Supporting Information

Electron Transfer Kinetics of a Series of Copper Complexes with Tripodal Tetradentate Guanidine Quinolinyl Ligands

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Data availability:

The obtained analytical Stopped-Flow and cyclic voltammetry data, as well as the optimized coordinates from DFT computations are provided in the RADAR4Chem repository available under the following link: https://www.radar-service.eu/radar/en/dataset/snmphx276tt041sa?token=QwPxHaoRvtRHZDfFgQFZ

Experimental data like NMR-, mass- and IR-spectra can be viewed in the Chemotion repository: https://dx.doi.org/10.14272/collection/ToS_2024-10-09

1. Experimental Part

1.1 General Aspects, Chemicals and Solvents

All reactions and manipulations that require inert conditions were carried out under nitrogen atmosphere (99.996 %), with the nitrogen gas being dried by passage through a column filled with SICAPENT®. If necessary, the solvents were dried by standard literature procedures and degassed by three circles of freeze pump thaw.[1] The Vilsmeier salts chloro-*N*,*N*,*N*',*N*'-tetramethylformamidinium chloride (TMG-VS) and *N*,*N*'-dimethylethylenechloroformamidinium chloride (DMEG-VS) were synthesized according to the literature.[2,3] All other chemicals were purchased from commercial suppliers and used without further purification.

1.2 Analytics and Compound Purification

1.2.1 Nuclear Magnetic Resonance Spectroscopy

The nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Avance III HD 400 or a Bruker Avance II 400 nuclear resonance spectrometer at 25 °C. The ^{1}H NMR spectra were referenced to the solvent residual signal and the $^{13}C\{^{1}H\}$ NMR spectra were referenced to the solvent signal. The solvent signals in the ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra were defined relative to

the external standard tetramethylsilane (TMS) as reported in the literature.[4] The chemical shifts of the compounds were assigned with the use of two-dimensional NMR spectroscopic experiments (COSY, HSQC, HMBC, APT). For the Bruker Avance III HD 400, the software Topspin (Version 3.5 pl 7) from Bruker Corporation and for the Bruker Avance II 400, the software TopSpin (Version 2.1) from Bruker Corporation were used for data acquisition. For visualization and examination of the NMR spectra the software MestReNova (Version 12.0.1-20560) from Mestrelab Research was used. Selected NMR spectroscopic data were deposited as original data in the Chemotion Repository and are published under an Open Access model.[5,6] The link to the original data is given in the analytical description.

1.2.2 Electron Spray Ionization High Resolution Mass Spectrometry

The electron spray ionization (ESI) high-resolution (HR) mass spectra were performed and recorded on an UHR-TOF Bruker Daltonik maXis II, an ESI-quadrupole time-of-flight (qToF) mass spectrometer capable of a resolution of at least 80.000 FWHM. Detection was either in positive or in the negative ion mode. The mass spectrometer was calibrated subsequently to every experiment via direct infusion of a L-proline sodium salt solution, which provided a *m*/*z* range of singly charged peaks up to 3000 Da in both ion modes. For the ThermoFisher Scientific LTQ Orbitrap XL the source voltage was 4.49 kV and the capillary temperature was 299.54 °C. The tube lens voltage was set between 110 and 130 V. For the Bruker Daltonik maXis II, the software otofControl (Version 6.3, Build 0.5) and Compass DataAnalysis (Version 5.3, Build 556.396.6383) from Bruker Corporation and for the ThermoFisher Scientific LTQ Orbitrap XL, the software Thermo Xcalibur (Version 4.5.445.18) were used for data acquisition and examination. Selected ESI-HRMS data were deposited as original data in the Chemotion Repository and are published under an Open Access model.[5,6] The link to the original data is given in the analytical description.

1.2.3 Fourier Transform Infrared Spectroscopy

The Fourier transform infrared (FTIR) spectra were recorded on a Shimadzu IRTracer 100 using a CsI beam splitter in combination with an attenuated total reflectance (ATR) unit (Quest model from Specac utilising a robust monolithic crystalline diamond) in a resolution of 2 cm^{-1}. For data acquisition, the software LabSolution IR (Version 2.15) from Shimadzu Corporation was used. Selected FTIR spectroscopic data were deposited as original data in the Chemotion

Repository and are published under an Open Access model.[5,6] The link to the original data is given in the analytical description.

1.2.4 Thin Layer Chromatography

Thin layer chromatography (TLC) was performed with TLC sheets from MACHEREY-NAGEL pre-coated with a layer of silica gel 60 with a thickness of 0.20 mm and a fluorescent indicator.

1.2.5 Column Chromatography

Column chromatography was performed with Geduran® Si 60 (40-63 µm) from Merck or with MP Alumina B - Super I from MP Biomedicals.

1.2.6 Single-Crystal X-Ray Diffraction

The ellipsoid plots and crystallographic data of **C1$_{DMEG}$**, **C3$_{TMG}$**, **C3$_{DMEG}$**, **C5$_{TMG}$** and **C5$_{DMEG}$** are presented in Fig. S12 to S16 and in Table S1 and S2. The data were collected with a four-circle goniometer Stoe Stadivari with Dectris Pilatus3 R 200 K hybrid pixel detector using GeniX 3D high flux Mo-K_α radiation (λ = 0.71073 Å) at 100 K. The temperature was controlled by an Oxford Cryostream 800. Crystals were mounted on cryoloops with perfluorinated oil. Data were collected with X-Area Pilatus[7], indexed with X-Area Recipe[8] and integrated with X-Area Integrate.[9] A spherical absorption correction was performed with STOE X-Red32 followed by a multi-scan absorption correction and scaling of reflections with X-Area LANA.[10]

The structures were solved by intrinsic phasing (ShelXT[11]) or direct methods (ShelXS[12]) and refined against F^2 with the full-matrix least-square method of ShelXL[13] using the graphical user interface ShelXle.[14] Non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were localized at idealized positions and refined with isotropic displacement parameters. All methyl groups were allowed to rotate but not to tip.

In **C3$_{TMG}$**, it was not possible to model the disordered molecule pentane per asymmetric unit adequately and the data sets were treated with the SQUEEZE routine as implemented in PLATON.[15,16]

Full crystallographic data of **C1$_{DMEG}$**, **C3$_{TMG}$**, **C3$_{DMEG}$**, **C5$_{TMG}$** and **C5$_{DMEG}$** have been deposited with the Cambridge Crystallographic Data Centre as supplementary no. CCDC – 2382527 for **C1$_{DMEG}$**, CCDC – 2382528 for **C3$_{TMG}$**, CCDC – 2382529 for **C3$_{DMEG}$**, CCDC – 2382530 for **C5$_{TMG}$** and CCDC – 2382531 for **C5$_{DMEG}$**. Copies of the data can be obtained free of charge on

application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: (+44)1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

1.2.7 Cyclic Voltammetry

The measurements were performed with a METROHM AUTOLAB PGSTAT 101 potentiostat using a three-electrode arrangement with a Pt disc working electrode (1 mm diameter), a Pt wire as counter electrode and an Ag/AgCl (in saturated ethanolic LiCl) reference electrode. The measurements were performed in MeCN and 100 mmol/L NBu_4PF_6 with a sample concentration of 1 mmol/L at room temperature. Ferrocene was added as an internal standard after the measurements of the sample and all potentials are referenced relative to the Fc/Fc^+ potential. Cyclic voltammograms were measured with 200 $mV \cdot s^{-1}$, 100 $mV \cdot s^{-1}$, 50 $mV \cdot s^{-1}$ and 20 $mV \cdot s^{-1}$. For data acquisition and examination, the software NOVA 2.1.5 (Build 7691) from Metrohm Autolab was used. For visualization of the cyclic voltammograms the software OriginPro 2021b (Version 9.8.5.212) from OriginLab was used. The cyclic voltammograms are depicted in Fig. S1 to S5.

1.2.8 UV/Vis Spectroscopy

The UV/Vis spectra were recorded with a Cary 60 spectrophotometer from Agilent Technologies in combination with quartz glass cuvettes (1 mm, QS) at room temperature. The solutions (c = 1 mM) were prepared from the corresponding complexes. For data acquisition, the software Cary WinUV (Version 5.1.3.1042) from Agilent Technologies was used. For visualization of the UV/Vis spectra, the software OriginPro 2021b (Version 9.8.5.212) from OriginLab was used. Figure S11 shows the UV/Vis spectra of $\mathbf{C3_{DMEG}}$ and the complex $[Co(bpy)_3](PF_6)_3$ used as a counter complex for the stopped-flow UV/Vis spectroscopic measurements (*vide infra*), with the Absorption of the Co-complex scaled to the employed equivalents in each standard stopped-flow measurement.

1.2.9 Stopped-Flow UV/Vis Spectroscopy

The stopped-flow measurements were performed with a HI-TECH Scientific SF-61SX2 device with a diode array detector. The optical light path for transmission of the quartz glass cuvette was 10 mm. The mixing time is given by HI-TECH to amount to 2 ms. UV/Vis spectra in a wavelength range of 300 nm to 800 nm were detected with a maximum temporal resolution of 375 s. The analyses were carried out with the TgK Scientific program Kinetic Studio

4.0.8.18533. UV/Vis spectra (300–800 nm) were detected. For visualization and examination of the results the software OriginPro 2021b (Version 9.8.5.212) from OriginLab was used.

The cross reactions of the Cu(I) complexes with the counter complex $[Co(bpy)_3](PF_6)_3$ were monitored. To measure the kinetic of the cross reaction a solution of each Cu(I) complex (0.4 mM) in MeCN was mixed with five differently concentrated solutions (with reactant in excess) of $[Co(bpy)_3](PF_6)_3$ complex (2 mM, 3 mM, 4 mM, 5 mM and 6 mM), corresponding to 5, 7.5, 10, 12.5 and 15 equivalents relative to [Cu(I)]. For every concentration of $[Co(bpy)_3](PF_6)_3$ 5 measurements were performed. Each measurement for each Cu(I) complex was repeated twice.

For $[Cu(I)(N(QuMe)(PhDMEG)_2)]PF_6$ (**C3$_{DMEG}$**), a jump in the k_{obs}-values was observed between $[Co(bpy)_3](PF_6)_3$ concentrations of 3 mM and 4 mM (see Fig. S8) that was apparent in both separately conducted measurements. The Cu(I) complex has a comparatively weak absorbance in a similar range where the employed counter-complex is active as well (see Fig. S11), rendering an interference of the counter-complex at higher concentrations a likely cause. Since only the relative position and not the slope seems to be affected, the cross-reaction rate k_{12} was evaluated from 3 mM to 6 mM to remain in the pseudo-first order regime. Two additional data points were collected with $[Co(bpy)_3](PF_6)_3$ concentrations of 4.5 mM and 5.5 mM.

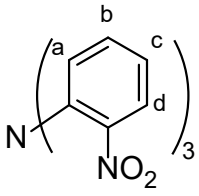
Due to the five differently concentrated solutions of the counter complex, the ionic strength was not the same for all analyzed cross reactions and varied for every solution of the counter complex with a specific concentration. The ionic strength influences the activity coefficients of the reactants. However, the influence on the activity coefficient is not significant for the determination of k_{12}. Therefore, for simplification the concentrations the activity coefficients were not considered for the determination of k_{12}. The resulting plots are depicted in Fig. S6 to S10.

1.3 Ligand Synthesis

1.3.1 Resynthesis of Tris(2-nitrophenyl)amine ($N(2\text{-}NO_2\text{-}Ph)_3$)

This molecule has been synthesized before and the synthesis was performed following a modified version of a literature-known procedure.[17]

2-Nitroaniline (25.00 g, 181.0 mmol, 1 eq.), 1-fluoro-2-nitrobenzene (76.6 g, 57.3 mL, 543 mmol, 3 eq.) and K_2CO_3 (150 g, 1086 mmol, 6 eq.) were combined in DMSO (140 mL). The mixture was heated to 130 °C under stirring for 3.5 d. After cooling to room temperature, water (500 mL) was given into the flask. The orange-brown precipitate was filtered off and washed with water (5x 100mL) and methanol (5x 100 mL), then dissolved in dichloromethane. Then, the solution was filtered over a small column filled with SiO_2, the solvent was evaporated under reduced pressure. Afterwards, the orange solid was suspended in methanol (500 mL), cooked in it for 1 h and filtered off under reduced pressure. The procedure was repeated twice. The product tris(2-nitrophenyl)amine (40.0 g, 105 mmol, 58 % yield) was obtained as an orange solid.



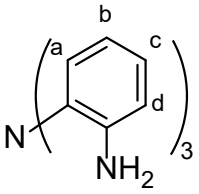
$C_{18}H_{12}N_4O_6$
380.32 g/mol

^{1}H-NMR (400 MHz, $CDCl_3$) δ [ppm] = 7.82 (dd, *J* = 8.2, 1.6 Hz, 3H, H-d), 7.53 (ddd, *J* = 8.2, 7.4, 1.7 Hz, 3H, H-b), 7.30 (ddd, *J* = 8.2, 7.3, 1.3 Hz, 3H, H-c), 7.21 (dd, *J* = 8.2, 1.3 Hz, 3H, H-a).

1.3.2 Resynthesis of Tris(2-aminophenyl)amine (N(2-NH_2-Ph)$_3$)

This molecule has been synthesized before and the synthesis was performed following a modified version of a literature-known procedure.[18]

Tris(2-nitrophenyl)amine (8.00 g, 21.0 mmol, 1.00 eq.) and palladium on activated charcoal (600 mg, 5.64 mmol, 0.268 eq.) were given into a round bottom flask which was subsequently evacuated and flushed with nitrogen three times. Methanol (250 mL) was added to the flask, which was then evacuated to the solvent's boiling point, then flushed with nitrogen for three times. The flask's atmosphere was substituted with molecular hydrogen and the reaction was stirred at room temperature for 16 hours. Afterwards, the grey precipitate was filtered off and suspended in degassed dichloromethane (300 mL) under nitrogen atmosphere. The suspension was filtered again under nitrogen atmosphere to remove the catalyst. The solvent was removed under reduced pressure, giving rise to the crude product in form of an off-white solid. The solid was then placed in a Büchner funnel and washed dropwise with cooled DCM (-30 °C) under reduced pressure to remove any remaining catalyst. After removal of remaining solvent in vacuo, the product tris(2-aminophenyl)amine (4.75 g, 16.4 mmol, 78 % yield) was obtained in form of a colorless solid.

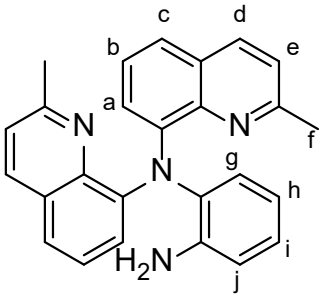


$C_{18}H_{18}N_4$
290.37 g/mol

^{1}H-NMR (400 MHz, $CDCl_3$) δ [ppm] = 6.99 (td, *J* = 7.6, 1.6 Hz, 3H, H-c), 6.91 (dd, *J* = 7.9, 1.5 Hz, 3H, H-a), 6.74 – 6.66 (m, 6H, H-b, H-d), 3.21 (s, 6H, H-N).

1.3.3 Resynthesis of N^1,N^1-bis(2-methylquinolin-8-yl)benzene-1,2-diamine

This molecule has been synthesized before and the synthesis was performed following a modified version of a literature-known procedure.[19]



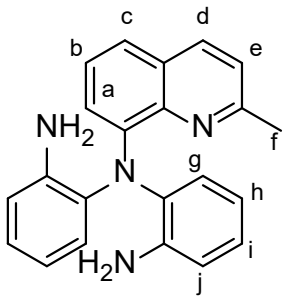
$C_{26}H_{22}N_4$
390.49 g/mol

Tris(2-aminophenyl)amine (2.80 g, 9.64 mmol, 1.00 eq.) was given into a round bottom flask and dissolved in HCl (6 M, 70 mL). The dissolution was heated to 80 °C, during which the crotonaldehyde (2.03 g, 2.40 mL, 28.9 mmol, 3.00 eq.) was dissolved in toluene (20 mL) in parallel. The dissolved aldehyde was then added to the heated HCl-solution via syringe and the reaction mixture was stirred at 80 °C for 3 hours. Afterwards, 100 mL of air were added to the solution via syringe, the heat was turned off and the flask was allowed to slowly cool to room temperature for an additional hour. The flask and its contents were subsequently cooled to 0 °C and KOH in water (50 % w/w) was added until a pH of 14 could be registered. The crude product was extracted from the aqueous layer with dichloromethane (3x 300 mL). The combined organic layers were dried over $MgSO_4$ and the solvent was removed under reduced pressure. The resulting crude product appeared as a black tar that was further purified via gradient elution column-chromatography (hexane:EtOAc 4:1 -> 3:2, R_F = 0.42 hexane/EtOAc 3:2). The product was obtained as a pale yellow solid (650 mg, 1.66 mmol, 17 % yield).

^{1}H-NMR (400 MHz, $CDCl_3$): δ [ppm] = 7.91 (d, *J* = 8.2 Hz, 2H, H-d), 7.39 (dd, *J* = 7.7 Hz, 1.5 Hz, 2H, H-c), 7.28-7.24 (m, 2H, H-b), 7.16 (dd, *J* = 7.7 Hz, 1.5 Hz, 1H, H-g), 7.11 (dd, *J* = 7.5 Hz, 1.3 Hz, 2H, H-a), 7.07-7.03 (m, 3H, H-2, H-i), 6.83 (dd, *J* = 7.9 Hz, 1.4 Hz, 1H, H-j), 6.69 (td, *J* = 7.6 Hz, 1.4 Hz, 1H, H-h), 4.63 (s, 2H, H-N), 2.14 (s, 6H, H-f).

1.3.4 Resynthesis of N^1-(2-aminophenyl)-N^1-(2-methylquinolin-8-yl)benzene-1,2-diamine

This molecule has been synthesized before and the synthesis was performed following a modified version of a literature-known procedure.[19]



$C_{22}H_{20}N_4$
340.43 g/mol

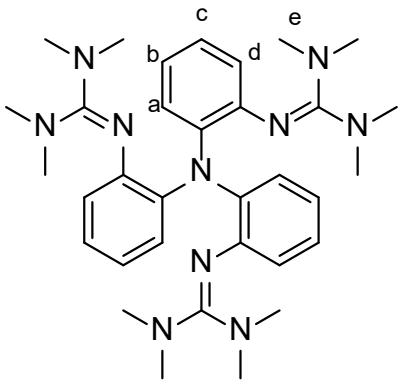
Tris(2-aminophenyl)amine (3.53 g, 12.2 mmol, 1.00 eq.) was dissolved in aqueous HCl (6 M, 73 mL) and heated to 80 °C. Crotonaldehyde (1.27 g, 1.50 mL, 18.1 mmol, 1.49 eq.), dissolved in toluene (21mL), was added and the reaction heated for 6 h with air (ca 100 mL) being injected after 3.5 h and after 6 h. In an ice bath 50 % w/w aqueous NaOH was added until a pH of 14 was reached. The mixture was diluted with water (300 mL) and extracted with DCM (4x 300 mL). The combined washings were dried with $MgSO_4$, filtered and the solvent was removed under reduced pressure. After drying on high vacuum, a black tar was obtained which was purified by column chromatography (hexane:EtOAc 4:1 -> 3:2, R_F = 0.25 hexane:EtOAc 3:2) yielding N^1-(2-aminophenyl)-N^1-(2-methylquinolin-8-yl)benzene-1,2-diamine (1.00 g, 2.94 mmol, 24 % yield) as a yellow solid.

^{1}H-NMR (400 MHz, $CDCl_3$): δ [ppm] = 7.95 (d, *J* = 8.4 Hz, 1H, H-d), 7.47 (dd, *J* = 8.1 Hz, *J*1.4 Hz, 1H, H-c), 7.33 (t, *J* = 7.8 Hz, 1H, H-b), 7.22 (dd, *J* = 7.5 Hz, 1.4 Hz, 1H, H-6), 7.17 (d, *J* = 8.2 Hz, 1H, H-e), 6.96 (td, *J* = 7.6 Hz, 1.5 Hz, 2H, H-i), 6.89 (dd, *J* = 7.8 Hz, 1.5 Hz, 2H, H-g), 6.75 (dd, *J* = 7.8 Hz, 1.4 Hz, 2H, H-j), 6.63 (td, *J* = 7.6 Hz, 1.4 Hz 2H, H-h), 3.64 (s, 4H, H-N), 2.47 (s, 3H, H-f).

1.3.5 General Procedure for the (Re-)Synthesis of Ligand Pair L1

Both syntheses (TMG_3trphen and $DMEG_3$trphen) were performed following a modified version of a literature-known procedure that was reported for TMG_3trphen (**$L1_{TMG}$**) by Stavropoulos and Cronin *et al*.[18]

Tris(2-aminophenyl)amine (1.00 g, 3.44 mmol, 1.00 eq.), together with the corresponding Vilsmeier salt (TMG-VS: 1.89 g, 11.02 mmol, 3.2 eq. or DMEG-VS: 2.04 g, 12.05 mmol, 3.5 eq.) and triethylamine (3.3 eq.) were placed into a preheated round-bottom flask and dissolved in dry acetonitrile (100 mL) under nitrogen counterflow. The reaction mixture was refluxed under a nitrogen atmosphere for 6 hours. Subsequently, the mixture was cooled to room temperature and treated with sodium hydroxide solution (100 mL, 1:1 w/w). The product was extracted with ethyl acetate (3 x 100 mL) from the aqueous phase, the combined organic phases were dried over $MgSO_4$, and the solvent was removed under reduced pressure. For purification, the product was recrystallized five times in acetonitrile. The product was stored under an inert atmosphere to avoid protonation.

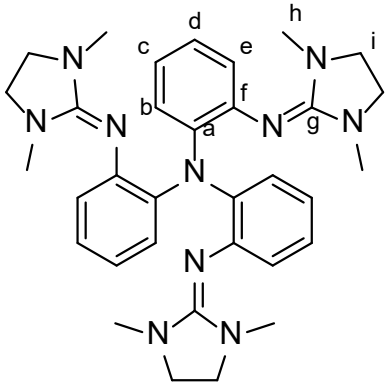


$C_{33}H_{48}N_{10}$
584.82 g/mol

TMG$_3$trphen (**L1$_{TMG}$**) was obtained in the form of colorless crystals (0.430 g, 0.74 mmol, 21 %).

^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm] = 7.00-6.89 (m, 3H, H-a), 6.80-6.89 (m, 3H, H-c), 6.64-6.60 (m, 3H, H-b), 6.27-6.20 (m, 3H, H-d), 2.44 (s, 36H, H-e).

DMEG$_3$trphen (**L1$_{DMEG}$**) was obtained in the form of light purple crystals (0.870 g, 1.50 mmol, 44 %).



$C_{33}H_{42}N_{10}$
578.77 g/mol

^{1}H NMR (400 MHz, CD_2Cl_2) δ [ppm] = 6.84 (dd, *J* = 7.7, 1.6 Hz, 3H, H-b), 6.74 (td, *J* = 7.5, 1.7 Hz, 3H, H-d), 6.65 – 6.57 (m, 6H, H-e, H-c), 3.03 (s, 12H, H-i), 2.37 (s, 18H, H-h).

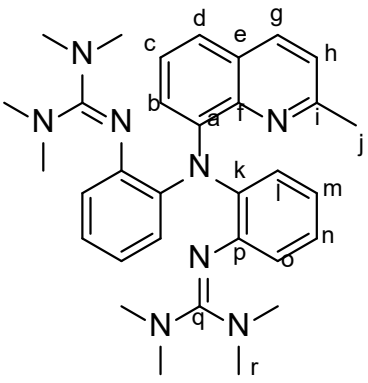
^{13}C NMR (101 MHz, CD_2Cl_2) δ [ppm] = 152.7 (g, 3C), 144.5 (a, 3C), 141.3 (f, 3C), 127.3 (b, 3C), 123.2 (c, 3C), 121.9 (d, 3C), 119.6 (e, 3C), 48.8 (i, 6C), 35.2 (h, 6C).

HR-ESI-MS (m/z (%) $[M+H]^+$, M+H = $C_{33}H_{43}N_{10}$) found: 579.3572 (100), 580.3600 (38), 581.3629 (7), calculated: 579.3672 (100) $[^{12}C_{33}{}^{1}H_{42}{}^{14}N_{10}]^+$, 580.3705 (36) $[^{12}C_{32}{}^{13}C^{1}H_{42}{}^{14}N_{10}]^+$, 581.3676 (1) $[^{12}C_{31}{}^{13}C_2{}^{1}H_{43}{}^{14}N_{10}]^+$.

IR (ATR, $\tilde{\nu}$) = 3047 (w), 3018 (w), 2971 (w), 2940 (w), 2867 (w), 2845 (w), 2767 (w), 2224 (w), 2201 (w), 2162 (w), 2158 (w), 2117 (w), 2087 (w), 2051 (w), 2029 (w), 1980 (w), 1973 (w), 1651 (vs), 1579 (vs), 1476 (vs), 1432 (vs), 1417 (m), 1394 (s), 1389 (s), 1309 (m), 1296 (m), 1281 (vs),

1278 (vs), 1260 (s), 1239 (s), 1201 (m), 1173 (w), 1154 (w), 1142 (m), 1121 (w), 1113 (m), 1105 (m), 1077 (w), 1074 (w), 1044 (m), 1033 (vs), 992 (w), 969 (s), 941 (w), 930 (w), 917 (m), 871 (w), 854 (w), 844 (w), 833 (w), 766 (m), 761 (m), 753 (m), 742 (s), 735 (vs), 720 (m), 712 (s), 697 (m), 687 (w), 650 (m), 643 (w), 628 (w), 619 (m), 598 (w), 587 (w), 560 (w), 545 (w), 536 (w), 530 (w), 529 (w), 507 (m), 485 (m), 472 (m), 462 (m), 445 (w), 429 (w), 426 (w), 405 (w), 398 (w), 385 (w), 366 (w), 357 (w) cm^{-1}.

1.3.6 Synthesis of N(QuMe)(PhTMG)$_2$ (L2$_{TMG}$)



$C_{32}H_{40}N_8$
536.73 g/mol

In a preheated round-bottom flask, N^1-(2-aminophenyl)-N^1- (2-methylquinolin-8-yl)benzene-1,2-diamine (603.0 mg, 1.77 mmol, 1.0 eq.), TMG-VS (696 mg, 4.07 mmol, 2.30 eq.), and triethylamine (0.73 mL, 5.3 mmol, 3.0 eq.) were added under a nitrogen counterflow and dissolved in dry acetonitrile (60 mL). The reaction mixture was connected to a reflux condenser and refluxed under a nitrogen atmosphere for five days. Subsequently, the reaction mixture was treated with an aqueous potassium hydroxide solution (100 mL, 1:1 w/w). The aqueous phase was extracted with diethyl ether (3 x 100 mL), and the combined organic phases were dried over $MgSO_4$. The solvent was removed under reduced pressure. The resulting orange oil was then heated under vacuum (<10^{-1} mbar), starting at 150 °C and rising to 250 °C, to remove any remaining urea derivative. The crude product was purified by repeated recrystallization in acetonitrile. N(QuMe)(PhTMG)$_2$ (**L2$_{TMG}$**) was obtained in the form of a brightly yellow solid (342 mg, 0.64 mmol, 36 %).

^{1}H NMR (400 MHz, CD_2Cl_2) δ [ppm] = 7.88 (d, *J* = 8.4 Hz, 1H, H-g), 7.36 (dd, *J* = 7.8, 1.6 Hz, 1H, H-d), 7.25 (t, *J* = 7.7 Hz, 1H, H-c), 7.18 (dd, *J* = 7.5, 1.5 Hz, 1H, H-b), 7.07 (d, *J* = 8.4 Hz, 1H, H-h), 6.97 (dd, *J* = 7.9, z1.6 Hz, 2H, h-O), 6.84 (td, *J* = 7.5, 1.6 Hz, 2H, H-m), 6.67 (td, *J* = 7.9, 1.6 Hz, 2H, H-n), 6.36 (dd, *J* = 7.8, 1.7 Hz, 2H, H-l), 2.34 – 2.24 (m, 27H, H-j, H.r).

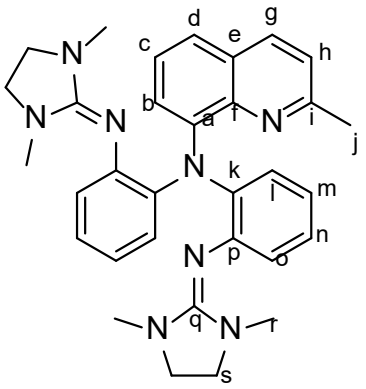
^{13}C NMR (101 MHz, CD_2Cl_2) δ [ppm] = 156.5 (q, 2C), 155.7 (i, 1C), 146.7 (a, 1C), 145.6 (k, 2C), 144.2 (f, 1C), 141.6 (p, 2C), 136.0 (g, 1C), 127.8 (e, 1C), 127.1 (o, 2C), 125.6 (c, b, 2C), 122.8 (m, 2C), 122.2 (l, 2C), 121.4 (d, 1C), 121.1 (h, 1C), 120.0 (n, 2C), 39.7 (r, 8C), 25.0 (j, 1C).

HR-ESI-MS (m/z (%) $[M+H]^+$, M+H = $C_{32}H_{41}N_8$) found: 537.34536 (100), 538.34790 (70), 539.35083 (12), calculated: 537.34541 (100) $[^{12}C_{32}{}^{1}H_{41}{}^{14}N_8]^+$, 538.34877 (36) $[^{12}C_{31}{}^{13}C^{1}H_{41}{}^{14}N_8]^+$, 539.34580 (2) $[^{12}C_{30}{}^{13}C_2{}^{1}H_{41}{}^{14}N_8]^+$.

IR (ATR, $\tilde{\nu}$) = 3050 (m), 3009 (m), 2922 (s), 2887 (s), 2880 (s), 2847 (s), 2803 (m), 1687 (m), 1609 (vs), 1601 (vs), 1574 (vs), 1563 (vs), 1497 (vs), 1482 (vs), 1459 (vs), 1450 (vs), 1425 (vs),

1367 (vs), 1328 (vs), 1278 (vs), 1271 (vs), 1235 (vs), 1206 (s), 1133 (vs), 1117 (vs), 1065 (s), 1058 (s), 1013 (vs), 925 (s), 922 (s), 917 (s), 853 (s), 849 (s), 841 (s), 827 (s), 795 (s), 772 (vs), 736 (vs), 713 (s), 702 (s), 674 (s), 671 (s), 666 (s), 630 (s), 624 (s), 618 (s), 584 (s), 563 (s), 552 (s), 546 (s), 538 (s) cm^{-1}.

1.3.7 Synthesis of N(QuMe)(PhDMEG)$_2$ (L2$_{DMEG}$)



$C_{32}H_{36}N_8$
532.70 g/mol

In a preheated round-bottom flask, *N*^{1}-(2-aminophenyl)-*N*^{1}-(2-methylquinolin-8-yl)benzene-1,2-diamine (1.14 g, 3.35 mmol, 1.0 eq.), DMEG-VS (1.30 g, 7.70 mmol, 2.30 eq.), and triethylamine (1.4 mL, 10.1 mmol, 3.0 eq.) were added under a nitrogen counterflow and dissolved in dry acetonitrile (100 mL). The reaction mixture was connected to a reflux condenser and refluxed under a nitrogen atmosphere for four days. Subsequently, the reaction mixture was cooled to room temperature and treated with an aqueous potassium hydroxide solution (100 mL, 1:1 w/w). The aqueous phase was extracted with diethyl ether (3 x 100 mL), and the combined organic phases were dried over $MgSO_4$. The solvent was removed under reduced pressure. The resulting brown oil was then heated under vacuum (<10^{-1} mbar), starting at 150 °C and rising to 250 °C, to remove any remaining urea derivative. The crude product was purified by repeated recrystallization in THF/hexane. N(QuMe)(PhDMEG)$_2$ (**L2$_{DMEG}$**) was obtained in the form of a yellow solid (374 mg, 0.70 mmol, 21 %).

^{1}H NMR (400 MHz, CD_2Cl_2) δ [ppm] = 7.86 (d, *J* = 8.3 Hz, 1H, H-g), 7.26 – 7.14 (m, 4H, H-b, H-c, H-l), 7.02 (d, *J* = 8.4 Hz, 1H, H-h), 6.97 (dd, *J* = 7.6, 1.6 Hz, 1H, H-d), 6.87 (td, *J* = 7.5, 1.7 Hz, 2H, H-m), 6.77 (td, *J* = 7.4, 1.7 Hz, 2H, H-n), 6.67 (dd, *J* = 7.7, 1.7 Hz, 2H, H-o), 2.73 (s, 8H, H-s), 2.32 (s, 3H, H-j), 2.01 (s, 12H, H-r).

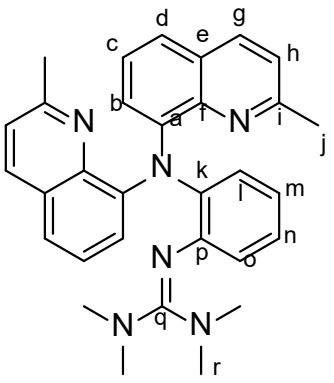
^{13}C NMR (101 MHz, CD_2Cl_2) δ [ppm] = 155.0 (q, 2C), 152.5 (i, 1C), 146.5 (a, 1C), 145.6 (k, 2C), 143.6 (f, 1C), 142.6 (p, 2C), 135.8 (g, 1C), 128.9 (e, 1C), 127.9 (b, 1C), 125.6 (c, 1C), 124.1 (o, 2C), 123.5 (m, 2C), 123.0 (d, 1C), 120.8 (h, 1C), 120.6 (n, 2C), 119.7 (l, 2C), 48.4 (s, 4C), 34.6 (r, 4C), 25.1 (j, 1C).

HR-ESI-MS (m/z (%) $[M+H]^+$, M+H = $C_{32}H_{37}N_8$) found: 533.31315 (100), 534.31612 (37), 535.31871 (7), calculated: 533.31411 (100) $[^{12}C_{32}{}^{1}H_{37}{}^{14}N_8]^+$, 534.31747 (35) $[^{12}C_{31}{}^{13}C^{1}H_{37}{}^{14}N_8]^+$, 535.31450 (1) $[^{12}C_{30}{}^{13}C_2{}^{1}H_{37}{}^{14}N_8]^+$.

IR (ATR, $\tilde{\nu}$) = 3055 (w), 2928 (w), 2861 (w), 1654 (vs), 1651 (vs), 1608 (vs), 1596 (s), 1577 (vs), 1560 (s), 1480 (vs), 1437 (vs), 1430 (s), 1420 (s), 1391 (m), 1368 (w), 1327 (w), 1313 (w), 1274 (vs), 1236 (s), 1160 (w), 1110 (w), 1081 (w), 1069 (w), 1038 (m), 1032 (s), 979 (w), 970

(m), 849 (w), 841 (w), 802 (w), 781 (w), 763 (s), 756 (vs), 742 (vs), 698 (m), 691 (s), 673 (w), 652 (m), 629 (w), 619 (m), 599 (w), 593 (m), 591 (m), 585 (w), 547 (m), 534 (m), 524 (m), 513 (m), 489 (m), 471 (m), 450 (m), 428 (m) cm^{-1}.

1.3.8 Synthesis of N(QuMe)$_2$(PhTMG) (L3$_{TMG}$)



$C_{31}H_{32}N_6$
488.64 g/mol

N^1,*N*^{1}-bis(2-methylquinolin-8-yl)benzene-1,2-diamine (509 mg, 1.3 mmol, 1.0 eq.), TMG-VS (325 mg, 1.9 mmol, 1.5 eq.), and triethylamine (0.4 mL, 3.0 mmol, 2.3 eq.) were added in a preheated flask under a nitrogen counterflow and dissolved in dry acetonitrile (80 mL). The reaction mixture was connected to a reflux condenser and refluxed under a nitrogen atmosphere for five days. Subsequently, the reaction mixture was cooled to room temperature and treated with potassium hydroxide solution (100 mL, 1:1 w/w). The aqueous phase was extracted with diethyl ether (3 x 100 mL), and the combined organic phases were dried over $MgSO_4$. The solvent was removed under reduced pressure. The resulting orange oil was then heated under vacuum (<10^{-1} mbar), starting at 100 °C and rising to 250 °C, to remove any remaining urea derivative. The remaining crude product was recrystallized in THF/hexane until no side product could be detected via NMR spectroscopy. N(QuMe)$_2$(PhTMG) (**L3$_{TMG}$**) was obtained as an orange solid (334 mg, 0.68 mmol, 52 %) and stored under a nitrogen atmosphere.

^{1}H NMR (400 MHz, CD_2Cl_2) δ [ppm] = 7.93 (d, *J* = 8.4 Hz, 2H, H-g), 7.41 (dd, *J* = 7.9, 1.6 Hz, 2H, H-d), 7.30 (t, *J* = 7.8 Hz, 2H, H-c), 7.21 (dd, *J* = 7.6, 1.6 Hz, 2H, H-b), 7.12 – 7.00 (m, 4H, H-h, H-m, H-o), 6.77 (td, *J* = 7.4, 1.6 Hz, 1H, H-n), 6.61 (dd, *J* = 7.9, 1.6 Hz, 1H, H-l), 2.36 (s, 12H, H-r), 2.11 (s, 6H, H-j).

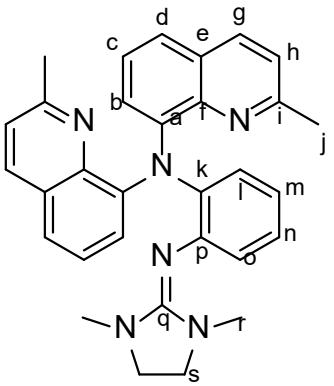
^{13}C NMR (101 MHz, CD_2Cl_2) δ [ppm] = 157.2 (q, 1C), 155.4 (i, 2C), 147.6 (k, 1C), 146.8 (a, 2C), 143.2 (f, 2C), 141.7 (p, 1C), 135.9 (g, 2C), 128.5 (o, 1C), 127.8 (e, 2C), 125.6 (c, 2C), 124.5 (m, 1C), 123.7 (b, 2C), 123.1 (l, 1C), 121.0 (h, 2C), 121.0 (d, 2C), 120.3 (n, 1C), 39.7 (r, 4C), 24.9 (j, 2C).

HR-ESI-MS (m/z (%) $[M+H]^+$, M+H = $C_{31}H_{33}N_6$) found: 489.27558 (100), 490.27873 (35), 491.28194 (6), calculated: 489.27667 (100) $[^{12}C_{31}{}^{1}H_{33}{}^{14}N_6]^+$, 490.28002 (33) $[^{12}C_{30}{}^{13}C^{1}H_{33}{}^{14}N_6]^+$, 491.28337 (5) $[^{12}C_{29}{}^{13}C_2{}^{1}H_{33}{}^{14}N_6]^+$.

IR (ATR, $\tilde{\nu}$) = 3050 (m), 3009 (m), 2923 (s), 2880 (m), 2800 (m), 1610 (vs), 1599 (vs), 1579 (vs), 1556 (vs), 1501 (vs), 1483 (vs), 1459 (vs), 1428 (vs), 1369 (vs), 1336 (vs), 1331 (vs), 1273 (vs), 1236 (vs), 1219 (s), 1197 (s), 1134 (vs), 1114 (vs), 1064 (s), 1060 (s), 1015 (vs), 966 (m), 926 (s),

851 (m), 831 (vs), 800 (s), 791 (vs), 749 (vs), 745 (vs), 702 (s), 666 (vs), 632 (s), 620 (s), 591 (m), 583 (m), 543 (m), 511 (m), 493 (m), 490 (m), 479 (m) cm^{-1}.

1.3.9 Synthesis of N(QuMe)$_2$(PhDMEG) (L3$_{DMEG}$)



$C_{31}H_{30}N_6$
486.62 g/mol

N^1,*N*^{1}-bis(2-methylquinolin-8-yl)benzene-1,2-diamine (786 mg, 2.0 mmol, 1.0 eq.), DMEG-VS (442 mg, 2.6 mmol, 1.3 eq.), and triethylamine (0.6 mL, 4.0 mmol, 2.0 eq.) were added in a preheated flask under a nitrogen counterflow and dissolved in dry acetonitrile (80 mL). The reaction mixture was connected to a reflux condenser and refluxed under a nitrogen atmosphere for five days. Subsequently, the reaction mixture was treated with a potassium hydroxide solution (100 mL, 1:1 w/w). The aqueous phase was extracted with diethyl ether (3 x 100 mL), and the combined organic phases were dried over $MgSO_4$. The solvent was removed under reduced pressure. The resulting orange oil was then heated under vacuum (<10^{-1} mbar), starting at 150 °C and rising to 250 °C, to remove any remaining urea derivative. Recrystallizations of the crude product in THF/hexane mixtures as well as acetonitrile were attempted but proved unsuccessful due to the crude product separating off as an oil. N(QuMe)$_2$(PhDMEG) (**L3$_{TMG}$**) was obtained as an orange solid (548 mg, 1.1 mmol, 56 %) and stored under a nitrogen atmosphere.

Since purification of the crude product was unsuccessful, it was not possible to obtain NMR spectra of a purer substance.

^{1}H NMR (400 MHz, CD_2Cl_2) δ [ppm] = 7.90 (d, *J* = 8.4 Hz, 2H, H-g), 7.36 (dd, *J* = 7.9, 1.5 Hz, 2H, H-b), 7.26 (t, *J* = 7.7 Hz, 2H, H-c), 7.19 (dd, *J* = 7.7, 1.5 Hz, 2H, H-d), 7.09 (dd, *J* = 7.8, 1.6 Hz, 1H, H-o), 7.03 – 6.94 (m, 3H, H-h, H-m), 6.81 – 6.74 (m, 2H, H-l, H-n), 2.75 (s, 4H, H-s), 2.12 – 2.09 (m, 12H, H-r, H-j).

^{13}C NMR (101 MHz, CD_2Cl_2) δ [ppm] = 155.6 (i, 2C), 152.9 (q, 1C), 147.5 (a, 2C), 143.2 (k, 1C), 142.6 (f,p, 3C), 135.9 (g, 2C), 129.1 (b, 2C), 127.8 (e, 2C), 125.7 (c, 2C), 124.4 (n, 1C), 124.3 (l, 1C), 123.9 (d, 2C), 121.0 (h, 2C), 121.0 (o, 1C), 120.7 (m, 1C), 48.3 (s, 2C), 34.7 (r, 2C), 25.0 (j, 2C).

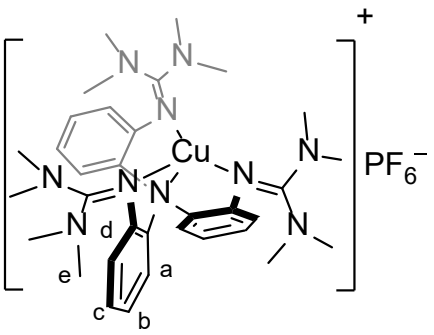
HR-ESI-MS (m/z (%) $[M+H]^+$, M+H = $C_{31}H_{31}N_6$) found: 487.25956 (100), 488.26265 (35), 489.26772 (6), calculated: 487.26102 (100) $[^{12}C_{31}{}^{1}H_{31}{}^{14}N_6]^+$, 488.26437 (34) $[^{12}C_{30}{}^{13}C^{1}H_{31}{}^{14}N_6]^+$, 491.28337 (5) $[^{12}C_{29}{}^{13}C_2{}^{1}H_{31}{}^{14}N_6]^+$.

IR (ATR, $\tilde{\nu}$) = 3043 (m), 2927 (s), 2854 (s), 1701 (s), 1649 (vs), 1594 (s), 1586 (vs), 1557 (s), 1502 (vs), 1477 (vs), 1460 (vs), 1428 (vs), 1396 (vs), 1368 (s), 1336 (vs), 1277 (vs), 1237 (vs), 1162 (s), 1132 (s), 1112 (s), 1071 (s), 1031 (vs), 993 (m), 970 (s), 933 (m), 830 (vs), 801 (s), 793 (s), 752 (vs), 702 (s), 665 (s), 649 (s), 630 (s), 595 (s), 581 (s), 520 (s), 488 (s), 447 (s) cm^{-1}.

1.4 Complex Synthesis

1.4.1 Resynthesis of [Cu(I){TMG_3trphen}]PF_6 ($C1_{TMG}$)

This molecule has been synthesized before.[18]



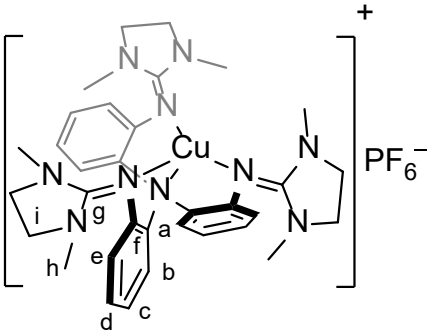
$C_{33}H_{48}N_{10}CuPF_6$
793.33 g/mol

A preheated Schlenk tube was charged with [Cu(MeCN)$_4$]PF_6 (40.7 mg, 108 µmol, 1.00 eq.) and TMG_3trphen (63.9 mg, 109 µmol, 1.01 eq.) in a nitrogen counterflow. The solids were dissolved in acetonitrile (2.5 mL) and stirred for 30 min at 30 °C. Afterwards, diethyl ether was added to the mixture and the resulting colorless precipitate was filtered off under reduced pressure. The product was washed with diethyl ether (3x 5 mL) and dried *in vacuo*. [Cu(I){TMG_3trphen}]PF_6 (**$C1_{TMG}$**) was obtained as a colorless powder (69.8 mg, 88.0 µmol, 81 % yield).

^{1}H NMR (400 MHz, CD_2Cl_2) δ [ppm] = 7.24 (dd, *J* = 7.8, 1.6 Hz, 3H, H-a), 7.05 – 6.95 (m, 3H, H-c), 6.82 (td, *J* = 7.5, 1.5 Hz, 3H, H-b), 6.42 (dd, *J* = 7.9, 1.5 Hz, 3H), 3.41 – 1.21 (m, 36H).

^{1}H NMR (400 MHz, CD_2Cl_2) δ [ppm] = 7.24 (dd, *J* = 7.8, 1.6 Hz, 3H, H-a), 7.05 – 6.95 (m, 3H, H-c), 6.82 (td, *J* = 7.5, 1.5 Hz, 3H, H-b), 6.42 (dd, *J* = 7.9, 1.5 Hz, 3H, H-d), 3.35 – 2.36 (m, 27H, H-e, H-e'), 1.52 (s, 9H, H-e'').

1.4.2 Synthesis of [Cu(I){$DMEG_3$trphen}]PF_6 ($C1_{DMEG}$)



$C_{33}H_{42}N_{10}CuPF_6$
787.28 g/mol

A preheated Schlenk tube was charged with [Cu(MeCN)$_4$]PF_6 (111 mg, 295 µmol, 1.00 eq.) and $DMEG_3$trphen (63.1 mg, 109 µmol, 1.00 eq.) in a nitrogen counterflow. The solids were dissolved in acetonitrile (2.5 mL) and stirred for 30 min at 30 °C. Afterwards, diethyl ether was added to the mixture and the resulting colorless

precipitate was filtered off under reduced pressure. The product was washed with diethyl ether (3x 5 mL) and dried *in vacuo*. [Cu(I){DMEG$_3$trphen}]PF_6 (**C1$_{DMEG}$**) was obtained as a colorless powder (49.1 mg, 62.4 µmol, 57 % yield).

^{1}H NMR (400 MHz, CD_3CN) δ [ppm] = 7.12 (dd, *J* = 7.8, 1.7 Hz, 3H, H-b), 7.07 – 6.97 (m, 3H, H-d), 6.91 – 6.78 (m, 6H, H-c, H-e), 3.28 (s, 12H, H-i), 2.48 (s, 18H, H-h).

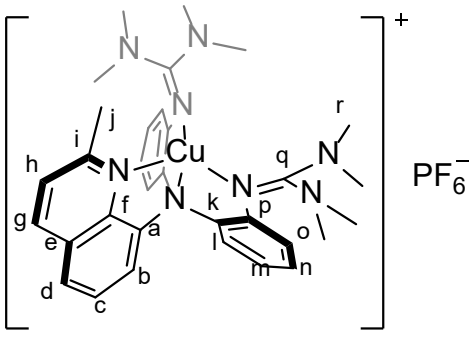
^{13}C NMR (101 MHz, CD_3CN) δ [ppm] = 163.5 (g, 3C), 147.5 (a, 3C), 140.2 (f, 3C), 129.2 (b, 3C), 126.1 (d, 3C), 123.6 (e, 3C), 121.7 (c, 3C), 48.9 (i, 6C), 35.8 (h, 6C).

HR-ESI-MS (m/z (%) $[M]^+$, M = $C_{33}H_{42}N_{10}Cu$) found: 641.2789 (100), 642.2819 (39), 643.2781 (49), 644.2804 (18), 645.2832 (3). calculated: 641.2889 (100) $[^{12}C_{33}{}^{1}H_{42}{}^{14}N_{10}{}^{63}Cu]^+$, 642.2923 (36) $[^{12}C_{32}{}^{13}C^{1}H_{42}{}^{14}N_{10}{}^{63}Cu]^+$, 643.2871 (45) $[^{12}C_{33}{}^{1}H_{42}{}^{14}N_{10}{}^{65}Cu]^+$, 644.2905 (16) $[^{12}C_{32}{}^{13}C^{1}H_{42}{}^{14}N_{10}{}^{65}Cu]^+$, 645.2938 (3) $[^{12}C_{31}{}^{13}C_2{}^{1}H_{42}{}^{14}N_{10}{}^{65}Cu]^+$.

IR (ATR, $\tilde{\nu}$) = 2974 (w), 2963 (w), 2960 (w), 1772 (w), 1602 (m), 1588 (w), 1574 (m), 1564 (m), 1506 (w), 1480 (m), 1465 (w), 1448 (w), 1442 (w), 1419 (w), 1398 (w), 1384 (w), 1287 (m), 1250 (w), 1235 (w), 1222 (w), 1198 (w), 1170 (w), 1151 (w), 1140 (w), 1108 (w), 1098 (w), 1071 (w), 1038 (w), 990 (w), 922 (w), 878 (w), 838 (vs), 797 (w), 754 (w), 747 (m), 738 (w), 722 (w), 704 (w), 649 (w), 622 (w), 607 (w), 592 (w), 557 (m), 545 (w), 533 (w), 494 (w), 481 (w), 479 (w), 469 (w), 462 (w), 449 (w), 419 (w) cm^{-1}.

1.4.3 Synthesis of [Cu(I){N(QuMe)(PhTMG)$_2$}]PF_6 (C3$_{TMG}$)

A preheated Schlenk tube was charged with $[Cu(MeCN)_4]PF_6$ (220 mg, 584 µmol, 1.00 eq.) and N(QuMe)(PhTMG)$_2$ (313 mg, 584 µmol, 1.00 eq.) in a nitrogen counterflow. The solids were dissolved in acetonitrile (5.00 mL) and stirred for 30 min at 30 °C. Afterwards, diethyl ether was added to the mixture and the resulting orange precipitate was filtered off under reduced pressure. The product was washed with diethyl ether (3x 10 mL) and dried in vacuo. [Cu(I){N(QuMe)(PhTMG)$_2$}]PF_6 (**C3$_{TMG}$**) was obtained as an orange powder (364 mg, 489 µmol, 84 % yield).



$C_{32}H_{40}N_8CuPF_6$
745.24 g/mol

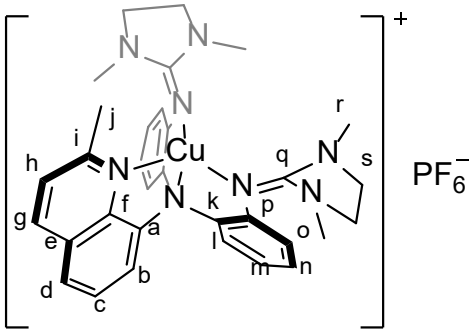
^{1}H NMR (400 MHz, CD_3CN) δ [ppm] = 8.27 (d, *J* = 8.6 Hz, 1H H-g), 7.79 – 7.76 (m, 2H, H-b, H-d), 7.52 (t, *J* = 7.8 Hz, 1H, H-c), 7.46 (d, *J* = 8.4 Hz, 1H, H-h), 7.28 (d, *J* = 7.9 Hz, 2H, H-o), 7.04 (td, *J* = 7.5, 1.6 Hz, 2H, H-m), 6.84 (t, *J* = 6.8 Hz, 2H, H-n), 6.54 (dd, *J* = 8.0, 1.5 Hz, 2H, H-l), 3.27 – 1.61 (m, 27H, H-j, H-r).

^{13}C NMR (101 MHz, CD_3CN) δ [ppm] = 164.2 (q, 2C), 158.4 (i, 1C), 149.4 (k, 2C), 144.2 (f, 1C), 144.1 (a, 1C), 138.2 (g, 1C), 131.0 (b, 1C), 129.5 (e, p, 3C), 129.3 (o, 2C), 127.3 (m, 2C), 126.9 (c, 1C), 126.7 (d, 1C), 124.2 (h, 1C), 122.6 (l, 2C), 121.9 (n, 2C), 39.8 (r, 8C), 28.1 (j, 1C).

HR-ESI-MS (m/z (%) $[M]^+$, M = $C_{32}H_{40}N_8Cu$) found: 599.2673 (100), 600.2704 (37), 601.2661 (49), 602.2688 (18). calculated: 599.2666 (100) $[^{12}C_{32}{}^{1}H_{40}{}^{14}N_8{}^{63}Cu]^+$, 600.2700 (34) $[^{12}C_{31}{}^{13}C^{1}H_{40}{}^{14}N_8{}^{63}Cu]^+$, 601.2648 (45) $[^{12}C_{32}{}^{1}H_{40}{}^{14}N_8{}^{65}Cu]^+$, 602.2687 (15) $[^{12}C_{31}{}^{13}C^{1}H_{40}{}^{14}N_8{}^{65}Cu]^+$, 603.2715 (3) $[^{12}C_{30}{}^{13}C_2{}^{1}H_{40}{}^{14}N_8{}^{65}Cu]^+$.

IR (ATR, $\tilde{\nu}$) = 3065 (m), 2941 (m), 2880 (m), 2803 (m), 1599 (m), 1534 (vs), 1476 (s), 1441 (s), 1425 (s), 1411 (s), 1394 (vs), 1341 (m), 1326 (m), 1317 (m), 1279 (m), 1267 (m), 1237 (s), 1211 (m), 1155 (s), 1144 (m), 1111 (m), 1064 (m), 1026 (s), 926 (m), 876 (m), 831 (vs), 798 (s), 751 (vs), 741 (s), 718 (m), 703 (m), 691 (m), 674 (s), 636 (m), 629 (m), 624 (m), 556 (vs), 531 (m), 486 (s) cm^{-1}.

1.4.4 Synthesis of [Cu(I){N(QuMe)(PhDMEG)$_2$}]PF$_6$ (C3$_{DMEG}$)



$C_{32}H_{36}N_8CuPF_6$
741.21 g/mol

A preheated Schlenk tube was charged with $[Cu(MeCN)_4]PF_6$ (105 mg, 278 µmol, 1.00 eq.) and N(QuMe)(PhDMEG)$_2$ (178 mg, 334 µmol, 1.20 eq.) in a nitrogen counterflow. The solids were dissolved in acetonitrile (5.00 mL) and stirred for 30 min at 30 °C. Afterwards, diethyl ether was added to the mixture and the resulting orange precipitate was filtered off under reduced pressure. The product was washed with diethyl ether (3x 10 mL) and dried *in vacuo*. [Cu(I){N(QuMe)(PhDMEG)$_2$}]PF$_6$ (**C3$_{DMEG}$**) was obtained as an orange powder (65.0 mg, 87.7 µmol, 31 % yield).

^{1}H NMR (400 MHz, CD_2Cl_2) δ [ppm] = 8.30 (d, *J* = 8.4 Hz, 1H, H-g), 7.80 (d, *J* = 8.1 Hz, 1H, H-d), 7.73 (d, *J* = 7.4 Hz, 1H, H-b), 7.54 (t, *J* = 7.8 Hz, 1H, H-c), 7.48 (d, *J* = 8.5 Hz, 1H, H-h), 7.15 (d, *J* = 7.9 Hz, 2H, H-o), 7.03 (t, *J* = 6.9 Hz, 2H, H-m), 6.91 – 6.76 (m, 4H, H-l, H-n), 3.18 (s, 8H, H-s), 2.81 (s, 3H, H-j), 2.45 (s, 12H, H-r).

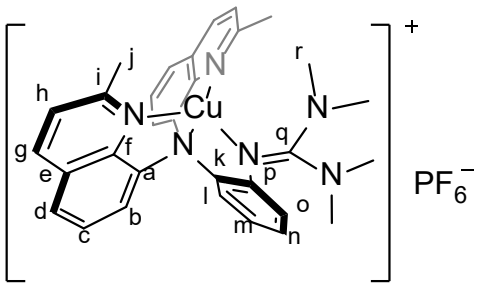
^{13}C NMR (101 MHz, CD_3CN) δ [ppm] = 162.92 (q, 2C), 158.8 (i, 1C), 147.5 (k, 2C), 144.1 (f, 1C), 143.5 (a, 1C), 140.7 (p, 2C), 138.5 (g, 1C), 131.5 (b, 1C), 129.6 (e, 1C), 128.4 (o, 2C), 127.0 (c, 1C), 126.8 (d, 1C), 126.7 (m, 2C), 124.2 (h, 1C), 123.7 (l, 2C), 121.9 (n, 2C) , 48.9 (s, 4C), 35.7 (r, 4C), 28.2 (j, 1C).

HR-ESI-MS (m/z (%) $[M]^+$, M = $C_{32}H_{36}N_8Cu$) found: 595.2270 (100), 596.2300 (37), 597.2260 (48), 598.2285 (17), 599.2314 (3). calculated: 595.2358 (100) $[^{12}C_{32}{}^{1}H_{36}{}^{14}N_8{}^{63}Cu]^+$, 596.2392 (35) $[^{12}C_{31}{}^{13}C^{1}H_{36}{}^{14}N_8{}^{63}Cu]^+$, 597.2340 (45) $[^{12}C_{32}{}^{1}H_{36}{}^{14}N_8{}^{65}Cu]^+$, 598.2374 (15) $[^{12}C_{31}{}^{13}C^{1}H_{36}{}^{14}N_8{}^{65}Cu]^+$, 599.24079 (3) $[^{12}C_{30}{}^{13}C_2{}^{1}H_{36}{}^{14}N_8{}^{65}Cu]^+$.

IR (ATR, $\tilde{\nu}$) = 2861 (w), 1697 (w), 1602 (w), 1566 (w), 1506 (w), 1479 (w), 1451 (w), 1413 (w), 1396 (w), 1288 (w), 1264 (w), 1238 (w), 1140 (w), 1117 (w), 1109 (w), 1076 (w), 1038 (w), 973 (w), 937 (w), 875 (w), 834 (s), 794 (w), 777 (w), 750 (w), 737 (w), 700 (w), 677 (w), 653 (w), 629 (w), 608 (w), 556 (m), 544 (w), 529 (w), 517 (w), 499 (w), 489 (w), 481 (w), 472 (w), 438 (w), 433 (w), 431 (w), 425 (w), 423 (w) cm^{-1}.

1.4.5 Synthesis of [Cu(I){N(QuMe)$_2$(PhTMG)}]PF$_6$ (C5$_{TMG}$)

A preheated Schlenk was charged with $[Cu(MeCN)_4]PF_6$ (163 mg, 432 µmol, 1.00 eq.) and $N(QuMe)_2(PhTMG)$ (234 mg, 478 µmol, 1.11 eq.) in a nitrogen counterflow. The solids were dissolved in acetonitrile (5.00 mL) and stirred for 30 min at 30 °C. Afterwards, diethyl ether was added to the mixture and the resulting yellow precipitate was filtered off under reduced pressure. The product was washed with diethyl ether (3x 10 mL) and dried *in vacuo*. [Cu(I){N(QuMe)$_2$(PhTMG)}]PF$_6$ (**C5$_{TMG}$**) was obtained as a yellow powder (216 mg, 310 µmol, 72 % yield).



$C_{31}H_{32}N_6CuPF_6$
697.15 g/mol

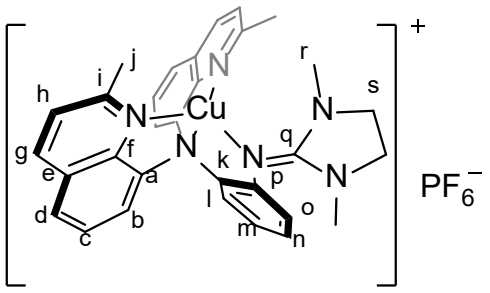
^{1}H NMR (400 MHz, CD_3CN) δ [ppm] = 8.28 (d, *J* = 8.5 Hz, 2H, H-g), 7.78 (d, *J* = 8.1 Hz, 2H, H-d), 7.69 (d, *J* = 7.6 Hz, 2H, H-b), 7.55 – 7.41 (m, 4H, H-h, H-c), 7.35 (dd, *J* = 8.0, 1.5 Hz, 1H, H-o), 7.11 (td, *J* = 7.6, 1.6 Hz, 1H, H-m), 6.89 (td, *J* = 7.5, 1.6 Hz, 1H, H-n), 6.61 (dd, *J* = 8.0, 1.5 Hz, 1H, H-l), 3.11 – 2.12 (m, *J* = 140.6 Hz, 18H, H-j, H-r).

^{13}C NMR (101 MHz, CD_3CN) δ [ppm] = 164.6 (q, 1C), 159.0 (i, 2C), 149.1 (k, 1C), 145.5 (a, 2C), 144.0 (f, 2C), 139.8 (p, 1C), 138.4 (g, 2C), 129.5 (b,o, 3C), 129.4 (e, 2C), 128.1 (m, 1C), 126.9 (c, 2C), 126.8 (d, 2C), 124.2 (h, 2C), 122.8 (l, 1C), 122.4 (n, 1C), 40.1 (r, 4C), 27.4 (j, 2C).

HR-ESI-MS (m/z (%) $[M]^+$, M = $C_{31}H_{32}N_6Cu$) found: 551.1979 (100), 552.2010 (33), 553.1967 (41), 554.1994 (15), 555.2023 (4), calculated: 551.1979 (100) $[^{12}C_{31}{}^{1}H_{32}{}^{14}N_6{}^{63}Cu]^+$, 552.2013 (34) $[^{12}C_{30}{}^{13}C^{1}H_{32}{}^{14}N_6{}^{63}Cu]^+$, 553.1961 (45) $[^{12}C_{31}{}^{1}H_{32}{}^{14}N_6{}^{65}Cu]^+$, 554.1995 (15) $[^{12}C_{30}{}^{13}C^{1}H_{32}{}^{14}N_6{}^{65}Cu]^+$, 555.2028 (2) $[^{12}C_{29}{}^{13}C_2{}^{1}H_{32}{}^{14}N_6{}^{65}Cu]^+$.

IR (ATR, $\tilde{\nu}$) = 3321 (w), 3302 (m), 3244 (w), 3159 (w), 2924 (w), 1636 (s), 1598 (s), 1532 (w), 1425 (w), 1376 (s), 1342 (vs), 1304 (vs), 1281 (vs), 1266 (vs), 1159 (w), 1146 (w), 1100 (vs), 1059 (vs), 1045 (s), 1032 (w), 1020 (w), 1012 (w), 989 (s), 867 (w), 826 (vs), 792 (w), 750 (m), 590 (w), 553 (s), 515 (w) cm^{-1}.

1.4.6 Synthesis of [Cu(I){N(QuMe)$_2$(PhDMEG)}]PF$_6$ (C5$_{DMEG}$)



A Schlenk tube was charged with [Cu(MeCN)$_4$]PF$_6$ (200 mg, 531 µmol, 1.00 eq.) and N(QuMe)$_2$(PhDMEG) (340 mg, 699 µmol, 1.32 eq.) in a nitrogen counterflow. The solids were dissolved in acetonitrile (1.50 mL) and stirred for 30 min at 30 °C. Afterwards, diethyl ether was added to the mixture and the resulting yellow precipitate was filtered off under reduced pressure. The product was washed with diethyl ether (3x 5 mL) and dried *in vacuo*. [Cu(I){N(QuMe)$_2$(PhDMEG)}]PF$_6$ (**C5$_{DMEG}$**) was obtained as a yellow powder (279 mg, 401 µmol, 75 % yield).

^{1}H NMR (400 MHz, CD_3CN) δ [ppm] = 8.28 (d, *J* = 8.5 Hz, 2H, H-g), 7.78 (dd, *J* = 8.1, 1.4 Hz, 2H, H-d), 7.60 (dd, *J* = 7.5, 1.3 Hz, 2H, H-b), 7.52 – 7.40 (m, 4H, H-c, H-h), 7.19 (dd, *J* = 8.0, 1.5 Hz, 1H, H-o), 7.11 – 7.02 (m, 1H, H-m), 6.91 (dd, *J* = 8.1, 1.6 Hz, 1H, H-l), 6.88 – 6.76 (m, 1H, H-n), 3.20 (s, 4H, H-s), 2.67 (s, 6H, H-j), 2.56 (s, 6H, H-r).

^{13}C NMR (101 MHz, CD_3CN) δ [ppm] = 163.4 (q, 1C), 159.0 (i, 2C), 147.5 (k, 1C), 145.4 (a, 2C), 143.7 (f, 2C), 139.9 (p, 1C), 138.4 (g, 2C), 129.3 (e, 2C), 128.8 (o, 1C), 128.9 (b, 2C), 127.5 (m, 1C), 126.9 (c, 2C), 126.6 (d, 2C), 124.2 (h, 2C), 123.7 (l, 1C), 122.0 (n, 1C), 48.9 (s, 2C), 35.9 (r, 2C), 27.2 (j, 2C).

HR-ESI-MS (m/z (%) $[M]^+$, M = $C_{31}H_{30}N_6Cu$) found: 549.1737 (100), 550.1769 (34), 551.1727 (47), 552.1752 (16), 553.1782 (3), calculated: 549.1828 (100) $[^{12}C_{31}{}^{1}H_{30}{}^{14}N_6{}^{63}Cu]^+$, 550.1891 (35) $[^{12}C_{30}{}^{13}C^{1}H_{30}{}^{14}N_6{}^{63}Cu]^+$, 551.1810 (45) $[^{12}C_{31}{}^{1}H_{30}{}^{14}N_6{}^{65}Cu]^+$, 552.1843 (15) $[^{12}C_{30}{}^{13}C^{1}H_{30}{}^{14}N_6{}^{65}Cu]^+$, 553.1876 (2) $[^{12}C_{29}{}^{13}C_2{}^{1}H_{30}{}^{14}N_6{}^{65}Cu]^+$.

IR (ATR, $\tilde{\nu}$) = 3050 (m), 2925 (s), 2868 (s), 2847 (s), 1695 (s), 1652 (vs), 1636 (vs), 1614 (s), 1596 (vs), 1586 (vs), 1557 (s), 1500 (vs), 1478 (vs), 1460 (vs), 1429 (vs), 1396 (vs), 1368 (s), 1338 (vs), 1325 (vs), 1276 (vs), 1250 (s), 1238 (vs), 1205 (s), 1162 (s), 1136 (s), 1111 (s), 1106 (s), 1075 (s), 1030 (vs), 990 (m), 969 (s), 927 (m), 863 (m), 830 (vs), 800 (s), 791 (s), 752 (vs), 701 (s), 667 (s), 647 (s), 631 (s), 620 (s), 593 (s), 579 (s), 541 (m), 533 (m), 519 (s), 505 (s), 484 (s), 477 (s), 468 (s), 447 (s), 437 (s), 368 (s) cm^{-1}.

1.4.7 Cu(II) Complexes

Synthesis of the Cu(II) salts was attempted in a similar fashion to the Cu(I) counterparts. Attempts for crystal structures resulted in crystals of $[Cu(I)(MeCN)_4]OTf$ with black precipitate. Attempted UV-vis spectra of the compounds resulted in precipitation of an unknown solid in the cuvette.

2. Results

2.1. Cyclic Voltammetry

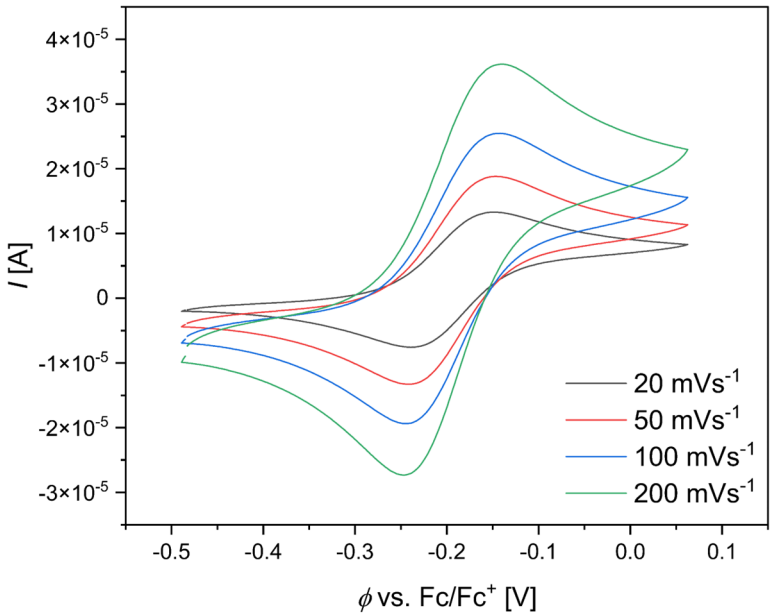


Figure S1: Cyclic voltammograms of the complex redox couple $[Cu(DMEG_3trphen)]^{+/2+}$ ($\mathbf{R1_{DMEG}}$) starting from $[Cu\{DMEG_3trphen\}]PF_6$ ($\mathbf{C1_{DMEG}}$) (c = 1 mM) in MeCN with $[NBu_4][PF_6]$ (c = 0.1 M).

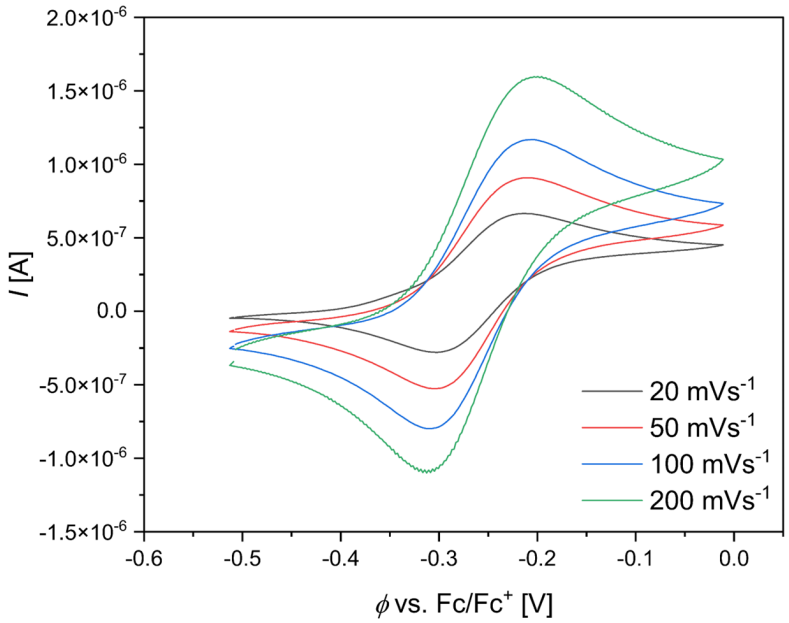


Figure S2: Cyclic voltammograms of the complex redox couple $[Cu\{N(QuMe)(PhTMG)_2\}]^{+/2+}$ (**R2$_{TMG}$**) starting from $[Cu(I)\{N(QuMe)(PhTMG)_2\}]PF_6$ (**C3$_{TMG}$**) (c = 1 mM) in MeCN with $[NBu_4][PF_6]$ (c = 0.1 M).

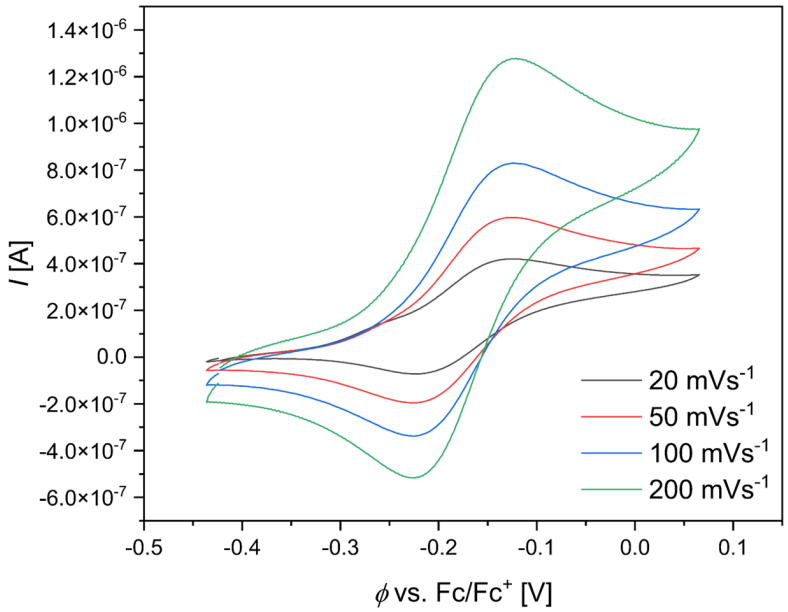


Figure S3: Cyclic voltammograms of the complex redox couple $[Cu\{N(QuMe)(PhDMEG)_2\}]^{+/2+}$ (**R2$_{DMEG}$**) starting from $[Cu(I)\{N(QuMe)(PhDMEG)_2\}]PF_6$ (**C3$_{DMEG}$**) (c = 1 mM) in MeCN with $[NBu_4][PF_6]$ (c = 0.1 M).

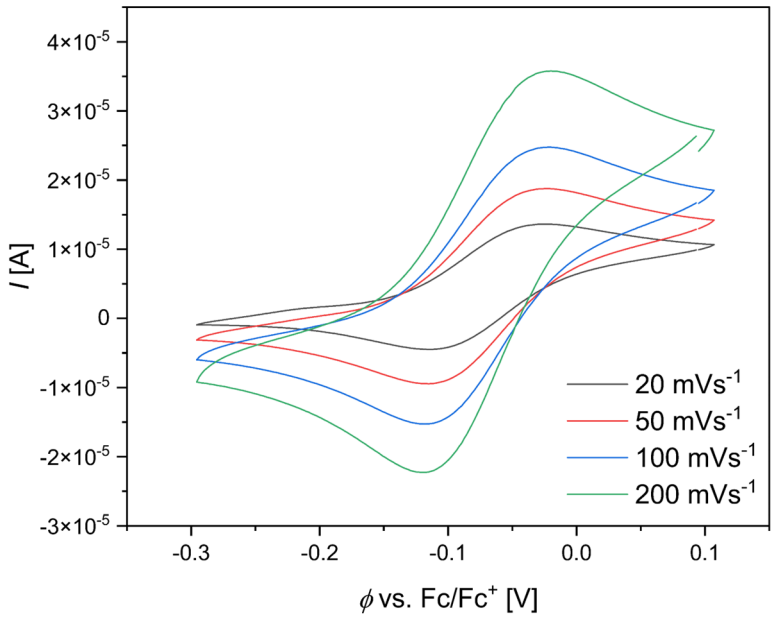


Figure S4: Cyclic voltammograms of the complex redox couple $[Cu\{N(QuMe)_2(PhTMG)\}]^{+/2+}$ (**R3$_{TMG}$**) starting from $[Cu(I)\{N(QuMe)_2(PhTMG)\}]PF_6$ (**C5$_{TMG}$**) (c = 1 mM) in MeCN with $[NBu_4][PF_6]$ (c = 0.1 M).

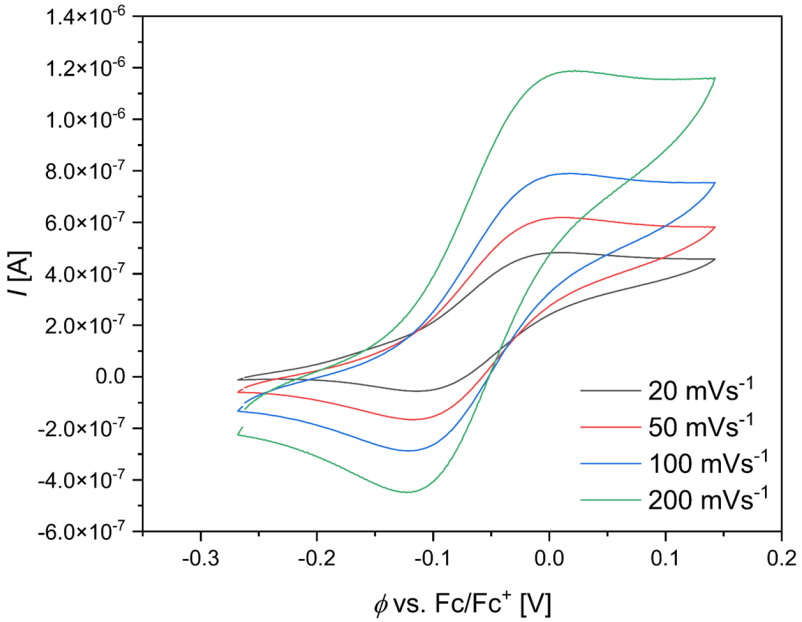


Figure S5: Cyclic voltammograms of the complex redox couple $[Cu\{N(QuMe)_2(PhDMEG)\}]^{+/2+}$ (**R3$_{DMEG}$**) starting from $[Cu(I)\{N(QuMe)_2(PhDMEG)\}]PF_6$ (**C5$_{DMEG}$**) (c = 1 mM) in MeCN with $[NBu_4][PF_6]$ (c = 0.1 M).

2.2. Kinetic Measurements via UV/Vis Stopped-Flow Spectroscopy

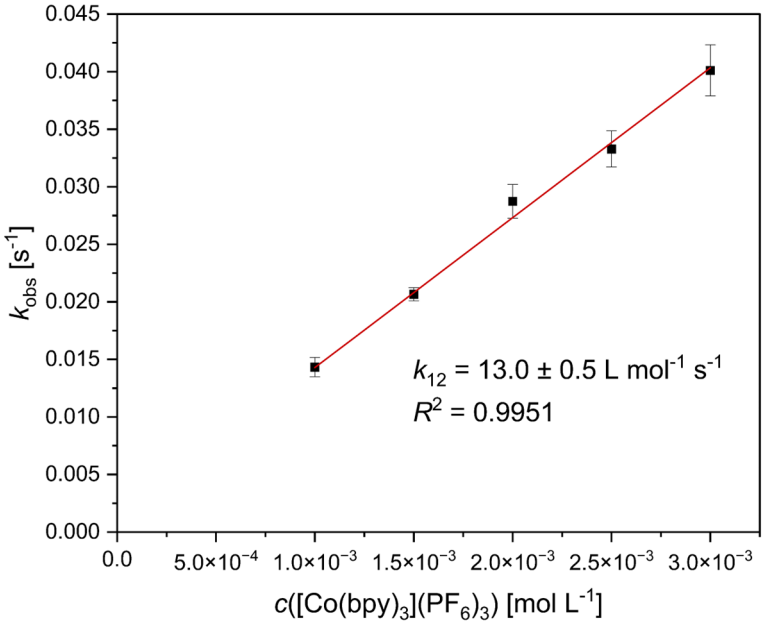


Figure S6: Plot of the reaction rate k_{obs} of the cross reaction between $[Cu(DMEG_3trphen)]PF_6$ (**C1$_{DMEG}$**) and $[Co(bpy)_3](PF_6)_3$ against the concentration of $[Co(bpy)_3](PF_6)_3$. Some error bars are too small to be visualized properly.

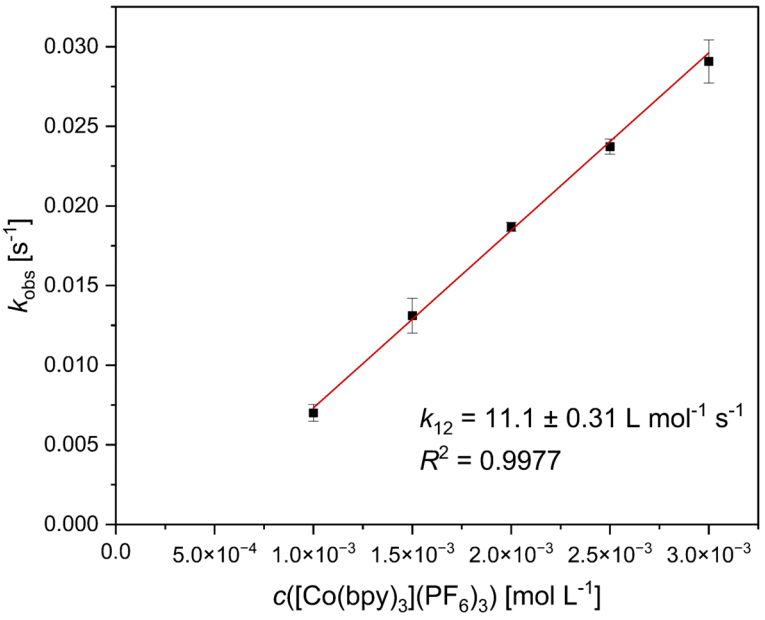


Figure S7: Plot of the reaction rate k_{obs} of the cross reaction between $[Cu(I)\{N(QuMe)(PhTMG)_2\}]PF_6$ (**C3$_{TMG}$**) and $[Co(bpy)_3](PF_6)_3$ against the concentration of $[Co(bpy)_3](PF_6)_3$. Some error bars are too small to be visualized properly.

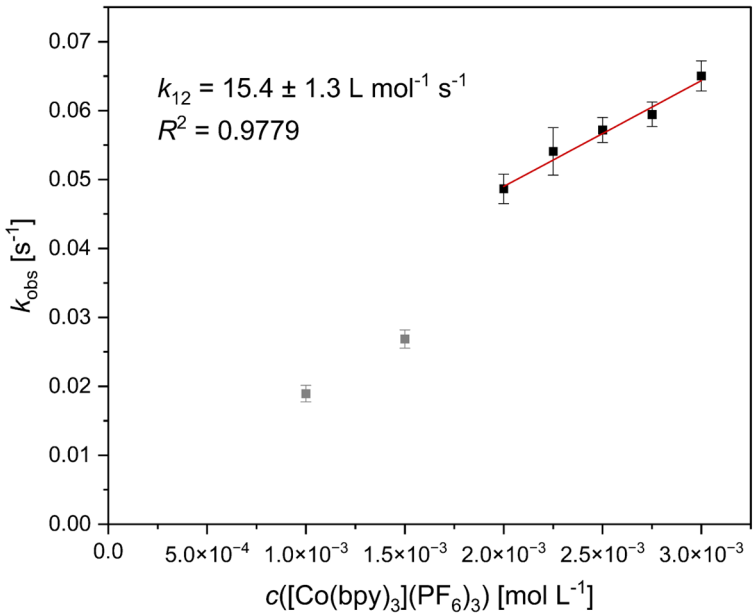


Figure S8: Plot of the reaction rate k_{obs} of the cross reaction between [Cu(I){N(QuMe)(PhDMEG)$_2$}]PF$_6$ (**C3$_{DMEG}$**) and [Co(bpy)$_3$](PF$_6$)$_3$ against the concentration of [Co(bpy)$_3$](PF$_6$)$_3$. Outliers are greyed out.

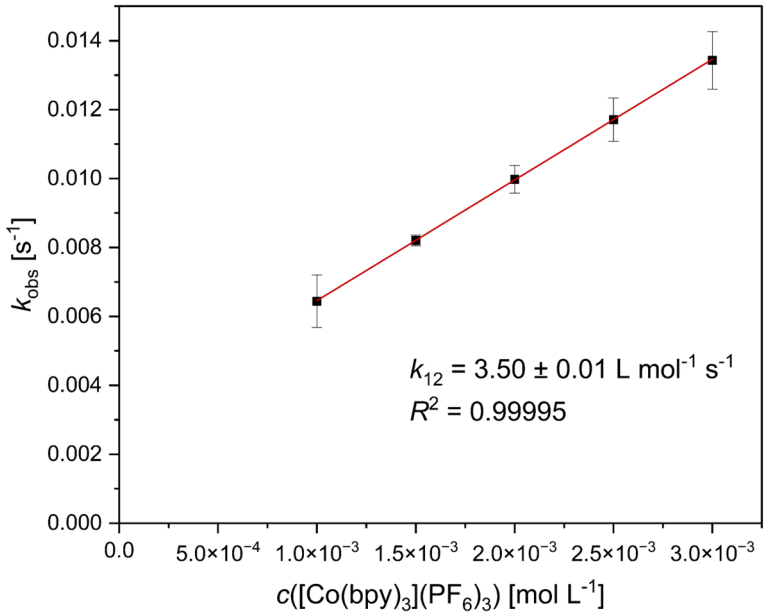


Figure S9: Plot of the reaction rate k_{obs} of the cross reaction between [Cu(I){N(QuMe)$_2$(PhTMG)}]PF$_6$ (**C5$_{TMG}$**) and [Co(bpy)$_3$](PF$_6$)$_3$ against the concentration of [Co(bpy)$_3$](PF$_6$)$_3$. Some error bars are too small to be visualized properly.

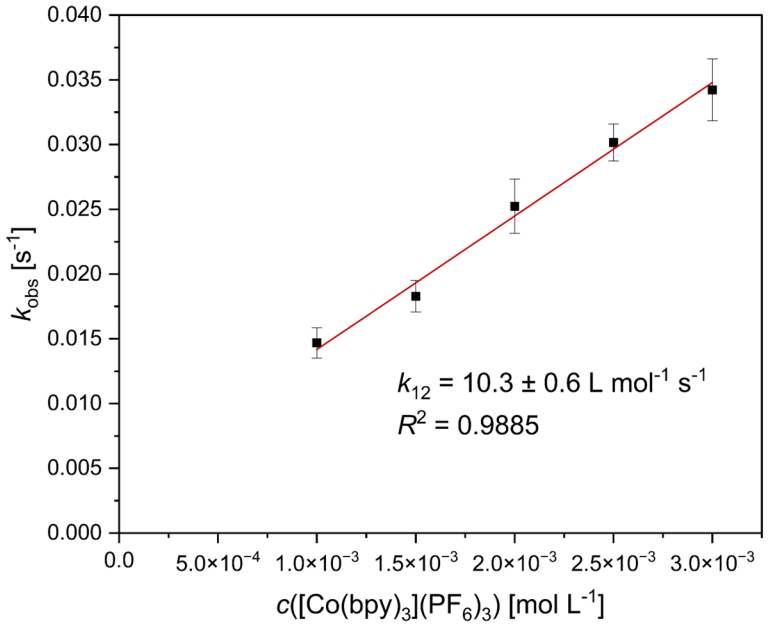


Figure S10: Plot of the reaction rate k_{obs} of the cross reaction between [Cu(I){N(QuMe)$_2$(PhDMEG)}]PF$_6$ (**C5$_{DMEG}$**) and [Co(bpy)$_3$](PF$_6$)$_3$ against the concentration of [Co(bpy)$_3$](PF$_6$)$_3$.

2.3. UV-vis Spectroscopic Measurements

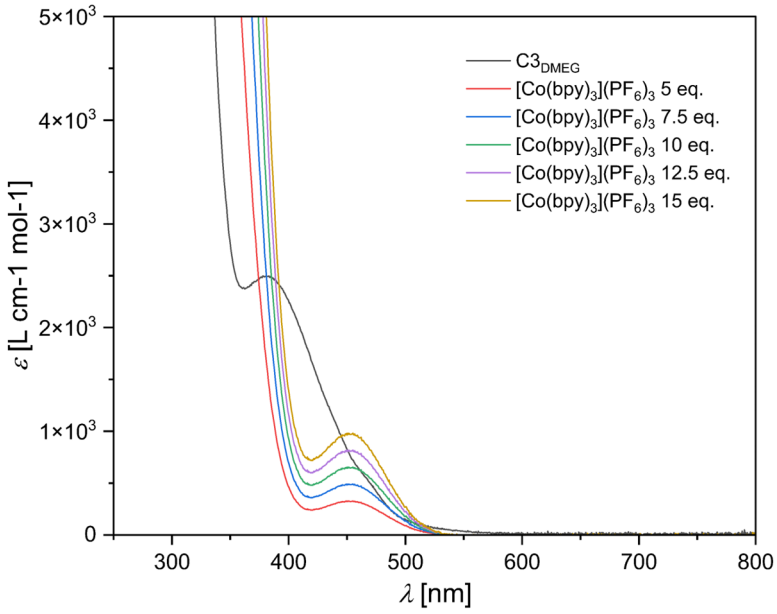


Figure S11: UV/Vis-spectra of **C3$_{DMEG}$** and [Co(bpy)$_3$](PF$_6$)$_3$. The latter are adjusted to the corresponding equivalents employed in the stopped-flow measurements.

2.4 Crystallographic Data

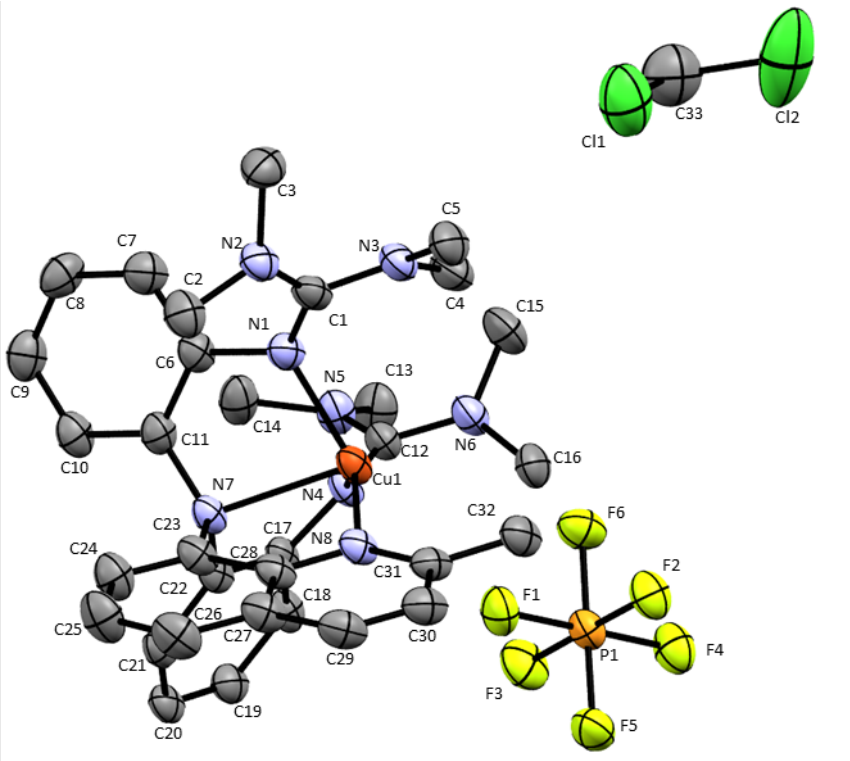


Figure S12: Molecular structure of [Cu{N(QuMe)(PhTMG)$_2$}]PF$_6$ (**C3$_{TMG}$**) in the solid state (ellipsoids drawn at 50 % probability level, asymmetric unit, H atoms are omitted for clarity). A strongly disordered molecules of pentane was removed via SQUEEZE.

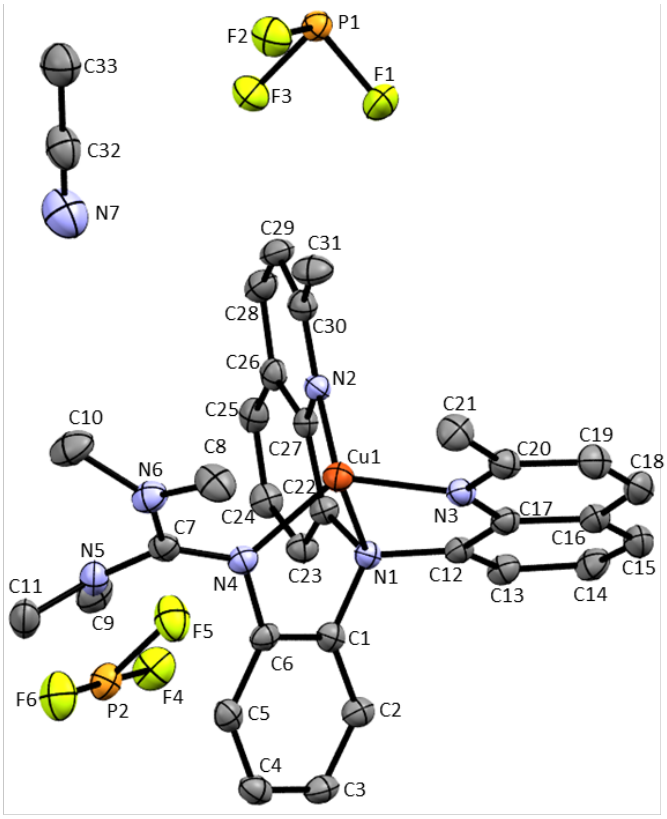


Figure S13: Molecular structure of [Cu{N(QuMe)$_2$(PhTMG)}]PF$_6$ (**C5$_{TMG}$**) in the solid state (50 % probability, asymmetric unit, H atoms are omitted for clarity).

Table S1: Crystallographic data of [Cu(N(QuMe)(PhTMG)$_2$)]PF_6 (**C3$_{TMG}$**) and [Cu(N(QuMe)$_2$(PhTMG))]PF_6 (**C5$_{TMG}$**). In **C3$_{TMG}$**, it was not possible to model the disordered molecule pentane per asymmetric unit adequately and the data sets were treated with the SQUEEZE routine as implemented in PLATON.

	C3$_{TMG}$	**C5$_{TMG}$**
Empirical formula	$C_{33}H_{42}Cl_2CuF_6N_8P$ [+C_5H_{12}]	$C_{33}H_{35}CuF_6N_7P$
Formular weight [g mol^{-1}]	830.15	738.19
Crystal size [mm]	0.320 x 0.310 x 0.280	0.220 x 0.150 x 0.070
Crystal system	monoclinic	monoclinic
Space group	$P2_1/n$	$P2/c$
a [Å]	10.622(2)	15.796(3)
b [Å]	28.710(6)	11.950(2)
c [Å]	13.779(3)	18.191(4)
α [°]	90	90
β [°]	103.09(3)	108.23(3)
γ [°]	90	90
V [Å^3]	4092.9(15)	3261.4(13)
Z	4	4
ρ [g cm^{-1}]	1.347	1.503
μ [mm^{-1}]	0.764	0.790
Wavelength[Å]	0.71073	0.71073
T [K]	100	100
F(000)	1712	1520
hkl range	$-12 \le h \le 12$,	$-15 \le h \le 20$,
	$-17 \le k \le 34$,	$-15 \le k \le 15$,
	$-16 \le l \le 16$	$-22 \le l \le 23$
Reflections collected	67893	49202
Independent reflections	7615	7117
$R_{int.}$	0.1157	0.0736
Number of parameters	469	441
Goodness-of-fit für F^2	1.059	0.956
R_1 [$I > 2\sigma(I)$]	0.0641	0.0516
wR_2 (all data)	0.1642	0.1371
Largest diff. Peak, hole [e Å^{-3}]	1.475, -1.391	0.877, -0.610

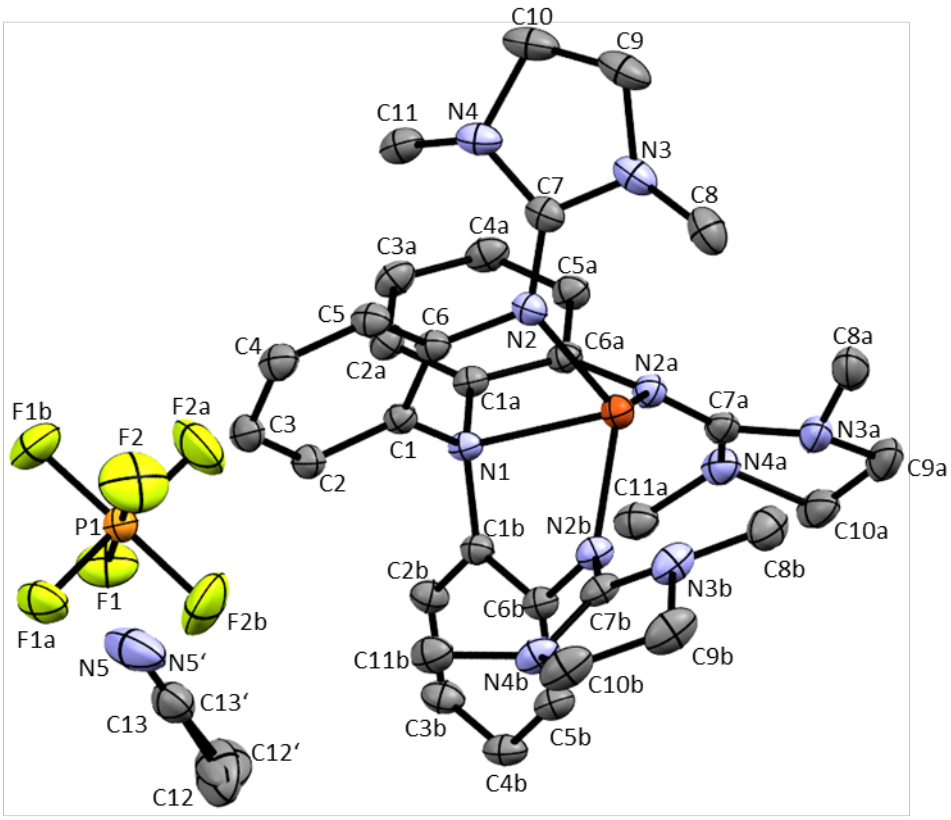


Figure S14: Molecular structure of [Cu(DMEG$_3$trphen)]PF$_6$ (**C1$_{DMEG}$**) in the solid state (50 % probability, H atoms are omitted for clarity).

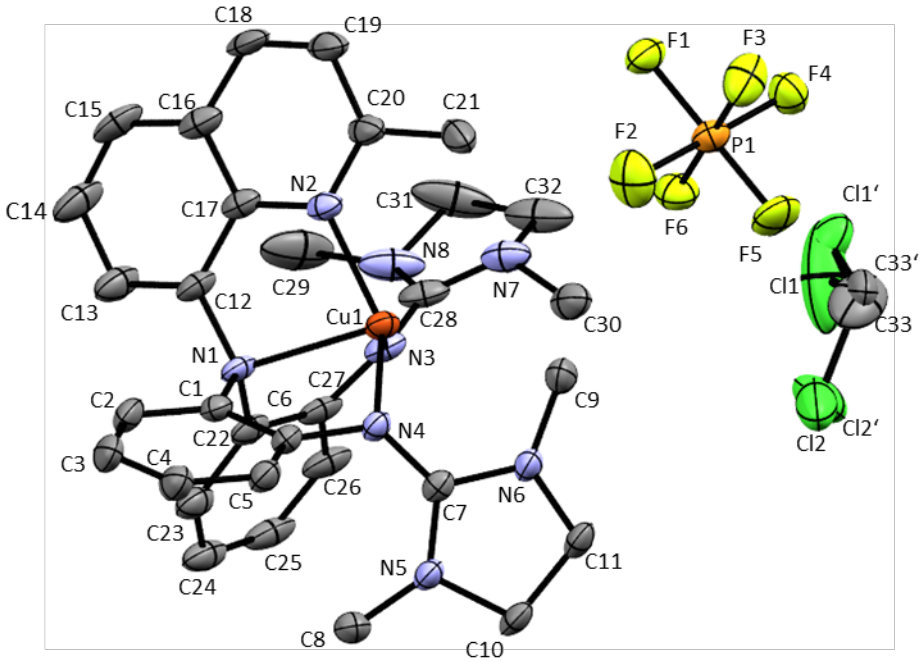


Figure S15: Molecular structure of [Cu{N(QuMe)(PhDMEG)$_2$}]PF$_6$ (**C3$_{DMEG}$**) in the solid state (50 % probability, asymmetric unit, H atoms are omitted for clarity).

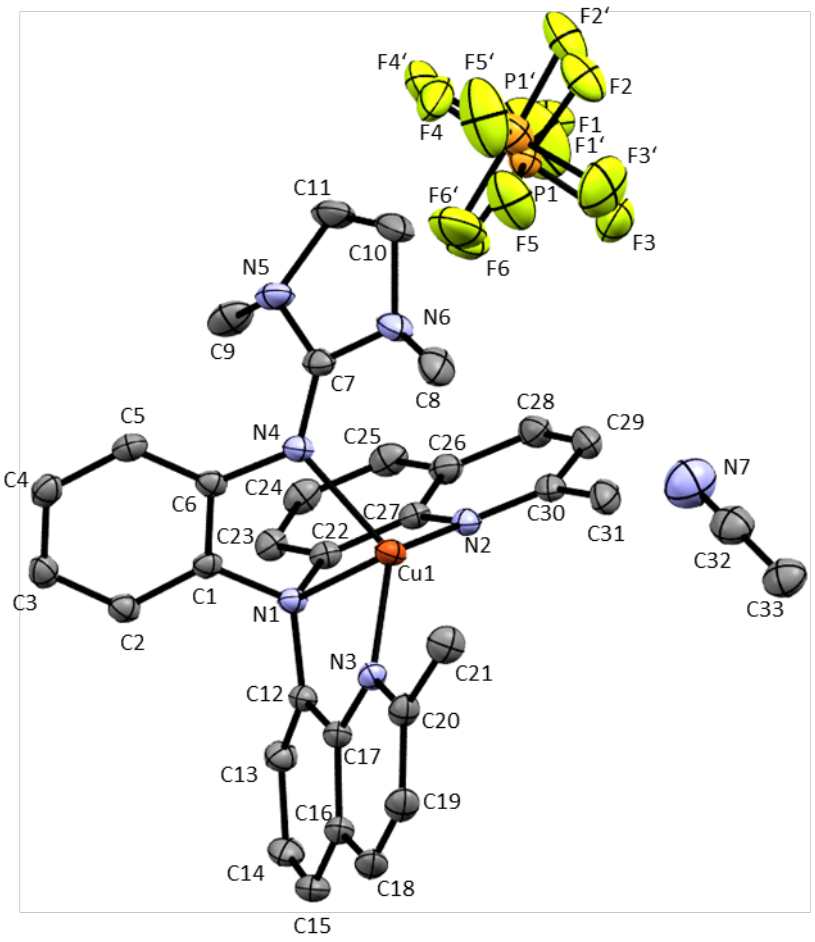


Figure S16: Molecular structure of [Cu{N(QuMe)$_2$(PhDMEG)}]PF_6 (**C5$_{DMEG}$**) in the solid state (50 % probability, asymmetric unit, H atoms are omitted for clarity).

Table S2: Crystallographic data of $[Cu(DMEG_3trphen)]PF_6$ (**C1$_{DMEG}$**), $[Cu\{N(QuMe)(PhDMEG)_2\}]PF_6$ (**C3$_{DMEG}$**) and $[Cu\{N(QuMe)_2(PhDMEG)\}]PF_6$ (**C5$_{DMEG}$**).

	C1$_{DMEG}$	**C3$_{DMEG}$**	**C5$_{DMEG}$**
Empirical formula	$C_{72}H_{93}Cu_2F_{12}N_{23}P_2$	$C_{33}H_{38}Cu_1F_6N_8P_1Cl_2$	$C_{33}H_{33}Cu_1F_6N_7P_1$
Formular weight [g mol^{-1}]	1697.71	826.12	736.17
Crystal size [mm]	0.230 x 0.150 x 0.120	0.147 x 0.073 x 0.060	0.220 x 0.200 x 0.110
Crystal system	trigonal	triclinic	triclinic
Space group	$R\bar{3}c$	$P\bar{1}$	$P\bar{1}$
a [Å]	14.977(2)	9.0207(18)	10.893(2)
b [Å]	14.977(2)	14.171(3)	12.015(2)
c [Å]	59.777(12)	15.375(3)	15.064(3)
α [°]	90	69.15(3)	66.91(3)
β [°]	90	81.46(3)	85.07(3)
γ [°]	120	73.01(3)	63.15(3)
V [Å^3]	11613(4)	1754.2(8)	1608.1(8)
Z	6	2	2
ρ [g cm^{-1}]	1.457	1.564	1.520
μ [mm^{-1}]	0.679	0.891	0.800
Wavelength[Å]	0.71073	0.71073	0.71073
T [K]	100	100	100
F(000)	5292	848	756
hkl range	$-22 \le h \le 22$, $-22 \le k \le 18$, $-88 \le l \le 88$	$-12 \le h \le 12$, $-19 \le k \le 19$, $-21 \le l \le 16$	$-15 \le h \le 15$, $-17 \le k \le 11$, $-21 \le l \le 21$
Reflections collected	84855	53162	59631
Independent reflections	4459	9063	8712
$R_{int.}$	0.0874	0.1238	0.0536
Number of parameters	172	493	502
Goodness-of-fit für F^2	1.067	0.963	1.052
R_1 [$I > 2\sigma(I)$]	0.0359	0.0494	0.0325
wR_2 (all data)	0.1030	0.0882	0.0895
Largest diff. Peak, hole [e Å^{-3}]	0.435, -0.713	0.696, -0.616	0.486, -0.337

3. Marcus Theory

The Marcus theory describes the outer-sphere electron-transfer between two metal complexes.[20] If two metal complexes that only differ in charge (C_1 and C_1^+ or C_2 and C_2^+) partake in such a reaction, it is called a self-exchange reaction, while a reaction between two different systems (e.g. C_1 and C_2^+) is referred to as a cross-reaction (see Scheme S1). In this work, complex C_1 corresponds to the $[Cu(I)L]^+$ complexes and complex C_2^+ corresponds to the counter complex $[Co(bpy)_3]^{3+}$.

$$C_1 + C_2^+ \xrightarrow{k_{12}} C_1^+ + C_2$$
$$C_2 + C_2^+ \xrightarrow{k_{22}} C_2^+ + C_2$$
$$C_1 + C_1^+ \xrightarrow{k_{11}} C_1^+ + C_1$$

Scheme S1: Schematic representations of the cross-reaction and the two self-exchange reaction that can occur between two redox couples.

Using the Marcus cross relation, which emerges from the Marcus theory, the cross-reaction rate (k_{12}) of an outer-sphere electron-transfer between two metal complexes can be utilized together with one self-exchange rate (e.g. k_{22}) to determine the remaining self-exchange rate (here: k_{11}).

$$k_{11} = \frac{{k_{12}}^2}{k_{22} \cdot K_{12} \cdot f_{12} \cdot {W_{12}}^2} \tag{1}$$

In this equation, K_{12} represents the equilibrium constant of the cross reaction. It depends on the difference between the redox potentials ΔE_{12} of the involved complexes' redox couples (C_1/C_1^+ and C_2/C_2^+).

$$K_{12} = \exp\left(\frac{\Delta E_{1/2} \cdot \mathrm{n} \cdot \mathrm{F}}{\mathrm{R} \cdot T}\right) \tag{2}$$

W_{12} is the work term and describes the electrostatic work that occurs during the cross reaction (Equation 3). It includes the electrostatic work w_{ij} that must be overcome for the approach of two complex cations and which is shown in Equation 5.

$$W_{12} = \exp\left(\frac{w_{11} + w_{22} - w_{12} - w_{21}}{2 \cdot \mathrm{R} \cdot T}\right) \tag{3}$$

f_{12} represents a correction term that adjusts the obtained rate constant to account for differences in reorganization energy and driving force between the self-exchange reactions and the cross-reaction.

$$f_{12} = \exp\left(\frac{\left(\ln K_{12} + \frac{w_{12} - w_{21}}{\mathrm{R} \cdot T}\right)^2}{4 \cdot \left(\ln\left(\frac{k_{22} \cdot k_{22}}{Z^2}\right) + \frac{w_{11} + w_{22}}{\mathrm{R} \cdot T}\right)}\right) \quad (4)$$

Z^2 represents the formation constant of the outer-sphere complex and is usually 10^{22} M^{-2} s^{-2}.[21,22]

The term w_{ij} must be considered for each possible permutation of the cation C_1, C_1^+, C_2 and C_2^+.

$$w_{ij} = \frac{Z_i \cdot Z_j \cdot e^2 \cdot N_A}{\varepsilon \cdot (a_i + a_j) \cdot (1 + \beta \cdot (a_i + a_j) \cdot \sqrt{\mu})} \quad (5)$$

$Z_{i/j}$ represents the cation's corresponding charge, $a_{i/j}$ is corresponding radius that has been determined for the employed complexes *via* the averaged collision diameter of the optimized DFT structures. ε is the permittivity of the solvent, μ is the ionic strength. The parameter β describes the Debye-Hückel constant and is described as follows:

$$\beta = \sqrt{\frac{8 \cdot \pi \cdot e^2 \cdot N_A}{1000 \cdot \varepsilon \cdot k_B \cdot T}} \quad (6)$$

The temperature T amounts to 298.15 K, $k_B = 1.38 \cdot 10^{-23}$. The constants and parameters used in this work are listed in Table S3.

Table S3: Used parameters and constants to determine the self-exchange rates of the studied complexes in this work.

r_{Cu}	[nm]	0.57
r_{Co}	[nm]	0.70
$E_{1/2}$ (Co)	[V] vs Fc/Fc^+	-0.056
k_{22}	[L mol^{-1} s^{-1}]	0.645
β	[$m^{0.5}$ mol^{-1}]	$4.88 \cdot 10^{-6}$
w_{11}	[J mol^{-1}]	$6.78 \cdot 10^{3}$
w_{12}	[J mol^{-1}]	$9.13 \cdot 10^{3}$
w_{21}	[J mol^{-1}]	$1.22 \cdot 10^{4}$
w_{22}	[J mol^{-1}]	$1.65 \cdot 10^{4}$
W_{12}	[ ]	1.51
k_B	[J K^{-1}]	$1.38 \cdot 10^{-23}$
E_{MeCN}	[C V^{-1} m^{-1}]	$3.97 \cdot 10^{-9}$
μ	[mol m^{-3}]	1.60

4. Computational Details

4.1 General

Density functional theory (DFT) calculations were performed with Gaussian 16, Revision B.01 using the default UltraFine grid (a 99,590 grid).[23] The geometry optimizations were started from the corresponding [Cu(I)L] solid state structures and conducted using the TPSSh functional[24,25] and with the Ahlrichs type basis set def2-TZVP[26–28] as implemented in Gaussian 16, Revision B.01. As solvent model, the Polarizable Continuum Model (PCM) was used as implemented in Gaussian 16. As empirical dispersion correction, the D3 dispersion with Becke–Johnson damping was used as implemented in Gaussian 16, Revision B.01.[29–31] Frequency calculations did not show imaginary values. For visualization and extraction of the calculated structural information Chemcraft (Version 1.8) was used. Calculated energy values were extracted directly from the output files using notepad++ (Version 7.8.1). The xyz-coordinates of every optimized geometry as well as their single point energies are listed under section 6.

4.2 Reorganization Energies

4.2.1 Theoretical Background

The total reorganization energy $\lambda_{11,T}$ of the whole electron self-exchange is divided in the internal reorganization energy $\lambda_{11,I}$ and the solvent reorganization energy $\lambda_{11,S}$ of the whole electron self-exchange (Equation 7).

$$\lambda_{11,T} = \lambda_{11,S} + \lambda_{11,I} \quad (7)$$

The total reorganization energy $\lambda_{11,T}$ and the internal reorganization energy $\lambda_{11,I}$ were calculated using DFT calculations and Nelsen's four-point method. The solvent reorganization energies $\lambda_{11,S}$ were obtained as the difference between the total and the internal reorganization energy.

The computations of the reorganization energies were performed using the tetra-coordinate Cu(I) and Cu(II) geometries of the redox pairs **P1**, **P2** and **P3**. Their coordinates are listed in section 6 under **[Cu(I)L]** and **[Cu(II)L]** for the corresponding oxidation state. The following explanation always refers to complexes of the same redox couple.

The total reorganization energy ($\lambda_{Cu(I),T}$ for Cu(I) and $\lambda_{Cu(II),T}$ for Cu(II)) of each complex is calculated with its optimized ground state energy ($E_{Cu(I)L(I)S(I)}$ for Cu(I) and $E_{Cu(II)L(II)S(II)}$ for Cu(II)) and the energy of the complex with the same oxidation state but structure and solvent sphere of the complementary complex ($E_{Cu(I)L(II)S(II)}$ for Cu(I) and $E_{Cu(II)L(I)S(I)}$ for Cu(II), Equation 8). The indices Cu(I) or Cu(II) represent the oxidation state, L(I) or L(II) represent the ground state complex structure of the appropriate oxidation state and S(I) or S(II) represent the ground state solvent sphere of the appropriate oxidation state. In Fig. S17 (left) the energies $E_{Cu(I)}(x)$ and $E_{Cu(II)}(x)$ of the Cu(I) and Cu(II) complex are functions of the complex structure and the solvent sphere which are represented by the variable x_{LS}. The ground state complex structures and ground state solvent spheres for each oxidation state are represented by $x_{L(I)S(I)}$ and $x_{L(II)S(II)}$.

$$\lambda_{11,T} = \lambda_{Cu(II),T} + \lambda_{Cu(I),T} = (E_{Cu(II)L(I)S(I)} - E_{Cu(II)L(II)S(II)}) + (E_{Cu(I)L(II)S(II)} - E_{Cu(I)L(I)S(I)}) \quad (8)$$

The internal reorganization energy $\lambda_{11,I}$ for the whole electron self-exchange is the sum of the internal reorganization energies $\lambda_{Cu(I),I}$ and $\lambda_{Cu(II),I}$. λ_I of each complex is calculated with its optimized ground state energy ($E_{Cu(I)L(I)S(I)}$ for Cu(I) and $E_{Cu(II)L(II)S(II)}$ for Cu(II)) and the energy of the complex with the same oxidation state but with the structure of the complementary

complex ($E_{Cu(I)L(II)S(I)}$ for Cu(I) and $E_{Cu(II)L(I)S(II)}$ for Cu(II)). In contrast to the total reorganization energy, the solvent sphere is allowed to relax for the calculated oxidation state.

$$\lambda_{11,I} = \lambda_{Cu(II),I} + \lambda_{Cu(I),I} = (E_{Cu(II)L(I)S(I_I)} - E_{Cu(II)L(II)S(II)}) + (E_{Cu(I)L(II)S(I)} - E_{Cu(I)L(I)S(I)}) \quad (9)$$

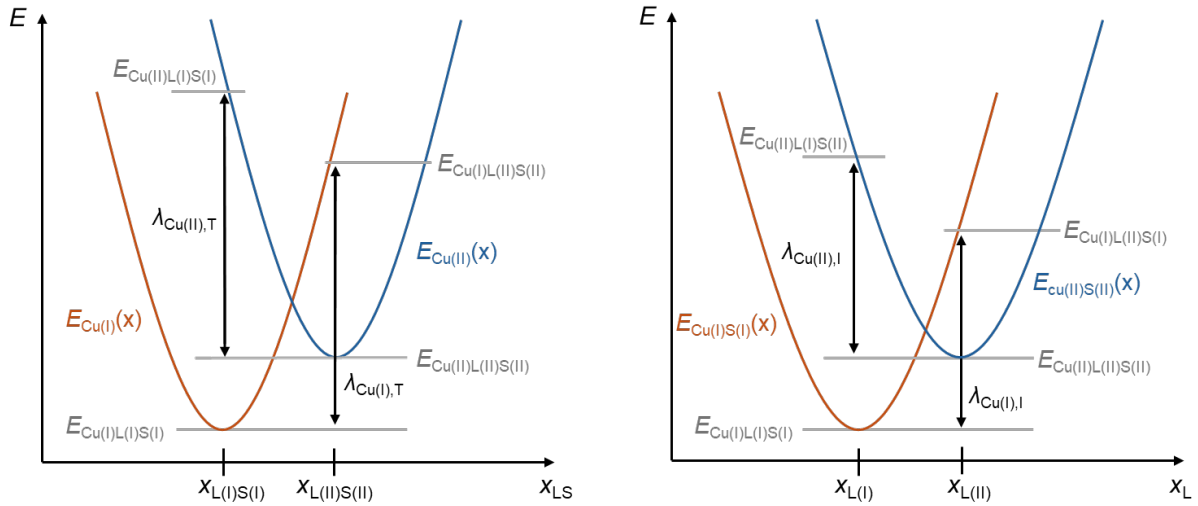


Figure S17: Schematic illustration of the Nelsen's four-point method for the calculation of the total reorganization energy $\lambda_{11,T}$ (left) and the internal reorganization energy $\lambda_{11,I}$ (right).

The keywords used in the computations of this procedure were chosen as described by Herres-Pawlis *et al.*[32]

4.3 Isodesmic Calculations

4.3.1 Cu(II) Systems

The isodesmic calculations of the Cu(II) systems were performed to determine whether tetra-coordinate [Cu(II)L] or penta-coordinate [Cu(II)LS] environments are preferred by the studied systems. For this, the reaction scheme shown in Scheme S2 was assumed. If more than one [Cu(II)L(MeCN)] species was available, the one lying lowest in energy was chosen.

$$[Cu(II)L] + MeCN \rightleftharpoons [Cu(II)L(MeCN)]$$

Scheme S2: Reaction equation for the coordination change of a [Cu(II)L] species by coordination of a MeCN molecule.

Each described species was optimized using DFT (*vide supra*) and the energy differences were subsequently calculated according to Equation 10.

$$\Delta E_{DFT} = E_{DFT,[Cu(II)L(MeCN)]} - E_{DFT,[Cu(II)L]} - E_{DFT,MeCN} \quad (10)$$

With $E_{DFT,X}$ being the single point energy of the species described in the above scheme. The resulting energy differences are listed in Table S4. The individual single point energies can be found in section 6.

Table S4: Obtained energy differences of the coordination of acetonitrile on a tetra-coordinate [Cu(II)L] species for the employed ligand L. The penta-coordinate [Cu(II)L(MeCN)] species was set as the product.

Employed ligand for [Cu(II)L]	ΔE_{DFT} [kJ/mol]
TMG_3trphen **($L1_{TMG}$)**	-57.57
$DMEG_3$trphen **($L1_{DMEG}$)**	-69.26
N(QuMe)$(PhTMG)_2$ **($L2_{TMG}$)**	-61.65
N(QuMe)$(PhDMEG)_2$ **($L2_{DMEG}$)**	-65.14
N(QuMe)$(PhTMG)_2$ **($L3_{TMG}$)**	-68.25
N(QuMe)$(PhTMG)_2$ **($L3_{DMEG}$)**	-67.00

4.3.2 Cu(I) Systems

The isodesmic calculations for the Cu(I) systems were performed to approximate the equilibrium constants of the reaction depicted in Scheme S3.

$$[Cu(I)L] + MeCN \rightleftharpoons [Cu(I)L(MeCN)]$$

Scheme S3: Reaction equation for the coordination change of a [Cu(I)L] species by coordination of a MeCN molecule.

Each side of the reaction was optimized using DFT (*vide supra*) and the energy differences were subsequently calculated according to Equation 11.

$$\Delta E_{DFT} = E_{DFT,[Cu(II)L(MeCN)]} - E_{DFT,[Cu(II)L] + MeCN} \quad (11)$$

Since smaller energy differences were expected compared to the Cu(II) systems, the acetonitrile was not added separately but included in the [Cu(I)L]+MeCN geometry to improve the accuracy of the calculation. To account for thermodynamic effects on the equilibrium, the electronic energy was converted into Gibb's free enthalpy at standard conditions using the correction terms from the frequency computations (see section 6). To approximate the equilibrium constant K_a, Equation (12) was used.

$$\Delta E_{DFT} = E_{DFT,[Cu(II)L(MeCN)]} - E_{DFT,[Cu(II)L] + MeCN} \quad (12)$$

The individual single point energies and correction terms can be found in section 6.

4.4 Scans

Scans of the [Cu(II)L(MeCN)] geometries were conducted to determine a potential energy barrier of the CN change from tetra-coordinate [Cu(II)L] to penta-coordinate [Cu(II)L(MeCN)] species.

The scans were performed using the previously optimized [Cu(II)L(MeCN)] geometries as a starting point, utilizing the above mentioned functional and dispersion correction together with the def2-SVP basis set. The optimization was performed using the opt=modredundant keyword, incrementally increasing the $Cu–N_{MeCN}$ bond by 0.4 Å in 15 steps, scanning a range of distance of up to 6 Å. The scans faced frequent crashes or failed to optimize certain geometries, yielding only incomplete results for the studied systems. Sub-dividing the scans into multiple computations of 4 steps each did not alleviate these problems. The described limitations were especially impeding the analysis of geometries featuring ligand $\mathbf{L1_{TMG}}$, leading to no results for $\mathbf{C2_{TMG}}$. Plots of the conducted scans are included below.

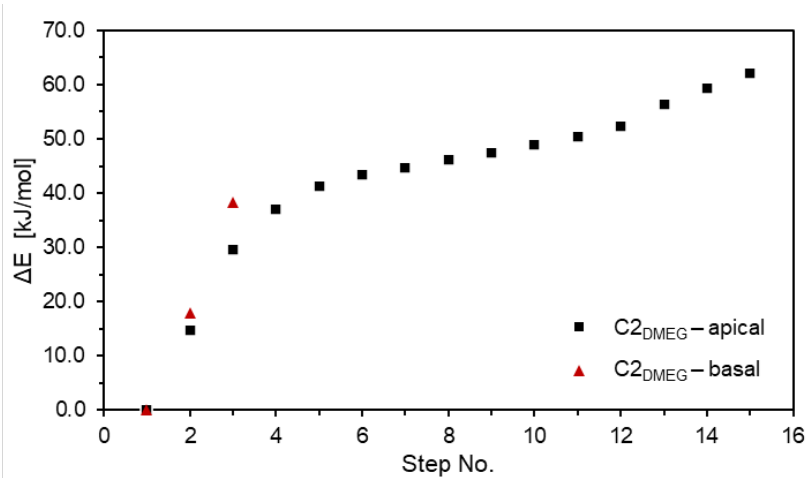


Figure S18: Plot of the difference in electronic energy of each scan step relative to the initial geometry (step 1) for all conformers of $[Cu(II)(DMEG_3trphen]^{2+}$ ($\mathbf{C2_{DMEG}}$).

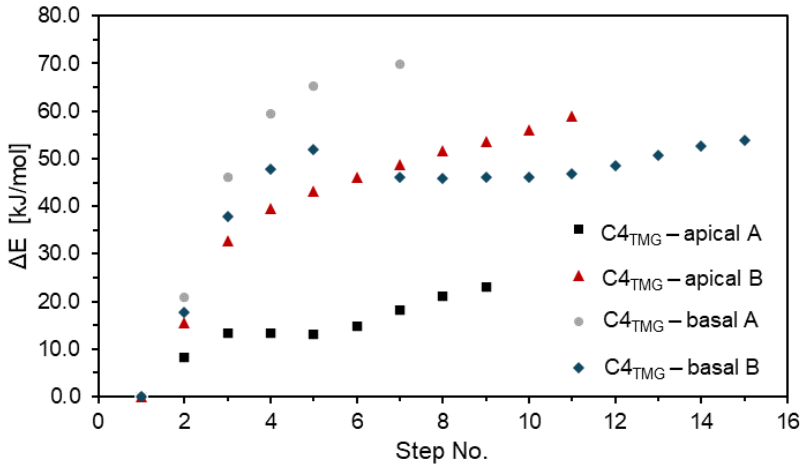


Figure S19: Plot of the difference in electronic energy of each scan step relative to the initial geometry (step 1) for all conformers of $[Cu\{N(QuMe)(PhTMG)_2\}]^{2+}$ (**$C4_{TMG}$**).

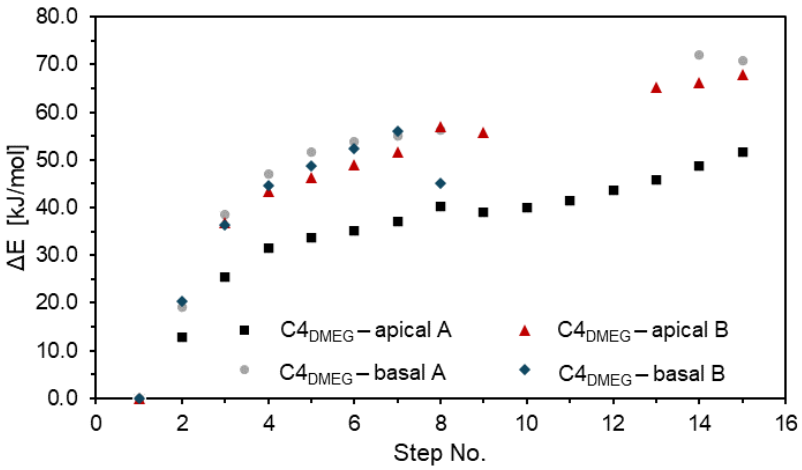


Figure S20: Plot of the difference in electronic energy of each scan step relative to the initial geometry (step 1) for all conformers of $[Cu\{N(QuMe)(PhDMEG)_2\}]^{2+}$ (**$C4_{DMEG}$**).

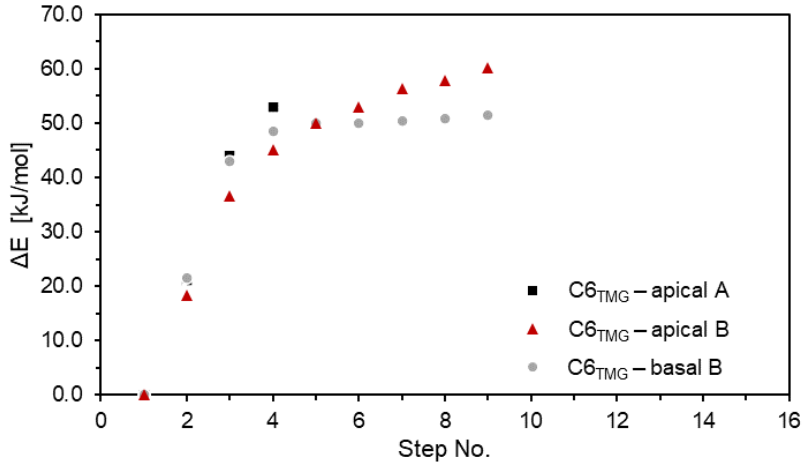


Figure S21: Plot of the difference in electronic energy of each scan step relative to the initial geometry (step 1) for all conformers of $[Cu\{N(QuMe)_2(PhTMG)\}]^{2+}$ (**$C6_{TMG}$**).

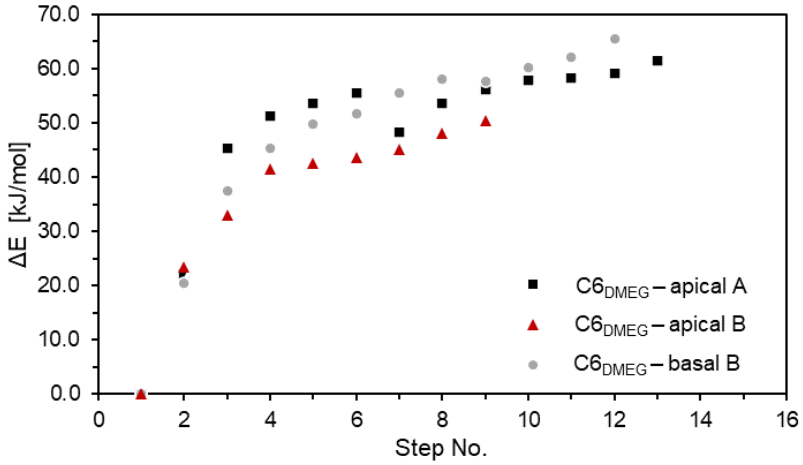


Figure S22: Plot of the difference in electronic energy of each scan step relative to the initial geometry (step 1) for all conformers of $[Cu\{N(QuMe)_2(PhDMEG)\}]^{2+}$ (**$C6_{DMEG}$**).

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6. Coordinates and Single-Point Energies

6.5.1 [Cu(I)L] Geometries

$[Cu(I)(TMG_3trphen)]^+$ ($C1_{TMG}$)

Cu	0.000381000	0.001604000	0.742798000
N	-0.004620000	-0.002000000	-1.579410000
C	-0.201402000	-1.398720000	-1.832288000
C	0.265848000	-2.319004000	-0.870045000
C	0.098179000	-3.687169000	-1.129994000
H	0.432917000	-4.405201000	-0.390083000
C	-0.528856000	-4.124731000	-2.289598000
H	-0.656725000	-5.187994000	-2.457437000
C	-1.016169000	-3.205996000	-3.218096000
H	-1.519156000	-3.543989000	-4.115922000
C	-0.846823000	-1.846068000	-2.982337000
H	-1.218464000	-1.114185000	-3.690009000
N	0.751172000	-1.843755000	0.352462000
C	1.742040000	-2.462059000	0.970762000
N	2.790714000	-3.050223000	0.327400000
C	3.191153000	-2.622996000	-1.002369000
H	2.824834000	-1.615928000	-1.187607000
H	2.803492000	-3.291300000	-1.778491000
H	4.282962000	-2.620776000	-1.051324000
C	3.423240000	-4.266132000	0.820639000
H	2.911839000	-4.607985000	1.717233000
H	4.480844000	-4.102059000	1.046378000
H	3.347750000	-5.043432000	0.053399000
N	1.754775000	-2.497294000	2.330262000
C	0.516953000	-2.287218000	3.058743000
H	-0.315262000	-2.690782000	2.487319000
H	0.332320000	-1.221483000	3.242022000
H	0.586301000	-2.799433000	4.020274000
C	2.984493000	-2.336441000	3.097859000
H	3.824497000	-2.210333000	2.419276000
H	3.165359000	-3.200630000	3.742137000
H	2.903874000	-1.444445000	3.726314000
C	-1.115978000	0.865936000	-1.834242000
C	-2.144441000	0.926668000	-0.870194000
C	-3.244879000	1.756406000	-1.131577000
H	-4.032311000	1.830061000	-0.390230000
C	-3.311985000	2.512786000	-2.294657000
H	-4.168418000	3.155497000	-2.463478000
C	-2.275008000	2.469491000	-3.225553000
H	-2.317504000	3.069817000	-4.126178000
C	-1.182336000	1.642934000	-2.987983000
H	-0.364147000	1.594229000	-3.697075000
N	-1.973929000	0.273555000	0.354759000
C	-3.004432000	-0.271760000	0.977174000
N	-4.039621000	-0.887911000	0.338215000
C	-3.871994000	-1.455282000	-0.988958000
H	-2.817134000	-1.643700000	-1.174591000
H	-4.257272000	-0.789124000	-1.768081000
H	-4.417121000	-2.401529000	-1.032247000
C	-5.408170000	-0.824249000	0.833121000
H	-5.447011000	-0.205258000	1.726233000
H	-5.795087000	-1.820679000	1.065184000
H	-6.044520000	-0.374185000	0.064334000
N	-3.038332000	-0.258529000	2.336639000
C	-2.234507000	0.711318000	3.058219000
H	-2.170097000	1.631668000	2.483056000
H	-1.218422000	0.339024000	3.238390000
H	-2.708569000	0.910848000	4.021123000
C	-3.511471000	-1.400172000	3.111187000
H	-3.825923000	-2.193490000	2.437642000
H	-4.347147000	-1.120622000	3.757765000
H	-2.696477000	-1.774725000	3.737715000
C	1.302125000	0.525839000	-1.838646000
C	1.871124000	1.389500000	-0.878781000
C	3.139463000	1.926432000	-1.144726000
H	3.598272000	2.574402000	-0.406663000
C	3.825947000	1.601620000	-2.307767000
H	4.810533000	2.021093000	-2.480081000
C	3.267995000	0.721872000	-3.234228000
H	3.807488000	0.454709000	-4.134729000
C	2.006014000	0.190409000	-2.992435000
H	1.553462000	-0.496659000	-3.697934000
N	1.223192000	1.572392000	0.347216000
C	1.269439000	2.738478000	0.967441000
N	1.251516000	3.942073000	0.326892000
C	0.672811000	4.078425000	-0.998945000
H	-0.018018000	3.258598000	-1.181385000
H	1.440321000	4.077714000	-1.780096000
H	0.125578000	5.023444000	-1.042463000
C	1.992182000	5.096454000	0.817667000
H	2.550786000	4.822135000	1.709284000
H	1.323209000	5.929866000	1.050666000
H	2.697214000	5.421505000	0.045784000
N	1.301882000	2.763208000	2.326853000
C	1.741914000	1.583343000	3.049082000
H	2.498943000	1.062048000	2.468466000
H	0.910632000	0.893620000	3.240433000
H	2.162461000	1.896246000	4.006706000
C	0.552815000	3.745654000	3.101997000
H	0.021533000	4.413906000	2.428835000
H	1.214922000	4.330434000	3.745634000
H	-0.177552000	3.228536000	3.731499000

E(RTPSSh) = -3475.32936825
Zero-point correction = 0.780535 (Hartree/Particle)
Thermal correction to Energy = 0.828723
Thermal correction to Enthalpy = 0.829667
Thermal correction to Gibbs Free Energy = 0.699859

$[Cu(I)(DMEG_3trphen)]^+$ ($C1_{DMEG}$)

Cu	-0.000197000	-0.000971000	0.812180000
N	-0.001568000	0.001310000	-1.552243000
N	-1.796352000	-0.843481000	0.364236000
N	-3.074357000	-0.165434000	2.203646000
N	-4.179052000	-0.459128000	0.280030000
C	-0.692515000	-1.230067000	-1.753355000
C	-0.409824000	-2.056231000	-2.837240000
H	0.354961000	-1.749234000	-3.541235000
C	-1.097782000	-3.251912000	-3.012351000
H	-0.872537000	-3.888715000	-3.859288000
C	-2.079461000	-3.618803000	-2.092753000
H	-2.621269000	-4.549347000	-2.217259000
C	-2.355704000	-2.808672000	-0.998048000
H	-3.095650000	-3.110977000	-0.265969000
C	-1.665127000	-1.605661000	-0.802331000
C	-2.952793000	-0.526696000	0.889147000
C	-2.141113000	-0.629769000	3.210370000
H	-2.119299000	0.077767000	4.039225000
H	-1.146167000	-0.693122000	2.765345000
H	-2.420636000	-1.621033000	3.586591000
C	-4.488781000	-0.064402000	2.560214000
H	-4.661285000	0.754814000	3.257616000
H	-4.825935000	-1.000836000	3.021252000
C	-5.139753000	0.159719000	1.202318000
H	-6.120062000	-0.307048000	1.113045000
H	-5.231460000	1.228270000	0.973986000
C	-4.338919000	-0.113932000	-1.126750000
H	-5.350530000	-0.383239000	-1.431263000
H	-3.631319000	-0.665193000	-1.738120000
H	-4.188424000	0.959585000	-1.283010000
N	1.628117000	-1.133522000	0.362185000
N	1.680384000	-2.581175000	2.200109000
N	2.489942000	-3.388047000	0.276444000
C	1.410280000	0.019215000	-1.753507000
C	1.983909000	0.678635000	-2.836739000
H	1.335395000	1.188242000	-3.539901000
C	3.363292000	0.681220000	-3.012315000
H	3.801807000	1.195812000	-3.858759000
C	4.172311000	0.013934000	-2.093534000
H	5.249083000	0.010762000	-2.218149000
C	3.609302000	-0.632113000	-0.999623000
H	4.241425000	-1.122267000	-0.268217000
C	2.222208000	-0.636624000	-0.803717000
C	1.933166000	-2.293596000	0.886068000
C	1.612144000	-1.542199000	3.208027000
H	0.985590000	-1.878326000	4.034189000
H	1.171136000	-0.648202000	2.762703000
H	2.608924000	-1.289004000	3.588209000
C	2.301538000	-3.856031000	2.556117000
H	1.678376000	-4.416510000	3.252345000
H	3.280391000	-3.678938000	3.018278000
C	2.435100000	-4.530310000	1.197732000
H	3.330274000	-5.144873000	1.108938000
H	1.556405000	-5.144652000	0.967838000
C	2.271376000	-3.698729000	-1.130486000
H	3.012538000	-4.437511000	-1.436303000
H	2.391753000	-2.809396000	-1.741068000
H	1.267595000	-4.108172000	-1.286446000
N	0.166918000	1.976411000	0.365738000
N	1.397616000	2.740751000	2.203533000
N	1.692961000	3.846489000	0.280729000
C	-0.722731000	1.215566000	-1.751297000
C	-1.580394000	1.384999000	-2.834300000
H	-1.697717000	0.569867000	-3.538944000
C	-2.271549000	2.579035000	-3.007913000
H	-2.936200000	2.703338000	-3.854287000
C	-2.097385000	3.611794000	-2.087546000
H	-2.632143000	4.546566000	-2.210856000
C	-1.256800000	3.444777000	-0.993687000
H	-1.147504000	4.236142000	-0.261148000
C	-0.560321000	2.244873000	-0.799659000
C	1.021192000	2.818273000	0.889907000
C	0.530405000	2.164812000	3.211743000
H	1.133851000	1.789020000	4.038062000
H	-0.025645000	1.337119000	2.767040000
H	-0.185335000	2.903542000	3.591634000
C	2.195262000	3.913246000	2.559783000
H	2.991992000	3.650557000	3.255059000
H	1.555361000	4.674072000	3.023212000
C	2.712535000	4.365743000	1.201340000
H	2.800647000	5.448045000	1.113316000
H	3.682213000	3.908997000	0.970083000
C	2.068980000	3.813797000	-1.126943000
H	2.346008000	4.824003000	-1.429149000
H	1.234828000	3.482752000	-1.737626000
H	2.919730000	3.142906000	-1.287082000

E(RTPSSh) = -3471.73863134
Zero-point correction = 0.719506 (Hartree/Particle)
Thermal correction to Energy = 0.762737
Thermal correction to Enthalpy = 0.763681
Thermal correction to Gibbs Free Energy = 0.64220

$[Cu(I)\{N(QuMe)(PhTMG)_2\}]^+$ ($C3_{TMG}$)

N	-0.024527000	1.329408000	0.690728000
C	0.294040000	-0.768531000	1.884577000
N	1.335937000	0.816087000	-1.704561000
N	-2.040640000	0.035683000	-0.690448000
C	-0.481810000	-1.002015000	4.172113000
H	-0.596203000	-1.616435000	5.057764000
N	0.792854000	-1.293919000	0.688360000
C	-0.981120000	0.299445000	4.155493000
H	-1.480418000	0.708250000	5.025488000
N	-3.096558000	-1.831329000	-1.558822000
C	-0.833151000	1.072848000	3.008952000
H	-1.218742000	2.085117000	2.971498000
N	-4.068464000	-0.749046000	0.247891000
C	-0.195156000	0.553713000	1.886316000
N	2.867078000	-2.041102000	1.570443000
C	1.846400000	-2.084610000	0.665886000
N	1.961713000	-2.996890000	-0.341419000
C	0.779670000	-3.344289000	-1.108176000
H	0.565201000	-2.591839000	-1.881259000
H	0.950407000	-4.305026000	-1.596360000
H	-0.080075000	-3.417590000	-0.446120000
C	3.236586000	-3.218659000	-1.018473000
H	3.176910000	-2.840157000	-2.043932000
H	4.026537000	-2.683607000	-0.498169000

H	3.479692000	-4.283061000	-1.050803000
C	3.194287000	-0.825837000	2.295990000
H	4.281889000	-0.719973000	2.320712000
H	2.769018000	0.032837000	1.782787000
H	2.816993000	-0.850115000	3.323324000
C	3.577979000	-3.239706000	1.994867000
H	4.640669000	-3.182675000	1.741663000
H	3.484784000	-3.343710000	3.080545000
H	3.140208000	-4.113236000	1.517984000
C	1.250073000	-0.289869000	-3.851250000
H	0.196185000	-0.398184000	-3.588271000
H	1.337346000	0.082379000	-4.873539000
H	1.715364000	-1.279910000	-3.821345000
Cu	-0.086857000	-0.331686000	-0.910076000
C	1.921763000	0.631804000	-2.883248000
C	3.151846000	1.247640000	-3.208280000
H	3.582960000	1.075083000	-4.186309000
C	3.792167000	2.022587000	-2.280591000
H	4.751791000	2.477323000	-2.497873000
C	3.194119000	2.236952000	-1.016007000
C	3.817042000	2.994075000	0.002519000
H	4.787128000	3.435782000	-0.193907000
C	3.204321000	3.149301000	1.221808000
H	3.686212000	3.714411000	2.010079000
C	1.931292000	2.593855000	1.449112000
H	1.444925000	2.730883000	2.407354000
C	1.280033000	1.874967000	0.469299000
C	1.925910000	1.641442000	-0.778176000
C	-2.217657000	1.388496000	-0.367740000
C	-3.352800000	2.114203000	-0.752411000
H	-4.167652000	1.592556000	-1.240888000
C	-3.420634000	3.489431000	-0.565241000
H	-4.305540000	4.027376000	-0.885519000
C	-2.349446000	4.177814000	0.000469000
H	-2.392412000	5.252247000	0.131414000
C	-1.222032000	3.470885000	0.406400000
H	-0.383969000	3.987812000	0.858704000
C	-1.156861000	2.090099000	0.247305000
C	-3.056558000	-0.811941000	-0.661454000
C	-3.879349000	-0.128213000	1.547726000
H	-2.818463000	-0.089846000	1.781710000
H	-4.288373000	0.886973000	1.575987000
H	-4.389233000	-0.736042000	2.299109000
C	-5.440320000	-1.106130000	-0.089484000
H	-6.087929000	-0.244708000	0.101107000
H	-5.503741000	-1.366270000	-1.143236000
H	-5.792943000	-1.946841000	0.514459000
C	-2.381225000	-1.721485000	-2.817844000
H	-2.303202000	-0.674147000	-3.099551000
H	-1.374506000	-2.149091000	-2.751365000
H	-2.938040000	-2.265061000	-3.584186000
C	-3.546371000	-3.169315000	-1.194056000
H	-2.732235000	-3.880044000	-1.363839000
H	-3.814151000	-3.190099000	-0.140567000
H	-4.407021000	-3.476203000	-1.793940000
C	0.145083000	-1.531102000	3.050436000
H	0.499005000	-2.555633000	3.055249000

E(RTPSSh) = -3322.84460714
Zero-point correction = 0.675854 (Hartree/Particle)
Thermal correction to Energy = 0.717472
Thermal correction to Enthalpy = 0.718416
Thermal correction to Gibbs Free Energy = 0.603211

$[Cu(I)\{N(QuMe)(PhDMEG)_2\}]^+$ ($C3_{DMEG}$)

N	0.069796000	1.250414000	0.791247000
C	1.131269000	2.088687000	0.328250000
N	-1.380901000	0.949836000	-1.584945000
C	1.133155000	3.463774000	0.536854000
H	0.298469000	3.917904000	1.057719000
N	-0.731980000	-1.358451000	0.563515000
C	2.198032000	4.241884000	0.092154000
H	2.194542000	5.311877000	0.260926000
N	2.046628000	0.121033000	-0.735566000
C	3.268999000	3.631854000	-0.557512000
H	4.105308000	4.227420000	-0.904997000
N	4.196445000	-0.664882000	-0.009280000
C	3.263560000	2.261404000	-0.791322000
H	4.076867000	1.797296000	-1.337023000
N	3.019506000	-1.889083000	-1.459057000
C	2.190784000	1.467141000	-0.370199000
N	-2.241699000	-2.696620000	-0.626038000
C	3.043201000	-0.730649000	-0.729766000
N	-2.778082000	-2.226862000	1.489851000
C	4.323169000	0.082637000	1.234289000
H	4.786136000	-0.565883000	1.979983000
H	3.339863000	0.379375000	1.595058000
H	4.940144000	0.973535000	1.101901000
C	2.242398000	-2.010870000	-2.676664000
H	1.991548000	-3.058521000	-2.842551000
H	2.794600000	-1.627455000	-3.542853000
H	1.319068000	-1.436426000	-2.568079000
C	4.960482000	-1.905863000	-0.169440000
H	4.808024000	-2.544654000	0.707395000
H	6.025453000	-1.701683000	-0.277028000
C	4.343449000	-2.513138000	-1.425160000
H	4.906522000	-2.236510000	-2.324575000
H	4.264741000	-3.598832000	-1.378725000
C	-1.270788000	1.733906000	0.699812000
C	-1.910442000	2.280894000	1.791334000
H	-1.382646000	2.328482000	2.736375000
Cu	0.090805000	-0.248138000	-0.982834000
C	-3.220241000	2.786895000	1.689109000
H	-3.693211000	3.217252000	2.563196000
C	-3.878382000	2.762139000	0.483955000
H	-4.875457000	3.175278000	0.384976000
C	-3.265914000	2.179563000	-0.649774000
C	-1.963429000	1.623899000	-0.539799000
C	-3.904271000	2.104432000	-1.910409000
H	-4.890865000	2.536430000	-2.032568000
C	-3.269382000	1.490584000	-2.955404000
H	-3.731930000	1.429258000	-3.932232000
C	-2.004714000	0.891217000	-2.756794000
C	-1.339431000	0.125442000	-3.856476000
H	-1.515304000	0.596144000	-4.825113000
H	-1.739496000	-0.891774000	-3.906171000
H	-0.265311000	0.062484000	-3.669048000
C	0.362667000	0.351419000	1.865907000
C	1.117479000	0.744669000	2.966143000
H	1.495361000	1.759933000	3.007317000
C	1.376905000	-0.153975000	3.996675000
H	1.965192000	0.156535000	4.851564000
C	0.868736000	-1.449417000	3.920804000

H	1.065365000	-2.157471000	4.717595000
C	0.125993000	-1.852874000	2.816804000
H	-0.238065000	-2.871193000	2.743763000
C	-0.131699000	-0.965334000	1.765437000
C	-1.840641000	-2.049832000	0.514035000
C	-1.287084000	-3.099195000	-1.638432000
H	-1.828532000	-3.363610000	-2.546143000
H	-0.678269000	-3.951665000	-1.314851000
H	-0.623882000	-2.258278000	-1.857828000
C	-2.998740000	-1.281314000	2.576141000
H	-4.065834000	-1.056587000	2.625860000
H	-2.458951000	-0.355714000	2.386600000
H	-2.674629000	-1.692417000	3.534188000
C	-3.348409000	-3.598423000	-0.305423000
H	-2.967221000	-4.605878000	-0.098194000
H	-4.061233000	-3.651381000	-1.127525000
C	-3.929944000	-2.954062000	0.947769000
H	-4.730736000	-2.246525000	0.703938000
H	-4.307573000	-3.683412000	1.663865000

E(RTPSSh) = -3320.45045156
Zero-point correction = 0.634712 (Hartree/Particle)
Thermal correction to Energy = 0.673339
Thermal correction to Enthalpy = 0.674283
Thermal correction to Gibbs Free Energy = 0.563025

$[Cu(I)\{N(QuMe)_2(PhTMG)\}]^+$ ($C5_{TMG}$)

N	0.750995000	0.872229000	0.737536000
C	2.034780000	-1.799844000	-3.244089000
H	2.609629000	-1.899800000	-4.164891000
H	1.134930000	-1.211877000	-3.435095000
H	1.719614000	-2.801218000	-2.932610000
Cu	0.257172000	-0.777746000	-0.760837000
N	2.178854000	-0.579799000	-1.167243000
C	2.844957000	-1.156727000	-2.163428000
N	-0.314297000	-1.702213000	0.948196000
C	4.256416000	-1.202138000	-2.182430000
H	4.755186000	-1.665893000	-3.023727000
N	-1.232170000	0.545559000	-1.126208000
C	4.969852000	-0.697512000	-1.128696000
H	6.051723000	-0.759195000	-1.106046000
N	-3.525226000	1.044327000	-0.774357000
C	4.287705000	-0.087451000	-0.050098000
N	-2.875513000	-0.795307000	-2.032764000
C	4.952899000	0.408594000	1.095058000
H	6.032352000	0.328161000	1.148549000
C	4.234486000	0.964422000	2.124705000
H	4.738886000	1.326887000	3.011864000
C	2.836823000	1.103912000	2.021408000
H	2.283969000	1.579490000	2.822093000
C	2.160186000	0.667374000	0.904043000
C	2.872350000	-0.000014000	-0.133780000
C	-0.418063000	-3.899647000	-0.055435000
H	-0.038673000	-4.848798000	0.328990000
H	0.322760000	-3.456344000	-0.723319000
H	-1.321543000	-4.119115000	-0.631550000
C	-0.726774000	-2.957337000	1.065520000
C	-1.460378000	-3.396492000	2.193276000
H	-1.767448000	-4.433163000	2.249319000
C	-1.795805000	-2.506479000	3.175666000
H	-2.385515000	-2.814909000	4.031213000
C	-1.367346000	-1.160729000	3.078270000
C	-1.704975000	-0.178304000	4.036824000
H	-2.311136000	-0.464843000	4.888360000
C	-1.281377000	1.118624000	3.876904000
H	-1.552773000	1.877342000	4.600329000
C	-0.471002000	1.468757000	2.780422000
H	-0.130846000	2.490731000	2.663888000
C	-0.098323000	0.530117000	1.842826000
C	-0.581680000	-0.803865000	1.950014000
C	0.344829000	2.013522000	-0.040510000
C	0.989615000	3.241622000	0.058930000
H	1.837734000	3.341662000	0.725848000
C	0.546234000	4.329912000	-0.686533000
H	1.051205000	5.284555000	-0.603469000
C	-0.552487000	4.181872000	-1.530537000
H	-0.906183000	5.023488000	-2.114836000
C	-1.186756000	2.951112000	-1.652502000
H	-2.012147000	2.828271000	-2.344087000
C	-0.741229000	1.841104000	-0.925181000
C	-2.515396000	0.296778000	-1.302388000
C	-1.904348000	-1.394715000	-2.930877000
H	-1.198351000	-2.046830000	-2.396142000
H	-1.342851000	-0.612552000	-3.437165000
H	-2.439434000	-1.994016000	-3.668921000
C	-3.967698000	-1.665942000	-1.606495000
H	-3.565595000	-2.645613000	-1.331285000
H	-4.697816000	-1.798646000	-2.408104000
H	-4.459546000	-1.237509000	-0.737113000
C	-3.348690000	1.821250000	0.440581000
H	-2.476210000	1.462967000	0.980504000
H	-4.232939000	1.687687000	1.068919000
H	-3.222951000	2.887289000	0.226559000
C	-4.789221000	1.241977000	-1.471805000
H	-4.745864000	0.768707000	-2.449685000
H	-4.957330000	2.315191000	-1.603999000
H	-5.626820000	0.826445000	-0.904219000

E(RTPSSh) = -3170.35897992
Zero-point correction = 0.570469 (Hartree/Particle)
Thermal correction to Energy = 0.605931
Thermal correction to Enthalpy = 0.606875
Thermal correction to Gibbs Free Energy = 0.503660

$[Cu(I)\{N(QuMe)_2(PhDMEG)\}]^+$ ($C5_{DMEG}$)

Cu	0.300672000	-1.023481000	-0.444343000
N	0.763281000	1.058033000	0.378371000
N	-0.525924000	-1.208481000	1.393996000
N	2.248168000	-1.018071000	-0.730398000
N	-1.096034000	0.122338000	-1.392217000
N	-3.427913000	0.755401000	-1.289112000
N	-2.858089000	-1.402385000	-1.460280000
C	0.509947000	1.823959000	-0.811656000
C	1.245886000	2.957872000	-1.138156000
H	2.055394000	3.269568000	-0.488809000
C	0.937581000	3.685992000	-2.283454000
H	1.511718000	4.570032000	-2.532572000

C	-0.116860000	3.275977000	-3.097357000
H	-0.365909000	3.839772000	-3.988863000
C	-0.839556000	2.129030000	-2.790027000
H	-1.634415000	1.788139000	-3.443122000
C	-0.529033000	1.374642000	-1.653044000
C	-2.380001000	-0.123578000	-1.388784000
C	-2.078015000	-2.474399000	-2.046085000
H	-2.529974000	-3.426517000	-1.771287000
H	-1.058991000	-2.441312000	-1.648275000
H	-2.030539000	-2.394458000	-3.138040000
C	-3.338594000	1.998629000	-0.532897000
H	-4.171123000	2.638535000	-0.825754000
H	-2.408911000	2.514081000	-0.752380000
H	-3.398650000	1.803049000	0.543539000
C	-4.304186000	-1.374665000	-1.675899000
H	-4.793649000	-2.196162000	-1.154078000
H	-4.528793000	-1.446357000	-2.746880000
C	-4.671929000	-0.007494000	-1.115617000
H	-5.495975000	0.468212000	-1.645925000
H	-4.919570000	-0.067211000	-0.048959000
C	2.132735000	0.882400000	0.759203000
C	2.736575000	1.663221000	1.719583000
H	2.149051000	2.407945000	2.242113000
C	4.108438000	1.525517000	2.007739000
H	4.557222000	2.160615000	2.761459000
C	4.876775000	0.624797000	1.311872000
H	5.940767000	0.538662000	1.498638000
C	4.282377000	-0.221479000	0.347305000
C	2.887636000	-0.129283000	0.098327000
C	5.013202000	-1.187771000	-0.383511000
H	6.084004000	-1.267449000	-0.235427000
C	4.360865000	-2.007277000	-1.264769000
H	4.899281000	-2.747180000	-1.842880000
C	2.956924000	-1.923213000	-1.398191000
C	2.202076000	-2.885343000	-2.259872000
H	2.818792000	-3.246548000	-3.083500000
H	1.303639000	-2.406662000	-2.655696000
H	1.889662000	-3.752991000	-1.669508000
C	-0.214083000	1.187223000	1.421798000
C	-0.599416000	2.423570000	1.891420000
H	-0.165284000	3.312017000	1.448793000
C	-1.540679000	2.545016000	2.930684000
H	-1.818060000	3.530362000	3.283998000
C	-2.087153000	1.421665000	3.502053000
H	-2.798662000	1.500839000	4.315691000
C	-1.740453000	0.138302000	3.022045000
C	-0.815508000	0.011779000	1.951465000
C	-2.294646000	-1.052248000	3.550532000
H	-2.993737000	-0.990673000	4.376630000
C	-1.943584000	-2.259232000	3.013082000
H	-2.348522000	-3.184302000	3.403498000
C	-1.062045000	-2.307866000	1.906867000
C	-0.732756000	-3.614665000	1.256698000
H	-0.444440000	-4.357135000	2.004068000
H	0.081962000	-3.483880000	0.542260000
H	-1.605337000	-4.006330000	0.726563000

E(RTPSSh) = -3169.16233403
Zero-point correction = 0.550390 (Hartree/Particle)
Thermal correction to Energy = 0.584009
Thermal correction to Enthalpy = 0.584953
Thermal correction to Gibbs Free Energy = 0.485687

6.5.2 [Cu(I)L] + S Geometries

[Cu(I)(TMG$_3$trphen)]$^+$ (C1$_{TMG}$) + MeCN

Cu	-0.210323000	0.011878000	0.707563000
N	-0.455460000	-0.054486000	-1.604571000
C	-1.513990000	0.897724000	-1.767088000
C	-2.433366000	1.058309000	-0.708425000
C	-3.484888000	1.970160000	-0.883203000
H	-4.185697000	2.121612000	-0.070087000
C	-3.608673000	2.707106000	-2.054152000
H	-4.424777000	3.413516000	-2.155176000
C	-2.677508000	2.561775000	-3.081501000
H	-2.763045000	3.145737000	-3.989873000
C	-1.634878000	1.654234000	-2.929875000
H	-0.898569000	1.524137000	-3.714610000
N	-2.196156000	0.412347000	0.509322000
C	-3.204584000	-0.036412000	1.237461000
N	-4.336830000	-0.581435000	0.707583000
C	-4.330993000	-1.190620000	-0.611432000
H	-3.315753000	-1.476419000	-0.875871000
H	-4.720286000	-0.510315000	-1.376104000
H	-4.958159000	-2.084950000	-0.581868000
C	-5.649489000	-0.385387000	1.308418000
H	-5.561583000	0.253483000	2.183815000
H	-6.101140000	-1.338277000	1.598399000
H	-6.304697000	0.103369000	0.580336000
N	-3.116784000	-0.003439000	2.593624000
C	-2.228782000	0.940453000	3.246390000
H	-2.017022000	1.763041000	2.568341000
H	-1.285615000	0.465709000	3.537742000
H	-2.714824000	1.320584000	4.148398000
C	-3.638209000	-1.072592000	3.435039000
H	-4.051434000	-1.860744000	2.810405000
H	-4.411814000	-0.704547000	4.114264000
H	-2.821156000	-1.488223000	4.032161000
C	0.856266000	0.362403000	-1.994682000
C	1.553390000	1.243062000	-1.138017000
C	2.815501000	1.697205000	-1.546239000
H	3.369487000	2.360995000	-0.893269000
C	3.381073000	1.265963000	-2.740046000
H	4.365840000	1.621560000	-3.021184000
C	2.705571000	0.357940000	-3.553704000
H	3.152257000	0.005458000	-4.475475000
C	1.441966000	-0.084701000	-3.176061000
H	0.892991000	-0.781699000	-3.798591000
N	1.021526000	1.522001000	0.125270000
C	1.188370000	2.707498000	0.685000000
N	1.229558000	3.880799000	-0.010157000
C	0.580417000	4.016908000	-1.302274000
H	-0.173508000	3.241547000	-1.414921000
H	1.296181000	3.940479000	-2.127503000
H	0.095181000	4.995347000	-1.345048000
C	2.090402000	4.987079000	0.386250000
H	2.676824000	4.702220000	1.256438000
H	1.507155000	5.882645000	0.618948000
H	2.772502000	5.220620000	-0.437514000
N	1.292290000	2.792976000	2.038009000
C	1.661309000	1.614550000	2.800946000
H	2.382259000	1.026287000	2.240459000
H	0.786181000	0.991660000	3.024002000
H	2.109555000	1.936722000	3.742431000
C	0.669241000	3.874245000	2.793441000
H	0.154512000	4.547523000	2.112415000
H	1.411573000	4.435622000	3.366396000
H	-0.061854000	3.453389000	3.489690000
C	-0.798045000	-1.432376000	-1.789018000
C	-0.333795000	-2.365557000	-0.838471000
C	-0.673111000	-3.714606000	-1.017514000
H	-0.344862000	-4.438686000	-0.280502000
C	-1.452145000	-4.120828000	-2.093236000
H	-1.708305000	-5.168763000	-2.199776000
C	-1.922600000	-3.187596000	-3.016038000
H	-2.540376000	-3.499716000	-3.849332000
C	-1.591301000	-1.846802000	-2.856132000
H	-1.952123000	-1.102779000	-3.556675000
N	0.329834000	-1.904146000	0.303084000
C	1.313285000	-2.600049000	0.844057000
N	2.208269000	-3.343226000	0.132024000
C	2.462084000	-3.078612000	-1.274013000
H	2.189408000	-2.052072000	-1.508721000
H	1.895442000	-3.753411000	-1.923647000
H	3.527929000	-3.220608000	-1.466051000
C	2.778969000	-4.579615000	0.651631000
H	2.358755000	-4.794393000	1.631037000
H	3.867738000	-4.511231000	0.730777000
H	2.530183000	-5.400378000	-0.028285000
N	1.476382000	-2.563775000	2.195682000
C	0.352213000	-2.162906000	3.022789000
H	-0.566774000	-2.585941000	2.623274000
H	0.244423000	-1.070852000	3.059725000
H	0.517981000	-2.533996000	4.035243000
C	2.793793000	-2.452479000	2.812869000
H	3.563286000	-2.534492000	2.050388000
H	2.941594000	-3.235899000	3.559750000
H	2.888979000	-1.478210000	3.301678000
C	5.128344000	0.182429000	0.759049000
N	4.998631000	0.936208000	1.624051000
C	5.291470000	-0.762965000	-0.331630000
H	6.223489000	-0.557764000	-0.859964000
H	4.458358000	-0.659651000	-1.027259000
H	5.319998000	-1.780123000	0.060469000

E(RTPSSh) = -3608.16010812
Zero-point correction = 0.827088 (Hartree/Particle)
Thermal correction to Energy = 0.880738
Thermal correction to Enthalpy = 0.881682
Thermal correction to Gibbs Free Energy = 0.736117

[Cu(I)(DMEG$_3$trphen)]$^+$ (C1$_{DMEG}$) + MeCN

Cu	0.073421000	-0.025805000	0.705963000
Cu	0.073421000	-0.025805000	0.705963000
N	0.530112000	0.172449000	-1.596182000
N	-1.611469000	0.860828000	-0.021977000
N	-2.268833000	2.155688000	1.816704000
N	-2.901555000	2.894414000	-0.194846000
C	-0.781385000	-0.110876000	-2.072906000
C	-0.997709000	-0.822038000	-3.249444000

H	-0.140940000	-1.176180000	-3.810760000
C	-2.291491000	-1.065325000	-3.698236000
H	-2.452091000	-1.619565000	-4.615064000
C	-3.373566000	-0.576279000	-2.968559000
H	-4.386490000	-0.749754000	-3.313129000
C	-3.166249000	0.118117000	-1.782503000
H	-4.010321000	0.474171000	-1.204673000
C	-1.871335000	0.343506000	-1.299662000
C	-2.234455000	1.901673000	0.474856000
C	-2.083860000	1.132939000	2.823651000
H	-1.593862000	1.564871000	3.696648000
H	-1.450928000	0.341539000	2.413964000
H	-3.041479000	0.698128000	3.128886000
C	-3.196364000	3.249876000	2.097343000
H	-2.819289000	3.887714000	2.896416000
H	-4.170284000	2.843290000	2.392779000
C	-3.263945000	3.957766000	0.750980000
H	-4.252147000	4.357035000	0.525168000
H	-2.528999000	4.768830000	0.687423000
C	-2.515402000	3.346088000	-1.525549000
H	-3.351252000	3.898639000	-1.955631000
H	-2.288279000	2.500761000	-2.166720000
H	-1.639102000	4.001005000	-1.471866000
N	0.502737000	-1.940315000	0.190952000
N	-0.709867000	-3.165938000	1.779304000
N	-0.395216000	-4.144236000	-0.205786000
C	1.530331000	-0.838694000	-1.707147000
C	2.564244000	-0.735645000	-2.633531000
H	2.596199000	0.131392000	-3.283055000
C	3.536541000	-1.725033000	-2.721704000
H	4.336806000	-1.637728000	-3.446527000
C	3.470162000	-2.826265000	-1.868975000
H	4.225811000	-3.601635000	-1.921363000
C	2.450288000	-2.929936000	-0.931659000
H	2.417545000	-3.772689000	-0.251141000
C	1.462180000	-1.941044000	-0.829931000
C	-0.143469000	-3.025307000	0.544247000
C	-0.243996000	-2.422675000	2.931479000
H	-1.056760000	-2.326364000	3.651497000
H	0.063961000	-1.427589000	2.604304000
H	0.610191000	-2.915572000	3.409757000
C	-1.169339000	-4.541605000	1.963887000
H	-2.103638000	-4.573181000	2.523928000
H	-0.411271000	-5.118329000	2.506883000
C	-1.319178000	-5.020675000	0.525328000
H	-1.048685000	-6.067531000	0.392103000
H	-2.339874000	-4.868607000	0.155726000
C	-0.578441000	-4.090931000	-1.650825000
H	-0.495404000	-5.104261000	-2.043940000
H	0.187237000	-3.473935000	-2.110331000
H	-1.565223000	-3.686454000	-1.901734000
N	1.719242000	1.203118000	0.667357000
N	2.791157000	0.618390000	2.664344000
N	4.112686000	1.283236000	0.986105000
C	0.959966000	1.533708000	-1.605100000
C	0.708480000	2.371020000	-2.687942000
H	0.170705000	1.973995000	-3.541153000
C	1.142458000	3.692024000	-2.673512000
H	0.944102000	4.337661000	-3.520466000
C	1.836273000	4.173717000	-1.564153000
H	2.177613000	5.202252000	-1.540583000
C	2.076308000	3.348811000	-0.471902000
H	2.587369000	3.732968000	0.403365000
C	1.638243000	2.018342000	-0.467440000
C	2.814752000	1.064180000	1.369754000
C	1.634297000	0.820036000	3.513144000
H	1.622876000	0.062369000	4.296531000
H	0.733349000	0.724497000	2.906356000
H	1.644511000	1.815897000	3.972284000
C	4.119147000	0.758611000	3.259942000
H	4.337068000	-0.068835000	3.934525000
H	4.180162000	1.699735000	3.820058000
C	5.014368000	0.778840000	2.029344000
H	5.882660000	1.427652000	2.139273000
H	5.354015000	-0.229703000	1.764683000
C	4.572125000	1.105697000	-0.385133000
H	5.541684000	1.594217000	-0.485697000
H	3.877166000	1.561073000	-1.083509000
H	4.677018000	0.042456000	-0.625216000
C	-4.700076000	-0.627107000	1.209013000
N	-5.436853000	0.256265000	1.313584000
C	-3.755276000	-1.722599000	1.079704000
H	-2.767411000	-1.320947000	0.847734000
H	-4.068063000	-2.389615000	0.275818000
H	-3.708209000	-2.280121000	2.015453000

E(RTPSSh) = -3604.57184464
Zero-point correction = 0.766340 (Hartree/Particle)
Thermal correction to Energy = 0.814824
Thermal correction to Enthalpy = 0.815768
Thermal correction to Gibbs Free Energy = 0.682048

$[Cu(I)\{N(QuMe)(PhTMG)_2\}]^+$ ($C3_{TMG}$) + MeCN

N	0.070166000	0.374702000	1.447526000
C	0.882581000	-1.894156000	1.100178000
N	1.035396000	1.663111000	-0.849719000
N	-1.964885000	-0.256603000	-0.316591000
C	0.573742000	-3.578010000	2.820921000
H	0.705889000	-4.600093000	3.156872000
N	1.223275000	-1.502294000	-0.198173000
C	-0.090697000	-2.657193000	3.629528000
H	-0.473953000	-2.951738000	4.598866000
N	-2.898010000	-1.462523000	-2.058903000
C	-0.258879000	-1.351530000	3.180663000
H	-0.777456000	-0.620622000	3.790264000
N	-3.683443000	-1.832576000	0.091473000
C	0.228548000	-0.965799000	1.935445000
N	3.502804000	-2.154673000	-0.076287000
C	2.351411000	-1.889628000	-0.759387000
N	2.404308000	-2.007511000	-2.115813000
C	1.162436000	-2.091054000	-2.861986000
H	0.732241000	-1.094692000	-3.036939000
H	1.365486000	-2.556526000	-3.827765000
H	0.442069000	-2.690436000	-2.310193000
C	3.563591000	-1.547363000	-2.874974000
H	3.274830000	-0.694489000	-3.496813000
H	4.346877000	-1.229058000	-2.192052000
H	3.946429000	-2.339440000	-3.522626000
C	3.787953000	-1.536380000	1.207113000
H	4.839392000	-1.238148000	1.221419000
H	3.169573000	-0.651082000	1.332206000

H	3.602362000	-2.221417000	2.040581000
C	4.426513000	-3.201852000	-0.491912000
H	5.412610000	-2.792001000	-0.728914000
H	4.537417000	-3.923984000	0.323272000
H	4.030107000	-3.714762000	-1.364795000
C	0.743959000	2.003298000	-3.226226000
H	-0.164593000	1.429486000	-3.036539000
H	0.490976000	2.910030000	-3.779286000
H	1.408971000	1.407721000	-3.858647000
Cu	-0.049486000	-0.006740000	-0.829485000
C	1.416151000	2.334694000	-1.931823000
C	2.441582000	3.306533000	-1.882418000
H	2.703355000	3.839589000	-2.787679000
C	3.107567000	3.535963000	-0.710004000
H	3.919713000	4.251909000	-0.659076000
C	2.734895000	2.826088000	0.456340000
C	3.412366000	2.976399000	1.687870000
H	4.243673000	3.669437000	1.745766000
C	3.029083000	2.240529000	2.782462000
H	3.558231000	2.338799000	3.722262000
C	1.925752000	1.371164000	2.698417000
H	1.614363000	0.806789000	3.569169000
C	1.218851000	1.225424000	1.523623000
C	1.647134000	1.917248000	0.354609000
C	-2.260309000	0.582765000	0.764976000
C	-3.525662000	1.155303000	0.952064000
H	-4.328675000	0.879890000	0.278650000
C	-3.744290000	2.102948000	1.944036000
H	-4.729622000	2.540893000	2.053689000
C	-2.700697000	2.511938000	2.771829000
H	-2.864165000	3.262789000	3.535069000
C	-1.440192000	1.946356000	2.609320000
H	-0.616658000	2.252225000	3.243340000
C	-1.216226000	0.982585000	1.629384000
C	-2.841778000	-1.154784000	-0.738089000
C	-3.355706000	-2.050883000	1.490058000
H	-2.284838000	-1.933784000	1.636063000
H	-3.884357000	-1.350629000	2.144848000
H	-3.642700000	-3.070694000	1.758008000
C	-5.035260000	-2.202839000	-0.306616000
H	-5.745309000	-1.764601000	0.401542000
H	-5.245257000	-1.813725000	-1.299881000
H	-5.168038000	-3.288375000	-0.305862000
C	-2.425859000	-0.513952000	-3.052765000
H	-2.523130000	0.498404000	-2.669329000
H	-1.379729000	-0.699324000	-3.320947000
H	-3.035756000	-0.621322000	-3.952629000
C	-3.113915000	-2.825691000	-2.528503000
H	-2.266164000	-3.127269000	-3.150439000
H	-3.180849000	-3.499725000	-1.677994000
H	-4.026919000	-2.901403000	-3.124895000
C	1.051495000	-3.203022000	1.571148000
H	1.533898000	-3.932065000	0.930367000
C	-2.231550000	3.506895000	-1.545043000
N	-2.802916000	3.061733000	-2.444397000
C	-1.515478000	4.071852000	-0.415478000
H	-2.093009000	4.891982000	0.012511000
H	-0.545198000	4.447271000	-0.742742000
H	-1.368527000	3.303014000	0.343936000

E(RTPSSh) = -3455.67866029
Zero-point correction = 0.722372 (Hartree/Particle)
Thermal correction to Energy = 0.769338
Thermal correction to Enthalpy = 0.770282
Thermal correction to Gibbs Free Energy = 0.642009

$[Cu(I)\{N(QuMe)(PhDMEG)_2\}]^+$ ($C3_{DMEG}$) + MeCN

N	-0.098195000	0.314211000	1.482271000
C	1.124832000	1.018731000	1.710319000
N	-1.187425000	1.663412000	-0.729322000
C	1.252567000	1.994959000	2.692082000
H	0.391234000	2.249081000	3.298224000
N	-1.136552000	-1.483874000	-0.307997000
C	2.475241000	2.627466000	2.900153000
H	2.568558000	3.386125000	3.667543000
N	1.979035000	-0.124353000	-0.236985000
C	3.575738000	2.264732000	2.126485000
H	4.533763000	2.746592000	2.283450000
N	3.854252000	-1.602683000	0.000417000
C	3.449400000	1.309928000	1.123962000
H	4.293578000	1.072089000	0.488227000
N	2.839601000	-1.441492000	-1.980813000
C	2.219955000	0.686759000	0.879819000
N	-2.544323000	-1.567366000	-2.177495000
C	2.856119000	-0.988709000	-0.691146000
N	-3.418861000	-2.247561000	-0.238879000
C	3.824745000	-1.798120000	1.443191000
H	4.039439000	-2.847325000	1.653951000
H	2.836133000	-1.560498000	1.832279000
H	4.566603000	-1.173060000	1.944153000
C	2.279269000	-0.658619000	-3.064629000
H	1.963540000	-1.327032000	-3.865474000
H	3.004038000	0.065378000	-3.451844000
H	1.408687000	-0.112050000	-2.692489000
C	4.496008000	-2.618615000	-0.839821000
H	4.116717000	-3.609648000	-0.567769000
H	5.578316000	-2.607172000	-0.714297000
C	4.057215000	-2.211286000	-2.243039000
H	4.802734000	-1.570345000	-2.728362000
H	3.850868000	-3.064094000	-2.888919000
C	-1.336305000	1.020777000	1.600802000
C	-2.062665000	0.990420000	2.772008000
H	-1.682436000	0.414020000	3.606795000
Cu	0.078338000	0.131585000	-0.813256000
C	-3.273472000	1.696536000	2.898236000
H	-3.816624000	1.657903000	3.834321000
C	-3.746991000	2.445530000	1.849276000
H	-4.666213000	3.012471000	1.939646000
C	-3.045472000	2.476268000	0.622272000
C	-1.842066000	1.735076000	0.477422000
C	-3.502276000	3.210783000	-0.497713000
H	-4.408217000	3.799650000	-0.412529000
C	-2.796966000	3.168895000	-1.668666000
H	-3.120693000	3.727984000	-2.537260000
C	-1.641877000	2.360722000	-1.766007000
C	-0.906284000	2.240691000	-3.062960000
H	-0.806468000	3.214328000	-3.546409000

H	-1.450190000	1.586150000	-3.749908000
H	0.084838000	1.814511000	-2.895220000
C	-0.119213000	-1.074369000	1.840072000
C	0.454287000	-1.535163000	3.020540000
H	0.936250000	-0.824894000	3.682605000
C	0.405118000	-2.888036000	3.343063000
H	0.853379000	-3.242527000	4.263207000
C	-0.229490000	-3.776574000	2.477079000
H	-0.273350000	-4.832361000	2.718433000
C	-0.790250000	-3.324111000	1.288052000
H	-1.251128000	-4.022273000	0.598821000
C	-0.735744000	-1.968701000	0.941868000
C	-2.293918000	-1.769987000	-0.845086000
C	-1.469262000	-1.550335000	-3.148677000
H	-1.846048000	-1.134631000	-4.082524000
H	-1.065796000	-2.553138000	-3.332559000
H	-0.664276000	-0.911616000	-2.778361000
C	-3.717558000	-2.050549000	1.173544000
H	-4.745204000	-1.693870000	1.261056000
H	-3.053671000	-1.300598000	1.599513000
H	-3.612417000	-2.979696000	1.736897000
C	-3.803685000	-2.220482000	-2.536667000
H	-3.609298000	-3.227312000	-2.926140000
H	-4.341365000	-1.646541000	-3.290514000
C	-4.528701000	-2.271690000	-1.196656000
H	-5.163698000	-1.391012000	-1.046947000
H	-5.133787000	-3.169734000	-1.075457000
C	2.782776000	3.206920000	-1.654939000
N	3.602285000	2.837549000	-2.380141000
C	1.744964000	3.664260000	-0.748540000
H	2.188074000	3.953650000	0.205006000
H	1.037897000	2.850822000	-0.574381000
H	1.219463000	4.515170000	-1.183924000

E(RTPSSh) = -3453.28441718
Zero-point correction = 0.681277 (Hartree/Particle)
Thermal correction to Energy = 0.725264
Thermal correction to Enthalpy = 0.726208
Thermal correction to Gibbs Free Energy = 0.601566

$[Cu(I)\{N(QuMe)_2(PhTMG)\}]^+$ ($C5_{TMG}$) + MeCN

N	0.496767000	-0.310395000	1.174766000
C	2.066604000	0.305742000	-3.516442000
H	2.750583000	0.902683000	-4.121349000
H	1.198961000	0.908126000	-3.240232000
H	1.717305000	-0.527632000	-4.134433000
Cu	0.050524000	-0.178626000	-1.052347000
N	2.009814000	-0.320195000	-1.182779000
C	2.743404000	-0.211466000	-2.287264000
N	-0.952735000	-1.900562000	-0.608664000
C	4.099929000	-0.602181000	-2.318645000
H	4.660226000	-0.477531000	-3.236355000
N	-1.172880000	1.251507000	-0.327228000
C	4.675458000	-1.155226000	-1.207995000
H	5.706286000	-1.489556000	-1.220787000
N	-3.411623000	1.808465000	0.222466000
C	3.917929000	-1.292116000	-0.021581000
N	-2.778224000	1.419111000	-1.976579000
C	4.438812000	-1.889101000	1.148641000
H	5.460318000	-2.250978000	1.140353000
C	3.653219000	-2.018540000	2.267043000
H	4.042738000	-2.491289000	3.160069000
C	2.340755000	-1.509923000	2.272478000
H	1.737799000	-1.594420000	3.167927000
C	1.811565000	-0.889306000	1.162274000
C	2.579929000	-0.815302000	-0.034294000
C	-1.197232000	-2.577606000	-2.916865000
H	-0.941149000	-3.553865000	-3.335246000
H	-0.346809000	-1.903274000	-3.030734000
H	-2.038755000	-2.186374000	-3.495058000
C	-1.562273000	-2.701935000	-1.470634000
C	-2.544047000	-3.632948000	-1.053798000
H	-3.009227000	-4.273521000	-1.792362000
C	-2.910905000	-3.690526000	0.262025000
H	-3.683087000	-4.373663000	0.596557000
C	-2.276184000	-2.846454000	1.205095000
C	-2.629170000	-2.823612000	2.573395000
H	-3.412202000	-3.486125000	2.923534000
C	-1.997067000	-1.961335000	3.436119000
H	-2.277403000	-1.928246000	4.481554000
C	-0.964451000	-1.124919000	2.971964000
H	-0.466747000	-0.450455000	3.658403000
C	-0.573685000	-1.143555000	1.650493000
C	-1.258466000	-1.979309000	0.725241000
C	0.383960000	1.085555000	1.508104000
C	1.170435000	1.684383000	2.485656000
H	1.921062000	1.094400000	2.997161000
C	0.994382000	3.027962000	2.802825000
H	1.612064000	3.488908000	3.563686000
C	0.016025000	3.767475000	2.142043000
H	-0.131058000	4.813563000	2.384353000
C	-0.754548000	3.182921000	1.143686000
H	-1.474363000	3.776612000	0.592685000
C	-0.569424000	1.841444000	0.790712000
C	-2.424922000	1.501197000	-0.665303000
C	-1.748793000	1.490992000	-2.998457000
H	-1.273339000	0.514359000	-3.167162000
H	-0.986210000	2.207180000	-2.700245000
H	-2.209281000	1.817544000	-3.932210000
C	-4.042022000	0.815599000	-2.389765000
H	-3.838043000	-0.083961000	-2.977519000
H	-4.626847000	1.507760000	-3.000011000
H	-4.617075000	0.532682000	-1.511954000
C	-3.361196000	1.367317000	1.605952000
H	-2.649191000	0.552228000	1.703916000
H	-4.352901000	1.007819000	1.891746000
H	-3.069642000	2.178684000	2.280207000
C	-4.492536000	2.728602000	-0.107567000
H	-4.330683000	3.143727000	-1.099273000
H	-4.498037000	3.544412000	0.621673000
H	-5.464891000	2.228833000	-0.077323000
C	3.434138000	2.677722000	-0.169220000
N	4.379091000	2.323570000	0.392152000
C	2.246980000	3.125538000	-0.875489000
H	1.544735000	2.294902000	-0.971511000
H	2.520955000	3.484968000	-1.868210000
H	1.767615000	3.928615000	-0.315294000

E(RTPSSh) = -3303.19277966
Zero-point correction = 0.617340 (Hartree/Particle)
Thermal correction to Energy = 0.657901
Thermal correction to Enthalpy = 0.658845
Thermal correction to Gibbs Free Energy = 0.544017

$[Cu(I)\{N(QuMe)_2(PhDMEG)\}]^+$ ($C5_{DMEG}$) + MeCN

Cu	0.916254000	1.012492000	-0.473990000
N	0.955832000	-1.029110000	0.548688000
N	-0.211865000	-0.032351000	-1.786491000
N	2.869416000	0.774408000	-0.366065000
N	-0.360502000	1.309592000	1.084810000
N	-2.705741000	1.443868000	1.651896000
N	-1.850174000	2.806936000	0.095433000
C	0.860164000	-0.596352000	1.916558000
C	1.498563000	-1.268713000	2.953149000
H	2.104406000	-2.137991000	2.726141000
C	1.353212000	-0.831556000	4.266246000
H	1.850249000	-1.360110000	5.070470000
C	0.559148000	0.281498000	4.536368000
H	0.437857000	0.627809000	5.556212000
C	-0.061082000	0.972647000	3.502182000
H	-0.647358000	1.860418000	3.708785000
C	0.089850000	0.556764000	2.174096000
C	-1.565326000	1.808665000	0.982377000
C	-0.826885000	3.704212000	-0.401814000
H	-1.218673000	4.235617000	-1.268112000
H	0.046323000	3.121751000	-0.712791000
H	-0.512569000	4.427537000	0.359067000
C	-2.943285000	0.064608000	2.064647000
H	-3.852881000	0.044464000	2.664231000
H	-2.119695000	-0.304039000	2.669232000
H	-3.071827000	-0.586944000	1.194090000
C	-3.195628000	3.321316000	0.347932000
H	-3.689386000	3.598186000	-0.582915000
H	-3.148416000	4.199593000	1.002964000
C	-3.852775000	2.134804000	1.040472000
H	-4.575579000	2.428112000	1.800885000
H	-4.338440000	1.471995000	0.316866000
C	2.232963000	-1.508285000	0.109584000
C	2.535374000	-2.850533000	0.050143000
H	1.771129000	-3.576907000	0.297568000
C	3.828434000	-3.287395000	-0.298369000
H	4.038340000	-4.349468000	-0.326605000
C	4.822145000	-2.376260000	-0.559254000
H	5.829775000	-2.701731000	-0.790080000
C	4.537544000	-0.990994000	-0.547785000
C	3.219815000	-0.548348000	-0.258029000
C	5.508876000	-0.003384000	-0.835060000
H	6.530179000	-0.305565000	-1.036209000
C	5.147900000	1.317104000	-0.856771000
H	5.875461000	2.091071000	-1.064610000
C	3.799335000	1.681989000	-0.647965000
C	3.347852000	3.101838000	-0.785097000
H	4.169629000	3.798212000	-0.617061000
H	2.542035000	3.307263000	-0.076890000
H	2.959210000	3.275533000	-1.794026000
C	-0.214258000	-1.655266000	0.002539000
C	-0.838504000	-2.699457000	0.648589000
H	-0.451714000	-3.033617000	1.603822000
C	-1.958602000	-3.336910000	0.082175000
H	-2.422298000	-4.162499000	0.607797000
C	-2.442095000	-2.929631000	-1.137406000
H	-3.286062000	-3.430290000	-1.597151000
C	-1.853382000	-1.833103000	-1.806729000
C	-0.746871000	-1.162822000	-1.221554000
C	-2.334509000	-1.342899000	-3.043917000
H	-3.171130000	-1.838932000	-3.521675000
C	-1.744507000	-0.249333000	-3.613736000
H	-2.091115000	0.142994000	-4.561339000
C	-0.686243000	0.409458000	-2.943804000
C	-0.089245000	1.658632000	-3.511349000
H	0.127687000	1.536501000	-4.574635000
H	0.830030000	1.910837000	-2.979347000
H	-0.790080000	2.492584000	-3.413922000
C	-5.640009000	-1.257702000	-0.572459000
N	-5.442487000	-0.374034000	-1.289013000
C	-5.886566000	-2.366891000	0.333908000
H	-6.031142000	-3.284969000	-0.237050000
H	-6.780924000	-2.167734000	0.925590000
H	-5.034141000	-2.493323000	1.002426000

E(RTPSSh) = -3301.99094760
Zero-point correction = 0.596324 (Hartree/Particle)
Thermal correction to Energy = 0.635801
Thermal correction to Enthalpy = 0.636745
Thermal correction to Gibbs Free Energy = 0.520943

6.5.3 [Cu(I)LS] Geometries

$[Cu(I)(TMG_3trphen)(MeCN)]^+$ ($C1_{TMG}$ + MeCN)

Cu	-0.054958000	-0.202739000	-0.733393000
N	0.575910000	0.108285000	1.701641000
N	1.803309000	-1.019621000	-0.496080000
N	-1.515242000	-1.483703000	1.003851000
N	0.104623000	1.840058000	-0.401799000
N	-3.695371000	-1.314737000	0.052354000
N	-2.402759000	-3.239500000	-0.181419000
N	2.516370000	-1.072456000	-2.709349000
N	4.091103000	-0.747914000	-1.044380000
N	-0.907123000	2.690556000	-2.308697000
N	-1.288028000	3.742988000	-0.274160000
N	-1.355838000	-0.589517000	-2.069993000
C	1.323849000	-1.097590000	1.871526000
C	2.016990000	-1.605923000	0.755714000
C	2.779364000	-2.770010000	0.922558000
H	3.295003000	-3.184916000	0.063752000
C	2.836654000	-3.421119000	2.149104000
H	3.424427000	-4.326939000	2.246694000
C	2.120182000	-2.928049000	3.238100000
H	2.149907000	-3.438581000	4.193488000
C	1.369042000	-1.765973000	3.091366000
H	0.808539000	-1.362522000	3.926840000
C	1.349437000	1.308099000	1.598081000
C	2.382817000	1.585877000	2.489043000

H	2.621547000	0.853343000	3.251673000
C	3.095214000	2.777254000	2.404290000
H	3.896863000	2.984902000	3.102761000
C	2.761621000	3.697713000	1.411276000
H	3.309266000	4.629764000	1.327077000
C	1.745865000	3.419208000	0.506177000
H	1.525282000	4.119252000	-0.291992000
C	1.022005000	2.216705000	0.573883000
C	-0.636143000	0.210188000	2.451248000
C	-0.764601000	1.088968000	3.522870000
H	0.068401000	1.734846000	3.772158000
C	-1.940457000	1.143403000	4.266564000
H	-2.027290000	1.834968000	5.096170000
C	-2.983102000	0.276985000	3.949014000
H	-3.894743000	0.280385000	4.536447000
C	-2.866438000	-0.597275000	2.874795000
H	-3.683761000	-1.268922000	2.640212000
C	-1.711313000	-0.627697000	2.072658000
C	2.786138000	-0.965562000	-1.380583000
C	4.450782000	-0.051798000	0.177726000
H	5.306698000	0.594831000	-0.031371000
H	4.720267000	-0.748416000	0.978812000
H	3.613891000	0.558058000	0.507034000
C	5.188376000	-1.411696000	-1.735340000
H	4.795648000	-2.072259000	-2.504322000
H	5.752375000	-2.011221000	-1.013492000
H	5.868127000	-0.686754000	-2.192050000
C	1.410680000	-1.877842000	-3.197215000
H	0.668226000	-1.255652000	-3.700980000
H	0.937185000	-2.381817000	-2.358991000
H	1.789511000	-2.617758000	-3.909888000
C	3.248344000	-0.322960000	-3.718617000
H	3.846674000	-0.979062000	-4.358179000
H	3.900978000	0.400018000	-3.234859000
H	2.532534000	0.211697000	-4.349664000
C	-2.530104000	-1.983263000	0.331070000
C	-1.313762000	-4.083147000	0.288104000
H	-1.614498000	-5.127355000	0.179765000
H	-1.106235000	-3.860898000	1.331017000
H	-0.400310000	-3.914695000	-0.293042000
C	-2.969240000	-3.640930000	-1.461061000
H	-2.162563000	-3.808009000	-2.182868000
H	-3.625220000	-2.864763000	-1.841483000
H	-3.539048000	-4.567544000	-1.356051000
C	-4.994201000	-1.971635000	0.021449000
H	-5.482689000	-1.844634000	-0.949670000
H	-5.638215000	-1.531407000	0.790766000
H	-4.877741000	-3.032405000	0.230374000
C	-3.734737000	0.136967000	0.036346000
H	-2.721150000	0.524143000	-0.047413000
H	-4.197824000	0.540181000	0.942985000
H	-4.315972000	0.462318000	-0.831171000
C	-0.664733000	2.754307000	-0.974599000
C	0.087571000	2.149823000	-3.221400000
H	-0.287726000	1.255720000	-3.722938000
H	0.980319000	1.891330000	-2.658457000
H	0.330482000	2.900599000	-3.979885000
C	-2.177452000	3.080803000	-2.899717000
H	-2.083839000	3.983870000	-3.510191000
H	-2.908548000	3.250923000	-2.112774000
H	-2.531832000	2.270150000	-3.541437000
C	-1.538737000	3.598300000	1.150179000
H	-2.507052000	4.049199000	1.379185000
H	-0.766869000	4.092816000	1.749099000
H	-1.561633000	2.542967000	1.410164000
C	-1.474848000	5.084086000	-0.813437000
H	-1.028681000	5.149570000	-1.802571000
H	-0.973878000	5.801444000	-0.156220000
H	-2.534538000	5.346554000	-0.873891000
C	-2.138178000	-0.720894000	-2.909824000
C	-3.115501000	-0.877224000	-3.968843000
H	-2.877323000	-0.202045000	-4.792685000
H	-4.111658000	-0.641552000	-3.590249000
H	-3.104515000	-1.903954000	-4.338084000

E(RTPSSh) = -3608.16051133
Zero-point correction = 0.828586 (Hartree/Particle)
Thermal correction to Energy = 0.880875
Thermal correction to Enthalpy = 0.881820
Thermal correction to Gibbs Free Energy = 0.744256

Cu(I)(DMEG$_3$trphen)(MeCN)]$^+$ (C1$_{DMEG}$ + MeCN)

Cu	-0.316291000	-0.095766000	-0.871751000
N	0.352803000	-0.043840000	1.451799000
N	-2.132836000	-0.373253000	0.240894000
N	-3.485681000	-1.239098000	-1.461482000
N	-3.763091000	-2.127139000	0.565741000
C	-0.839241000	0.383390000	2.131957000
C	-0.761273000	1.035465000	3.359463000
H	0.215869000	1.211094000	3.793437000
C	-1.909426000	1.458588000	4.018321000
H	-1.835367000	1.965341000	4.972769000
C	-3.152617000	1.223944000	3.431179000
H	-4.059431000	1.554840000	3.924980000
C	-3.240191000	0.584792000	2.203052000
H	-4.206784000	0.428230000	1.737993000
C	-2.088232000	0.148455000	1.523532000
C	-3.079865000	-1.186650000	-0.163799000
C	-3.368730000	-0.109687000	-2.360999000
H	-3.045547000	-0.445955000	-3.347110000
H	-2.633039000	0.582154000	-1.955280000
H	-4.333074000	0.402822000	-2.455706000
C	-4.597273000	-2.171432000	-1.617134000
H	-4.497664000	-2.757829000	-2.530978000
H	-5.543546000	-1.618442000	-1.654228000
C	-4.483168000	-3.017147000	-0.353395000
H	-5.449520000	-3.305001000	0.059182000
H	-3.888801000	-3.921597000	-0.530759000
C	-3.198447000	-2.742165000	1.757512000
H	-3.986639000	-3.310205000	2.251706000
H	-2.838868000	-1.978322000	2.440969000
H	-2.372424000	-3.415784000	1.504254000
N	0.183820000	1.839463000	-0.527759000
N	-1.260066000	2.852850000	-2.072555000
N	-0.915202000	3.953865000	-0.153110000
C	1.371760000	0.961419000	1.378473000
C	2.468821000	0.965846000	2.231048000
H	2.574161000	0.164054000	2.952763000

C	3.415000000	1.982645000	2.153124000
H	4.269883000	1.981313000	2.818698000
C	3.248464000	3.004555000	1.219270000
H	3.979681000	3.801766000	1.149349000
C	2.157479000	2.999086000	0.358041000
H	2.044819000	3.775789000	-0.389660000
C	1.204411000	1.975391000	0.419176000
C	-0.594456000	2.834191000	-0.876257000
C	-0.739274000	2.164300000	-3.240105000
H	-1.524204000	2.118609000	-3.994449000
H	-0.453857000	1.147862000	-2.964586000
H	0.133256000	2.681449000	-3.655439000
C	-1.890302000	4.159603000	-2.261731000
H	-2.851957000	4.062119000	-2.764688000
H	-1.238745000	4.807872000	-2.860221000
C	-2.011991000	4.658743000	-0.828938000
H	-1.896325000	5.738073000	-0.737305000
H	-2.969458000	4.362770000	-0.383484000
C	-0.961416000	3.946229000	1.304410000
H	-1.073183000	4.976041000	1.643603000
H	-0.040245000	3.541507000	1.712757000
H	-1.805850000	3.350660000	1.667472000
N	2.101375000	-1.065861000	-0.350985000
N	3.601515000	-0.129037000	-1.860694000
N	4.519299000	-1.301611000	-0.191800000
C	0.756434000	-1.399239000	1.601772000
C	0.216337000	-2.230534000	2.578668000
H	-0.489082000	-1.817688000	3.288970000
C	0.569827000	-3.576625000	2.638624000
H	0.134853000	-4.213145000	3.400132000
C	1.479386000	-4.092631000	1.719530000
H	1.755756000	-5.140465000	1.752044000
C	2.034220000	-3.263973000	0.748785000
H	2.734159000	-3.662163000	0.022633000
C	1.695857000	-1.906920000	0.671059000
C	3.319723000	-0.872241000	-0.737165000
C	2.599531000	0.119581000	-2.873453000
H	2.910226000	0.977121000	-3.471881000
H	1.655792000	0.343443000	-2.378628000
H	2.459036000	-0.746423000	-3.533176000
C	4.991370000	-0.321352000	-2.250246000
H	5.404099000	0.584407000	-2.694925000
H	5.084316000	-1.144726000	-2.971635000
C	5.628484000	-0.673671000	-0.914883000
H	6.471637000	-1.358940000	-1.005384000
H	5.959066000	0.227940000	-0.382383000
C	4.737368000	-1.486981000	1.234566000
H	5.539477000	-2.214024000	1.376064000
H	3.838538000	-1.861424000	1.712988000
H	5.029110000	-0.541845000	1.706175000
C	-0.594811000	-2.427922000	-2.794107000
N	-0.409415000	-1.481655000	-2.160725000
C	-0.848939000	-3.622169000	-3.574119000
H	-1.743286000	-4.120159000	-3.194887000
H	0.001199000	-4.301657000	-3.496848000
H	-1.002166000	-3.356346000	-4.621200000

E(RTPSSh) = -3604.57341730
Zero-point correction = 0.766312 (Hartree/Particle)
Thermal correction to Energy = 0.814518
Thermal correction to Enthalpy = 0.815462
Thermal correction to Gibbs Free Energy = 0.682926

$[Cu(I)\{N(QuMe)(PhTMG)_2\}(MeCN)]^+$ ($C3_{TMG}$ + MeCN)

N	-0.004718000	-0.782801000	1.420332000
C	0.125200000	1.654965000	1.601154000
N	-1.052174000	-2.385571000	-0.516613000
N	1.863149000	-0.507231000	-0.600269000
C	1.180453000	2.658448000	3.552342000
H	1.495323000	3.550018000	4.082838000
N	-0.396753000	1.739603000	0.316013000
C	1.443008000	1.396988000	4.085501000
H	1.954374000	1.293598000	5.034730000
N	2.927292000	0.534259000	-2.375700000
C	1.043773000	0.268714000	3.379193000
H	1.245958000	-0.722348000	3.767428000
N	4.017360000	0.433156000	-0.327373000
C	0.386788000	0.386347000	2.157065000
N	-2.097938000	3.324840000	0.774802000
C	-1.162718000	2.758285000	-0.040160000
N	-1.069996000	3.254253000	-1.300807000
C	0.155672000	3.107599000	-2.066347000
H	0.054029000	2.325520000	-2.824483000
H	0.379199000	4.053709000	-2.567023000
H	0.968383000	2.848977000	-1.392822000
C	-2.228680000	3.726667000	-2.045699000
H	-2.279475000	3.188054000	-2.996097000
H	-3.134895000	3.526439000	-1.478982000
H	-2.162352000	4.797297000	-2.258559000
C	-2.677122000	2.582995000	1.880721000
H	-3.738330000	2.833839000	1.949083000
H	-2.573788000	1.516985000	1.693803000
H	-2.193052000	2.827022000	2.832211000
C	-2.387564000	4.752977000	0.753450000
H	-3.429125000	4.945746000	0.481846000
H	-2.205210000	5.165824000	1.750483000
H	-1.731330000	5.251089000	0.044096000
C	-0.588427000	-3.430153000	-2.639202000
H	0.444286000	-3.462191000	-2.292270000
H	-0.839170000	-4.369814000	-3.133476000
H	-0.666737000	-2.628412000	-3.380891000
Cu	-0.026515000	0.086084000	-0.918489000
C	-1.512966000	-3.150298000	-1.490233000
C	-2.837140000	-3.654161000	-1.481871000
H	-3.173118000	-4.287697000	-2.294084000
C	-3.679868000	-3.324508000	-0.452093000
H	-4.702365000	-3.685834000	-0.432334000
C	-3.215646000	-2.501040000	0.600027000
C	-4.029063000	-2.083913000	1.681742000
H	-5.059829000	-2.416261000	1.729487000
C	-3.503953000	-1.260152000	2.646658000
H	-4.118703000	-0.932669000	3.476912000
C	-2.159898000	-0.835955000	2.587640000
H	-1.763313000	-0.195422000	3.365219000
C	-1.338281000	-1.226764000	1.550364000
C	-1.864242000	-2.068489000	0.521354000
C	2.021986000	-1.552289000	0.314209000
C	3.063949000	-2.485527000	0.221690000
H	3.828850000	-2.345596000	-0.533716000
C	3.098237000	-3.604588000	1.045134000

H	3.910987000	-4.315047000	0.944895000
C	2.082991000	-3.828660000	1.973649000
H	2.099242000	-4.707593000	2.606851000
C	1.049061000	-2.904825000	2.085623000
H	0.250992000	-3.052431000	2.804815000
C	1.023108000	-1.773463000	1.278497000
C	2.924825000	0.124545000	-1.081221000
C	3.917984000	0.563351000	1.117130000
H	2.888745000	0.780022000	1.393359000
H	4.239400000	-0.349299000	1.629670000
H	4.557616000	1.390626000	1.433438000
C	5.370909000	0.393528000	-0.865903000
H	5.960845000	-0.327406000	-0.291130000
H	5.345054000	0.073000000	-1.904456000
H	5.854761000	1.371854000	-0.799254000
C	2.083040000	-0.130809000	-3.355173000
H	1.892539000	-1.151280000	-3.033339000
H	1.122455000	0.381207000	-3.478454000
H	2.604921000	-0.138965000	-4.314576000
C	3.555050000	1.777142000	-2.805706000
H	2.820354000	2.379659000	-3.346096000
H	3.895349000	2.334376000	-1.935964000
H	4.402537000	1.589635000	-3.470589000
C	0.537167000	2.784722000	2.329504000
H	0.375864000	3.767793000	1.902374000
C	-2.424448000	0.035219000	-2.779370000
N	-1.431732000	0.076877000	-2.191163000
C	-3.677526000	-0.032807000	-3.503734000
H	-3.496025000	0.089677000	-4.572660000
H	-4.347366000	0.756948000	-3.159264000
H	-4.144319000	-1.003335000	-3.327013000

E(RTPSSh) = -3455.68193840
Zero-point correction = 0.722319 (Hartree/Particle)
Thermal correction to Energy = 0.769185
Thermal correction to Enthalpy = 0.770129
Thermal correction to Gibbs Free Energy = 0.641859

$[Cu(I)\{N(QuMe)(PhDMEG)_2\}(MeCN)]^+$ ($C3_{DMEG}$ + MeCN)

N	-0.009170000	-0.996608000	1.307485000
C	-0.880167000	-2.075382000	0.952474000
N	1.387789000	-2.099906000	-0.740106000
C	-0.791746000	-3.317632000	1.569642000
H	-0.014721000	-3.481825000	2.307889000
N	0.175446000	1.658070000	0.531094000
C	-1.692057000	-4.328655000	1.248397000
H	-1.620554000	-5.294804000	1.733348000
N	-1.789285000	-0.634494000	-0.755639000
C	-2.692301000	-4.079650000	0.309911000
H	-3.403759000	-4.856512000	0.053857000
N	-4.068854000	0.054905000	-0.477080000
C	-2.772582000	-2.844659000	-0.323161000
H	-3.525963000	-2.668726000	-1.082562000
N	-2.894468000	0.865353000	-2.196584000
C	-1.860567000	-1.824413000	-0.024163000
N	0.954373000	3.397406000	-0.845529000
C	-2.866184000	0.026206000	-1.112299000
N	1.669214000	3.388585000	1.263196000
C	-4.233813000	-0.273931000	0.931478000
H	-4.865702000	0.487339000	1.391293000
H	-3.266011000	-0.274462000	1.431239000
H	-4.701456000	-1.252354000	1.058988000
C	-2.062622000	0.618943000	-3.362582000
H	-1.979028000	1.541246000	-3.937339000
H	-2.493998000	-0.163717000	-3.998092000
H	-1.068246000	0.310318000	-3.039120000
C	-4.936932000	1.067557000	-1.083084000
H	-4.928264000	1.973267000	-0.466573000
H	-5.962496000	0.709230000	-1.169530000
C	-4.273387000	1.298224000	-2.436938000
H	-4.725545000	0.672873000	-3.215994000
H	-4.307791000	2.339152000	-2.757170000
C	1.360381000	-1.275394000	1.496932000
C	2.044059000	-0.942273000	2.648291000
H	1.509264000	-0.478380000	3.467812000
Cu	0.078080000	0.128223000	-0.929216000
C	3.422612000	-1.213777000	2.772816000
H	3.927688000	-0.941120000	3.692012000
C	4.116877000	-1.832311000	1.761585000
H	5.172954000	-2.054956000	1.862920000
C	3.448393000	-2.175844000	0.561590000
C	2.067698000	-1.879844000	0.413979000
C	4.088169000	-2.782844000	-0.545320000
H	5.140527000	-3.036326000	-0.477543000
C	3.376698000	-3.032911000	-1.689179000
H	3.848770000	-3.496689000	-2.547177000
C	2.011653000	-2.656726000	-1.762578000
C	1.223339000	-2.870152000	-3.021130000
H	0.976709000	-3.930028000	-3.140350000
H	1.797370000	-2.567942000	-3.900007000
H	0.297007000	-2.298928000	-2.977061000
C	-0.602688000	0.020375000	2.124160000
C	-1.341277000	-0.313499000	3.256009000
H	-1.463901000	-1.361024000	3.505558000
C	-1.911374000	0.674411000	4.050795000
H	-2.483968000	0.405116000	4.929850000
C	-1.731319000	2.012037000	3.699995000
H	-2.172103000	2.796808000	4.304546000
C	-1.008000000	2.353231000	2.565933000
H	-0.902265000	3.394251000	2.282893000
C	-0.430825000	1.367483000	1.745540000
C	0.877761000	2.756611000	0.354439000
C	-0.113309000	3.334782000	-1.825265000
H	0.304449000	3.275747000	-2.830820000
H	-0.749808000	4.224493000	-1.752411000
H	-0.714245000	2.447489000	-1.632656000
C	2.187553000	2.742967000	2.456655000
H	3.265390000	2.909714000	2.507255000
H	2.000800000	1.671731000	2.404665000
H	1.720280000	3.143126000	3.359198000
C	1.708477000	4.642443000	-0.708066000
H	1.012775000	5.488228000	-0.662113000
H	2.383469000	4.791522000	-1.551129000
C	2.447665000	4.446613000	0.615988000
H	3.475472000	4.100352000	0.461813000
H	2.469977000	5.350726000	1.224372000
C	2.353486000	0.727275000	-2.865255000
N	1.432099000	0.497284000	-2.210101000
C	3.520987000	1.007542000	-3.675927000
H	4.002137000	1.922012000	-3.324986000
H	3.227470000	1.132270000	-4.719356000

H	4.225034000	0.177334000	-3.597368000

E(RTPSSh) = -3453.28699691
Zero-point correction = 0.680989 (Hartree/Particle)
Thermal correction to Energy = 0.725040
Thermal correction to Enthalpy = 0.725984
Thermal correction to Gibbs Free Energy = 0.600603

[Cu(I){N(QuMe)$_2$(PhTMG)}(MeCN)]$^+$ (C5$_{TMG}$ + MeCN)

N	0.586471000	-0.763261000	-1.093694000
C	0.925605000	-0.896369000	3.867562000
H	1.412708000	-0.879589000	4.842156000
H	0.117073000	-1.632171000	3.899301000
H	0.476458000	0.080568000	3.669150000
Cu	-0.083070000	0.121106000	1.078212000
N	1.516824000	-1.003978000	1.526005000
C	1.894581000	-1.240831000	2.780627000
N	1.663180000	1.674283000	-0.547263000
C	3.164905000	-1.774287000	3.086578000
H	3.421777000	-1.956904000	4.122033000
N	-1.776397000	-0.766848000	0.363157000
C	4.066426000	-2.009045000	2.082751000
H	5.063082000	-2.375215000	2.301390000
N	-3.978557000	-0.299699000	-0.377410000
C	3.697689000	-1.758241000	0.742709000
N	-3.347005000	0.141634000	1.805734000
C	4.593859000	-1.922027000	-0.340199000
H	5.601019000	-2.267306000	-0.137619000
C	4.188892000	-1.633392000	-1.619417000
H	4.875735000	-1.741589000	-2.449952000
C	2.863332000	-1.226495000	-1.867807000
H	2.538642000	-1.028695000	-2.882628000
C	1.960051000	-1.087111000	-0.839605000
C	2.374200000	-1.298398000	0.501487000
C	2.987662000	2.901876000	1.052302000
H	4.027562000	3.170358000	0.844271000
H	2.962099000	1.935744000	1.554016000
H	2.585130000	3.666444000	1.722602000
C	2.192197000	2.837203000	-0.218852000
C	2.011530000	3.994352000	-1.019768000
H	2.466711000	4.930034000	-0.717102000
C	1.256259000	3.916421000	-2.159562000
H	1.095224000	4.790111000	-2.781673000
C	0.670844000	2.682642000	-2.532714000
C	-0.147431000	2.519576000	-3.676368000
H	-0.336567000	3.371479000	-4.319552000
C	-0.691725000	1.289370000	-3.952156000
H	-1.318357000	1.153838000	-4.825736000
C	-0.440428000	0.180079000	-3.117623000
H	-0.871222000	-0.783232000	-3.359103000
C	0.348127000	0.307143000	-1.993956000
C	0.921950000	1.575953000	-1.678600000
C	-0.298148000	-1.900518000	-1.174616000
C	0.049241000	-3.030641000	-1.908670000
H	1.005463000	-3.053540000	-2.416689000
C	-0.815953000	-4.115421000	-1.997059000
H	-0.535397000	-4.988755000	-2.572960000
C	-2.042412000	-4.062183000	-1.337653000
H	-2.725775000	-4.902159000	-1.389505000
C	-2.389311000	-2.946389000	-0.588913000
H	-3.324994000	-2.930935000	-0.042463000
C	-1.526616000	-1.843453000	-0.485059000
C	-3.011693000	-0.337779000	0.581332000
C	-2.660724000	-0.312963000	3.003167000
H	-1.967032000	0.446221000	3.374489000
H	-2.109720000	-1.221667000	2.775532000
H	-3.402594000	-0.519948000	3.779405000
C	-4.243044000	1.276093000	1.982213000
H	-3.732130000	2.038010000	2.577593000
H	-5.160512000	0.987691000	2.502688000
H	-4.494589000	1.698441000	1.012380000
C	-3.643496000	-0.219487000	-1.788032000
H	-2.637249000	0.176341000	-1.898459000
H	-4.349541000	0.457976000	-2.274082000
H	-3.698348000	-1.198461000	-2.275271000
C	-5.381974000	-0.554764000	-0.077069000
H	-5.490916000	-0.824344000	0.970464000
H	-5.727651000	-1.390276000	-0.693286000
H	-6.002573000	0.318818000	-0.294650000
C	-0.727577000	3.015380000	1.806069000
N	-0.466094000	1.906563000	1.623925000
C	-1.043229000	4.413177000	2.019279000
H	-1.027560000	4.636324000	3.087159000
H	-2.034452000	4.633189000	1.619581000
H	-0.302935000	5.033444000	1.510933000

E(RTPSSh) = -3303.19590183
Zero-point correction = 0.617247 (Hartree/Particle)
Thermal correction to Energy = 0.657817
Thermal correction to Enthalpy = 0.658761
Thermal correction to Gibbs Free Energy = 0.542715

[Cu(I){N(QuMe)$_2$(PhDMEG)}(MeCN)]$^+$ (C5$_{DMEG}$ + MeCN)

Cu	-0.058699000	0.045100000	1.095000000
N	0.614020000	-0.695334000	-1.116152000
N	1.457754000	1.831758000	-0.553352000
N	1.638923000	-0.965716000	1.446535000
N	-1.698512000	-0.975561000	0.384549000
N	-3.993498000	-0.668125000	-0.297439000
N	-3.357437000	-0.026482000	1.743414000
C	-0.131922000	-1.926036000	-1.186922000
C	0.331070000	-3.008993000	-1.928247000
H	1.273410000	-2.920435000	-2.454670000
C	-0.403736000	-4.187084000	-1.999238000
H	-0.034648000	-5.023150000	-2.580426000
C	-1.617243000	-4.274735000	-1.319036000
H	-2.200731000	-5.187360000	-1.361357000
C	-2.078311000	-3.205746000	-0.563889000
H	-3.006963000	-3.288284000	-0.011285000
C	-1.345309000	-2.011532000	-0.474937000
C	-2.944984000	-0.604014000	0.580006000
C	-2.718201000	-0.292658000	3.018141000
H	-2.749461000	0.602611000	3.639411000

H	-1.680364000	-0.568260000	2.842719000
H	-3.227496000	-1.111845000	3.538735000
C	-3.818454000	-0.642671000	-1.742133000
H	-4.770476000	-0.906561000	-2.202416000
H	-3.072590000	-1.370280000	-2.047044000
H	-3.516407000	0.352880000	-2.084536000
C	-4.805645000	0.171954000	1.724251000
H	-5.079059000	1.123532000	2.179670000
H	-5.295705000	-0.638541000	2.276540000
C	-5.118934000	0.110554000	0.234847000
H	-6.067729000	-0.377495000	0.015178000
H	-5.118832000	1.109163000	-0.217237000
C	2.023650000	-0.863353000	-0.924743000
C	2.904543000	-0.845054000	-1.980434000
H	2.529803000	-0.636228000	-2.975601000
C	4.274922000	-1.107295000	-1.782571000
H	4.946005000	-1.090786000	-2.632649000
C	4.747545000	-1.416687000	-0.531379000
H	5.792991000	-1.654249000	-0.372611000
C	3.869678000	-1.419615000	0.578984000
C	2.497990000	-1.099968000	0.391562000
C	4.295058000	-1.709111000	1.894204000
H	5.330961000	-1.973892000	2.073056000
C	3.395939000	-1.643979000	2.926127000
H	3.695802000	-1.865093000	3.942321000
C	2.067417000	-1.238271000	2.677024000
C	1.087549000	-1.069584000	3.795936000
H	1.569710000	-1.179354000	4.766716000
H	0.291780000	-1.815591000	3.715423000
H	0.622130000	-0.081236000	3.736648000
C	0.196786000	0.369312000	-1.955161000
C	-0.660162000	0.188961000	-3.019247000
H	-0.999412000	-0.808685000	-3.265957000
C	-1.095648000	1.287501000	-3.788857000
H	-1.770791000	1.109223000	-4.617471000
C	-0.667146000	2.561920000	-3.508803000
H	-0.997160000	3.406139000	-4.103352000
C	0.215667000	2.780809000	-2.424097000
C	0.650239000	1.684234000	-1.632877000
C	0.691306000	4.060253000	-2.048928000
H	0.389754000	4.928404000	-2.624940000
C	1.518341000	4.188479000	-0.964819000
H	1.892018000	5.159635000	-0.662298000
C	1.881595000	3.035998000	-0.221252000
C	2.760112000	3.150869000	0.990343000
H	3.753157000	3.516967000	0.713134000
H	2.860714000	2.177286000	1.467760000
H	2.342744000	3.863155000	1.707356000
C	-0.867503000	2.839999000	2.017263000
N	-0.542654000	1.769320000	1.738536000
C	-1.261543000	4.192745000	2.353712000
H	-0.748479000	4.893617000	1.692952000
H	-0.990696000	4.409248000	3.388252000
H	-2.339853000	4.305338000	2.231393000

E(RTPSSh) = -3301.99861826
Zero-point correction = 0.596793 (Hartree/Particle)
Thermal correction to Energy = 0.635832
Thermal correction to Enthalpy = 0.636776
Thermal correction to Gibbs Free Energy = 0.5237

6.5.4 [Cu(II)L] Geometries

$[Cu(II)(TMG_3trphen)]^{2+}$ ($C2_{TMG}$ - MeCN)

Cu	-0.018047000	-0.121928000	0.598894000
N	0.147089000	-0.405809000	-1.562333000
C	-1.237382000	-0.456268000	-1.990078000
C	-2.220092000	-0.668077000	-1.008978000
C	-3.561819000	-0.687026000	-1.406174000
H	-4.333222000	-0.814841000	-0.656447000
C	-3.906717000	-0.508004000	-2.740003000
H	-4.952364000	-0.517128000	-3.023398000
C	-2.924763000	-0.285163000	-3.701930000
H	-3.195292000	-0.123161000	-4.737576000
C	-1.587893000	-0.252878000	-3.318977000
H	-0.811482000	-0.056487000	-4.048102000
N	-1.831845000	-0.762426000	0.337715000
C	-2.468275000	-1.595271000	1.171474000
N	-2.915108000	-2.808105000	0.773074000
C	-2.295194000	-3.519201000	-0.338082000
H	-1.289368000	-3.139343000	-0.501068000
H	-2.876277000	-3.409895000	-1.257969000
H	-2.238619000	-4.577191000	-0.075687000
C	-4.150505000	-3.391319000	1.289390000
H	-4.652244000	-2.675802000	1.935792000
H	-3.953822000	-4.312309000	1.842765000
H	-4.803892000	-3.620673000	0.443612000
N	-2.630097000	-1.237797000	2.460194000
C	-2.659964000	0.164125000	2.849704000
H	-2.839765000	0.777211000	1.971153000
H	-1.717845000	0.460535000	3.318462000
H	-3.465545000	0.311739000	3.571646000
C	-2.606283000	-2.206301000	3.551845000
H	-2.288532000	-3.174691000	3.173602000
H	-3.586314000	-2.299853000	4.025104000
H	-1.887813000	-1.864621000	4.300131000
C	0.859623000	0.790350000	-1.950548000
C	0.691920000	1.943045000	-1.157706000
C	1.372168000	3.109130000	-1.541648000
H	1.276338000	3.998359000	-0.930126000
C	2.184672000	3.119548000	-2.665148000
H	2.699758000	4.032365000	-2.940051000
C	2.364444000	1.961671000	-3.423396000
H	3.010964000	1.967547000	-4.291777000
C	1.706190000	0.796004000	-3.055594000
H	1.840564000	-0.116339000	-3.623630000
N	-0.026169000	1.839543000	0.029848000
C	-0.713450000	2.881300000	0.498664000
N	-1.457534000	3.670777000	-0.314599000
C	-1.953755000	3.177088000	-1.592234000
H	-2.022430000	2.092435000	-1.562682000
H	-1.301481000	3.474862000	-2.418718000
H	-2.948112000	3.595868000	-1.756186000
C	-1.581495000	5.110588000	-0.105787000
H	-0.955022000	5.418559000	0.727099000
H	-2.617826000	5.396343000	0.088477000

H	-1.238645000	5.622151000	-1.009159000
N	-0.717267000	3.138134000	1.823806000
C	0.405195000	2.748673000	2.664634000
H	1.233779000	2.436041000	2.035709000
H	0.125669000	1.931766000	3.334832000
H	0.708701000	3.604010000	3.272866000
C	-1.853252000	3.738487000	2.513512000
H	-2.721006000	3.737583000	1.858505000
H	-1.636370000	4.760667000	2.833151000
H	-2.075514000	3.140883000	3.400314000
C	0.942461000	-1.605705000	-1.611908000
C	1.867293000	-1.765373000	-0.560807000
C	2.739929000	-2.857644000	-0.602058000
H	3.449119000	-3.009221000	0.201944000
C	2.651799000	-3.783158000	-1.634629000
H	3.322027000	-4.634319000	-1.639992000
C	1.691289000	-3.646486000	-2.635411000
H	1.616029000	-4.381666000	-3.426656000
C	0.833910000	-2.551498000	-2.622616000
H	0.090432000	-2.420979000	-3.398864000
N	1.745412000	-0.908404000	0.551200000
C	2.805903000	-0.630229000	1.333721000
N	4.040595000	-0.442782000	0.828436000
C	4.240870000	0.030820000	-0.536875000
H	3.316418000	0.455360000	-0.918245000
H	4.566164000	-0.782865000	-1.189759000
H	5.009951000	0.805179000	-0.519703000
C	5.253728000	-0.816902000	1.551502000
H	4.993857000	-1.403899000	2.428411000
H	5.829812000	0.061350000	1.850043000
H	5.866013000	-1.428959000	0.885363000
N	2.606707000	-0.503156000	2.658432000
C	1.510363000	-1.189771000	3.335260000
H	1.099675000	-1.956781000	2.684595000
H	0.724396000	-0.484838000	3.616512000
H	1.899170000	-1.653025000	4.244224000
C	3.395446000	0.401511000	3.490616000
H	3.960068000	1.081837000	2.858207000
H	4.075731000	-0.144569000	4.147492000
H	2.706880000	0.980503000	4.109041000

E(UTPSSh) = -3475.16189274
Zero-point correction = 0.785346 (Hartree/Particle)
Thermal correction to Energy = 0.831933
Thermal correction to Enthalpy = 0.832877
Thermal correction to Gibbs Free Energy = 0.708624

$Cu(II)(DMEG_3trphen)]^{2+}$ ($C2_{DMEG}$ - MeCN)

Cu	0.049319000	-0.204572000	-0.557485000
N	0.233558000	0.049901000	1.570314000
N	-0.322895000	1.822458000	-0.448113000
N	-1.553727000	2.339350000	-2.372821000
N	-2.192716000	3.323459000	-0.474072000
C	0.777969000	1.387841000	1.640481000
C	1.656643000	1.758448000	2.654371000
H	1.960899000	1.022422000	3.388497000
C	2.116450000	3.066450000	2.726938000
H	2.786803000	3.360109000	3.524645000
C	1.698527000	3.997300000	1.773622000
H	2.052464000	5.020070000	1.826179000
C	0.852406000	3.623482000	0.740576000
H	0.563498000	4.338728000	-0.020239000
C	0.381779000	2.305274000	0.644907000
C	-1.290676000	2.486094000	-1.048924000
C	-0.522630000	2.003243000	-3.341217000
H	-0.944353000	1.375539000	-4.125752000
H	0.279133000	1.467071000	-2.838918000
H	-0.113868000	2.913432000	-3.792490000
C	-2.625235000	3.255310000	-2.773564000
H	-3.317118000	2.772391000	-3.462515000
H	-2.188611000	4.132085000	-3.263710000
C	-3.266467000	3.613773000	-1.435308000
H	-3.571927000	4.657083000	-1.373308000
H	-4.128669000	2.974871000	-1.216557000
C	-2.558504000	3.241536000	0.934400000
H	-3.102828000	4.147854000	1.196720000
H	-1.668829000	3.179106000	1.554399000
H	-3.193446000	2.369628000	1.122270000
N	1.896391000	-0.756531000	-0.390436000
N	2.816231000	-0.740778000	-2.555875000
N	4.085666000	0.058751000	-0.926922000
C	1.173823000	-0.990457000	1.888729000
C	1.174537000	-1.677800000	3.094833000
H	0.400365000	-1.478632000	3.824956000
C	2.191095000	-2.587329000	3.362079000
H	2.208455000	-3.113515000	4.308029000
C	3.200717000	-2.798641000	2.420654000
H	3.997590000	-3.501120000	2.632895000
C	3.180710000	-2.147325000	1.195917000
H	3.935445000	-2.361999000	0.449161000
C	2.138489000	-1.261535000	0.893029000
C	2.909042000	-0.500322000	-1.240719000
C	1.844967000	-1.615417000	-3.186267000
H	1.302182000	-1.076076000	-3.963918000
H	1.147287000	-1.973380000	-2.432007000
H	2.358857000	-2.469593000	-3.633780000
C	4.064850000	-0.390754000	-3.240619000
H	3.868413000	0.270369000	-4.084636000
H	4.536836000	-1.303757000	-3.610453000
C	4.892156000	0.284131000	-2.133536000
H	5.883745000	-0.153490000	-2.020289000
H	4.996532000	1.359358000	-2.293035000
C	4.383662000	0.773938000	0.302173000
H	5.170010000	0.263983000	0.861481000
H	3.488880000	0.841413000	0.914944000
H	4.715744000	1.782810000	0.049439000
N	-1.659276000	-1.056720000	-0.108123000
N	-2.193930000	-2.284033000	-2.029734000
N	-2.464725000	-3.324970000	-0.080068000
C	-1.137854000	-0.066205000	2.034161000
C	-1.522507000	0.447574000	3.266050000
H	-0.786694000	0.942608000	3.887885000
C	-2.843241000	0.332620000	3.685615000
H	-3.143521000	0.733176000	4.645394000
C	-3.773174000	-0.286490000	2.853266000
H	-4.808418000	-0.367109000	3.162595000
C	-3.396281000	-0.776048000	1.609076000
H	-4.131234000	-1.223078000	0.950799000
C	-2.068145000	-0.676541000	1.177374000
C	-2.100514000	-2.167979000	-0.689642000

C	-2.302987000	-1.153451000	-2.932337000
H	-1.584945000	-1.251001000	-3.747269000
H	-2.109772000	-0.238056000	-2.376475000
H	-3.313008000	-1.108782000	-3.350279000
C	-2.774149000	-3.576175000	-2.398320000
H	-2.228093000	-4.031106000	-3.224019000
H	-3.815739000	-3.429023000	-2.700703000
C	-2.659192000	-4.371020000	-1.097380000
H	-3.546509000	-4.963072000	-0.878488000
H	-1.784420000	-5.028708000	-1.103415000
C	-1.919717000	-3.753728000	1.203464000
H	-2.531749000	-4.575770000	1.572211000
H	-1.955252000	-2.943448000	1.925137000
H	-0.885728000	-4.095809000	1.089332000

E(UTPSSh) = -3471.56499398
Zero-point correction = 0.722362 (Hartree/Particle)
Thermal correction to Energy = 0.765433
Thermal correction to Enthalpy = 0.766377
Thermal correction to Gibbs Free Energy = 0.645359

$[Cu(II)\{N(QuMe)(PhTMG)_2\}]^{2+}$ ($C4_{TMG}$ - MeCN)

N	-0.018371000	1.508130000	0.309833000
C	0.284918000	-0.315177000	1.921272000
N	1.557869000	0.355487000	-1.671964000
N	-1.989277000	-0.006680000	-0.747168000
C	-0.401754000	-0.020909000	4.228232000
H	-0.495227000	-0.423805000	5.229647000
N	0.712865000	-1.094667000	0.852361000
C	-0.860329000	1.267721000	3.950102000
H	-1.305152000	1.873659000	4.729012000
N	-2.996503000	-1.975692000	-1.446542000
C	-0.746850000	1.769089000	2.660939000
H	-1.113404000	2.759311000	2.420414000
N	-3.902388000	-0.829232000	0.361082000
C	-0.161428000	0.996190000	1.662660000
N	2.751425000	-1.804045000	1.795336000
C	1.672957000	-2.005722000	0.997160000
N	1.609107000	-3.153873000	0.290614000
C	0.331645000	-3.691416000	-0.153035000
H	0.207441000	-3.563768000	-1.231732000
H	0.298580000	-4.759818000	0.072290000
H	-0.473740000	-3.184792000	0.371076000
C	2.797469000	-3.841704000	-0.201635000
H	2.667101000	-4.038097000	-1.268227000
H	3.669398000	-3.207189000	-0.063671000
H	2.952200000	-4.794492000	0.310501000
C	3.215267000	-0.464193000	2.126467000
H	4.306516000	-0.461511000	2.097094000
H	2.839625000	0.245552000	1.394396000
H	2.884782000	-0.160085000	3.123962000
C	3.372629000	-2.887359000	2.551915000
H	4.403312000	-3.057171000	2.231321000
H	3.374375000	-2.613868000	3.610447000
H	2.796486000	-3.800679000	2.428582000
C	1.655719000	-1.384116000	-3.359423000
H	0.743165000	-1.720849000	-2.867760000
H	1.412256000	-1.119107000	-4.391615000
H	2.368765000	-2.209661000	-3.389545000
Cu	-0.094201000	-0.295644000	-0.858207000
C	2.244523000	-0.204142000	-2.658753000
C	3.504308000	0.306270000	-3.048945000
H	4.032923000	-0.177258000	-3.859761000
C	4.041278000	1.378226000	-2.393001000
H	5.015579000	1.765822000	-2.666233000
C	3.323351000	1.993010000	-1.339578000
C	3.828815000	3.078933000	-0.591576000
H	4.806387000	3.473744000	-0.840207000
C	3.098853000	3.605980000	0.446125000
H	3.493253000	4.424797000	1.033754000
C	1.827147000	3.089187000	0.754457000
H	1.265936000	3.501794000	1.583060000
C	1.291735000	2.056327000	0.018489000
C	2.048159000	1.461210000	-1.019337000
C	-2.261000000	1.362853000	-0.566743000
C	-3.478618000	1.956661000	-0.916541000
H	-4.305842000	1.336239000	-1.237425000
C	-3.602913000	3.339455000	-0.924029000
H	-4.545742000	3.784207000	-1.218462000
C	-2.520413000	4.154369000	-0.596375000
H	-2.618269000	5.232152000	-0.622740000
C	-1.311792000	3.579331000	-0.218922000
H	-0.470165000	4.202699000	0.053344000
C	-1.195895000	2.197169000	-0.170847000
C	-2.976065000	-0.924581000	-0.609314000
C	-3.631954000	-0.131490000	1.614522000
H	-2.561398000	0.000651000	1.739091000
H	-4.126559000	0.842458000	1.633092000
H	-4.013948000	-0.743416000	2.433273000
C	-5.274960000	-1.303039000	0.191005000
H	-5.944576000	-0.495150000	0.493403000
H	-5.457422000	-1.538494000	-0.853923000
H	-5.477652000	-2.178348000	0.811159000
C	-2.503237000	-1.880132000	-2.818197000
H	-2.213763000	-0.855382000	-3.031990000
H	-1.650054000	-2.545791000	-2.963957000
H	-3.300981000	-2.185000000	-3.499453000
C	-3.501685000	-3.287151000	-1.048651000
H	-2.783964000	-4.037757000	-1.384295000
H	-3.583304000	-3.333729000	0.034203000
H	-4.470056000	-3.504683000	-1.503981000
C	0.151322000	-0.806532000	3.228806000
H	0.464665000	-1.821422000	3.441522000

E(UTPSSh) = -3322.67228708
Zero-point correction = 0.679849 (Hartree/Particle)
Thermal correction to Energy = 0.720227
Thermal correction to Enthalpy = 0.721171
Thermal correction to Gibbs Free Energy = 0.60984

$[Cu(II)\{N(QuMe)(PhDMEG)_2\}]^{2+}$ ($C4_{DMEG}$ - MeCN)

N	0.042316000	1.528047000	0.246629000
C	1.194270000	2.217972000	-0.288337000
N	-1.601639000	0.282545000	-1.622028000
C	1.298170000	3.598376000	-0.382746000
H	0.453326000	4.224416000	-0.127464000
N	-0.626353000	-1.069384000	0.906966000
C	2.504768000	4.167868000	-0.775080000
H	2.595993000	5.244881000	-0.833978000
N	1.992124000	0.014887000	-0.830407000
C	3.599188000	3.351694000	-1.063612000
H	4.542020000	3.796608000	-1.357563000
N	3.867292000	-0.916156000	0.337816000
C	3.487301000	1.969534000	-1.016221000
H	4.323354000	1.341946000	-1.299697000
N	3.054456000	-2.005066000	-1.411131000
C	2.265582000	1.380967000	-0.669190000
N	-1.601051000	-3.118579000	0.308419000
C	2.954049000	-0.913644000	-0.639691000
N	-2.666530000	-1.899382000	1.836060000
C	3.836322000	-0.100240000	1.539819000
H	3.848847000	-0.757936000	2.410984000
H	2.927158000	0.493659000	1.560212000
H	4.703826000	0.560954000	1.572587000
C	2.487143000	-2.150478000	-2.740076000
H	1.903087000	-3.069748000	-2.799307000
H	3.291876000	-2.188206000	-3.478387000
H	1.850224000	-1.293914000	-2.949130000
C	4.668969000	-2.146557000	0.296493000
H	4.444365000	-2.742354000	1.183637000
H	5.732840000	-1.911282000	0.288586000
C	4.196899000	-2.828637000	-0.997934000
H	4.957166000	-2.798495000	-1.781483000
H	3.888877000	-3.862507000	-0.844869000
C	-1.287458000	2.050945000	-0.010758000
C	-1.802844000	3.105701000	0.707558000
H	-1.211018000	3.558833000	1.492630000
Cu	0.099352000	-0.294023000	-0.855244000
C	-3.095004000	3.593271000	0.437817000
H	-3.472914000	4.431808000	1.008223000
C	-3.866417000	3.010605000	-0.537996000
H	-4.861853000	3.379658000	-0.753377000
C	-3.381340000	1.899091000	-1.261847000
C	-2.081292000	1.402777000	-0.987551000
C	-4.142261000	1.225250000	-2.246066000
H	-5.135317000	1.586120000	-2.486333000
C	-3.622720000	0.129699000	-2.877622000
H	-4.185902000	-0.400738000	-3.633887000
C	-2.334298000	-0.341006000	-2.535431000
C	-1.783134000	-1.575248000	-3.172865000
H	-2.020309000	-1.596125000	-4.237074000
H	-2.232584000	-2.459878000	-2.712959000
H	-0.700961000	-1.633843000	-3.049550000
C	0.236297000	1.060241000	1.612318000
C	0.843234000	1.873930000	2.564017000
H	1.203674000	2.853416000	2.274643000
C	0.977303000	1.430674000	3.872572000
H	1.437874000	2.069220000	4.615373000
C	0.509585000	0.161632000	4.218108000
H	0.611620000	-0.192981000	5.236869000
C	-0.063640000	-0.666690000	3.266110000
H	-0.387374000	-1.665736000	3.531970000
C	-0.206296000	-0.239668000	1.936463000
C	-1.574218000	-1.978890000	1.043487000
C	-0.404810000	-3.736826000	-0.236074000
H	-0.607413000	-4.126738000	-1.233877000
H	-0.073031000	-4.557274000	0.408632000
H	0.386529000	-2.992360000	-0.291774000
C	-3.197602000	-0.655222000	2.371230000
H	-4.244563000	-0.564893000	2.075102000
H	-2.644876000	0.189347000	1.965965000
H	-3.128963000	-0.636973000	3.460404000
C	-2.702926000	-3.976658000	0.753081000
H	-2.303670000	-4.783138000	1.376598000
H	-3.226370000	-4.414394000	-0.096155000
C	-3.578388000	-3.015326000	1.560080000
H	-4.427278000	-2.646750000	0.976067000
H	-3.950376000	-3.457136000	2.483830000

E(UTPSSh) = -3320.27552869
Zero-point correction = 0.637476 (Hartree/Particle)
Thermal correction to Energy = 0.675727
Thermal correction to Enthalpy = 0.676671
Thermal correction to Gibbs Free Energy = 0.566411

$[Cu(II)\{N(QuMe)_2(PhTMG)\}]^{2+}$ ($C6_{TMG}$ - MeCN)

N	0.774388000	1.087884000	0.123977000
C	1.980374000	-3.244640000	-1.930708000
H	2.614705000	-4.001259000	-2.387970000
H	1.319891000	-2.830755000	-2.696451000
H	1.359919000	-3.732792000	-1.176305000
Cu	0.261425000	-0.839962000	-0.549885000
N	2.180786000	-1.120410000	-0.774148000
C	2.807696000	-2.160823000	-1.316802000
N	-0.210253000	-1.165591000	1.461124000
C	4.216617000	-2.236948000	-1.318574000
H	4.688564000	-3.099081000	-1.769571000
N	-1.308495000	0.063864000	-1.191597000
C	4.961289000	-1.242594000	-0.743626000
H	6.042803000	-1.302135000	-0.718941000
N	-3.594980000	0.454119000	-0.730144000
C	4.316868000	-0.118837000	-0.180599000
N	-2.853030000	-1.638299000	-1.409910000
C	5.014974000	0.943415000	0.436708000
H	6.096074000	0.897961000	0.485955000
C	4.328887000	2.003547000	0.974758000
H	4.859073000	2.811570000	1.461607000
C	2.924709000	2.058706000	0.888373000
H	2.398402000	2.901647000	1.315972000
C	2.221885000	1.053698000	0.266820000
C	2.899986000	-0.078331000	-0.243418000
C	-0.445340000	-3.576618000	1.388425000
H	0.027314000	-4.303805000	2.051356000
H	0.163280000	-3.464036000	0.493941000
H	-1.420731000	-3.979265000	1.104308000
C	-0.610785000	-2.265309000	2.081546000

C	-1.204561000	-2.210379000	3.365575000
H	-1.499174000	-3.134321000	3.845756000
C	-1.424077000	-1.001711000	3.964260000
H	-1.907989000	-0.938756000	4.931820000
C	-1.022234000	0.188384000	3.313136000
C	-1.254243000	1.474856000	3.846855000
H	-1.747369000	1.561487000	4.807469000
C	-0.875360000	2.594268000	3.146178000
H	-1.070648000	3.582704000	3.541125000
C	-0.220413000	2.467202000	1.908086000
H	0.063190000	3.354803000	1.356829000
C	0.055723000	1.224269000	1.384496000
C	-0.375618000	0.052749000	2.056488000
C	0.204820000	1.907059000	-0.936290000
C	0.742583000	3.115268000	-1.353017000
H	1.672362000	3.473865000	-0.931708000
C	0.063948000	3.866945000	-2.307204000
H	0.471257000	4.816273000	-2.630531000
C	-1.138634000	3.400380000	-2.834422000
H	-1.663836000	3.983502000	-3.580977000
C	-1.659217000	2.172630000	-2.444392000
H	-2.561188000	1.790583000	-2.904808000
C	-0.977313000	1.397205000	-1.503921000
C	-2.588774000	-0.353490000	-1.115617000
C	-2.061928000	-2.388845000	-2.381326000
H	-1.490127000	-3.177304000	-1.887760000
H	-1.390238000	-1.712784000	-2.903013000
H	-2.741756000	-2.850383000	-3.100887000
C	-3.922087000	-2.383259000	-0.751292000
H	-3.521547000	-3.355097000	-0.458339000
H	-4.772921000	-2.544313000	-1.416627000
H	-4.244288000	-1.849248000	0.139082000
C	-3.396475000	1.566060000	0.193279000
H	-2.414811000	1.496689000	0.650972000
H	-4.157607000	1.503207000	0.973275000
H	-3.490583000	2.522784000	-0.325201000
C	-4.949428000	0.318693000	-1.264061000
H	-4.940277000	-0.342139000	-2.126764000
H	-5.283182000	1.309333000	-1.579555000
H	-5.642013000	-0.062313000	-0.510790000

E(UTPSSh) = -3170.17901200
Zero-point correction = 0.574910 (Hartree/Particle)
Thermal correction to Energy = 0.608909
Thermal correction to Enthalpy = 0.609853
Thermal correction to Gibbs Free Energy = 0.511599

$[Cu(II)\{N(QuMe)_2(PhDMEG)\}]^{2+}$ ($C6_{DMEG}$ - MeCN)

Cu	0.166123000	-0.920280000	-0.365416000
N	0.808340000	1.097223000	-0.122340000
N	-0.193586000	-0.840406000	1.662282000
N	2.051555000	-1.338319000	-0.583786000
N	-1.349155000	-0.101451000	-1.206553000
N	-3.624918000	0.234176000	-0.516630000
N	-3.054107000	-1.711275000	-1.405802000
C	0.186600000	1.745584000	-1.261770000
C	0.697674000	2.871277000	-1.890302000
H	1.659694000	3.270187000	-1.597193000
C	-0.049482000	3.501081000	-2.880723000
H	0.339605000	4.389512000	-3.361275000
C	-1.305441000	3.004331000	-3.230157000
H	-1.890985000	3.503228000	-3.992583000
C	-1.802534000	1.853234000	-2.637398000
H	-2.752217000	1.438736000	-2.952895000
C	-1.039043000	1.181415000	-1.674565000
C	-2.639418000	-0.490095000	-1.059382000
C	-2.350611000	-2.621404000	-2.292266000
H	-2.200674000	-3.582146000	-1.797990000
H	-1.389061000	-2.186468000	-2.554191000
H	-2.940030000	-2.771043000	-3.199690000
C	-3.471200000	1.442543000	0.275395000
H	-4.120231000	2.225675000	-0.118224000
H	-2.440573000	1.781619000	0.239329000
H	-3.743943000	1.231715000	1.312146000
C	-4.492593000	-1.861078000	-1.155914000
H	-4.690041000	-2.766748000	-0.583581000
H	-5.014067000	-1.925854000	-2.113410000
C	-4.843756000	-0.577699000	-0.386286000
H	-5.700203000	-0.051272000	-0.805356000
H	-5.026906000	-0.767802000	0.673650000
C	2.260078000	1.012047000	-0.079729000
C	3.053805000	2.086505000	0.248508000
H	2.600083000	3.032294000	0.513525000
C	4.456477000	1.969662000	0.249091000
H	5.057410000	2.834218000	0.499465000
C	5.053432000	0.774881000	-0.069524000
H	6.132352000	0.677848000	-0.078662000
C	4.264640000	-0.357168000	-0.372008000
C	2.850818000	-0.243749000	-0.359792000
C	4.814860000	-1.624773000	-0.673317000
H	5.891601000	-1.742369000	-0.697321000
C	3.988803000	-2.685592000	-0.923244000
H	4.388242000	-3.663685000	-1.155384000
C	2.587001000	-2.520745000	-0.862853000
C	1.670135000	-3.669018000	-1.133959000
H	2.081958000	-4.596716000	-0.736200000
H	1.544462000	-3.792189000	-2.213787000
H	0.686664000	-3.500750000	-0.694645000
C	0.193576000	1.481242000	1.143894000
C	0.013817000	2.807288000	1.464371000
H	0.288055000	3.571087000	0.747849000
C	-0.522883000	3.183502000	2.709789000
H	-0.641011000	4.234893000	2.937577000
C	-0.877315000	2.225950000	3.627457000
H	-1.273235000	2.503931000	4.596830000
C	-0.749329000	0.855123000	3.310434000
C	-0.231964000	0.468385000	2.044559000
C	-1.140074000	-0.178245000	4.191311000
H	-1.523627000	0.078504000	5.171727000
C	-1.044889000	-1.485230000	3.795314000
H	-1.340073000	-2.290850000	4.454141000
C	-0.590161000	-1.795060000	2.494044000
C	-0.550901000	-3.208505000	2.004536000
H	-0.998086000	-3.887667000	2.728109000
H	0.483566000	-3.516246000	1.831532000
H	-1.093928000	-3.297286000	1.060275000

E(UTPSSh) = -3168.98136512
Zero-point correction = 0.553396 (Hartree/Particle)
Thermal correction to Energy = 0.586492
Thermal correction to Enthalpy = 0.587436
Thermal correction to Gibbs Free Energy = 0.489292

6.5.5 [Cu(II)LS] Geometries

[Cu(II)(TMG_3trphen)(MeCN)]$^{2+}$ ($C2_{TMG}$) Basal

Cu	-0.239857000	0.018491000	-0.342982000
N	0.393904000	-0.293268000	1.613419000
N	1.439926000	-1.281204000	-0.695209000
N	-1.844523000	-0.987769000	0.463792000
N	0.613808000	1.833607000	-0.050469000
N	-4.059405000	-0.775694000	-0.341594000
N	-2.664269000	-2.498275000	-1.061353000
N	2.212873000	-1.054003000	-2.875120000
N	3.753335000	-1.350026000	-1.169798000
N	0.122338000	3.256109000	-1.818696000
N	-0.268876000	3.974888000	0.357407000
N	-1.215672000	0.397801000	-2.028625000
C	0.873963000	-1.674323000	1.601747000
C	1.500682000	-2.110560000	0.423196000
C	2.024476000	-3.410228000	0.406181000
H	2.489806000	-3.776980000	-0.501131000
C	1.906129000	-4.237550000	1.515602000
H	2.308302000	-5.243096000	1.473927000
C	1.251105000	-3.796541000	2.663945000
H	1.144502000	-4.448021000	3.522163000
C	0.730840000	-2.506734000	2.702809000
H	0.219056000	-2.143688000	3.585395000
C	1.446237000	0.677534000	1.877909000
C	2.363897000	0.503456000	2.905292000
H	2.328072000	-0.395934000	3.507317000
C	3.324496000	1.480390000	3.142660000
H	4.044525000	1.349708000	3.940357000
C	3.356423000	2.617954000	2.337352000
H	4.110122000	3.378286000	2.505043000
C	2.452157000	2.777507000	1.295542000
H	2.517663000	3.642595000	0.646488000
C	1.476763000	1.801423000	1.046183000
C	-0.818403000	-0.113088000	2.400768000
C	-0.817030000	0.396506000	3.689090000
H	0.101583000	0.773945000	4.118643000
C	-1.999146000	0.398830000	4.425577000
H	-2.008649000	0.797927000	5.431798000
C	-3.151325000	-0.148053000	3.867861000
H	-4.067375000	-0.184205000	4.445834000
C	-3.156608000	-0.638511000	2.566066000
H	-4.064373000	-1.059824000	2.156767000
C	-1.995581000	-0.577201000	1.783826000
C	2.451806000	-1.250016000	-1.555321000
C	4.184343000	-0.947413000	0.159634000
H	5.154851000	-0.454453000	0.070628000
H	4.282453000	-1.805338000	0.832085000
H	3.466990000	-0.246756000	0.577913000
C	4.743755000	-2.078655000	-1.954403000
H	4.267445000	-2.543441000	-2.813841000
H	5.174683000	-2.864856000	-1.327647000
H	5.548648000	-1.421270000	-2.293431000
C	0.992096000	-1.525713000	-3.508036000
H	0.475592000	-0.699455000	-3.998896000
H	0.344115000	-1.957185000	-2.752615000
H	1.235921000	-2.280412000	-4.262070000
C	3.152861000	-0.369239000	-3.752081000
H	3.643735000	-1.059635000	-4.443728000
H	3.905185000	0.140633000	-3.155263000
H	2.602742000	0.369641000	-4.339558000
C	-2.868458000	-1.416510000	-0.288670000
C	-1.603999000	-3.448478000	-0.738525000
H	-1.981244000	-4.458034000	-0.911237000
H	-1.313391000	-3.329289000	0.300621000
H	-0.728856000	-3.284688000	-1.370980000
C	-3.321298000	-2.708301000	-2.346399000
H	-2.552317000	-2.873870000	-3.104516000
H	-3.900381000	-1.830268000	-2.615678000
H	-3.978392000	-3.580088000	-2.318143000
C	-5.329759000	-1.465469000	-0.553662000
H	-5.784769000	-1.182238000	-1.505518000
H	-6.010811000	-1.187060000	0.254396000
H	-5.173814000	-2.540580000	-0.525837000
C	-4.159992000	0.649954000	-0.054414000
H	-3.166406000	1.089645000	-0.032477000
H	-4.652067000	0.825652000	0.905647000
H	-4.748342000	1.120997000	-0.844870000
C	0.169738000	3.018197000	-0.493488000
C	1.068594000	2.623139000	-2.728342000
H	0.542422000	2.011878000	-3.463042000
H	1.746155000	1.997850000	-2.155235000
H	1.631248000	3.396791000	-3.257300000
C	-0.860435000	4.142256000	-2.429424000
H	-0.412106000	5.083329000	-2.757142000
H	-1.659449000	4.344855000	-1.720479000
H	-1.278492000	3.641751000	-3.304660000
C	-0.764689000	3.626242000	1.682988000
H	-1.610028000	4.276705000	1.913703000
H	0.007760000	3.761209000	2.445710000
H	-1.096029000	2.590831000	1.688966000
C	-0.050126000	5.399541000	0.121993000
H	0.571280000	5.537084000	-0.758916000
H	0.473620000	5.813454000	0.987484000
H	-0.994721000	5.932992000	-0.006357000
C	-1.909668000	0.606298000	-2.921207000
C	-2.769231000	0.877426000	-4.053111000
H	-2.191020000	1.366611000	-4.838371000
H	-3.585742000	1.529175000	-3.739095000
H	-3.175603000	-0.058709000	-4.437451000

E(UTPSSh) = -3608.00677694
Zero-point correction = 0.832396 (Hartree/Particle)
Thermal correction to Energy = 0.883711
Thermal correction to Enthalpy = 0.884655
Thermal correction to Gibbs Free Energy = 0.749857

Cu(II)(DMEG$_3$trphen)(MeCN)]]$^{2+}$ (C2$_{DMEG}$) Apical

Cu	-0.103905000	-0.232545000	-0.651449000
N	0.274773000	-0.139178000	1.632000000
N	1.761247000	-1.051389000	-0.378502000
N	2.958521000	-0.475912000	-2.318722000
N	4.153062000	-1.014706000	-0.509331000
C	0.703718000	-1.495369000	1.728991000
C	0.285737000	-2.376800000	2.717289000
H	-0.401185000	-2.034311000	3.481562000
C	0.759352000	-3.687098000	2.719082000
H	0.433826000	-4.374018000	3.490625000
C	1.655528000	-4.107325000	1.738164000
H	2.027347000	-5.124882000	1.742299000
C	2.053223000	-3.237517000	0.728287000
H	2.709887000	-3.576244000	-0.064333000
C	1.575892000	-1.924912000	0.702774000
C	2.899936000	-0.877879000	-1.014471000
C	1.955389000	-0.882221000	-3.292323000
H	2.054136000	-0.253348000	-4.175911000
H	0.956749000	-0.759532000	-2.884344000
H	2.090518000	-1.930931000	-3.579446000
C	4.352910000	-0.511059000	-2.777954000
H	4.573048000	0.342064000	-3.418091000
H	4.526056000	-1.434329000	-3.341756000
C	5.133927000	-0.498103000	-1.471323000
H	6.022033000	-1.128219000	-1.495394000
H	5.424332000	0.517220000	-1.180151000
C	4.496255000	-0.898138000	0.899623000
H	5.416302000	-1.455802000	1.076580000
H	3.708772000	-1.314129000	1.519425000
H	4.649679000	0.150723000	1.169253000
N	-1.995868000	0.005602000	-0.015263000
N	-3.356045000	-0.479106000	-1.883764000
N	-3.768299000	-1.613496000	-0.039407000
C	-0.983211000	0.289730000	2.186462000
C	-1.075488000	0.716452000	3.508504000
H	-0.190346000	0.683223000	4.131845000
C	-2.277308000	1.187319000	4.021784000
H	-2.338392000	1.512187000	5.052835000
C	-3.394720000	1.246454000	3.191060000
H	-4.336091000	1.626355000	3.570245000
C	-3.306826000	0.846548000	1.866104000
H	-4.168512000	0.929163000	1.213839000
C	-2.103586000	0.353501000	1.338782000
C	-3.000123000	-0.654394000	-0.596589000
C	-2.701505000	0.399443000	-2.823390000
H	-1.995778000	-0.152098000	-3.452794000
H	-2.170989000	1.170405000	-2.268752000
H	-3.451602000	0.868637000	-3.461552000
C	-4.312752000	-1.501810000	-2.304281000
H	-3.808215000	-2.282286000	-2.883638000
H	-5.095555000	-1.057574000	-2.917088000
C	-4.834553000	-2.018590000	-0.958662000
H	-5.781951000	-1.550146000	-0.676426000
H	-4.952339000	-3.100951000	-0.938756000
C	-3.579878000	-2.236998000	1.253955000
H	-4.215788000	-1.785393000	2.020306000
H	-2.538780000	-2.144410000	1.555784000
H	-3.825997000	-3.295179000	1.158873000
N	0.509426000	1.682019000	-0.395889000
N	-0.453548000	2.873579000	-2.173882000
N	-0.662890000	3.768826000	-0.150973000
C	1.318097000	0.849295000	1.720677000
C	2.225646000	0.872949000	2.772888000
H	2.184653000	0.094546000	3.525996000
C	3.171249000	1.889063000	2.852365000
H	3.875296000	1.911998000	3.674883000
C	3.206865000	2.872600000	1.864437000
H	3.943884000	3.665417000	1.915489000
C	2.319679000	2.835099000	0.795965000
H	2.370360000	3.582400000	0.012826000
C	1.359871000	1.819748000	0.709712000
C	-0.162052000	2.733429000	-0.858367000
C	0.365261000	2.284609000	-3.219153000
H	-0.253971000	1.749589000	-3.940082000
H	1.070307000	1.598941000	-2.755866000
H	0.917572000	3.071831000	-3.740407000
C	-1.120128000	4.154668000	-2.422253000
H	-1.992801000	4.026756000	-3.062229000
H	-0.417076000	4.831435000	-2.916594000
C	-1.479764000	4.630959000	-1.012645000
H	-1.245615000	5.681862000	-0.845434000
H	-2.536080000	4.463599000	-0.781675000
C	-0.951130000	3.762371000	1.273780000
H	-0.732692000	4.749349000	1.683334000
H	-0.336279000	3.026199000	1.779876000
H	-2.005137000	3.524885000	1.442955000
C	-0.868096000	-3.105316000	-1.567159000
N	-0.629020000	-1.986986000	-1.449183000
C	-1.176273000	-4.510868000	-1.700790000
H	-0.868297000	-4.861542000	-2.686543000
H	-2.250076000	-4.657655000	-1.576706000
H	-0.638336000	-5.065820000	-0.930392000

E(UTPSSh) = -3604.41141209
Zero-point correction = 0.769922 (Hartree/Particle)
Thermal correction to Energy = 0.817291
Thermal correction to Enthalpy = 0.818235
Thermal correction to Gibbs Free Energy = 0.689311

Cu(II)(DMEG$_3$trphen)(MeCN)]]$^{2+}$ (C2$_{DMEG}$) Basal

Cu	-0.277853000	0.175772000	-0.247763000
N	0.348359000	-1.303897000	1.059965000
N	0.944589000	1.342426000	0.856854000
N	0.703463000	3.618736000	0.282318000
N	0.356447000	3.068968000	2.398901000
C	1.554859000	-0.811490000	1.714805000
C	2.434654000	-1.666698000	2.364081000
H	2.254702000	-2.734417000	2.343767000
C	3.537350000	-1.146046000	3.031939000
H	4.226385000	-1.808647000	3.539787000
C	3.744288000	0.232820000	3.035390000
H	4.603573000	0.649467000	3.547760000
C	2.880319000	1.084565000	2.360248000
H	3.076009000	2.150024000	2.332523000
C	1.771166000	0.571190000	1.671290000
C	0.693602000	2.617160000	1.179097000

C	1.425053000	3.568051000	-0.974861000
H	0.832904000	4.038072000	-1.760803000
H	1.611621000	2.528475000	-1.231874000
H	2.377191000	4.100488000	-0.884304000
C	0.431948000	4.905022000	0.930200000
H	-0.376704000	5.431359000	0.422421000
H	1.331865000	5.523490000	0.889661000
C	0.070924000	4.506136000	2.372429000
H	0.665540000	5.035426000	3.117462000
H	-0.987690000	4.664685000	2.591077000
C	-0.076572000	2.233050000	3.502319000
H	0.661606000	2.236068000	4.307142000
H	-0.218087000	1.213599000	3.149326000
H	-1.026247000	2.613373000	3.883729000
N	1.155362000	-0.881316000	-1.501841000
N	2.045495000	0.704976000	-2.971756000
N	3.506292000	-0.662006000	-1.983509000
C	0.600748000	-2.465235000	0.209249000
C	0.362952000	-3.761799000	0.643446000
H	-0.075722000	-3.928655000	1.619431000
C	0.703005000	-4.833742000	-0.175634000
H	0.524379000	-5.847362000	0.160482000
C	1.276647000	-4.591723000	-1.423018000
H	1.544086000	-5.422215000	-2.065895000
C	1.485563000	-3.292140000	-1.866735000
H	1.894207000	-3.105408000	-2.852843000
C	1.138280000	-2.200137000	-1.060051000
C	2.186946000	-0.345103000	-2.115528000
C	0.835490000	0.903775000	-3.750178000
H	0.621930000	1.969240000	-3.839327000
H	0.011614000	0.409214000	-3.244983000
H	0.956117000	0.478932000	-4.752800000
C	3.333096000	1.033836000	-3.584135000
H	3.469744000	2.112325000	-3.659204000
H	3.381248000	0.599615000	-4.589041000
C	4.323596000	0.371415000	-2.632456000
H	5.177666000	-0.071703000	-3.142934000
H	4.687079000	1.074937000	-1.875027000
C	4.062691000	-1.279472000	-0.787369000
H	5.058260000	-1.650428000	-1.030108000
H	3.448002000	-2.116079000	-0.469588000
H	4.136819000	-0.554182000	0.029568000
N	-1.990827000	-0.920828000	-0.038538000
N	-4.163271000	0.053802000	-0.388147000
N	-3.176203000	-1.009507000	-2.052969000
C	-0.808667000	-1.476401000	1.930805000
C	-0.712908000	-1.817176000	3.269535000
H	0.258675000	-1.876051000	3.742495000
C	-1.872403000	-2.101783000	3.988659000
H	-1.807468000	-2.365588000	5.036490000
C	-3.102634000	-2.075140000	3.338120000
H	-4.006406000	-2.327623000	3.880380000
C	-3.200389000	-1.710502000	1.998724000
H	-4.167681000	-1.689647000	1.514187000
C	-2.052608000	-1.348513000	1.282476000
C	-3.077281000	-0.647216000	-0.767408000
C	-4.228711000	0.940204000	0.757533000
H	-4.519270000	1.937062000	0.418656000
H	-3.247412000	0.992811000	1.224096000
H	-4.956791000	0.587934000	1.491474000
C	-5.154422000	0.104097000	-1.469868000
H	-5.481272000	1.131935000	-1.624099000
H	-6.023500000	-0.506084000	-1.215322000
C	-4.378296000	-0.456215000	-2.676582000
H	-4.927454000	-1.244144000	-3.191375000
H	-4.109497000	0.316775000	-3.401859000
C	-2.248895000	-1.871760000	-2.753647000
H	-2.783560000	-2.725564000	-3.175448000
H	-1.499865000	-2.216490000	-2.044504000
H	-1.758207000	-1.325092000	-3.562467000
C	-1.789190000	2.495516000	-1.682124000
N	-1.179786000	1.627000000	-1.241028000
C	-2.551141000	3.591046000	-2.237172000
H	-2.517532000	4.436864000	-1.548914000
H	-3.585858000	3.277863000	-2.380785000
H	-2.121045000	3.881948000	-3.196506000

E(UTPSSh) = -3604.41433353
Zero-point correction = 0.769912 (Hartree/Particle)
Thermal correction to Energy = 0.817498
Thermal correction to Enthalpy = 0.818443
Thermal correction to Gibbs Free Energy = 0.688514

$[Cu(II)\{N(QuMe)(PhTMG)_2\}(MeCN)]]^{2+}$ ($C4_{TMG}$) Apical A

N	0.023067000	1.182830000	1.059794000
C	-2.154153000	1.476669000	-0.034893000
N	-0.369778000	-1.561633000	0.579585000
N	2.062288000	-0.132792000	-0.084961000
C	-3.670954000	3.233479000	0.686521000
H	-4.600587000	3.773097000	0.549606000
N	-1.855045000	0.396635000	-0.876218000
C	-2.816823000	3.559344000	1.737681000
H	-3.078300000	4.337430000	2.443571000
N	2.968309000	-2.257120000	-0.150615000
C	-1.613118000	2.880044000	1.866910000
H	-0.956475000	3.117537000	2.692736000
N	3.932900000	-0.634813000	-1.485255000
C	-1.247962000	1.882883000	0.963521000
N	-3.920860000	-0.713345000	-0.573281000
C	-2.846760000	-0.380120000	-1.331600000
N	-2.765862000	-0.884142000	-2.579579000
C	-1.986625000	-0.214210000	-3.613958000
H	-1.031426000	-0.719462000	-3.781097000
H	-2.559246000	-0.233101000	-4.543203000
H	-1.803609000	0.812937000	-3.315972000
C	-3.388121000	-2.142655000	-2.975529000
H	-2.649561000	-2.738080000	-3.515862000
H	-3.712154000	-2.687892000	-2.092906000
H	-4.243351000	-1.973958000	-3.633932000
C	-3.855412000	-0.738206000	0.881482000
H	-4.346207000	-1.648015000	1.232935000
H	-2.819473000	-0.744975000	1.204395000
H	-4.359488000	0.131110000	1.312412000
C	-5.267681000	-0.815307000	-1.129532000
H	-5.664003000	-1.828122000	-1.029206000
H	-5.917934000	-0.127666000	-0.581944000
H	-5.259570000	-0.527197000	-2.177203000
C	-0.632455000	-3.263635000	-1.128869000
H	-0.395191000	-2.431748000	-1.792566000
H	0.120616000	-4.042769000	-1.266275000

H	-1.593226000	-3.694394000	-1.413946000
Cu	0.092719000	-0.110656000	-0.718160000
C	-0.655923000	-2.822474000	0.297995000
C	-0.930490000	-3.750594000	1.330668000
H	-1.192226000	-4.766185000	1.064547000
C	-0.812591000	-3.367487000	2.637649000
H	-0.978083000	-4.076466000	3.440231000
C	-0.443649000	-2.038525000	2.954982000
C	-0.211740000	-1.597300000	4.275781000
H	-0.338003000	-2.298021000	5.092162000
C	0.191242000	-0.304550000	4.508898000
H	0.398081000	0.030806000	5.517288000
C	0.309576000	0.606686000	3.443003000
H	0.606520000	1.629074000	3.641332000
C	0.039225000	0.224475000	2.148762000
C	-0.278960000	-1.130351000	1.875215000
C	2.348671000	1.171037000	0.334953000
C	3.610156000	1.780181000	0.309830000
H	4.469946000	1.217834000	-0.024258000
C	3.775824000	3.103957000	0.701096000
H	4.762823000	3.549053000	0.655130000
C	2.685768000	3.854379000	1.121195000
H	2.799578000	4.896920000	1.390703000
C	1.438323000	3.243417000	1.231250000
H	0.597838000	3.818884000	1.589213000
C	1.269849000	1.910175000	0.887061000
C	2.992037000	-0.975429000	-0.577501000
C	3.727070000	0.423744000	-2.461953000
H	2.708839000	0.784158000	-2.392502000
H	4.420366000	1.250076000	-2.288318000
H	3.902907000	0.018461000	-3.461222000
C	5.255571000	-1.257119000	-1.516501000
H	5.998515000	-0.460261000	-1.590616000
H	5.423743000	-1.810369000	-0.596559000
H	5.370280000	-1.921239000	-2.375935000
C	2.645290000	-2.585650000	1.232841000
H	2.393790000	-1.673741000	1.764741000
H	1.810585000	-3.285867000	1.279250000
H	3.516072000	-3.056161000	1.698258000
C	3.348096000	-3.381965000	-0.997654000
H	2.601512000	-4.168149000	-0.869948000
H	3.355730000	-3.068453000	-2.038730000
H	4.325251000	-3.790551000	-0.728681000
C	-3.345329000	2.207011000	-0.184719000
H	-4.018051000	1.951956000	-0.994182000
C	0.598657000	2.342057000	-2.509827000
N	0.499153000	1.272694000	-2.097379000
C	0.739554000	3.685692000	-3.021829000
H	-0.162838000	3.966082000	-3.566463000
H	1.601425000	3.732178000	-3.689022000
H	0.889574000	4.368155000	-2.183526000

E(UTPSSh) = -3455.50031496
Zero-point correction = 0.727145 (Hartree/Particle)
Thermal correction to Energy = 0.772115
Thermal correction to Enthalpy = 0.773059
Thermal correction to Gibbs Free Energy = 0.651087

$[Cu(II)\{N(QuMe)(PhTMG)_2\}(MeCN)]]^{2+}$ ($C4_{TMG}$) Apical B

N	0.049100000	1.181193000	1.035646000
C	0.156945000	-1.179256000	1.648728000
N	1.881525000	0.755948000	-1.041811000
N	-1.951197000	0.022182000	-0.342537000
C	-0.517671000	-1.906171000	3.859086000
H	-0.671837000	-2.711408000	4.567429000
N	0.579932000	-1.435339000	0.336931000
C	-0.811842000	-0.592104000	4.220891000
H	-1.191307000	-0.365604000	5.209284000
N	-2.939922000	-1.734643000	-1.499683000
C	-0.634790000	0.426289000	3.292411000
H	-0.894639000	1.448337000	3.541194000
N	-3.872144000	-1.042523000	0.505787000
C	-0.146152000	0.137472000	2.022634000
N	2.573413000	-2.516675000	0.998950000
C	1.558339000	-2.318954000	0.122433000
N	1.571970000	-3.029630000	-1.027256000
C	0.339526000	-3.387726000	-1.711489000
H	0.313406000	-2.948719000	-2.712021000
H	0.282660000	-4.474744000	-1.812781000
H	-0.503655000	-3.028953000	-1.128865000
C	2.804464000	-3.503857000	-1.645792000
H	2.748956000	-3.302013000	-2.716897000
H	3.652440000	-2.967910000	-1.226247000
H	2.942566000	-4.578709000	-1.505480000
C	3.036220000	-1.469374000	1.898765000
H	4.128065000	-1.477505000	1.900382000
H	2.691266000	-0.501928000	1.547596000
H	2.674808000	-1.632701000	2.917638000
C	3.124449000	-3.844122000	1.259316000
H	4.171282000	-3.908542000	0.953472000
H	3.058994000	-4.037341000	2.333218000
H	2.541433000	-4.596158000	0.734372000
C	2.225702000	-0.289296000	-3.205285000
H	1.371576000	-0.903512000	-2.921457000
H	1.912566000	0.366238000	-4.022916000
H	3.024238000	-0.929066000	-3.580962000
Cu	-0.003842000	0.036768000	-0.912343000
C	2.705603000	0.537178000	-2.055987000
C	4.004263000	1.094764000	-2.073298000
H	4.651541000	0.886217000	-2.914764000
C	4.422171000	1.874225000	-1.031561000
H	5.418589000	2.300096000	-1.021301000
C	3.551806000	2.129888000	0.053198000
C	3.935517000	2.904606000	1.169349000
H	4.929841000	3.334265000	1.189793000
C	3.063966000	3.091402000	2.213417000
H	3.358595000	3.672038000	3.078177000
C	1.776345000	2.527470000	2.168262000
H	1.106797000	2.666031000	3.007006000
C	1.353078000	1.792203000	1.082391000
C	2.251647000	1.555123000	0.007294000
C	-2.196348000	1.308179000	0.168046000
C	-3.385861000	2.006825000	-0.055398000
H	-4.203707000	1.508944000	-0.562499000
C	-3.502482000	3.341060000	0.317503000
H	-4.429629000	3.868400000	0.127406000
C	-2.425090000	4.006162000	0.895613000
H	-2.505278000	5.052806000	1.161794000
C	-1.236904000	3.321238000	1.139468000

H	-0.397811000	3.833755000	1.591433000
C	-1.127021000	1.979504000	0.801583000
C	-2.915248000	-0.890755000	-0.441553000
C	-3.652988000	-0.641149000	1.885882000
H	-2.587120000	-0.604985000	2.086421000
H	-4.094555000	0.338592000	2.092667000
H	-4.115809000	-1.384447000	2.537795000
C	-5.249404000	-1.384593000	0.161972000
H	-5.908942000	-0.621562000	0.583479000
H	-5.371211000	-1.392578000	-0.917898000
H	-5.531806000	-2.357643000	0.570757000
C	-2.532143000	-1.299032000	-2.828451000
H	-2.389012000	-0.223711000	-2.825489000
H	-1.608300000	-1.787349000	-3.146739000
H	-3.321276000	-1.557195000	-3.539304000
C	-3.422598000	-3.106587000	-1.395162000
H	-2.710444000	-3.764360000	-1.898235000
H	-3.488170000	-3.391106000	-0.347578000
H	-4.398840000	-3.231082000	-1.870997000
C	-0.050272000	-2.200415000	2.585555000
H	0.143465000	-3.227054000	2.299063000
C	-0.784916000	2.233892000	-2.987100000
N	-0.485006000	1.301910000	-2.384910000
C	-1.172904000	3.405087000	-3.740503000
H	-1.654076000	3.096779000	-4.669614000
H	-0.288489000	4.002185000	-3.966042000
H	-1.871894000	3.994910000	-3.145485000

E(UTPSSh) = -3455.51865773
Zero-point correction = 0.726655 (Hartree/Particle)
Thermal correction to Energy = 0.771971
Thermal correction to Enthalpy = 0.772916
Thermal correction to Gibbs Free Energy = 0.649912

$[Cu(II)\{N(QuMe)(PhTMG)_2\}(MeCN)]]^{2+}$ ($C4_{TMG}$) Basal A

N	0.075768000	-1.579780000	-0.593759000
C	2.354704000	-0.858192000	-1.075779000
N	0.407141000	-0.583916000	1.945428000
N	-1.924704000	0.100239000	-0.494321000
C	4.037466000	-2.483169000	-1.718549000
H	5.043584000	-2.690266000	-2.063656000
N	1.873240000	0.429412000	-0.842065000
C	3.163373000	-3.533909000	-1.448476000
H	3.479811000	-4.562227000	-1.566640000
N	-3.270336000	1.171029000	1.037463000
C	1.864691000	-3.245933000	-1.045820000
H	1.160116000	-4.044707000	-0.851799000
N	-3.411995000	1.803268000	-1.196436000
C	1.463744000	-1.925129000	-0.898254000
N	3.844421000	1.355312000	0.084305000
C	2.719503000	1.457548000	-0.659911000
N	2.407037000	2.648901000	-1.203432000
C	1.549539000	2.737811000	-2.380063000
H	0.575550000	3.154491000	-2.114072000
H	2.024112000	3.395516000	-3.111365000
H	1.415287000	1.747244000	-2.803917000
C	2.784749000	3.921923000	-0.598839000
H	1.910431000	4.575150000	-0.610369000
H	3.096150000	3.762925000	0.430933000
H	3.584710000	4.415513000	-1.154739000
C	3.988801000	0.337333000	1.117604000
H	4.365887000	0.814929000	2.024079000
H	3.025093000	-0.120566000	1.321958000
H	4.693806000	-0.435977000	0.802139000
C	5.061412000	2.106300000	-0.217886000
H	5.285630000	2.836863000	0.562055000
H	5.890290000	1.397200000	-0.282380000
H	4.956803000	2.609682000	-1.175133000
C	1.296103000	1.266178000	3.250810000
H	1.633673000	1.619559000	2.280148000
H	0.573368000	1.983017000	3.651136000
H	2.142309000	1.239493000	3.940261000
Cu	0.035109000	0.390416000	-0.018791000
C	0.669839000	-0.089633000	3.146610000
C	0.348744000	-0.805664000	4.326620000
H	0.593412000	-0.369798000	5.286841000
C	-0.287694000	-2.013360000	4.242991000
H	-0.569898000	-2.557440000	5.136840000
C	-0.590238000	-2.558941000	2.973321000
C	-1.291835000	-3.772539000	2.791681000
H	-1.602726000	-4.335460000	3.663700000
C	-1.589658000	-4.213057000	1.525539000
H	-2.143662000	-5.131856000	1.381159000
C	-1.166031000	-3.485225000	0.395226000
H	-1.398323000	-3.846786000	-0.598336000
C	-0.451307000	-2.322313000	0.548827000
C	-0.182826000	-1.809517000	1.840104000
C	-1.961944000	-0.755045000	-1.594352000
C	-3.001593000	-0.900378000	-2.521381000
H	-3.911825000	-0.328164000	-2.408937000
C	-2.864304000	-1.770215000	-3.598427000
H	-3.673043000	-1.848842000	-4.315417000
C	-1.703844000	-2.517121000	-3.774845000
H	-1.593189000	-3.172477000	-4.629230000
C	-0.692192000	-2.444543000	-2.819634000
H	0.196661000	-3.053900000	-2.913137000
C	-0.843331000	-1.600396000	-1.732597000
C	-2.878373000	1.011374000	-0.239008000
C	-2.657049000	2.156811000	-2.391546000
H	-1.625993000	1.833821000	-2.280474000
H	-3.086260000	1.687148000	-3.279928000
H	-2.687010000	3.241823000	-2.513488000
C	-4.794284000	2.275529000	-1.162154000
H	-5.264453000	2.026940000	-2.116673000
H	-5.334753000	1.773289000	-0.364261000
H	-4.845482000	3.357355000	-1.020281000
C	-3.089030000	0.105589000	2.017817000
H	-2.910731000	-0.832937000	1.502334000
H	-2.244653000	0.328516000	2.674334000
H	-3.994896000	0.032383000	2.622479000
C	-3.731749000	2.443659000	1.581918000
H	-3.169229000	2.646438000	2.495949000
H	-3.552346000	3.241674000	0.866678000
H	-4.794497000	2.410942000	1.830465000
C	3.644730000	-1.164236000	-1.538579000
H	4.341847000	-0.364196000	-1.750287000
C	-0.391749000	3.358448000	0.854703000
N	-0.187668000	2.286904000	0.492324000
C	-0.642015000	4.705499000	1.316948000

H	0.308130000	5.208606000	1.500647000
H	-1.216076000	4.669983000	2.243672000
H	-1.204218000	5.250524000	0.557378000

E(UTPSSh) = -3455.51784888
Zero-point correction = 0.727164 (Hartree/Particle)
Thermal correction to Energy = 0.772209
Thermal correction to Enthalpy = 0.773154
Thermal correction to Gibbs Free Energy = 0.651389

$[Cu(II)\{N(QuMe)(PhTMG)_2\}(MeCN)]]^{2+}$ ($C4_{TMG}$) Basal B

N	-0.768148000	-0.939073000	1.001471000
C	0.548224000	0.796601000	2.064033000
N	-1.923359000	-0.647547000	-1.352712000
N	1.330086000	-1.279289000	-0.716418000
C	1.354816000	0.532133000	4.331475000
H	1.917480000	0.924051000	5.170419000
N	0.493248000	1.452936000	0.831411000
C	0.768242000	-0.729760000	4.415427000
H	0.863919000	-1.322965000	5.315734000
N	3.179148000	-0.557067000	-1.916908000
C	0.071032000	-1.231750000	3.322773000
H	-0.371701000	-2.219173000	3.356751000
N	3.519058000	-1.793496000	0.013819000
C	-0.043966000	-0.464875000	2.170836000
N	-0.247942000	3.524065000	1.660975000
C	0.510272000	2.797217000	0.809947000
N	1.274243000	3.434755000	-0.093228000
C	2.463774000	2.802820000	-0.648452000
H	2.311471000	2.557563000	-1.701416000
H	3.303282000	3.496523000	-0.566758000
H	2.677248000	1.896098000	-0.091201000
C	0.934638000	4.744894000	-0.636928000
H	1.063570000	4.709504000	-1.720326000
H	-0.102194000	4.978741000	-0.407911000
H	1.585648000	5.527537000	-0.241475000
C	-1.459719000	2.964115000	2.247225000
H	-2.213684000	3.751596000	2.289109000
H	-1.823518000	2.151386000	1.623705000
H	-1.276542000	2.590752000	3.258773000
C	0.198904000	4.793641000	2.229329000
H	-0.430976000	5.622460000	1.899101000
H	0.141914000	4.719263000	3.318114000
H	1.231259000	4.981202000	1.946261000
C	-1.468646000	-0.832213000	-3.731485000
H	-0.444186000	-0.692099000	-3.399154000
H	-1.555475000	-1.820266000	-4.192417000
H	-1.711765000	-0.095337000	-4.499132000
Cu	-0.166085000	0.256859000	-0.631712000
C	-2.415500000	-0.744777000	-2.579553000
C	-3.815397000	-0.786324000	-2.796885000
H	-4.179303000	-0.864662000	-3.813179000
C	-4.685607000	-0.695000000	-1.743857000
H	-5.756630000	-0.679198000	-1.908285000
C	-4.180090000	-0.635452000	-0.423639000
C	-4.975408000	-0.535228000	0.742959000
H	-6.052947000	-0.487510000	0.642788000
C	-4.381662000	-0.487594000	1.981637000
H	-4.990416000	-0.396609000	2.872168000
C	-2.980618000	-0.596544000	2.123848000
H	-2.532792000	-0.609946000	3.108758000
C	-2.195930000	-0.711884000	1.003634000
C	-2.775579000	-0.667139000	-0.283226000
C	0.740295000	-2.432447000	-0.201481000
C	1.143663000	-3.731769000	-0.540553000
H	2.009790000	-3.862481000	-1.178434000
C	0.425323000	-4.836260000	-0.102432000
H	0.754125000	-5.829576000	-0.384720000
C	-0.724808000	-4.676900000	0.669106000
H	-1.294346000	-5.538030000	0.994907000
C	-1.139978000	-3.396880000	1.018689000
H	-2.031773000	-3.250479000	1.616111000
C	-0.401348000	-2.297199000	0.603478000
C	2.650583000	-1.229241000	-0.868192000
C	3.156189000	-2.002825000	1.407173000
H	2.351932000	-1.324935000	1.680548000
H	2.837233000	-3.033105000	1.592512000
H	4.030273000	-1.786075000	2.024783000
C	4.750495000	-2.446942000	-0.416592000
H	4.734629000	-3.483679000	-0.068091000
H	4.809245000	-2.446648000	-1.501921000
H	5.632172000	-1.951839000	-0.001818000
C	2.435513000	-0.400866000	-3.156634000
H	1.632500000	-1.131935000	-3.181197000
H	2.017759000	0.604831000	-3.250969000
H	3.111147000	-0.577027000	-3.996601000
C	4.466067000	0.124298000	-1.855805000
H	4.344626000	1.136773000	-2.247213000
H	4.802660000	0.181724000	-0.823563000
H	5.221969000	-0.387017000	-2.457598000
C	1.257624000	1.286133000	3.169993000
H	1.758775000	2.243744000	3.100716000
C	-0.530707000	2.382069000	-2.878566000
N	-0.273655000	1.632824000	-2.045548000
C	-0.845058000	3.316443000	-3.936196000
H	-1.274880000	4.222004000	-3.506300000
H	-1.564543000	2.860671000	-4.617758000
H	0.066931000	3.565544000	-4.480718000

E(UTPSSh) = -3455.51713594
Zero-point correction = 0.726200 (Hartree/Particle)
Thermal correction to Energy = 0.771818
Thermal correction to Enthalpy = 0.772762
Thermal correction to Gibbs Free Energy = 0.649188

$[Cu(II)\{N(QuMe)(PhDMEG)_2\}(MeCN)]]^{2+}$ ($C4_{DMEG}$) Apical A

N	-0.127226000	1.434505000	0.568249000
C	0.973297000	2.289927000	0.185938000
N	-0.989500000	0.253623000	-1.777587000
C	0.957616000	3.657874000	0.440374000
H	0.099923000	4.095442000	0.935490000
N	-1.281315000	-0.934755000	0.862130000
C	2.029986000	4.458648000	0.068300000
H	2.012590000	5.521064000	0.275894000

N	2.033433000	0.335298000	-0.812945000
C	3.119062000	3.878287000	-0.579320000
H	3.959397000	4.490159000	-0.885592000
N	4.077467000	-0.267794000	0.285092000
C	3.128163000	2.520776000	-0.862736000
H	3.961746000	2.082717000	-1.399594000
N	3.596511000	-1.242532000	-1.630214000
C	2.056096000	1.698115000	-0.482989000
N	-2.699297000	-2.379388000	-0.324543000
C	3.190310000	-0.341402000	-0.724574000
N	-3.621197000	-1.202971000	1.331792000
C	3.906385000	0.450981000	1.529813000
H	4.339949000	-0.144167000	2.334085000
H	2.845068000	0.588296000	1.726540000
H	4.394431000	1.429015000	1.499566000
C	3.010230000	-1.451570000	-2.933744000
H	2.492213000	-2.412720000	-2.983793000
H	3.796809000	-1.434388000	-3.690524000
H	2.307496000	-0.643475000	-3.122484000
C	5.277816000	-1.051724000	-0.017890000
H	5.577496000	-1.628048000	0.856130000
H	6.100342000	-0.392120000	-0.308717000
C	4.802176000	-1.939742000	-1.177841000
H	5.527490000	-1.994288000	-1.988256000
H	4.555819000	-2.955276000	-0.854496000
C	-1.392883000	1.819669000	0.001287000
C	-2.227708000	2.722137000	0.618689000
H	-1.959654000	3.113934000	1.592325000
Cu	0.292426000	-0.582741000	-0.398367000
C	-3.420092000	3.141110000	-0.001551000
H	-4.054378000	3.860606000	0.500446000
C	-3.764434000	2.654261000	-1.238803000
H	-4.668147000	2.985657000	-1.736020000
C	-2.947083000	1.695496000	-1.879006000
C	-1.759104000	1.251381000	-1.242801000
C	-3.262783000	1.128142000	-3.134970000
H	-4.156443000	1.452065000	-3.655340000
C	-2.445057000	0.173754000	-3.670752000
H	-2.663406000	-0.278556000	-4.629182000
C	-1.312750000	-0.274599000	-2.950553000
C	-0.469701000	-1.371448000	-3.512741000
H	-1.094895000	-2.179418000	-3.894995000
H	0.208890000	-1.770530000	-2.761398000
H	0.124022000	-0.992380000	-4.349073000
C	-0.189588000	0.921995000	1.909497000
C	0.403508000	1.529988000	3.006601000
H	0.944504000	2.459210000	2.879405000
C	0.299204000	0.933197000	4.262020000
H	0.763556000	1.405747000	5.118668000
C	-0.399273000	-0.262272000	4.413997000
H	-0.477934000	-0.724553000	5.390457000
C	-0.973483000	-0.887565000	3.311918000
H	-1.482968000	-1.837946000	3.416293000
C	-0.874128000	-0.303497000	2.048271000
C	-2.468020000	-1.468354000	0.661895000
C	-1.677732000	-3.291708000	-0.807802000
H	-1.992884000	-3.685600000	-1.772870000
H	-1.526689000	-4.121958000	-0.109195000
H	-0.733845000	-2.769868000	-0.934193000
C	-3.930497000	0.039017000	2.025351000
H	-4.401104000	0.747239000	1.337009000
H	-3.033091000	0.484074000	2.440498000
H	-4.621987000	-0.182165000	2.839030000
C	-4.057076000	-2.917894000	-0.192365000
H	-4.018127000	-3.885312000	0.320140000
H	-4.517591000	-3.052000000	-1.170073000
C	-4.747422000	-1.859167000	0.654952000
H	-5.273228000	-1.122670000	0.037763000
H	-5.444184000	-2.275961000	1.380866000
C	1.767704000	-2.849322000	1.152115000
N	1.246039000	-2.099013000	0.455312000
C	2.430213000	-3.786476000	2.030336000
H	3.489501000	-3.533813000	2.093569000
H	2.317613000	-4.797108000	1.635793000
H	1.979222000	-3.728308000	3.022000000

E(UTPSSh) = -3453.11835839
Zero-point correction = 0.684996 (Hartree/Particle)
Thermal correction to Energy = 0.727817
Thermal correction to Enthalpy = 0.728761
Thermal correction to Gibbs Free Energy = 0.608670

$[Cu(II)\{N(QuMe)(PhDMEG)_2\}(MeCN)]]^{2+}$ ($C4_{DMEG}$) Apical B

N	0.023060000	1.289604000	0.902158000
C	1.144967000	2.113094000	0.539473000
N	-1.910731000	0.585828000	-1.000610000
C	1.215926000	3.485126000	0.733820000
H	0.377728000	4.015048000	1.166908000
N	-0.423797000	-1.408215000	0.459979000
C	2.369482000	4.176789000	0.369379000
H	2.422429000	5.247493000	0.522712000
N	1.984626000	0.084855000	-0.434613000
C	3.449183000	3.490779000	-0.180967000
H	4.348837000	4.026472000	-0.459138000
N	3.884152000	-0.990076000	0.551285000
C	3.368882000	2.122162000	-0.411951000
H	4.187076000	1.594177000	-0.887162000
N	2.884234000	-1.944097000	-1.202206000
C	2.213038000	1.416979000	-0.067003000
N	-1.557470000	-3.075527000	-0.736995000
C	2.885251000	-0.875114000	-0.357154000
N	-2.543851000	-2.343434000	1.111564000
C	3.868731000	-0.369796000	1.867389000
H	3.286002000	-0.973274000	2.569385000
H	3.441668000	0.626449000	1.811534000
H	4.896398000	-0.292914000	2.222260000
C	2.455037000	-1.821677000	-2.588029000
H	2.183563000	-2.806482000	-2.965323000
H	3.259973000	-1.409313000	-3.206395000
H	1.593716000	-1.163120000	-2.652098000
C	4.503252000	-2.317177000	0.441569000
H	4.103762000	-2.965600000	1.228445000
H	5.584837000	-2.251210000	0.550913000
C	4.067439000	-2.774488000	-0.946061000
H	4.830658000	-2.557551000	-1.700986000
H	3.817657000	-3.833599000	-0.989249000
C	-1.305027000	1.844498000	0.979156000
C	-1.693522000	2.663517000	2.017008000
H	-0.976486000	2.918749000	2.786276000

Cu	0.013317000	-0.013325000	-0.934148000
C	-3.006154000	3.160299000	2.104566000
H	-3.274026000	3.809764000	2.928052000
C	-3.936977000	2.816674000	1.155804000
H	-4.953652000	3.186573000	1.211968000
C	-3.585853000	1.954831000	0.094568000
C	-2.257881000	1.455838000	0.000607000
C	-4.516890000	1.535705000	-0.883642000
H	-5.536270000	1.899735000	-0.832218000
C	-4.127622000	0.677565000	-1.872611000
H	-4.822204000	0.340825000	-2.630737000
C	-2.794237000	0.209018000	-1.913932000
C	-2.360553000	-0.705209000	-3.014259000
H	-2.273897000	-0.140314000	-3.946803000
H	-3.100157000	-1.491541000	-3.170461000
H	-1.396101000	-1.161129000	-2.799511000
C	0.312141000	0.341005000	1.962366000
C	0.852366000	0.753999000	3.174843000
H	1.114664000	1.796592000	3.311322000
C	1.059872000	-0.165395000	4.195551000
H	1.477888000	0.157959000	5.140529000
C	0.733708000	-1.505328000	3.986991000
H	0.897986000	-2.232046000	4.773760000
C	0.223703000	-1.927096000	2.766858000
H	0.002070000	-2.973869000	2.596321000
C	0.003194000	-1.007806000	1.732538000
C	-1.459495000	-2.233665000	0.316358000
C	-0.403565000	-3.560431000	-1.471517000
H	-0.564508000	-3.460100000	-2.545946000
H	-0.232081000	-4.615039000	-1.236377000
H	0.466265000	-2.981183000	-1.169541000
C	-3.013773000	-1.348968000	2.061018000
H	-3.940884000	-0.903856000	1.690013000
H	-2.270847000	-0.568853000	2.188970000
H	-3.203670000	-1.819163000	3.027224000
C	-2.744772000	-3.924513000	-0.616119000
H	-2.431258000	-4.941691000	-0.364235000
H	-3.304703000	-3.952030000	-1.550640000
C	-3.524409000	-3.264424000	0.525592000
H	-4.376216000	-2.684644000	0.158913000
H	-3.879114000	-3.979884000	1.267079000
C	0.715684000	1.775252000	-3.387132000
N	0.405119000	1.018597000	-2.580184000
C	1.118351000	2.726344000	-4.398297000
H	1.515068000	2.190621000	-5.261749000
H	1.890309000	3.378150000	-3.986286000
H	0.257071000	3.323152000	-4.700755000

E(UTPSSh) = -3453.12329767
Zero-point correction= 0.685318
(Hartree/Particle)
Thermal correction to Energy= 0.727929
Thermal correction to Enthalpy= 0.728873
Thermal correction to Gibbs Free Energy= 0.609793

[Cu(II){N(QuMe)(PhDMEG)$_2$}(MeCN)]]$^{2+}$ (C4$_{DMEG}$) Basal A

N	0.930553000	-1.261828000	0.564297000
C	0.495329000	-2.532860000	-0.006442000
N	1.870333000	0.071782000	-1.621122000
C	1.235273000	-3.700430000	0.107977000
H	2.223025000	-3.673768000	0.550530000
N	0.365098000	1.227242000	1.225830000
C	0.685706000	-4.902614000	-0.326948000
H	1.253804000	-5.819713000	-0.238298000
N	-1.340830000	-1.272687000	-0.877054000
C	-0.602155000	-4.914454000	-0.860581000
H	-1.039648000	-5.848242000	-1.193898000
N	-3.530465000	-1.585226000	0.036030000
C	-1.326519000	-3.737930000	-1.006147000
H	-2.306809000	-3.752401000	-1.467701000
N	-3.314533000	-0.401253000	-1.825656000
C	-0.772396000	-2.514782000	-0.605847000
N	-1.091473000	3.033945000	1.864893000
C	-2.669297000	-1.117320000	-0.882359000
N	0.828415000	3.494560000	0.879158000
C	-3.163379000	-2.097747000	1.342076000
H	-3.708764000	-1.543138000	2.108558000
H	-2.096356000	-1.961021000	1.498919000
H	-3.408185000	-3.158727000	1.422986000
C	-2.795669000	-0.229756000	-3.171128000
H	-2.995225000	0.781215000	-3.525207000
H	-3.272884000	-0.942984000	-3.850523000
H	-1.724327000	-0.409652000	-3.152627000
C	-4.893289000	-1.117053000	-0.231175000
H	-5.181545000	-0.403230000	0.544857000
H	-5.599592000	-1.947155000	-0.224726000
C	-4.764780000	-0.453181000	-1.611134000
H	-5.220368000	-1.058703000	-2.399055000
H	-5.199295000	0.545729000	-1.641507000
C	2.360361000	-1.004266000	0.451637000
C	3.253650000	-1.359993000	1.432191000
H	2.896103000	-1.806248000	2.351152000
Cu	0.029627000	0.206885000	-0.565596000
C	4.634869000	-1.156724000	1.237005000
H	5.324659000	-1.451642000	2.017393000
C	5.102643000	-0.609309000	0.067332000
H	6.164644000	-0.466645000	-0.092957000
C	4.197320000	-0.204803000	-0.940379000
C	2.805906000	-0.378876000	-0.734033000
C	4.592381000	0.395407000	-2.158276000
H	5.646449000	0.539827000	-2.364647000
C	3.640062000	0.783480000	-3.060460000
H	3.918151000	1.233224000	-4.004750000
C	2.265089000	0.626275000	-2.759109000
C	1.228845000	1.117149000	-3.719177000
H	1.569923000	0.985945000	-4.746562000
H	1.050157000	2.185135000	-3.562612000
H	0.288561000	0.588861000	-3.578373000
C	0.422330000	-1.032713000	1.918260000
C	0.248249000	-2.060286000	2.831978000
H	0.413157000	-3.085497000	2.526223000
C	-0.130653000	-1.759039000	4.137292000
H	-0.273908000	-2.555027000	4.856528000
C	-0.296893000	-0.426628000	4.507915000
H	-0.568213000	-0.179941000	5.527792000
C	-0.133652000	0.602038000	3.587220000
H	-0.270028000	1.630356000	3.896380000
C	0.189400000	0.314017000	2.253119000
C	0.040199000	2.516828000	1.348836000
C	-2.311409000	2.297031000	2.125946000

H	-3.133224000	2.768722000	1.582409000
H	-2.547852000	2.283762000	3.192343000
H	-2.192556000	1.274965000	1.774166000
C	2.126963000	3.298288000	0.272402000
H	2.071741000	3.432807000	-0.811692000
H	2.456589000	2.285845000	0.494731000
H	2.835753000	4.017107000	0.686378000
C	-1.045762000	4.500379000	1.856735000
H	-0.918643000	4.880336000	2.872817000
H	-1.972672000	4.899293000	1.446064000
C	0.174419000	4.799575000	0.966017000
H	-0.105142000	5.155272000	-0.029669000
H	0.848142000	5.526789000	1.417816000
C	-1.566808000	2.615236000	-1.716406000
N	-0.931755000	1.715597000	-1.388642000
C	-2.370417000	3.746176000	-2.122981000
H	-1.718802000	4.553640000	-2.459126000
H	-2.968341000	4.083941000	-1.274950000
H	-3.030530000	3.449666000	-2.939149000

E(UTPSSh) = -3453.12214931
Zero-point correction = 0.685136 (Hartree/Particle)
Thermal correction to Energy = 0.727934
Thermal correction to Enthalpy = 0.728879
Thermal correction to Gibbs Free Energy = 0.609512

$[Cu(II)\{N(QuMe)(PhDMEG)_2\}(MeCN)]]^{2+}$ ($C4_{DMEG}$) Basal B

N	-1.170032000	0.565469000	0.913413000
C	-1.507914000	1.888303000	0.390365000
N	-2.019283000	-0.470156000	-1.352729000
C	-2.687715000	2.530731000	0.738920000
H	-3.410680000	2.025474000	1.367989000
N	1.125227000	-0.886500000	0.889582000
C	-2.925271000	3.823788000	0.285346000
H	-3.841242000	4.332390000	0.557992000
N	0.505702000	1.712263000	-0.903812000
C	-1.973860000	4.454784000	-0.514768000
H	-2.150222000	5.462901000	-0.871194000
N	2.284078000	3.182811000	-0.256955000
C	-0.808648000	3.796750000	-0.886079000
H	-0.091334000	4.277798000	-1.540466000
N	2.644628000	1.698251000	-1.876314000
C	-0.556652000	2.488993000	-0.449239000
N	2.857561000	-2.344035000	0.200174000
C	1.725683000	2.199822000	-1.003988000
N	1.525673000	-3.056635000	1.806738000
C	1.787659000	3.594906000	1.047528000
H	2.633882000	3.660866000	1.732812000
H	1.085966000	2.856497000	1.431351000
H	1.292226000	4.566271000	0.994574000
C	2.259857000	1.062212000	-3.122836000
H	2.991654000	0.297690000	-3.384282000
H	2.204512000	1.797786000	-3.933002000
H	1.288093000	0.596511000	-2.994204000
C	3.714202000	3.305842000	-0.555815000
H	4.292241000	2.848067000	0.253285000
H	4.008453000	4.350556000	-0.652032000
C	3.850861000	2.529058000	-1.864953000
H	3.842039000	3.195415000	-2.734354000
H	4.749881000	1.914407000	-1.902110000
C	-2.310391000	-0.322478000	0.995471000
C	-2.952536000	-0.694103000	2.149596000
H	-2.576283000	-0.375016000	3.112707000
Cu	-0.074337000	-0.352449000	-0.622524000
C	-4.129515000	-1.472024000	2.067255000
H	-4.628266000	-1.759876000	2.983955000
C	-4.664490000	-1.827724000	0.852013000
H	-5.587592000	-2.392019000	0.797716000
C	-4.003994000	-1.469650000	-0.348062000
C	-2.787398000	-0.760155000	-0.259765000
C	-4.461875000	-1.776672000	-1.651595000
H	-5.394832000	-2.312857000	-1.779287000
C	-3.729899000	-1.377702000	-2.738447000
H	-4.078841000	-1.571572000	-3.744517000
C	-2.481006000	-0.730344000	-2.567177000
C	-1.663828000	-0.321935000	-3.749730000
H	-2.283562000	0.252172000	-4.442066000
H	-1.297238000	-1.196507000	-4.292190000
H	-0.820606000	0.290996000	-3.438470000
C	-0.309015000	0.619880000	2.086885000
C	-0.598618000	1.441122000	3.168835000
H	-1.467465000	2.086371000	3.134007000
C	0.233120000	1.431393000	4.282596000
H	0.012683000	2.068461000	5.129361000
C	1.352852000	0.600672000	4.290335000
H	2.014236000	0.593032000	5.148696000
C	1.655689000	-0.198601000	3.196730000
H	2.553217000	-0.805874000	3.198609000
C	0.826629000	-0.197318000	2.064807000
C	1.807029000	-2.040800000	0.974242000
C	3.594970000	-1.409977000	-0.622336000
H	3.634483000	-1.759470000	-1.655676000
H	4.615896000	-1.310033000	-0.245061000
H	3.096339000	-0.444597000	-0.586282000
C	0.362420000	-3.162856000	2.661126000
H	-0.013607000	-4.185680000	2.615105000
H	-0.408630000	-2.484114000	2.302493000
H	0.606584000	-2.913778000	3.697419000
C	3.328317000	-3.707948000	0.458453000
H	4.405608000	-3.702027000	0.621010000
H	3.104297000	-4.355692000	-0.392421000
C	2.545604000	-4.104888000	1.722889000
H	2.069267000	-5.080126000	1.629483000
H	3.169293000	-4.099519000	2.620534000
C	0.888433000	-2.548160000	-2.612469000
N	0.580127000	-1.697633000	-1.904182000
C	1.290307000	-3.611501000	-3.505233000
H	2.226373000	-3.336556000	-3.993495000
H	0.516004000	-3.764856000	-4.258069000
H	1.431138000	-4.529829000	-2.933546000

E(UTPSSh) = -3453.12175382
Zero-point correction = 0.684854 (Hartree/Particle)
Thermal correction to Energy = 0.727723
Thermal correction to Enthalpy = 0.728667
Thermal correction to Gibbs Free Energy = 0.609549

$[Cu(II)\{N(QuMe)_2(PhTMG)\}(MeCN)]]^{2+}$ ($C6_{TMG}$) Apical A

N	0.595298000	1.316298000	0.154103000
C	1.959122000	-2.653721000	-2.246705000
H	2.613865000	-3.301588000	-2.826468000
H	1.211540000	-2.217774000	-2.911805000
H	1.439921000	-3.263190000	-1.502770000
Cu	0.246304000	-0.910313000	0.162755000
N	2.070631000	-0.662845000	-0.872030000
C	2.738006000	-1.570233000	-1.573258000
N	-1.045407000	-0.403686000	1.631238000
C	4.148613000	-1.531809000	-1.652337000
H	4.656702000	-2.274295000	-2.253123000
N	-1.035539000	-0.369442000	-1.273332000
C	4.853803000	-0.603702000	-0.931960000
H	5.937555000	-0.605716000	-0.936391000
N	-3.330573000	0.120964000	-1.552294000
C	4.163212000	0.365933000	-0.171083000
N	-2.615000000	-2.070331000	-1.319560000
C	4.798145000	1.334423000	0.642384000
H	5.880108000	1.352334000	0.691753000
C	4.043212000	2.224017000	1.366184000
H	4.525135000	2.951208000	2.007457000
C	2.636044000	2.243257000	1.253268000
H	2.065958000	2.988981000	1.791281000
C	1.997675000	1.337536000	0.440797000
C	2.749066000	0.333599000	-0.224986000
C	-1.664858000	-2.720503000	2.066276000
H	-1.017952000	-3.173035000	2.822890000
H	-1.229283000	-2.917714000	1.088657000
H	-2.639503000	-3.203282000	2.135835000
C	-1.791601000	-1.254088000	2.324125000
C	-2.695070000	-0.795049000	3.310034000
H	-3.284160000	-1.522311000	3.852437000
C	-2.825328000	0.543509000	3.547586000
H	-3.527587000	0.912861000	4.285516000
C	-2.044686000	1.466621000	2.815473000
C	-2.166772000	2.863373000	2.981365000
H	-2.872646000	3.240056000	3.711691000
C	-1.417806000	3.721547000	2.214790000
H	-1.522421000	4.792979000	2.326337000
C	-0.502903000	3.210853000	1.277249000
H	0.073466000	3.892649000	0.664965000
C	-0.332208000	1.853577000	1.115757000
C	-1.128135000	0.946985000	1.861116000
C	0.287974000	1.644978000	-1.229331000
C	0.857746000	2.745709000	-1.857316000
H	1.561772000	3.365058000	-1.314072000
C	0.528009000	3.039327000	-3.175141000
H	0.967828000	3.899311000	-3.664298000
C	-0.365875000	2.217088000	-3.859433000
H	-0.622741000	2.434107000	-4.889389000
C	-0.913698000	1.100589000	-3.241899000
H	-1.576407000	0.441337000	-3.789444000
C	-0.591649000	0.796747000	-1.914577000
C	-2.310899000	-0.754985000	-1.389533000
C	-1.700548000	-3.091342000	-1.812270000
H	-1.270193000	-3.676084000	-0.994609000
H	-0.905898000	-2.612815000	-2.374485000
H	-2.251897000	-3.770000000	-2.467033000
C	-3.886040000	-2.552559000	-0.790008000
H	-3.683018000	-3.396095000	-0.128356000
H	-4.554055000	-2.892888000	-1.585019000
H	-4.368021000	-1.761496000	-0.220317000
C	-3.281741000	1.483389000	-1.040393000
H	-2.492873000	1.572667000	-0.300578000
H	-4.239518000	1.705690000	-0.565541000
H	-3.104430000	2.202043000	-1.844817000
C	-4.469663000	-0.174408000	-2.417821000
H	-4.288725000	-1.095812000	-2.964824000
H	-4.574507000	0.644399000	-3.133837000
H	-5.395323000	-0.261303000	-1.844274000
C	2.046375000	-2.602482000	2.057292000
N	1.316416000	-2.048098000	1.364603000
C	2.962556000	-3.302154000	2.928532000
H	3.234263000	-2.651128000	3.760711000
H	3.857774000	-3.572757000	2.367097000
H	2.481222000	-4.203459000	3.310734000

E(UTPSSh) = -3303.02613925
Zero-point correction = 0.620928 (Hartree/Particle)
Thermal correction to Energy = 0.660301
Thermal correction to Enthalpy = 0.661246
Thermal correction to Gibbs Free Energy = 0.549571

$[Cu(II)\{N(QuMe)_2(PhTMG)\}(MeCN)]]^{2+}$ ($C6_{TMG}$) Apical B

N	0.665773000	0.122407000	1.244756000
C	2.393891000	-0.197050000	-3.450681000
H	2.985303000	0.469033000	-4.081440000
H	1.383409000	0.200735000	-3.381688000
H	2.362964000	-1.171624000	-3.944060000
Cu	0.305399000	0.158531000	-0.951496000
N	2.293039000	-0.209675000	-1.010664000
C	3.034788000	-0.318465000	-2.105270000
N	-0.267981000	-1.768525000	-0.575989000
C	4.428767000	-0.541653000	-2.024604000
H	4.994041000	-0.632622000	-2.942642000
N	-1.450721000	0.841308000	-0.221419000
C	5.035462000	-0.635330000	-0.805278000
H	6.101908000	-0.810009000	-0.724999000
N	-3.725544000	0.583504000	0.338451000
C	4.269452000	-0.489321000	0.373560000
N	-3.019969000	0.312794000	-1.849097000
C	4.843661000	-0.561878000	1.660841000
H	5.909142000	-0.737969000	1.746468000
C	4.058522000	-0.419979000	2.777349000
H	4.490971000	-0.484790000	3.767421000
C	2.678497000	-0.188929000	2.641639000
H	2.070670000	-0.098382000	3.531850000
C	2.087451000	-0.087194000	1.401250000
C	2.872791000	-0.261465000	0.232470000
C	-0.281445000	-2.476150000	-2.906656000
H	0.570762000	-3.102007000	-3.187013000
H	-0.021731000	-1.439020000	-3.105170000
H	-1.122254000	-2.762383000	-3.539354000
C	-0.606328000	-2.691752000	-1.465666000

C	-1.262386000	-3.882829000	-1.072944000
H	-1.517023000	-4.608641000	-1.833884000
C	-1.589915000	-4.084238000	0.237346000
H	-2.122569000	-4.975123000	0.548481000
C	-1.231810000	-3.117341000	1.205218000
C	-1.554994000	-3.246577000	2.573811000
H	-2.095747000	-4.126370000	2.900910000
C	-1.197366000	-2.265299000	3.466230000
H	-1.458800000	-2.352541000	4.512903000
C	-0.475987000	-1.140926000	3.026655000
H	-0.204193000	-0.367002000	3.733586000
C	-0.123347000	-1.000767000	1.703217000
C	-0.528590000	-1.969015000	0.754159000
C	0.075710000	1.408928000	1.546949000
C	0.599878000	2.315484000	2.456227000
H	1.516973000	2.087667000	2.982678000
C	-0.054234000	3.524483000	2.684253000
H	0.358652000	4.230376000	3.393970000
C	-1.232363000	3.817547000	2.003938000
H	-1.743067000	4.756516000	2.180147000
C	-1.743608000	2.926225000	1.067266000
H	-2.628447000	3.178492000	0.495667000
C	-1.093400000	1.716067000	0.818310000
C	-2.713709000	0.599338000	-0.563613000
C	-2.294087000	0.901941000	-2.965082000
H	-1.711778000	0.149046000	-3.502281000
H	-1.634993000	1.682239000	-2.597703000
H	-3.013496000	1.338043000	-3.662937000
C	-4.067041000	-0.640573000	-2.199320000
H	-3.664697000	-1.342779000	-2.932702000
H	-4.937169000	-0.143652000	-2.635808000
H	-4.368483000	-1.192037000	-1.312034000
C	-3.510926000	0.280390000	1.744295000
H	-2.561215000	-0.229821000	1.866703000
H	-4.314449000	-0.377431000	2.081679000
H	-3.513226000	1.188853000	2.353721000
C	-5.061766000	1.066071000	-0.000283000
H	-5.053608000	1.511213000	-0.991776000
H	-5.346623000	1.830335000	0.727228000
H	-5.796588000	0.258189000	0.033298000
C	0.914120000	3.106633000	-1.763000000
N	0.678752000	1.986566000	-1.657931000
C	1.198790000	4.517988000	-1.888017000
H	0.744065000	4.900454000	-2.802807000
H	2.278276000	4.669499000	-1.923289000
H	0.782132000	5.041275000	-1.025893000

E(UTPSSh) = -3303.02796505
Zero-point correction = 0.621147 (Hartree/Particle)
Thermal correction to Energy = 0.660416
Thermal correction to Enthalpy = 0.661360
Thermal correction to Gibbs Free Energy = 0.550009

$[Cu(II)\{N(QuMe)_2(PhTMG)\}(MeCN)]]^{2+}$ ($C6_{TMG}$) Basal B

N	-0.768389000	-1.181503000	-0.166682000
C	-0.482963000	3.174395000	-2.452751000
H	-0.448162000	3.540136000	-3.480007000
H	0.471895000	2.723275000	-2.196633000
H	-0.645154000	4.039045000	-1.801879000
Cu	0.107876000	0.700533000	-0.028978000
N	-1.386394000	1.115502000	-1.537708000
C	-1.595853000	2.189518000	-2.285929000
N	-1.098076000	0.640395000	1.719543000
C	-2.850822000	2.428293000	-2.898605000
H	-2.972928000	3.311764000	-3.511859000
N	1.707048000	-0.278964000	-0.750011000
C	-3.891856000	1.566644000	-2.689201000
H	-4.866352000	1.753216000	-3.125299000
N	3.710328000	-1.021579000	0.235892000
C	-3.695769000	0.413916000	-1.893006000
N	3.585013000	1.094335000	-0.710062000
C	-4.719054000	-0.514271000	-1.595082000
H	-5.710885000	-0.349140000	-1.998534000
C	-4.458361000	-1.597456000	-0.791728000
H	-5.244151000	-2.300282000	-0.546487000
C	-3.160252000	-1.819304000	-0.290885000
H	-2.962707000	-2.683201000	0.331202000
C	-2.144437000	-0.947216000	-0.598009000
C	-2.395309000	0.213043000	-1.364727000
C	-1.760089000	2.961581000	2.030362000
H	-2.799163000	3.233430000	2.233798000
H	-1.588086000	3.012283000	0.958384000
H	-1.132176000	3.695659000	2.540158000
C	-1.503598000	1.585799000	2.555305000
C	-1.717101000	1.296148000	3.926916000
H	-2.044961000	2.095086000	4.579367000
C	-1.487807000	0.038762000	4.417064000
H	-1.610184000	-0.176913000	5.471831000
C	-1.107714000	-0.997045000	3.530886000
C	-0.855968000	-2.336544000	3.911677000
H	-0.934384000	-2.610300000	4.956859000
C	-0.509018000	-3.271659000	2.965595000
H	-0.306734000	-4.293388000	3.260239000
C	-0.445694000	-2.933633000	1.596072000
H	-0.217292000	-3.690383000	0.857189000
C	-0.694784000	-1.640395000	1.211053000
C	-0.971515000	-0.643614000	2.170699000
C	0.028972000	-1.953778000	-1.115392000
C	-0.464756000	-3.081041000	-1.756376000
H	-1.491463000	-3.386716000	-1.602496000
C	0.370803000	-3.812915000	-2.593073000
H	-0.006219000	-4.693947000	-3.096214000
C	1.687363000	-3.396977000	-2.781062000
H	2.341644000	-3.954341000	-3.440793000
C	2.167923000	-2.251589000	-2.160242000
H	3.176941000	-1.910574000	-2.356923000
C	1.337699000	-1.503647000	-1.314692000
C	2.995809000	-0.078401000	-0.415562000
C	3.194844000	1.863518000	-1.885299000
H	2.813027000	2.843894000	-1.595197000
H	2.430214000	1.317803000	-2.430457000
H	4.070770000	2.006446000	-2.523059000
C	4.652907000	1.665694000	0.102641000
H	4.432847000	2.722558000	0.263069000
H	5.624268000	1.589996000	-0.391157000
H	4.689105000	1.160424000	1.064535000
C	3.052668000	-2.025119000	1.063254000
H	2.093731000	-1.643414000	1.403053000

H	3.686967000	-2.222443000	1.928465000
H	2.898929000	-2.957597000	0.512679000
C	5.132937000	-1.244145000	-0.013914000
H	5.459333000	-0.637779000	-0.854642000
H	5.271860000	-2.297996000	-0.266537000
H	5.734460000	-1.010063000	0.866964000
C	1.447977000	3.344111000	0.897922000
N	0.999232000	2.364229000	0.499861000
C	2.006261000	4.582673000	1.391368000
H	1.197380000	5.237898000	1.717616000
H	2.568789000	5.069765000	0.593567000
H	2.668455000	4.371369000	2.232064000

E(UTPSSh) = -3303.02707760
Zero-point correction = 0.621010 (Hartree/Particle)
Thermal correction to Energy = 0.660248
Thermal correction to Enthalpy = 0.661192
Thermal correction to Gibbs Free Energy = 0.551246

$[Cu(II)\{N(QuMe)_2(PhDMEG)\}(MeCN)]]^{2+}$ ($C6_{DMEG}$) Apical A

Cu	-0.267770000	-0.915710000	-0.057564000
N	-0.617593000	1.279255000	-0.298071000
N	1.174750000	-0.559360000	-1.414511000
N	-2.126792000	-0.598036000	0.828887000
N	0.901949000	-0.233085000	1.432013000
N	3.257055000	0.254736000	1.556736000
N	2.584898000	-1.863684000	1.530485000
C	-0.406620000	1.761620000	1.059309000
C	-1.011051000	2.924833000	1.520654000
H	-1.687176000	3.469334000	0.872163000
C	-0.746976000	3.378838000	2.807192000
H	-1.213764000	4.287262000	3.166497000
C	0.119736000	2.657106000	3.627393000
H	0.329535000	3.003986000	4.632163000
C	0.699334000	1.478169000	3.179236000
H	1.344996000	0.899282000	3.828612000
C	0.438620000	1.009455000	1.886449000
C	2.186483000	-0.567496000	1.514172000
C	1.734152000	-2.943856000	1.997185000
H	2.078779000	-3.879321000	1.558373000
H	0.709654000	-2.761189000	1.685412000
H	1.763999000	-3.023509000	3.088816000
C	3.304624000	1.626382000	1.073752000
H	3.819806000	2.252851000	1.803016000
H	2.303459000	2.013884000	0.921601000
H	3.849155000	1.657069000	0.125954000
C	4.024074000	-1.946307000	1.798587000
H	4.496352000	-2.693988000	1.162969000
H	4.180908000	-2.220195000	2.846606000
C	4.500449000	-0.524908000	1.505671000
H	5.221030000	-0.156697000	2.234820000
H	4.931072000	-0.435401000	0.503487000
C	-1.999475000	1.253735000	-0.677231000
C	-2.598330000	2.062853000	-1.611835000
H	-2.007138000	2.760119000	-2.190569000
C	-3.997280000	2.007251000	-1.798319000
H	-4.450421000	2.656889000	-2.536484000
C	-4.784124000	1.184980000	-1.029121000
H	-5.861514000	1.182686000	-1.140687000
C	-4.187583000	0.315113000	-0.085542000
C	-2.779549000	0.312225000	0.043488000
C	-4.904963000	-0.578556000	0.743096000
H	-5.987549000	-0.597623000	0.695624000
C	-4.228463000	-1.407419000	1.599561000
H	-4.759319000	-2.083942000	2.256232000
C	-2.814514000	-1.431743000	1.596366000
C	-2.052038000	-2.423957000	2.414087000
H	-2.658342000	-2.794314000	3.239511000
H	-1.141988000	-1.969590000	2.806328000
H	-1.771529000	-3.281109000	1.793278000
C	0.387385000	1.725739000	-1.231174000
C	0.549071000	3.059200000	-1.536331000
H	-0.105497000	3.790031000	-1.078960000
C	1.558777000	3.485509000	-2.416617000
H	1.654693000	4.538971000	-2.645446000
C	2.416267000	2.569208000	-2.973620000
H	3.202180000	2.881741000	-3.650451000
C	2.299932000	1.198473000	-2.657226000
C	1.277275000	0.763572000	-1.771225000
C	3.187071000	0.222956000	-3.167443000
H	3.978163000	0.528410000	-3.841964000
C	3.044056000	-1.084002000	-2.799934000
H	3.711597000	-1.849564000	-3.172376000
C	2.014621000	-1.461088000	-1.906221000
C	1.867764000	-2.899236000	-1.527963000
H	1.458574000	-3.458321000	-2.374405000
H	1.202626000	-3.030830000	-0.678617000
H	2.843040000	-3.326364000	-1.291490000
C	-1.866691000	-2.848955000	-1.902996000
N	-1.215491000	-2.197253000	-1.216602000
C	-2.684623000	-3.671765000	-2.764353000
H	-2.646828000	-3.278043000	-3.780920000
H	-3.713896000	-3.658055000	-2.403395000
H	-2.305220000	-4.694449000	-2.753210000

E(UTPSSh) = -3301.82881233
Zero-point correction = 0.599883 (Hartree/Particle)
Thermal correction to Energy = 0.638113
Thermal correction to Enthalpy = 0.639057
Thermal correction to Gibbs Free Energy = 0.528272

$[Cu(II)\{N(QuMe)_2(PhDMEG)\}(MeCN)]]^{2+}$ ($C6_{DMEG}$) Apical B

Cu	0.345279000	0.373870000	-0.899810000
N	0.654230000	-0.119570000	1.256680000
N	-0.414022000	-1.517298000	-0.898643000
N	2.290213000	-0.158002000	-1.016919000
N	-1.361966000	1.041336000	-0.024114000
N	-3.679827000	0.656290000	0.460881000

N	-2.990243000	0.644205000	-1.660907000
C	0.194088000	1.138164000	1.797331000
C	0.797492000	1.816133000	2.845699000
H	1.689177000	1.417236000	3.310768000
C	0.251195000	3.017266000	3.294273000
H	0.723701000	3.545916000	4.112646000
C	-0.896852000	3.530199000	2.696231000
H	-1.322660000	4.461973000	3.048221000
C	-1.484390000	2.872096000	1.621737000
H	-2.348592000	3.291705000	1.121024000
C	-0.942063000	1.673284000	1.154024000
C	-2.615096000	0.812694000	-0.364705000
C	-2.314352000	1.304495000	-2.765392000
H	-2.451764000	0.717167000	-3.671989000
H	-1.251893000	1.394020000	-2.552016000
H	-2.720878000	2.309539000	-2.921719000
C	-3.596400000	0.227097000	1.849106000
H	-4.461557000	0.617286000	2.385270000
H	-2.694877000	0.611638000	2.314363000
H	-3.599550000	-0.865351000	1.909993000
C	-4.449561000	0.521596000	-1.744530000
H	-4.735038000	-0.248370000	-2.459881000
H	-4.875565000	1.479216000	-2.062030000
C	-4.835876000	0.178420000	-0.310395000
H	-5.750560000	0.670425000	0.017066000
H	-4.939531000	-0.902000000	-0.165089000
C	2.043554000	-0.497335000	1.370814000
C	2.592657000	-0.898698000	2.568597000
H	1.973723000	-0.924553000	3.455537000
C	3.941296000	-1.284357000	2.660699000
H	4.343534000	-1.585326000	3.619403000
C	4.734646000	-1.277088000	1.540835000
H	5.776501000	-1.569188000	1.593479000
C	4.199759000	-0.895732000	0.291485000
C	2.834722000	-0.509597000	0.193555000
C	4.974386000	-0.882111000	-0.890699000
H	6.017529000	-1.171622000	-0.843220000
C	4.405376000	-0.497477000	-2.070329000
H	4.978513000	-0.466158000	-2.987488000
C	3.040537000	-0.129235000	-2.110779000
C	2.445374000	0.303749000	-3.412254000
H	3.079385000	1.065104000	-3.871056000
H	1.447932000	0.718309000	-3.285169000
H	2.396203000	-0.540895000	-4.103814000
C	-0.258553000	-1.219970000	1.485332000
C	-0.668023000	-1.569011000	2.751551000
H	-0.348009000	-0.973512000	3.597633000
C	-1.499355000	-2.685061000	2.958256000
H	-1.799603000	-2.943400000	3.965604000
C	-1.913906000	-3.444455000	1.891295000
H	-2.539638000	-4.316423000	2.038296000
C	-1.542457000	-3.087202000	0.576058000
C	-0.722772000	-1.947474000	0.364116000
C	-1.967838000	-3.804398000	-0.565685000
H	-2.589254000	-4.683098000	-0.439599000
C	-1.599460000	-3.377879000	-1.810337000
H	-1.911617000	-3.907735000	-2.700406000
C	-0.827817000	-2.201546000	-1.956715000
C	-0.463109000	-1.717884000	-3.320774000
H	0.411376000	-2.265534000	-3.683791000
H	-0.220454000	-0.657024000	-3.310445000
H	-1.278555000	-1.889373000	-4.023173000
C	1.052769000	3.372913000	-1.347248000
N	0.809519000	2.250114000	-1.331950000
C	1.350655000	4.786743000	-1.361074000
H	2.431587000	4.930173000	-1.383429000
H	0.937005000	5.245675000	-0.461690000
H	0.901241000	5.242383000	-2.244485000

E(UTPSSh) = -3301.82984418
Zero-point correction = 0.600262 (Hartree/Particle)
Thermal correction to Energy = 0.638186
Thermal correction to Enthalpy = 0.639130
Thermal correction to Gibbs Free Energy = 0.529889

$[Cu(II)\{N(QuMe)_2(PhDMEG)\}(MeCN)]]^{2+}$ ($C6_{DMEG}$) Basal B

Cu	-0.174285000	-0.658077000	-0.051427000
N	0.871416000	1.145684000	-0.065086000
N	1.094808000	-0.901793000	1.591048000
N	1.252212000	-1.101487000	-1.629323000
N	-1.653295000	0.479245000	-0.767330000
N	-3.693281000	1.043134000	0.348256000
N	-3.687788000	-0.701313000	-0.999819000
C	0.117768000	2.089835000	-0.886500000
C	0.672310000	3.270100000	-1.362241000
H	1.717113000	3.488857000	-1.184225000
C	-0.124112000	4.171104000	-2.059993000
H	0.301604000	5.094770000	-2.430137000
C	-1.468552000	3.871639000	-2.274764000
H	-2.096669000	4.565829000	-2.820449000
C	-2.012773000	2.676048000	-1.827004000
H	-3.046979000	2.434117000	-2.041794000
C	-1.217577000	1.751877000	-1.133435000
C	-2.956859000	0.296207000	-0.487791000
C	-3.295597000	-1.539452000	-2.111950000
H	-3.268811000	-2.590264000	-1.816901000
H	-2.307965000	-1.224819000	-2.439759000
H	-4.008979000	-1.420103000	-2.930473000
C	-3.203792000	2.106135000	1.199622000
H	-3.439277000	3.088252000	0.780985000
H	-2.125186000	2.011340000	1.304663000
H	-3.667941000	2.011532000	2.182077000
C	-5.039245000	-0.711506000	-0.432308000
H	-5.167882000	-1.571404000	0.229172000
H	-5.775985000	-0.770632000	-1.232559000
C	-5.098752000	0.628031000	0.324808000
H	-5.704673000	1.375727000	-0.193206000
H	-5.469513000	0.515602000	1.342768000
C	2.200513000	0.836856000	-0.588267000
C	3.295071000	1.604029000	-0.270200000
H	3.195106000	2.423896000	0.430019000
C	4.546593000	1.334684000	-0.857454000
H	5.393661000	1.958119000	-0.601732000
C	4.684262000	0.305527000	-1.756157000

H	5.638797000	0.103878000	-2.227403000
C	3.581431000	-0.522416000	-2.064647000
C	2.324985000	-0.276383000	-1.452356000
C	3.659705000	-1.623588000	-2.948519000
H	4.597158000	-1.839537000	-3.447755000
C	2.557369000	-2.406433000	-3.151964000
H	2.592431000	-3.256168000	-3.821361000
C	1.355884000	-2.135747000	-2.452356000
C	0.169138000	-3.027340000	-2.639012000
H	-0.382598000	-2.723842000	-3.534207000
H	-0.503600000	-2.967375000	-1.786286000
H	0.481778000	-4.062332000	-2.780308000
C	0.899557000	1.449399000	1.358006000
C	0.782121000	2.702884000	1.903135000
H	0.583314000	3.559262000	1.272359000
C	0.951378000	2.869743000	3.296046000
H	0.856048000	3.862726000	3.716261000
C	1.269788000	1.806457000	4.106842000
H	1.432203000	1.949701000	5.168175000
C	1.374601000	0.503631000	3.563382000
C	1.130655000	0.328175000	2.184429000
C	1.695340000	-0.661809000	4.299969000
H	1.899936000	-0.584988000	5.361335000
C	1.757542000	-1.871979000	3.661564000
H	2.030800000	-2.770073000	4.200292000
C	1.430962000	-1.978383000	2.286427000
C	1.471193000	-3.302679000	1.594208000
H	2.473316000	-3.728782000	1.687746000
H	1.230016000	-3.199107000	0.538814000
H	0.777104000	-4.005962000	2.059825000
C	-1.996277000	-2.971776000	0.943631000
N	-1.314371000	-2.163184000	0.494635000
C	-2.856711000	-3.991213000	1.499095000
H	-2.262961000	-4.672796000	2.109488000
H	-3.330751000	-4.544554000	0.687206000
H	-3.621773000	-3.518572000	2.116615000

E(UTPSSh) = -3301.82863509
Zero-point correction = 0.599946 (Hartree/Particle)
Thermal correction to Energy = 0.638076
Thermal correction to Enthalpy = 0.639020
Thermal correction to Gibbs Free Energy = 0.529622

6.5.6 Acetonitrile

C	0.000000000	0.000000000	0.277715000
N	0.000000000	0.000000000	1.432453000
C	0.000000000	0.000000000	-1.176267000
H	0.000000000	1.026456000	-1.545289000
H	-0.888937000	-0.513228000	-1.545289000
H	0.888937000	-0.513228000	-1.545289000

E(RTPSSh) = -132.822958520
Zero-point correction = 0.045124 (Hartree/Particle)
Thermal correction to Energy = 0.048717
Thermal correction to Enthalpy = 0.049661
Thermal correction to Gibbs Free Energy = 0.022163