	6.82894700	2.82925100	-0.53459700
C	8.10675600	0.68027900	-0.65514800
C	4.42161200	2.70215500	-0.30516500
H	9.03684400	-1.23707400	-0.74628900
H	7.74638500	-3.40443800	-0.62583100
C	5.60997300	3.46471800	-0.42122100
H	7.74867500	3.40121300	-0.62545600
H	9.03767000	1.23300200	-0.74614600
H	5.53950600	4.54744900	-0.42175000
C	-0.04947800	0.00034500	-0.19550600
C	0.73794900	0.00052900	-2.37331400

C	0.23971300	0.00020000	1.22802900
C	-1.39433600	0.00041900	-0.63576800
C	-0.56622700	0.00061900	-2.89722400
H	1.59930400	0.00056000	-3.03544200
C	-0.82796100	0.00012200	2.16562800
C	-2.48823800	0.00033000	0.32354400
C	-1.64130700	0.00055200	-2.02477700
H	-0.71351100	0.00072900	-3.97261700
C	-0.49133000	-0.00001900	3.53639100
C	-2.20691200	0.00018800	1.71278400
C	1.82995900	-0.00000200	2.91502800
H	-2.67486100	0.00058700	-2.36043000
C	0.84028800	-0.00008100	3.91323200
H	-1.29662300	-0.00007400	4.26318800
H	2.88426700	-0.00005300	3.17827300
H	1.13045700	-0.00018700	4.95922400
N	0.99641400	0.00038700	-1.06531300
N	1.54225000	0.00013900	1.61315100
N	4.45354100	1.36437300	-0.29932400
N	4.45264100	-1.36541200	-0.29937700
C	3.09445000	3.38496200	-0.19657600
C	2.61250700	3.78729900	1.06563800
C	2.34755900	3.64511400	-1.36453500
C	1.36905800	4.42614800	1.13890700
C	1.11086500	4.28797000	-1.24344200
C	0.59762500	4.67905300	-0.00097300
H	0.99209900	4.72889500	2.11329500
H	0.53124100	4.48367000	-2.14288400
C	3.09219700	-3.38509800	-0.19667200
C	2.61005400	-3.78709000	1.06560200
C	2.34510200	-3.64482400	-1.36456500
C	1.36623500	-4.42515400	1.13895700
C	1.10799400	-4.28691700	-1.24338500

C	0.59457600	-4.67762700	-0.00089800
H	0.98912400	-4.72762000	2.11337800
H	0.52819200	-4.48226400	-2.14278500
C	2.86660100	3.25606300	-2.73175800
H	3.79596300	3.78439700	-2.97752200
H	3.08187700	2.18385900	-2.79082400
H	2.13408800	3.49551800	-3.50688800
C	3.41278500	3.54528300	2.32700100
H	3.65346800	2.48433500	2.45258700
H	4.36280200	4.09336800	2.31740800
H	2.85301500	3.86791300	3.20866300
C	-0.76089800	5.33097500	0.10676000
H	-1.55265500	4.57447700	0.17256500
H	-0.83355500	5.95948800	0.99942000
H	-0.97700300	5.95246900	-0.76783200
C	3.41061500	-3.54563100	2.32689300
H	4.35975400	-4.09525400	2.31765200
H	3.65299200	-2.48501100	2.45193600
H	2.85027800	-3.86691200	3.20868800
C	2.86431200	-3.25618600	-2.73184300
H	3.08083000	-2.18423000	-2.79082300
H	3.79300200	-3.78558600	-2.97786900
H	2.13136300	-3.49469100	-3.50685400
C	-0.76437700	-5.32860900	0.10706500
H	-0.83559100	-5.96113500	0.99702000
H	-1.55515700	-4.57157700	0.17829700
H	-0.98323000	-5.94583200	-0.76984200
N	-3.73637300	0.00038900	-0.15557900
C	-4.46913500	0.00017500	2.15130300
C	-4.76080000	0.00029100	0.72452400
C	-5.53983500	0.00009100	3.08268200
C	-6.12776900	0.00022500	0.27681500
C	-6.84227100	0.00011400	2.63912900

H	-5.29410900	0.00001700	4.14029900
C	-6.47768900	0.00016600	-1.15903800
C	-7.16180600	0.00017700	1.26169600
H	-7.67244200	0.00006500	3.33791800
C	-7.93687300	0.00027500	-1.50484500
C	-8.59263600	0.00018100	0.91816800
C	-8.30410000	0.00035400	-2.86163900
C	-8.94494500	0.00028100	-0.52109000
C	-9.64509400	0.00045000	-3.23208100
H	-7.51149700	0.00033500	-3.60244700
C	-10.29798300	0.00036700	-0.90269200
C	-10.64819400	0.00045600	-2.24824000
H	-9.91679100	0.00051900	-4.28458500
H	-11.04872200	0.00035900	-0.11909300
H	-11.69563400	0.00052800	-2.53827400
N	-3.20119200	0.00012200	2.61898800
O	-9.47962000	0.00011800	1.79022700
O	-5.65161400	0.00002500	-2.08309300

Cu^{+}-AnQ^{2-} no solvent correction

Cu	2.85323200	-0.01140100	-0.05854000
C	5.62858500	-0.84217800	-0.42317400
C	4.34249700	-2.78817900	-0.19723200
C	5.67727300	0.58368500	-0.48393600
C	6.83269600	-1.60243500	-0.54835100
C	5.48804000	-3.59855800	-0.31673600
C	6.93150200	1.24575000	-0.66134300
C	8.07874100	-0.90795200	-0.72634200
C	6.73805900	-3.00078500	-0.49131900
H	5.38047300	-4.67718300	-0.27041400
C	6.93552800	2.64737200	-0.71514600
C	8.12612100	0.45370300	-0.77842900
C	4.52926400	2.62697200	-0.43173300

H	8.98904600	-1.49595600	-0.81856800
H	7.63667900	-3.60591900	-0.58433900
C	5.72862500	3.34258200	-0.60070900
H	7.87430800	3.17925000	-0.84925900
H	9.07491000	0.96813000	-0.91284400
H	5.69675400	4.42623400	-0.64416100
C	-0.04891500	0.00440700	-0.19918600
C	0.74476800	-0.18635000	-2.36533300
C	0.23444900	0.13259500	1.21390400
C	-1.39717900	-0.03400800	-0.64139100
C	-0.55991800	-0.22667800	-2.89263800
H	1.60932000	-0.25144200	-3.02096300
C	-0.84278100	0.22285500	2.14421000
C	-2.49651000	0.05166000	0.30667400
C	-1.63779300	-0.15134700	-2.02680400
H	-0.70365500	-0.31442300	-3.96541200
C	-0.50720700	0.33858700	3.51202900
C	-2.21824900	0.18535400	1.69218900
C	1.81846600	0.27629700	2.89952000
H	-2.67116600	-0.17677900	-2.36294600
C	0.82241400	0.36423400	3.89234800
H	-1.31568300	0.40279000	4.23277500
H	2.87254300	0.30419800	3.16362800
H	1.10929000	0.44901500	4.93644900
N	0.99979900	-0.07085500	-1.06319800
N	1.53523700	0.15943200	1.60335500
N	4.49511000	1.28594000	-0.37036200
N	4.40251500	-1.44918200	-0.24507200
C	3.22558100	3.35979200	-0.32626500
C	2.79856600	3.86806400	0.91679500
C	2.43449700	3.54890800	-1.47850900
C	1.57165200	4.53975200	0.99005900
C	1.21689400	4.22904200	-1.36195500

C	0.76036200	4.72320600	-0.13460500
H	1.23608900	4.91641400	1.95433900
H	0.60327500	4.36365300	-2.25051000
C	2.99422200	-3.41710400	-0.01077100
C	2.50232100	-3.65422100	1.28865300
C	2.22651900	-3.77958400	-1.13631700
C	1.23668800	-4.23413400	1.43963500
C	0.96546600	-4.35516300	-0.94079800
C	0.44615000	-4.58181200	0.33883000
H	0.85392200	-4.40475300	2.44390100
H	0.36789600	-4.61941500	-1.81101700
C	2.88595000	3.03415500	-2.82750400
H	3.84436400	3.47573500	-3.12622300
H	3.02693400	1.94868200	-2.80962200
H	2.14777200	3.26888900	-3.59959600
C	3.63947300	3.70045800	2.16411000
H	3.93799000	2.65710300	2.30685300
H	4.56054400	4.29387000	2.11355000
H	3.08329100	4.01819500	3.05078100
C	-0.58606300	5.40073000	-0.02260900
H	-1.38235300	4.66397000	0.14109400
H	-0.61234900	6.10292600	0.81693800
H	-0.83509100	5.95061200	-0.93621700
C	3.31583500	-3.28783100	2.51039000
H	4.28948700	-3.79196100	2.51404800
H	3.51189200	-2.21117600	2.54455900
H	2.78590500	-3.56359800	3.42656900
C	2.74403200	-3.55791500	-2.54116300
H	3.04777000	-2.51725700	-2.69434700
H	3.62188200	-4.18105100	-2.75103200
H	1.97460800	-3.79986400	-3.27990400
C	-0.94218400	-5.14960500	0.52439000
H	-1.03372400	-5.67969400	1.47788300

H	-1.69478600	-4.35138400	0.51974500
H	-1.20148800	-5.84555900	-0.28026500
N	-3.74409900	0.00529600	-0.17457500
C	-4.48662400	0.22171300	2.11995300
C	-4.77548200	0.09056300	0.69689500
C	-5.56210100	0.30411900	3.04146900
C	-6.14064200	0.05190500	0.24477400
C	-6.86597000	0.26223300	2.59609400
H	-5.31959900	0.40041600	4.09608900
C	-6.47981200	-0.07170300	-1.17926000
C	-7.18990500	0.13899800	1.22867800
H	-7.69646000	0.32414000	3.29264800
C	-7.93824000	-0.10247300	-1.52228800
C	-8.61154300	0.10774000	0.89124700
C	-8.30527500	-0.22030900	-2.87612900
C	-8.95203900	-0.01818900	-0.54367000
C	-9.64325700	-0.25398800	-3.25270800
H	-7.50638200	-0.28317200	-3.60812300
C	-10.30455900	-0.05317600	-0.93427600
C	-10.65176500	-0.16984400	-2.27456000
H	-9.91023400	-0.34536100	-4.30331100
H	-11.05579100	0.01420900	-0.15345500
H	-11.69914100	-0.19599200	-2.56710800
N	-3.21966400	0.26801300	2.59081100
O	-9.51813700	0.18263500	1.75330600
O	-5.65541000	-0.15111100	-2.11070900

Cu^{+}-AnQ-H^{1+} no solvent correction

Cu	2.85589000	-0.00018900	-0.04062100
C	5.60608800	-0.72245700	-0.59562100
C	4.40287000	-2.70742500	-0.35121400
C	5.60533900	0.72550800	-0.59546400
C	6.82007800	-1.41448200	-0.83758100

C	5.57470000	-3.46705900	-0.58461100
C	6.81864000	1.41882700	-0.83719700
C	8.02863700	-0.67900100	-1.07937400
C	6.77253700	-2.82742700	-0.82594000
H	5.51194100	-4.54997900	-0.56912800
C	6.76966200	2.83171900	-0.82517100
C	8.02794900	0.68463900	-1.07917200
C	4.40008200	2.70916900	-0.35066300
H	8.94562100	-1.23130500	-1.26205200
H	7.67972200	-3.39756800	-1.00618800
C	5.57115800	3.47006300	-0.58374100
H	7.67627100	3.40283400	-1.00523100
H	8.94437800	1.23792100	-1.26167800
H	5.50729800	4.55291600	-0.56797400
C	-0.09295400	-0.00036000	-0.23396900
C	0.76208700	-0.00024400	-2.38181600
C	0.18595100	-0.00045100	1.20370500
C	-1.42388500	-0.00036500	-0.71550000
C	-0.51861400	-0.00024900	-2.95071400
H	1.64624900	-0.00020400	-3.01169900
C	-0.87062200	-0.00052700	2.13517300
C	-2.52520100	-0.00041200	0.23927800
C	-1.61929500	-0.00031300	-2.11031500
H	-0.63340700	-0.00021100	-4.02902600
C	-0.55516000	-0.00065700	3.50603800
C	-2.25246100	-0.00047100	1.66048500
C	1.76442100	-0.00061900	2.88863500
H	-2.61900900	-0.00033300	-2.52784700
C	0.77812100	-0.00071200	3.88451800
H	-1.35352600	-0.00071200	4.23929800
H	2.81684600	-0.00066000	3.15436300
H	1.06599900	-0.00082900	4.93018100
N	0.97410600	-0.00029900	-1.06328600

N	1.48395600	-0.00048300	1.58189900
N	4.42791200	1.37124500	-0.35917800
N	4.42934700	-1.36946600	-0.35936900
C	3.09826800	3.39979000	-0.08689700
C	2.74139800	3.73753900	1.23592700
C	2.26518900	3.75861000	-1.16716200
C	1.53697500	4.41683400	1.45606600
C	1.06994800	4.43804000	-0.89949200
C	0.68941900	4.78286200	0.40303600
H	1.26590700	4.68603300	2.47473000
H	0.43251000	4.72522500	-1.73315600
C	3.10179000	-3.39942600	-0.08745900
C	2.74539100	-3.73784800	1.23532400
C	2.26897900	-3.75884300	-1.16772900
C	1.54168900	-4.41841400	1.45541700
C	1.07444100	-4.43953500	-0.90009900
C	0.69438400	-4.78503300	0.40238100
H	1.27099900	-4.68813700	2.47404500
H	0.43720500	-4.72716400	-1.73376000
C	2.65811200	3.46027000	-2.59823100
H	3.51660100	4.06600800	-2.91187600
H	2.94516700	2.41234000	-2.73640100
H	1.83621700	3.68401200	-3.28345600
C	3.65020200	3.41722800	2.40312400
H	3.96160600	2.36728500	2.40609000
H	4.56682700	4.01819000	2.37211100
H	3.15463600	3.63037100	3.35379700
C	-0.57030800	5.57662200	0.66148600
H	-1.01516900	5.32395700	1.62916500
H	-0.35474500	6.65198000	0.67694500
H	-1.31967000	5.40895400	-0.11833200
C	3.65398900	-3.41687700	2.40250000
H	4.57122600	-4.01689200	2.37127900

H	3.96431600	-2.36661400	2.40565100
H	3.15872900	-3.63071900	3.35317700
C	2.66145600	-3.45977000	-2.59876900
H	2.94725100	-2.41147100	-2.73677500
H	3.52065200	-4.06442100	-2.91257800
H	1.83978600	-3.68437300	-3.28398100
C	-0.56454300	-5.58005700	0.66083900
H	-1.01098100	-5.32608000	1.62746000
H	-1.31315700	-5.41499200	-0.12023800
H	-0.34748100	-6.65507300	0.67877000
N	-3.78996800	-0.00040900	-0.18741700
C	-4.51006000	-0.00047400	2.11567600
C	-4.79829300	-0.00043100	0.71778800
C	-5.58127100	-0.00050100	3.05198100
C	-6.16470900	-0.00042300	0.27609000
C	-6.89017000	-0.00049500	2.61492600
H	-5.33600200	-0.00053900	4.10934700
C	-6.49430700	-0.00038900	-1.13809500
C	-7.18705700	-0.00046100	1.23348500
H	-7.71883300	-0.00051900	3.31504500
C	-7.85833500	-0.00042700	-1.60269400
C	-8.63049700	-0.00046000	0.80568600
C	-8.14798900	-0.00042600	-2.98221300
C	-8.91693600	-0.00045600	-0.65532400
C	-9.47387500	-0.00045200	-3.41025200
H	-7.33677200	-0.00040500	-3.70156100
C	-10.23684900	-0.00047600	-1.09843000
C	-10.51400700	-0.00047600	-2.47296500
H	-9.69870400	-0.00045200	-4.47171600
H	-11.03740900	-0.00049400	-0.36605500
H	-11.54573900	-0.00049400	-2.81077000
N	-3.23288800	-0.00049800	2.55246100
O	-9.51649300	-0.00045400	1.64490200

O	-5.53763000	-0.00033300	-2.01414400
H	-4.63376500	-0.00027700	-1.50793100

Cu^{+}-AnQH no solvent correction

Cu	-2.84271900	0.00012800	-0.03943500
C	-5.61172600	0.72299600	-0.59978600
C	-4.40887800	2.70572400	-0.35118600
C	-5.61109100	-0.72557100	-0.59980200
C	-6.82478800	1.41526200	-0.84726800
C	-5.57968200	3.46624100	-0.58997400
C	-6.82352400	-1.41888800	-0.84743600
C	-8.03204700	0.67949400	-1.09437300
C	-6.77698400	2.82789400	-0.83610300
H	-5.51468900	4.54908900	-0.57465300
C	-6.77445100	-2.83147800	-0.83645300
C	-8.03143400	-0.68416900	-1.09447700
C	-4.40652500	-2.70723800	-0.35118400
H	-8.94818100	1.23218100	-1.28129800
H	-7.68339400	3.39810500	-1.02074200
C	-5.57660500	-3.46878200	-0.59027100
H	-7.68033100	-3.40247900	-1.02125700
H	-8.94707000	-1.23765000	-1.28149900
H	-5.51064300	-4.55157300	-0.57507300
C	0.07629500	0.00046800	-0.23582100
C	-0.77340700	0.00071900	-2.38844100
C	-0.19769100	0.00030700	1.19858800
C	1.41071200	0.00056100	-0.70803300
C	0.51164200	0.00081600	-2.94809100
H	-1.65430500	0.00080200	-3.02317800
C	0.86785000	0.00033100	2.12246600
C	2.51079600	0.00049100	0.24710600
C	1.60880900	0.00073700	-2.10317400
H	0.63325400	0.00096100	-4.02598200

C	0.55713000	0.00022300	3.49512200
C	2.24762400	0.00044100	1.64381900
C	-1.76732700	0.00005500	2.89641500
H	2.61294500	0.00083200	-2.50948000
C	-0.77214400	0.00009200	3.88454200
H	1.36613900	0.00024800	4.21693100
H	-2.81798100	-0.00006100	3.17057600
H	-1.05211000	0.00000400	4.93262500
N	-0.98948500	0.00055400	-1.07230300
N	-1.49596900	0.00014900	1.59032500
N	-4.43478500	-1.36949200	-0.35869900
N	-4.43594800	1.36794600	-0.35882700
C	-3.10602000	-3.39762800	-0.08197300
C	-2.75012600	-3.72634600	1.24285300
C	-2.26704900	-3.75369900	-1.15817600
C	-1.54062200	-4.39360600	1.46926200
C	-1.06683200	-4.42064300	-0.88424200
C	-0.68502400	-4.75297500	0.42086100
H	-1.26476100	-4.64642900	2.49075800
H	-0.41843800	-4.69471700	-1.71366500
C	-3.10892300	3.39725200	-0.08225400
C	-2.75311000	3.72642200	1.24250200
C	-2.27044900	3.75395900	-1.15860800
C	-1.54418400	4.39478300	1.46865400
C	-1.07077000	4.42200800	-0.88492200
C	-0.68906300	4.75481500	0.42007100
H	-1.26838500	4.64795000	2.49008300
H	-0.42275400	4.69657300	-1.71447600
C	-2.65232500	-3.45109800	-2.59021300
H	-3.52741800	-4.03349300	-2.90286300
H	-2.90678600	-2.39513000	-2.72986500
H	-1.83484500	-3.69664400	-3.27306400
C	-3.65929800	-3.39581300	2.40676700

H	-3.93970100	-2.33728600	2.41773900
H	-4.59163200	-3.97174100	2.36426500
H	-3.17370500	-3.62855100	3.35798000
C	0.59232400	-5.51494000	0.68760300
H	1.02260300	-5.25063500	1.65848200
H	0.40613900	-6.59609800	0.69804800
H	1.34371800	-5.32198200	-0.08402800
C	-3.66177400	3.39511100	2.40659200
H	-4.59471800	3.97005400	2.36415800
H	-3.94106800	2.33629000	2.41774400
H	-3.17628100	3.62847700	3.35770200
C	-2.65570900	3.45100800	-2.59057700
H	-2.91002500	2.39498600	-2.73005000
H	-3.53089400	4.03323500	-2.90329600
H	-1.83829000	3.69657200	-3.27349600
C	0.58761800	5.51797300	0.68659700
H	1.01954100	5.25236600	1.65639900
H	1.33824000	5.32751900	-0.08639500
H	0.39999100	6.59885600	0.69942700
N	3.78158700	0.00046900	-0.19819700
C	4.50594300	0.00051500	2.10509500
C	4.79122100	0.00045300	0.69105200
C	5.58304300	0.00058300	3.03714000
C	6.16413600	0.00041700	0.23506400
C	6.88584900	0.00057600	2.59005100
H	5.34102200	0.00063400	4.09456100
C	6.48992500	0.00030600	-1.14640900
C	7.20202100	0.00048900	1.21131100
H	7.71711200	0.00064200	3.28756600
C	7.85981100	0.00020500	-1.59613700
C	8.62141200	0.00047900	0.81055200
C	8.17065000	0.00002400	-2.97401400
C	8.91108500	0.00028300	-0.64164300

C	9.49576800	-0.00008300	-3.38802100
H	7.36438600	-0.00003100	-3.69858800
C	10.24262600	0.00017900	-1.08092000
C	10.53516700	-0.00000700	-2.44131400
H	9.72920300	-0.00022700	-4.44843000
H	11.02846600	0.00024800	-0.33298900
H	11.56912300	-0.00009300	-2.77281300
N	3.23531700	0.00047800	2.54586000
O	9.52765600	0.00061800	1.65530600
O	5.53922000	0.00026700	-2.07848900
H	4.65609400	0.00032300	-1.59865200

Cu^{+}-AnQH^{-} no solvent correction

Cu	2.82664100	0.00021600	-0.03802900
C	5.59470600	-0.72404900	-0.68218200
C	4.40108900	-2.70291900	-0.37631500
C	5.59456900	0.72446700	-0.68209800
C	6.79493400	-1.41779600	-0.98340900
C	5.55892400	-3.46548200	-0.66798800
C	6.79465800	1.41846200	-0.98334600
C	7.98971200	-0.68153000	-1.28450900
C	6.74541800	-2.83005700	-0.96944500
H	5.49172800	-4.54822700	-0.64752300
C	6.74487000	2.83070600	-0.96933800
C	7.98957100	0.68243500	-1.28449300
C	4.40061700	2.70309900	-0.37597100
H	8.89657700	-1.23454200	-1.51281500
H	7.64177000	-3.40196600	-1.19470100
C	5.55826800	3.46588300	-0.66775900
H	7.64108000	3.40281300	-1.19465400
H	8.89632000	1.23564100	-1.51279400
H	5.49086600	4.54861400	-0.64724600
C	-0.05509600	-0.00004500	-0.23877700

C	0.78899700	0.00027500	-2.39936700
C	0.21308200	-0.00030400	1.18616900
C	-1.40448000	0.00009200	-0.69939500
C	-0.50583200	0.00049500	-2.94976500
H	1.66707700	0.00027200	-3.03855800
C	-0.86454200	-0.00049100	2.10537200
C	-2.49317000	-0.00008900	0.23927200
C	-1.59858500	0.00040500	-2.10516800
H	-0.63280400	0.00072900	-4.02780300
C	-0.55666300	-0.00077500	3.47940400
C	-2.24693200	-0.00039300	1.63438300
C	1.77293100	-0.00068400	2.90154100
H	-2.60509600	0.00056600	-2.50567200
C	0.76857900	-0.00088700	3.88227800
H	-1.37809700	-0.00090700	4.18788700
H	2.82207200	-0.00078200	3.18424700
H	1.04016000	-0.00111500	4.93307500
N	1.00594800	0.00002000	-1.08363600
N	1.51147400	-0.00037600	1.59517000
N	4.42977400	1.36525600	-0.38803500
N	4.43000600	-1.36508800	-0.38828500
C	3.11298200	3.38762500	-0.03970100
C	2.80918100	3.68068100	1.30574900
C	2.22815700	3.76278100	-1.07158600
C	1.60361900	4.32854300	1.59803100
C	1.03363600	4.40820100	-0.73222800
C	0.69696800	4.69364600	0.59606600
H	1.36598100	4.55058700	2.63607700
H	0.34672400	4.69097900	-1.52682600
C	3.11347500	-3.38762700	-0.04031600
C	2.80960100	-3.68115000	1.30500500
C	2.22869600	-3.76241100	-1.07238400
C	1.60399000	-4.32905700	1.59700900

C	1.03412800	-4.40788300	-0.73330800
C	0.69735600	-4.69373100	0.59488300
H	1.36631000	-4.55147100	2.63496900
H	0.34725800	-4.69039600	-1.52803400
C	2.55213900	3.48770400	-2.52384900
H	3.44844100	4.02949300	-2.84968500
H	2.73691300	2.42273600	-2.69937300
H	1.72580000	3.79475600	-3.16999900
C	3.76510400	3.32305100	2.42313700
H	4.00359200	2.25417900	2.42331600
H	4.71495400	3.86414100	2.33217000
H	3.33415300	3.57203000	3.39636200
C	-0.61788000	5.35349300	0.93967800
H	-1.40266800	4.60280900	1.09513300
H	-0.54214700	5.94196100	1.85916600
H	-0.95519800	6.01586700	0.13659000
C	3.76548800	-3.32399400	2.42257800
H	4.71493700	-3.86586100	2.33199400
H	4.00482200	-2.25531400	2.42259900
H	3.33408500	-3.57243600	3.39574000
C	2.55280700	-3.48691500	-2.52453700
H	2.73754100	-2.42188800	-2.69975800
H	3.44917800	-4.02855900	-2.85042000
H	1.72655300	-3.79384200	-3.17085500
C	-0.61766200	-5.35337600	0.93822000
H	-0.54246300	-5.94124100	1.85813400
H	-1.40249700	-4.60254400	1.09277100
H	-0.95458700	-6.01622300	0.13536300
N	-3.78009200	0.00001900	-0.21876700
C	-4.51311300	-0.00046000	2.09544100
C	-4.78838500	-0.00017400	0.66612300
C	-5.58978100	-0.00065400	2.99836800
C	-6.16077100	-0.00009600	0.19721500

C	-6.90525700	-0.00057300	2.53504000
H	-5.36558000	-0.00086400	4.06032800
C	-6.45637100	0.00016500	-1.17152700
C	-7.22893500	-0.00030400	1.17699200
H	-7.73441800	-0.00072200	3.23669100
C	-7.82139500	0.00022300	-1.63327100
C	-8.63124900	-0.00025000	0.77193400
C	-8.12190300	0.00047400	-3.01644900
C	-8.88654800	0.00002400	-0.69099500
C	-9.43929200	0.00052700	-3.44966000
H	-7.30356400	0.00062300	-3.72814500
C	-10.21338500	0.00008200	-1.15533600
C	-10.49396500	0.00033200	-2.51580900
H	-9.65739200	0.00072000	-4.51455900
H	-11.00293500	-0.00007400	-0.41052900
H	-11.52464300	0.00037500	-2.86041200
N	-3.22809000	-0.00057000	2.54338200
O	-9.57786400	-0.00043100	1.58631600
O	-5.48743100	0.00036200	-2.10833600
H	-4.61654800	0.00026300	-1.59969900

Cu^{+}-$AnQH_2$ no solvent correction

Cu	2.86332800	-0.00069100	-0.03703900
C	5.63652300	-0.73117700	-0.57862900
C	4.42673000	-2.71048700	-0.33868600
C	5.63944900	0.71741000	-0.57957500
C	6.84971200	-1.42662500	-0.81662400
C	5.59737100	-3.47416600	-0.56813300
C	6.85540100	1.40762700	-0.81868600
C	8.06059700	-0.69393400	-1.05502200
C	6.79824300	-2.83908500	-0.80522100
H	5.52927000	-4.55683500	-0.55310100
C	6.80962500	2.82029700	-0.80935600

C	8.06332500	0.66972900	-1.05605000
C	4.43771700	2.70193600	-0.34211600
H	8.97675800	-1.24900900	-1.23473200
H	7.70458400	-3.41168700	-0.98275000
C	5.61136400	3.46055100	-0.57299100
H	7.71823500	3.38898300	-0.98786900
H	8.98169500	1.22086300	-1.23660800
H	5.54763000	4.54350700	-0.55951600
C	-0.05155100	0.00259200	-0.24352700
C	0.80421600	0.00166100	-2.39395300
C	0.21659600	0.00252700	1.19045700
C	-1.38469500	0.00362000	-0.71948200
C	-0.47969500	0.00266900	-2.95695200
H	1.68659000	0.00083900	-3.02678200
C	-0.85481500	0.00344600	2.10915400
C	-2.48806300	0.00433300	0.23215800
C	-1.57912900	0.00359100	-2.11515600
H	-0.59828400	0.00263800	-4.03522600
C	-0.54934100	0.00346200	3.48379400
C	-2.22910600	0.00429100	1.62315500
C	1.77843500	0.00163400	2.89601400
H	-2.58294200	0.00414000	-2.52223200
C	0.77771700	0.00256800	3.87930000
H	-1.36201100	0.00416200	4.20149500
H	2.82770600	0.00090100	3.17565700
H	1.05278000	0.00255800	4.92875100
N	1.01720200	0.00157500	-1.07781100
N	1.51339200	0.00159900	1.58910500
N	4.46288400	1.36411600	-0.34792000
N	4.45731600	-1.37279600	-0.34636000
C	3.13660400	3.39545700	-0.08429300
C	2.77129000	3.72795100	1.23693800
C	2.30573100	3.74899800	-1.16756000

C	1.56052400	4.39638500	1.45268900
C	1.10392400	4.41720000	-0.90422900
C	0.71260400	4.75283500	0.39716300
H	1.27674700	4.65097200	2.47157000
H	0.46107900	4.68808700	-1.73898000
C	3.12269200	-3.39832900	-0.08041100
C	2.75584000	-3.72819400	1.24103200
C	2.29038700	-3.74915900	-1.16348400
C	1.54215600	-4.39122000	1.45720800
C	1.08570300	-4.41195800	-0.89973700
C	0.69281100	-4.74486200	0.40190500
H	1.25717700	-4.64375000	2.47626400
H	0.44175600	-4.68072200	-1.73433000
C	2.70059200	3.44072900	-2.59573700
H	3.58157000	4.01711900	-2.90299700
H	2.94960000	2.38284100	-2.73049000
H	1.88975200	3.68897100	-3.28547900
C	3.67089300	3.39817300	2.40843900
H	3.94489300	2.33807200	2.42609300
H	4.60672000	3.96869900	2.36968900
H	3.17990500	3.63762200	3.35520900
C	-0.56761600	5.51386800	0.65256700
H	-1.00280400	5.25355000	1.62232300
H	-0.38373100	6.59549700	0.65812200
H	-1.31429000	5.31474100	-0.12206100
C	3.65670400	-3.40130200	2.41237500
H	4.58986600	-3.97623800	2.37450900
H	3.93564400	-2.34247200	2.42890700
H	3.16438400	-3.63738600	3.35929800
C	2.68679500	-3.44386500	-2.59187100
H	2.94098800	-2.38731800	-2.72740800
H	3.56495600	-4.02481400	-2.89862500
H	1.87479200	-3.68867500	-3.28147200

C	-0.59072600	-5.50015600	0.65768900
H	-1.02258300	-5.24057700	1.62911200
H	-1.33798700	-5.29491600	-0.11479300
H	-0.41233200	-6.58271800	0.65953000
N	-3.75818100	0.00475800	-0.22161100
C	-4.48708500	0.00575400	2.07639700
C	-4.77180000	0.00485600	0.66059800
C	-5.57420700	0.00902700	3.01344900
C	-6.14279100	0.00475300	0.19507000
C	-6.86447100	0.00935400	2.57715200
H	-5.32800200	0.01206900	4.06983700
C	-6.46317500	0.00803700	-1.17158600
C	-7.20190700	0.00506500	1.17779800
H	-7.67955200	0.01264700	3.29179300
C	-7.82518400	0.00537000	-1.59583100
C	-8.53346300	0.00186900	0.76515800
C	-8.15446500	0.00819500	-2.97644200
C	-8.87562100	-0.00450400	-0.61944000
C	-9.47052700	-0.00120500	-3.38809800
H	-7.34663500	0.01701400	-3.69896000
C	-10.22049800	-0.02101100	-1.08229000
C	-10.51216800	-0.01777400	-2.43057500
H	-9.71093400	0.00137500	-4.44664900
H	-11.05110200	-0.04407900	-0.38104200
H	-11.54720200	-0.03124700	-2.75796900
N	-3.22794200	0.00533100	2.52288800
O	-9.48434900	-0.00356900	1.74586700
O	-5.51604100	0.01236800	-2.12858700
H	-4.63760100	0.01081600	-1.65917500
H	-10.37021200	0.07845700	1.37343400

$FeCp_2^{1+}$ no solvent correction

Fe	-0.00024200	0.00001900	0.00012100

C	1.71470900	0.32264900	-1.17407500
H	1.68928600	0.60919600	-2.21685800
C	1.71477100	-1.01702700	-0.66964000
H	1.68920000	-1.92022400	-1.26442100
C	1.71511700	-0.95129900	0.76033100
H	1.68945000	-1.79618900	1.43537700
C	1.71532700	0.42896900	1.13968900
H	1.68964300	0.81014100	2.15171200
C	1.71507500	1.21632500	-0.05580100
H	1.68960000	2.29663400	-0.10538500
C	-1.71411200	0.32352500	-1.17419200
C	-1.71444600	-1.01650200	-0.67058300
C	-1.71550100	-0.95164400	0.75951600
H	-1.69039600	-1.79693700	1.43408600
C	-1.71559100	0.42839300	1.13970000
H	-1.69023100	0.80907100	2.15193500
C	-1.71455500	1.21654200	-0.05538500
H	-1.68912800	-1.91935200	-1.26594700
H	-1.68695700	0.61066200	-2.21680600
H	-1.68894200	2.29691200	-0.10419500

$FeCp_2$ no solvent correction

Fe	-0.00004000	-0.00020300	-0.00004600
C	1.69046200	1.20603300	-0.15641200
H	1.66246800	2.27819100	-0.29554200
C	1.69068600	0.22395200	-1.19525000
H	1.66315500	0.42294500	-2.25795400
C	1.69092200	-1.06750700	-0.58226600
H	1.66363000	-2.01667800	-1.09996300
C	1.69082000	-0.88362200	0.83540800
H	1.66333300	-1.66934500	1.57807700
C	1.69051600	0.52150700	1.09861100
H	1.66271600	0.98505700	2.07535200

C	-1.69037600	1.20605000	-0.15645700
C	-1.69066400	0.22392000	-1.19525900
C	-1.69094300	-1.06752200	-0.58222400
H	-1.66360000	-2.01670800	-1.09989300
C	-1.69082700	-0.88358100	0.83544700
H	-1.66326600	-1.66922600	1.57819600
C	-1.69047200	0.52156300	1.09859500
H	-1.66309200	0.42289900	-2.25796400
H	-1.66244900	2.27821000	-0.29559100
H	-1.66260600	0.98516200	2.07531200

$[Co(dppe)_2H_2]^+$ no solvent correction

Co	0.00009700	0.46415600	-0.00014600
P	1.11095700	-1.03886100	-1.41521800
P	-1.39226200	0.93922100	-1.70619700
P	-1.11118500	-1.03808000	1.41549700
P	1.39246400	0.93949500	1.70583800
C	2.59582300	-0.44253500	-2.35952100
C	3.52534500	-1.34761000	-2.90081300
C	4.58475700	-0.89374000	-3.69066800
C	4.73000600	0.46956200	-3.96089100
C	3.81064600	1.37823700	-3.43113600
C	2.75645200	0.92576100	-2.63285300
C	1.59793200	-2.75617400	-0.94927400
C	2.57187400	-2.92558500	0.05056100
C	3.00748700	-4.20091900	0.41397500
C	2.47407700	-5.33125100	-0.21329100
C	1.50368800	-5.17480700	-1.20454000
C	1.06881200	-3.89747400	-1.57195400
C	-0.10384000	-1.27639100	-2.81987900
C	-0.68386300	0.08822300	-3.20888800
C	-1.52510100	2.69563900	-2.27026600
C	-0.59996100	3.66624800	-1.85912000

C	-0.67021700	4.97208900	-2.35394100
C	-1.66749200	5.32533800	-3.26525800
C	-2.59653700	4.36626200	-3.67992600
C	-2.52830400	3.06231800	-3.18590700
C	-3.16738700	0.42951300	-1.65491900
C	-3.73331900	-0.49284000	-2.55024500
C	-5.09220300	-0.81752300	-2.47495800
C	-5.90384000	-0.22512200	-1.50537000
C	-5.35054300	0.69523400	-0.60953300
C	-3.99522900	1.01756200	-0.68301500
C	-1.59886200	-2.75534200	0.95010200
C	-2.57354800	-2.92465000	-0.04904300
C	-3.00957800	-4.19993100	-0.41211100
C	-2.47587200	-5.33032200	0.21481100
C	-1.50477200	-5.17398000	1.20536800
C	-1.06945000	-3.89669000	1.57242600
C	-2.59566700	-0.44090300	2.35986200
C	-3.52506300	-1.34556800	2.90208700
C	-4.58417200	-0.89111000	3.69200000
C	-4.72924600	0.47239100	3.96134500
C	-3.81000300	1.38065000	3.43068500
C	-2.75609600	0.92757400	2.63235600
C	0.10367000	-1.27564400	2.82009300
C	0.68407100	0.08890500	3.20876100
C	3.16756000	0.42970700	1.65452200
C	3.73352700	-0.49243800	2.55003300
C	5.09241300	-0.81713000	2.47479000
C	5.90401700	-0.22491700	1.50506400
C	5.35068400	0.69523700	0.60903800
C	3.99536700	1.01755300	0.68246300
C	1.52552400	2.69602100	2.26950000
C	2.52850300	3.06264400	3.18540900
C	2.59695000	4.36669700	3.67910500

C	1.66836300	5.32595000	3.26381600
C	0.67132700	4.97276400	2.35221400
C	0.60084900	3.66680800	1.85772900
H	3.43168500	-2.41064300	-2.70698400
H	5.29456700	-1.60909700	-4.09582700
H	5.55200800	0.82008700	-4.57802800
H	3.91266400	2.44053700	-3.63420900
H	2.06151000	1.64568900	-2.21345300
H	3.01238500	-2.05936200	0.53251800
H	3.77040800	-4.30977100	1.17953700
H	2.81607100	-6.32373700	0.06495900
H	1.08415500	-6.04535400	-1.70006500
H	0.31919300	-3.81069900	-2.35007500
H	0.39244600	-1.74935200	-3.67355700
H	-0.89583800	-1.94578300	-2.46724100
H	-1.42575500	0.00587300	-4.00849700
H	0.10456100	0.74790700	-3.58483600
H	0.17584400	3.40319900	-1.14933100
H	0.05360400	5.71105800	-2.02248600
H	-1.72392100	6.34019100	-3.64762000
H	-3.37780000	4.63236600	-4.38580400
H	-3.26645100	2.33557400	-3.51038700
H	-3.13075400	-0.96766000	-3.31714400
H	-5.51322800	-1.52832900	-3.18019800
H	-6.95894000	-0.47545000	-1.44936500
H	-5.97277300	1.16243900	0.14774900
H	-3.58327600	1.73663600	0.01727200
H	-3.01427400	-2.05839000	-0.53074000
H	-3.77305800	-4.30871500	-1.17712400
H	-2.81819500	-6.32276600	-0.06318100
H	-1.08499600	-6.04456300	1.70062500
H	-0.31925600	-3.81000800	2.35000700
H	-3.43153700	-2.40873900	2.70892200

H	-5.29388400	-1.60614500	4.09789700
H	-5.55102500	0.82339200	4.57850900
H	-3.91188600	2.44308800	3.63310000
H	-2.06118900	1.64714500	2.21229000
H	-0.39267700	-1.74830900	3.67390400
H	0.89548200	-1.94531200	2.46756900
H	1.42601700	0.00653100	4.00831100
H	-0.10416100	0.74885700	3.58465700
H	3.13097700	-0.96707700	3.31706300
H	5.51345500	-1.52779300	3.18016400
H	6.95912400	-0.47522600	1.44909000
H	5.97289600	1.16229600	-0.14834800
H	3.58337700	1.73644200	-0.01798800
H	3.26632100	2.33576900	3.51034700
H	3.37802100	4.63275200	4.38521200
H	1.72496900	6.34089100	3.64591800
H	-0.05213300	5.71187100	2.02027500
H	-0.17477400	3.40379600	1.14773500
H	0.76341200	1.52939900	-0.64134400
H	-0.76294700	1.52990000	0.64056700

[$Co(dppe)_2H$] no solvent correction

Co	-0.08836100	-0.24161700	0.02749100
P	0.50519000	1.35546300	-1.43288300
P	-0.41629800	-1.54651700	-1.69709400
P	-1.72493100	0.68072400	1.21784300
P	1.31824200	-0.13814200	1.74432300
C	0.15739000	3.17039400	-1.26265800
C	-0.84669800	3.83201400	-1.98523700
C	-1.07000300	5.20228900	-1.81128400
C	-0.29295900	5.93472500	-0.91251100
C	0.70884600	5.28571300	-0.18289100
C	0.92811700	3.91820800	-0.35455200

C	2.26260900	1.41975200	-2.06540300
C	3.12891900	0.35412500	-1.78901700
C	4.41748400	0.31692600	-2.33246300
C	4.86021600	1.35213500	-3.15795300
C	4.00708500	2.42568800	-3.43671600
C	2.71991400	2.45821200	-2.89605500
C	-0.35785000	0.89361400	-3.03297600
C	-0.08763400	-0.59328000	-3.29395200
C	0.58376900	-3.10765500	-1.91662200
C	1.84236600	-3.11992900	-2.54179400
C	2.60380500	-4.29088400	-2.60923400
C	2.13018700	-5.47566200	-2.04008500
C	0.88580400	-5.47628600	-1.40236900
C	0.12449000	-4.30706900	-1.34131900
C	-2.10782100	-2.25887000	-2.07543500
C	-3.16648100	-2.08176100	-1.17821500
C	-4.44095100	-2.59183100	-1.45544700
C	-4.67364000	-3.28478000	-2.64435100
C	-3.62257300	-3.47506100	-3.54964100
C	-2.35228300	-2.97238600	-3.26339500
C	-2.96413300	-0.37831900	2.15216200
C	-2.62959200	-1.69887800	2.49747100
C	-3.49673600	-2.48881500	3.25830500
C	-4.72607400	-1.97815300	3.68187700
C	-5.07735000	-0.66930600	3.33981200
C	-4.20496700	0.12199600	2.58680100
C	-2.84638000	2.04807000	0.64947200
C	-3.63031000	1.80792800	-0.49410100
C	-4.52372600	2.76842100	-0.97043900
C	-4.63690500	4.00417500	-0.32390500
C	-3.85145100	4.26437600	0.80069800
C	-2.96913000	3.29277400	1.28662100
C	-0.84741200	1.43408100	2.70529000

C	0.23923100	0.45896800	3.18318000
C	2.02446300	-1.69185200	2.49066100
C	2.64432400	-1.69274300	3.75319600
C	3.15501100	-2.87274500	4.29706600
C	3.06417100	-4.07223200	3.58103800
C	2.45852400	-4.08135700	2.32304100
C	1.94011500	-2.89821700	1.78371700
C	2.81137200	0.96918400	1.93122900
C	4.07542700	0.51344600	1.51666000
C	5.20445000	1.32888000	1.60782800
C	5.09800400	2.62768500	2.11473000
C	3.85054300	3.09764900	2.53056400
C	2.72096700	2.27731700	2.43688800
H	-0.42424600	-1.49770900	0.73974900
H	-1.46715800	3.28958400	-2.69003400
H	-1.85450500	5.69281400	-2.38084300
H	-0.46441700	6.99952700	-0.78115400
H	1.32498200	5.84517800	0.51614000
H	1.72070500	3.43417700	0.20839500
H	2.78168200	-0.44565300	-1.14131800
H	5.07485500	-0.51778600	-2.10317000
H	5.86204500	1.32752500	-3.57810600
H	4.34399200	3.23865800	-4.07447400
H	2.07240700	3.30113400	-3.11925400
H	-1.43085600	1.06470700	-2.89524300
H	-0.01140700	1.51586900	-3.86597800
H	0.95905200	-0.72950400	-3.57845100
H	-0.70436200	-0.97073300	-4.11464600
H	2.24782000	-2.21491900	-2.98174700
H	3.56886600	-4.27336800	-3.10895100
H	2.72117800	-6.38567400	-2.09361200
H	0.50183300	-6.38954700	-0.95506200
H	-0.84350500	-4.33321000	-0.84926400

H	-2.98885400	-1.54860800	-0.25221600
H	-5.24455200	-2.44617900	-0.73866900
H	-5.66189800	-3.67918100	-2.86484100
H	-3.79114800	-4.02081200	-4.47437300
H	-1.54315400	-3.15349200	-3.96614800
H	-1.68922100	-2.11629100	2.15165800
H	-3.21066800	-3.50627100	3.51142700
H	-5.40392200	-2.59303200	4.26763300
H	-6.03212600	-0.25911400	3.65868000
H	-4.50102000	1.13534000	2.33682000
H	-3.54433200	0.85561500	-1.01077000
H	-5.12842700	2.55341400	-1.84768100
H	-5.32777500	4.75598400	-0.69543900
H	-3.92610100	5.22253800	1.30814200
H	-2.38378600	3.51731500	2.17216700
H	-0.40167100	2.37670300	2.36781000
H	-1.54863900	1.65895700	3.51751100
H	-0.22712400	-0.43997300	3.60021900
H	0.84766700	0.90221400	3.97847600
H	2.74023100	-0.76647300	4.31308400
H	3.62786500	-2.85589700	5.27556800
H	3.46580900	-4.99003900	4.00215400
H	2.38697600	-5.00477700	1.75499100
H	1.46298800	-2.90715500	0.80945500
H	4.18434400	-0.49764800	1.13533900
H	6.16921600	0.94763500	1.28418400
H	5.97634700	3.26272200	2.18757200
H	3.75223100	4.10199100	2.93472600
H	1.76721100	2.67014300	2.77469300

$[Co(dppe)_2]^-$ no solvent correction

Co	-0.02585500	-0.00535400	-0.02288100
P	0.31667800	1.75837100	-1.18338500

P	-0.14253300	-1.18695700	-1.82538100
P	-1.70756200	0.22827400	1.27812000
P	1.24870800	-0.34292000	1.67819900
C	-0.40492400	3.44705800	-0.82856300
C	-1.57117500	3.94488600	-1.43286700
C	-2.10187700	5.18865100	-1.07128400
C	-1.47613400	5.96888100	-0.09698700
C	-0.31462800	5.48608100	0.51925200
C	0.20612800	4.24251600	0.16104700
C	2.03273400	2.35057300	-1.72810500
C	3.14270200	1.54791900	-1.43700200
C	4.42421000	1.89356100	-1.88205300
C	4.61579100	3.05421300	-2.63499000
C	3.51710300	3.86921000	-2.93341300
C	2.24189500	3.52008100	-2.48116000
C	-0.35603400	1.39803300	-2.91481700
C	0.13334100	-0.00109400	-3.30183600
C	1.08094300	-2.54307500	-2.29676600
C	2.42061000	-2.22211500	-2.59142700
C	3.37627200	-3.21411900	-2.82270700
C	3.02652700	-4.56696600	-2.74526400
C	1.70710300	-4.90713100	-2.43235300
C	0.75156400	-3.90980300	-2.21310300
C	-1.70051900	-2.05589900	-2.48084600
C	-2.81131500	-2.19381700	-1.64043500
C	-3.99478700	-2.79776700	-2.08389600
C	-4.08983900	-3.27275400	-3.39372500
C	-2.98834500	-3.14885800	-4.24933100
C	-1.80941800	-2.55345000	-3.79326100
C	-2.71304300	-1.22449800	1.98052000
C	-2.12047300	-2.49750800	1.95593300
C	-2.76247200	-3.60864800	2.51146900
C	-4.02612300	-3.47133700	3.09365200

C	-4.63554800	-2.21239600	3.11846200
C	-3.98293200	-1.10229300	2.57159100
C	-3.13371700	1.41140700	1.00639600
C	-3.91151400	1.24274700	-0.15499100
C	-4.99259800	2.07943200	-0.43458700
C	-5.31129200	3.13247300	0.43161400
C	-4.53680800	3.32984600	1.57633500
C	-3.46633100	2.47378200	1.86331600
C	-1.01588700	0.83452600	2.93351300
C	0.21576500	-0.01617100	3.26179700
C	1.98800100	-1.99834200	2.21482800
C	2.53728000	-2.21920400	3.49119600
C	3.02438400	-3.47583000	3.86009900
C	2.98363900	-4.53928500	2.94978400
C	2.44903400	-4.33286900	1.67581000
C	1.95102000	-3.07345000	1.31861900
C	2.75532400	0.71382200	2.07571700
C	4.06950300	0.27207900	1.83912400
C	5.16869900	1.10891300	2.05368700
C	4.98404600	2.41605000	2.51402300
C	3.68396200	2.87504300	2.75051700
C	2.58917800	2.03613400	2.52702500
H	-2.08287200	3.36248100	-2.19178400
H	-3.01063900	5.54247500	-1.55261700
H	-1.88816200	6.93504400	0.18369800
H	0.18632100	6.08057500	1.28029400
H	1.11033800	3.88413300	0.64647500
H	2.98547800	0.64824200	-0.84896600
H	5.27086600	1.25941500	-1.63040500
H	5.61006700	3.32665700	-2.98149900
H	3.65445800	4.77802800	-3.51577900
H	1.40151300	4.16977500	-2.71212800
H	-1.44989200	1.40544300	-2.85314600

H	-0.04480800	2.15068400	-3.65068300
H	1.20714100	0.03123400	-3.51167400
H	-0.36604900	-0.36095100	-4.20746200
H	2.73073800	-1.18196300	-2.62549200
H	4.39955600	-2.92809000	-3.05588700
H	3.77044000	-5.34043000	-2.91907800
H	1.41542900	-5.95298900	-2.36086400
H	-0.26712100	-4.20283300	-1.97649400
H	-2.74135200	-1.82510800	-0.62348200
H	-4.83643900	-2.89398000	-1.40218000
H	-5.00781400	-3.73776100	-3.74559300
H	-3.04579700	-3.52158600	-5.26998600
H	-0.95852400	-2.49240100	-4.46673900
H	-1.14905200	-2.60788800	1.47899400
H	-2.27682600	-4.58118700	2.48044700
H	-4.53262300	-4.33471800	3.51879600
H	-5.62104800	-2.09243900	3.56402200
H	-4.47364700	-0.13373500	2.60285100
H	-3.65958400	0.44650900	-0.85016700
H	-5.58064700	1.91570300	-1.33491000
H	-6.14539400	3.79403500	0.21067500
H	-4.76312400	4.15096900	2.25295600
H	-2.89226500	2.64539300	2.76807400
H	-0.73425700	1.88379200	2.78810000
H	-1.75679100	0.78248500	3.74230800
H	-0.10481200	-0.99852000	3.62584900
H	0.82387600	0.44143700	4.05092000
H	2.59444600	-1.40013300	4.20377000
H	3.43976800	-3.62497900	4.85470200
H	3.36635800	-5.51707900	3.23336700
H	2.41666500	-5.14569600	0.95460300
H	1.52292000	-2.91445500	0.33397300
H	4.23928300	-0.74261600	1.48943700

H	6.17256900	0.73596000	1.86153600
H	5.83755100	3.06849500	2.68002200
H	3.52067800	3.89034800	3.10558900
H	1.58764300	2.41984100	2.70275000

$[Co(dppe)_2H]^+$ no solvent correction

Co	-0.06973900	-0.37991100	0.10207500
P	1.00169400	0.74356300	-1.64524600
P	-1.31500300	-1.43585500	-1.54961800
P	-1.31648100	1.45896500	1.13754900
P	1.41376100	-0.25961800	1.89555000
C	1.62130000	2.47729900	-1.64884100
C	0.84977900	3.53694700	-2.15354500
C	1.34720200	4.84335300	-2.14486700
C	2.61570600	5.11079700	-1.62623700
C	3.38647300	4.06365500	-1.11181600
C	2.89471100	2.75738600	-1.12119600
C	2.39482400	-0.22045300	-2.38333200
C	2.60753600	-1.54238100	-1.96371700
C	3.59547500	-2.33198500	-2.55978900
C	4.38884900	-1.80261300	-3.58004300
C	4.18789400	-0.48457500	-4.00478300
C	3.19649900	0.30093600	-3.41364900
C	-0.24908600	0.68821700	-3.03232400
C	-0.73316700	-0.75957300	-3.19823100
C	-1.05231700	-3.26429500	-1.64526300
C	-0.61672700	-3.93061100	-2.80104400
C	-0.48264600	-5.32313400	-2.81020600
C	-0.78871200	-6.06800800	-1.66995000
C	-1.23018200	-5.41377100	-0.51529900
C	-1.35450900	-4.02412500	-0.50117900
C	-3.15784800	-1.32171500	-1.63639500
C	-3.89338300	-0.95342200	-0.50248200

C	-5.29149600	-0.91938100	-0.54044600
C	-5.96859700	-1.25545200	-1.71365100
C	-5.24346800	-1.63690700	-2.84811100
C	-3.84925300	-1.67592400	-2.80912600
C	-2.71610200	1.08562500	2.30408000
C	-2.78676500	-0.17353200	2.92532800
C	-3.78367100	-0.45325900	3.86458600
C	-4.73356700	0.51789500	4.19059600
C	-4.67969200	1.77009400	3.57195100
C	-3.67940800	2.05353300	2.63818300
C	-1.92278100	2.96119200	0.25582900
C	-2.82922200	2.77550200	-0.80476200
C	-3.34624200	3.86853900	-1.50274700
C	-2.95762700	5.16794800	-1.15931700
C	-2.05393100	5.36413000	-0.11280000
C	-1.54143800	4.26973200	0.59166000
C	-0.05166100	2.11048400	2.35420900
C	0.60962500	0.93061900	3.08649100
C	1.66983800	-1.78320900	2.90245100
C	2.42928200	-1.73672000	4.08560500
C	2.61435300	-2.88744100	4.85239000
C	2.05917400	-4.10372700	4.43882000
C	1.31641000	-4.16183300	3.25823000
C	1.11924100	-3.00623400	2.49492600
C	3.15138000	0.36252300	1.74071000
C	4.10263300	-0.46892200	1.12248000
C	5.43000400	-0.06112800	0.98811900
C	5.83386700	1.18814800	1.47149100
C	4.89921800	2.02349500	2.08580100
C	3.56689100	1.61640600	2.21542800
H	-0.77605000	-1.29831000	1.02996600
H	-0.14069600	3.36101100	-2.55842500
H	0.73981900	5.64841800	-2.54731600

H	3.00302200	6.12536900	-1.62640300
H	4.37606400	4.25931700	-0.70970500
H	3.51461200	1.95615200	-0.73265500
H	1.99745600	-1.96163300	-1.16751000
H	3.74384500	-3.35464900	-2.22527200
H	5.16032400	-2.41141500	-4.04223600
H	4.80302600	-0.06777100	-4.79690000
H	3.05572800	1.32356800	-3.75090900
H	-1.08244100	1.34602200	-2.76531700
H	0.19314200	1.05912200	-3.96308600
H	0.09909700	-1.37861500	-3.54331300
H	-1.52277100	-0.81819700	-3.95141900
H	-0.38338000	-3.38333000	-3.70789900
H	-0.14431500	-5.82195800	-3.71370600
H	-0.68889900	-7.14919600	-1.68099800
H	-1.47962000	-5.98552200	0.37393000
H	-1.69924000	-3.52722900	0.40105200
H	-3.37996900	-0.69881500	0.41581000
H	-5.84386800	-0.63033700	0.34868100
H	-7.05375500	-1.22844100	-1.74548100
H	-5.76338800	-1.91302200	-3.76078900
H	-3.31120700	-2.00273100	-3.69397600
H	-2.06937300	-0.94532400	2.66352600
H	-3.81893700	-1.43178800	4.33482300
H	-5.51098200	0.30034300	4.91698800
H	-5.41611400	2.53067000	3.81510100
H	-3.65727700	3.03178500	2.16950100
H	-3.15049600	1.77298300	-1.07441000
H	-4.05489000	3.70580000	-2.30982000
H	-3.36013700	6.01926500	-1.70031300
H	-1.74938600	6.36947600	0.16352500
H	-0.84802000	4.45328300	1.40551200
H	0.68974600	2.68484000	1.78787100

H	-0.52506500	2.78337200	3.07706700
H	-0.14207400	0.35304800	3.63326900
H	1.33399300	1.28020000	3.82835000
H	2.88717100	-0.80541800	4.40704300
H	3.19699200	-2.83704600	5.76748800
H	2.21024500	-5.00009200	5.03303700
H	0.89052200	-5.10459800	2.92740900
H	0.53333300	-3.05422500	1.58295200
H	3.81314000	-1.44950000	0.75725800
H	6.14928500	-0.72150300	0.51294500
H	6.86858300	1.50302500	1.37448100
H	5.20206500	2.99315300	2.47037200
H	2.86652900	2.29146400	2.69503900

[$Co(dppe)_2$] no solvent correction

Co	0.02554400	-0.14205900	-0.00344600
P	-0.16283400	1.77918700	-1.26134400
P	0.15501600	-1.37025600	-1.88835900
P	-1.76273700	-0.13158000	1.36101500
P	1.39263200	0.10130100	1.76693200
C	-1.29557900	3.21827400	-0.95830800
C	-2.57118900	3.33157000	-1.53240700
C	-3.40386700	4.41306100	-1.22417600
C	-2.97739100	5.40182700	-0.33623100
C	-1.70980500	5.29884400	0.24790800
C	-0.88249300	4.21749900	-0.05675700
C	1.35266200	2.68449800	-1.87250100
C	2.62126300	2.18025100	-1.55684500
C	3.77960400	2.78713600	-2.05515300
C	3.68295400	3.90953400	-2.87972300
C	2.42195900	4.42541300	-3.20039800
C	1.26831900	3.81863600	-2.69995200
C	-0.76813600	1.09542700	-2.90081100

C	0.11249600	-0.10070300	-3.28502700
C	1.66124800	-2.37915900	-2.34599800
C	2.87928600	-1.74038400	-2.64386300
C	4.04209300	-2.47607900	-2.88180600
C	4.02290500	-3.87251600	-2.80347200
C	2.82687100	-4.52091600	-2.48587800
C	1.66027700	-3.78296100	-2.26165700
C	-1.18615300	-2.54770900	-2.45712600
C	-2.19150100	-2.93378200	-1.56152600
C	-3.22094200	-3.79623100	-1.95746000
C	-3.26299500	-4.28017900	-3.26614700
C	-2.26359500	-3.90705500	-4.17256300
C	-1.23332100	-3.05577500	-3.76854700
C	-2.25721100	-1.75306200	2.15066200
C	-1.34589300	-2.82061200	2.10239000
C	-1.63044200	-4.03968300	2.72487700
C	-2.84262400	-4.21579200	3.39717400
C	-3.76363100	-3.16430000	3.44578400
C	-3.47215800	-1.94338700	2.83095900
C	-3.42930400	0.62541100	1.05722000
C	-4.16268400	0.16367400	-0.05141600
C	-5.43001200	0.67176100	-0.33845000
C	-5.98429800	1.67373700	0.46611000
C	-5.25961900	2.15647700	1.55717500
C	-3.99583700	1.63308500	1.85367300
C	-1.15490500	0.76906800	2.89617100
C	0.23766400	0.24254700	3.27301500
C	2.50200600	-1.27955900	2.35408600
C	3.04246600	-1.32385800	3.65213500
C	3.84625400	-2.39163800	4.05525700
C	4.13056500	-3.43270400	3.16291000
C	3.60580000	-3.39742500	1.86974700
C	2.79504200	-2.32769200	1.47084300

C	2.51893800	1.55796900	2.03335500
C	3.90640800	1.46074200	1.83202700
C	4.73283500	2.57898400	1.97108500
C	4.19045800	3.82063100	2.31357200
C	2.81177500	3.93294500	2.51359300
C	1.98638600	2.81476400	2.36918600
H	-2.93196000	2.57837100	-2.22453500
H	-4.38741600	4.47756100	-1.68145800
H	-3.62332700	6.24291500	-0.10030500
H	-1.36351600	6.06402000	0.93790500
H	0.10418200	4.15864400	0.39524500
H	2.69640300	1.31132200	-0.91029200
H	4.75402000	2.38617300	-1.78979000
H	4.58098000	4.38382900	-3.26627400
H	2.33742700	5.30147600	-3.83815100
H	0.29708700	4.23709200	-2.94928500
H	-1.80542600	0.76974400	-2.77060200
H	-0.74494400	1.86345400	-3.68307000
H	1.13600900	0.23675600	-3.47109900
H	-0.24772400	-0.56819000	-4.20641100
H	2.93168200	-0.65631100	-2.68178100
H	4.96549300	-1.95602500	-3.12308200
H	4.92791200	-4.44540800	-2.98508200
H	2.79525000	-5.60538500	-2.41771700
H	0.74108900	-4.31081500	-2.02660400
H	-2.16605000	-2.55862000	-0.54437000
H	-3.98486400	-4.08570500	-1.24088300
H	-4.06302700	-4.94552800	-3.57919400
H	-2.28326700	-4.28433400	-5.19170600
H	-0.45282800	-2.80052000	-4.48027500
H	-0.40823900	-2.69862100	1.56539300
H	-0.90772100	-4.84965200	2.67714400
H	-3.07006000	-5.16420200	3.87611800

H	-4.71105900	-3.29336300	3.96267700
H	-4.19985300	-1.13858800	2.87697100
H	-3.73690600	-0.60204100	-0.69421100
H	-5.98178300	0.29011000	-1.19356800
H	-6.96816300	2.07592400	0.24077600
H	-5.67583300	2.93995100	2.18490200
H	-3.46088500	2.02070300	2.71423000
H	-1.11473900	1.83448500	2.64301600
H	-1.84638200	0.64413300	3.73828500
H	0.14717000	-0.76850400	3.68374200
H	0.69535300	0.86733700	4.04722800
H	2.84413500	-0.51662700	4.35212200
H	4.25415600	-2.41072300	5.06256500
H	4.75834700	-4.26247600	3.47641200
H	3.82355200	-4.19674400	1.16676500
H	2.38671700	-2.30223200	0.46444500
H	4.34987600	0.50294300	1.57633400
H	5.80373000	2.47630700	1.81590500
H	4.83320800	4.68941600	2.42347100
H	2.37634300	4.89180400	2.78284600
H	0.91731800	2.92833800	2.52434400

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