ELECTRONIC SUPPLEMENTARY INFORMATION

FOR

Aerobic Intramolecular Carbon-Hydrogen Bond Oxidation Promoted by Cu(I) Complexes

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1- General methods and materials.

Most of the reactions and operations have been carried out under air, with the exception of the synthesis of Cu(I) complexes, that were carried out using standard Schlenk techniques under an inert atmosphere of nitrogen. All solvents were dried using a SPS-MBraun system. THF was carefully distilled before use in oxygenation reactions, which was preformed using 100% oxygen gas. The reactants were purchased from Sigma-Aldrich and used without further purification.

NMR spectra were recorded on Agilent 500 DD2, ^{1}H and ^{13}C NMR shifts reported relative to tetramethylsilane. FT-IR spectra were collected on a Alpha Bruker FTIR spectrometer. UV-Visible spectra were run using a Varian Cary 50 spectrophotometer. Elemental analyses were performed on a Perkin Elmer Series II CHNS/O Analyzer 2400. Crystal structure determinations were carried out using a BRUKER D8 FIXED-CHI diffractometer equipped with an Oxford Cryosystem low-temperature device.

The compounds $TlTp^{Ms}$ (H-B),[1] $Tl(Me\text{-}Tp^{Ms})$[2] and $Tp^{Ms}Cu(THF)$[3] were prepared according to literature procedures.

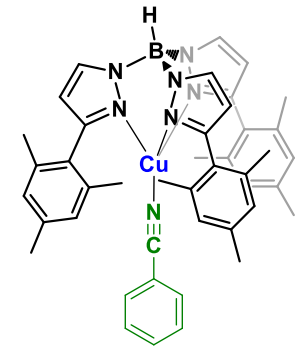
CCDC 1998194 (**1a**), 1998192 (**1b**), 1998369 (**2a**), 1998208 (**2b**), 1998370 (**3a**) 1998191 (**3b**), contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre.

2- Synthesis and characterization of complexes 1-3.

Complexes Tp^{x}Cu(NCPh) (1a,b)

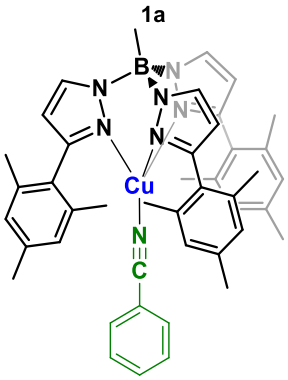
In a Schlenk tube, TlTp^{Ms} (0.385 g, 0.5 mmol) or Tl(Me-Tp^{Ms}) (0.39 g, 0.5 mmol) was dissolved in 10 mL of dichloromethane, then four equivalents of benzonitrile (206 µL, 2 mmol) were added. CuCl (0.049 g, 0.5 mmol) was added and the mixture was stirred for 4 h, before being filtered through celite, under nitrogen. The volume of the yellow solution was concentrated under vacuum to approximately one third of the initial. After adding 1 ml of hexane, the solutions were cooled to -30°C, which led to the isolation of both complexes as yellow crystals with yields of 90% for **1a** and 70% for **1b**.

Analysis calculated for $C_{43}H_{45}BCuN_7$ (**1a**): C, 70.40; H, 6.18; N, 13.35 %. Found: C, 70.63; H, 6.33; N, 13.10 %. Analysis calculated for $C_{44}H_{47}BCuN_7$ (**1b**): C, 70.40; H, 5.91; N, 13.40 %. Found: C, 70.26; H, 6.19; N, 13.0 %.



1a

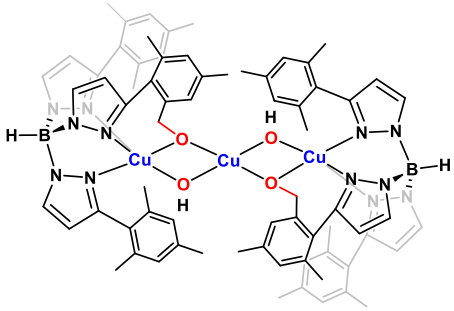
^{1}H NMR (500 MHz, C_6D_6) δ 1.94 (s, 9H, C*H*$_{3Mes}$), 2.19 (s, 18H, C*H*$_{3Mes}$), 6.02 (d, 3H, *J* = 2 Hz, C*H*$_{pz}$), 6.54 (m, 2H, C*H*$_{bznit}$), 6.64 (s, 6H, C*H*$_{Mes}$), 6.67 (m, 1H, C*H*$_{bznit}$), 6.80 (m, 2H, C*H*$_{bznit}$), 7.74 (d, 3H, *J* = 2 Hz, C*H*$_{pz}$). ^{13}C{^{1}H} (125 MHz, C_6D_6) δ 20.5 (*C*H$_{3Mes}$), 20.6 (*C*H$_{3Mes}$), 104.2 (*C*H$_{pz}$), 127.6 (*C*H$_{Mes}$), 131.2 (*C*H$_{bznit}$), 131.6 (*C*H$_{bznit}$), 132.3 (*C*$_{qMes}$), 134.2 (*C*H$_{pz}$), 135.9 (*C*$_{qMes}$), 137.8 (*C*$_{qMes}$), 150.1 (*C*$_{qpz}$).). ^{11}B{^{1}H} (160 MHz, C_6D_6) δ -3.06 (*B*H).



1b

^{1}H NMR (500 MHz, C_6D_6) δ 1.05 (s, 3H, BC*H*$_3$), 1.92 (s, 9H, C*H*$_{3Mes}$), 2.18 (s, 18H, C*H*$_{3Mes}$), 6.03 (d, 3H, *J* = 2 Hz, C*H*$_{pz}$), 6.63 (s, 6H, C*H*$_{Mes}$), 6.69 (t, 2H, *J* = 7 Hz, C*H*$_{bznit}$), 6.78 (s, 1H, C*H*$_{bznit}$), 6.85 (t, 2H, *J* = 7 Hz, C*H*$_{bznit}$), 7.65 (d, 3H, *J* = 2 Hz, C*H*$_{pz}$). ^{13}C{^{1}H} (125 MHz, C_6D_6) δ 20.6 (*C*H$_{3Mes}$), 20.7 (*C*H$_{3Mes}$), 103.9 (*C*H$_{pz}$), 127.5 (*C*H$_{Mes}$), 131.2 (*C*H$_{bznit}$), 131.6 (*C*H$_{bznit}$), 131.9 (*C*H$_{pz}$), 132.4 (*C*$_{qMes}$), 135.8 (*C*$_{qMes}$), 137.9 (*C*$_{qMes}$), 148.7 (*C*$_{qpz}$). ^{11}B{^{1}H} (160 MHz, C_6D_6) δ -1.35 (*B*Me)

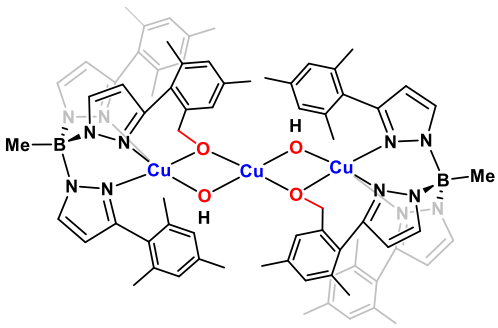
Complex 2a



$Tp^{Ms}Cu(THF)$ (0.015 g, 0.021 mmol) was dissolved in oxygenated THF (upon bubbling O2 for one hour, adding THF to maintaing 0.6 mL of volume). The colorless solution was transferred into a NMR tube. After 24 h stading at room temperature, green crystals corresponding to complex **2a** appeared. This reaction was carried out on a larger scale using a Schlenk tube (0.35 g of $Tp^{Ms}Cu(THF)$, 0.5 mmol) in oxygenated THF (10 mL) again obtaining complex **2a** as a crystalline green solid (0.158 g, 68% yield). When using complex $Tp^{Ms}Cu(NCPh)$ **1a** (0.2 g, 0.02 mmol) as starting material, **2a** crystallized after 72 h at room temperature giving 90 mg (71% yield).

Analysis calculated for $C_{72}H_{80}B_2Cu_3N_{12}O_4$ (**2a**): C, 62.23; H, 5.80; N, 12.09 %. Found: C, 62.66; H, 6.04; N, 11.51 %.

Complex 2b



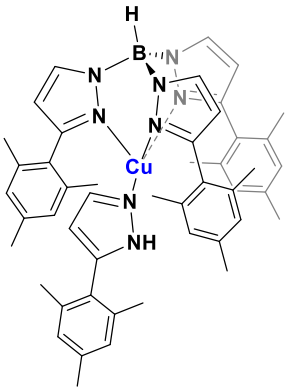
Complex **2b** was obtained following the above procedure, using complex **1b** (0.25 g, 0.33 mmol) in acetone as solvent, previously oxygenated for one hour (10 mL) in a Schlenk tube. After 72 h, the appearance of green crystals of complex **2b** was observed, with a final yield of 24 mg (25%).

Analysis calculated for $C_{74}H_{84}B_2Cu_3N_{12}O_4$ (**2b**): C, 62.69; H, 5.97; N, 11.86 %. Found: C, 62.68; H, 6.33; N, 11.52 %.

Complexes $Tp^{x}Cu(Hpz^{Ms})$ (3a,b)

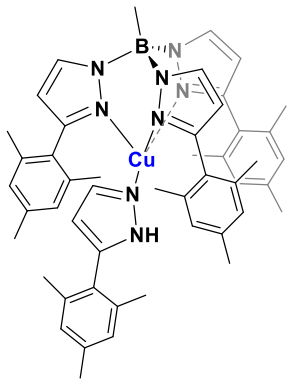
These complexes were detected by in situ NMR studies as by-products in the reaction of complexes **2a** and **2b**. For their characterization, they were independently synthesized following this procedure. The compounds $Tp^{Ms}Tl$ (0.385 g, 0.5 mmol) or Me-$Tp^{Ms}Tl$ (0.393 g, 0.5 mmol) were dissolved in 10 mL of dichloromethane along with one equiv of 3-mesitylpyrazole (0.093 g, 0.5 mmol), before adding CuCl (0.049 g, 0.5 mmol). After 12 h of stirring, the reaction mixtures were filtered through celite, and the filtrates were concentrated under vacuum to ca 50% of the initial volume. Then 1.5 mL of hexane was added before cooling to -30 °C. The expected complexes were obtained as colorless crystals with yields of 60% for **3a** and 55% for **3b**

Analysis calculated for $C_{48}H_{53}BCuN_8$ (**3a**): C, 70.62; H, 6.54; N, 13.73 %. Found: C, 70.36; H, 6.61; N, 13.57 %. Analysis calculated for $C_{49}H_{55}BCuN_8$ (**3b**): C, 70.87; H, 6.88; N, 13.49 %. Found C, 70.45; H, 6.88; N, 13.06 %.



3a

^{1}H NMR (500 MHz, THF-d_8) δ 1.79 (s, 6H, C*H*$_{3Mes}$), 1.89 (s, 9H, C*H*$_{3Mes}$), 1.92 (s, 18H, C*H*$_{3Mes}$), 2.31 (s, 3H, C*H*$_{3Mes}$), 5.44 (s, 1H, C*H*$_{pz}$), 5.90 (s, 1H, C*H*$_{pz}$), 5.97 (d, 3H, *J* = 2 Hz, C*H*$_{pz}$), 6.59 (s, 6H, C*H*$_{Mes}$), 6.94 (s, 2H, C*H*$_{Mes}$), 7.64 (s, 1H, C*H*$_{pz}$), 7.74 (d, 3H, *J* = 2 Hz, C*H*$_{pz}$). ^{13}C{^{1}H} (125 MHz, THF-d_8) δ 18.9 (*C*H$_{3Mes}$), 19.8 (*C*H$_{3Mes}$), 19.9 (*C*H$_{3Mes}$), 20.1 (*C*H$_{3Mes}$), 103.3 (*C*H$_{pz}$), 104.0 (*C*H$_{pz}$), 126.3 (*C*$_{qMes}$), 127.2 (*C*H$_{Mes}$), 127.9 (*C*H$_{Mes}$), 132.4 (*C*H$_{pz}$), 133.6 (*C*H$_{pz}$), 136.6 (*C*$_{qMes}$), 137.4 (*C*$_{qMes}$), 137.5 (*C*$_{qMes}$), 138.4 (*C*$_{qMes}$), 138.7 (*C*$_{qMes}$), 140.2 (*C*$_{qpz}$), 148.3 (*C*$_{qpz}$). ^{11}B{^{1}H} (160 MHz, THF-d_8) δ -3.35 (BH).



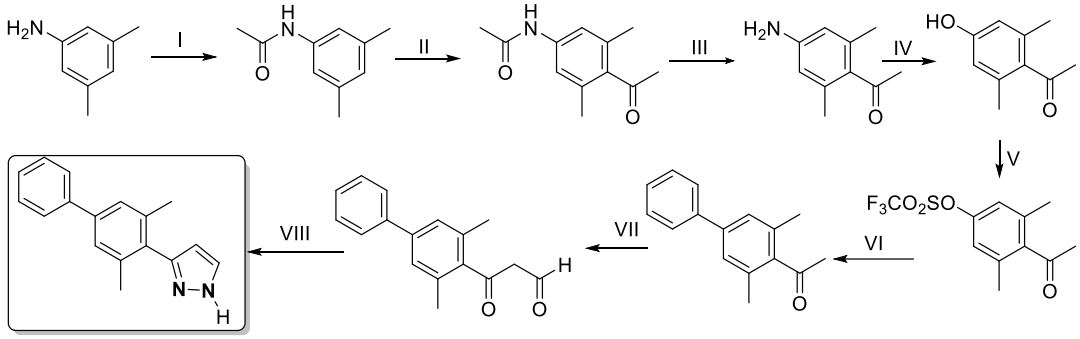
3b

^{1}H NMR (500 MHz, THF-d_8) δ 1.11 (s, 3H, BC*H*$_3$), 1.77 (s, 6H, C*H*$_{3Mes}$), 1.85 (s, 9H, C*H*$_{3Mes}$), 1.89 (s, 18H, C*H*$_{3Mes}$), 2.29 (s, 3H, C*H*$_{3Mes}$), 5.37 (s, 1H, C*H*$_{pz}$), 5.83 (s, 1H, C*H*$_{pz}$), 5.93 (d, 3H, *J* = 2 Hz, C*H*$_{pz}$), 6.55 (s, 6H, C*H*$_{Mes}$), 6.92 (s, 2H, C*H*$_{Mes}$), 7.56 (s, 1H, C*H*$_{pz}$),7.75 (d, 3H, *J* = 2 Hz, C*H*$_{pz}$). ^{13}C{^{1}H} (125 MHz, THF-d_8) δ 20.7 (*C*H$_{3Mes}$), 21.6 (*C*H$_{3Mes}$), 21.8 (*C*H$_{3Mes}$), 21.9 (*C*H$_{3Mes}$), 104.9 (*C*H$_{pz}$), 105.7 (*C*H$_{pz}$), 128.3 (*C*$_{qMes}$), 129.0 (*C*H$_{Mes}$), 129.7 (*C*H$_{Mes}$), 133.2 (*C*H$_{pz}$), 134.3 (*C*H$_{pz}$), 138.4 (*C*$_{qMes}$), 139.2 (*C*$_{qMes}$), 139.3 (*C*$_{qMes}$), 140.2 (*C*$_{qMes}$), 140.3 (*C*$_{qMes}$), 142.3 (*C*$_{qpz}$), 150.8 (*C*$_{qpz}$). ^{11}B{^{1}H} (160 MHz, THF-d_8) δ – 1.38 (*B*-Me).

3. Synthesis and characterization of complex Me-Tp$^{Me2\text{-}biphen}$Cu(NCPh) (4).

Step A: Synthesis of 3-(3,5-dimethyl-[1,1'-biphenyl]-4-yl)-pyrazole)

The preparation of the pyrazole was carried out following a procedure consisting of 8 steps.[4]



I:

In a three-necked round bottom flask under N_2, K_2CO_3 (44.2 g, 328 mmol) was placed and suspended in dry DCM (100 mL). Then 3,5-dimethylaniline (10 mL, 164 mmol) was added and the mixture was cooled to 0°C. After stirring at that temperature for 30 min, acetyl chloride (22.7 mL, 328 mmol, previously distilled) was added dropwise. After 2 h, 10 mL of H_2O were added and organics were extracted with DCM (3 x 60 mL). The organic phases were combined and dried with MgSO4, before filtering and removing volatiles to isolate the desired product as a white solid (53.9 g, 99% yield).

II:

The substituted aniline obtained above (13.59 g, 0.192 mol) and $AlCl_3$ (50.38 g, 0.465 mol) were placed into a 500 mL three-necked flask under N_2, along with DCM (200 mL), before cooling at 0 °C. Then, acetyl chloride (17.50 mL, 0.253 mol) was added dropwise under N2, the mixture being stirred for 3 h at 0° C. After this time, the flask was opened to air and its content was poured into a beaker containing 600 g of H_2O and 30 mL of HCl. Organics were extracted with DCM (3 x 50 mL) and the organic phase was dried with $MgSO_4$. After filtration and solvent evaporation, the desired product was obtained as a pale yellow solid (38.6g, 98% yield).

III:

In a 250 mL ampoule, 9 g of the compound obtained in step II, 60 mL of H_2O and 5 mL of HCl were placed. The mixture was heated at 95 °C for 20 h. After this time, it was allowed to cool and the resulting brown solution was transferred to a beaker, pH being brought 8 with a saturated solution of Na_2CO_3. The resulting yellow solid was filtered on a sintered glass funnel and subsequently dissolved in DCM (100 mL). The solution was

treated with $MgSO_4$ before filtering and evaporating the solvent. The targeted compound was obtained as a yellow solid (7 g, 98% yield).

IV:

In one-round botton flask 72.5 g of ice and 22.5 mL of H_2SO_4 were placed before the product obtained in step II was added portion-wise (2.29 g, 14 mmol). The mixture was stirred until it was dissolved (10 min). Then 97.5 mL of CPME (cyclopentyl methyl ether) and a solution of $NaNO_2$ (1.06 g, 15.3 mmol in 39 mL of H_2O) were added dropwise, before heating at 110 ° C for 5 h. After this time, the resulting yellow solution was extracted with ethyl acetate (3 x 60 mL). The extracts were combined and dried with MgSO4. Filtration and evaporation led to the desired product as a brown solid. This product was purified by chromatography on a silica column with ethyl acetate (2.2 g, 95% yield).

V:

In a 250 mL Schlenk flask, the above compound (2.53 g, 15 mmol) was placed and dissolved in dry DCM (20 mL). Et_3N (4.30 mL, 31 mmol) was added and the reaction was cooled to 0°C. Then triflic acid (3.11 mL, 18.5 mmol) was added dropwise, turning the color to dark brown. After stirring for 16 h, H_2O (60 mL) was added and extracted with ethyl acetate (3 x 80 mL). The extract was dried with $MgSO_4$, filtered and taken to dryness to yield the desired product. This product was purified by column chromatography (silica; 5: 1 petroleum ether: ethyl acetate) affording a brown oil (4.2 g, 95% yield).

VI:

The product obtained in the previous step (4.2 g, 14.2 mmol), KF (2.66 g, 45.01 mmol), PCy_3 (47 mg, 0.16 mmol), $Pd(OAc)_2$, (31 mg, 0.12 mmol) and phenyl boronic acid (2.02 g, 16.5 mol) were placed in a 500 mL ampoule, and was dissolved in dioxane (20 mL). The mixture was heated at 110 ° C for 12 h. After this time, the volatiles were evaporated and the residue was dissolved in ethyl acetate (200 mL). After filtering through celite, the brown solution was taken to dryness and purified by column chromatography (silica; 15: 1, petroleum ether: ethyl acetate) obtaining the desired product as a white solid (2.9 g, yield).

VII:

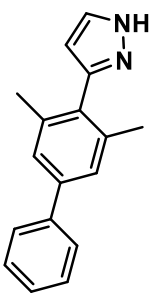
In a round bottom Schlenk flask, sodium ethoxide (1.07 g, 15.7 mmol) was weighed inside a dry box and dissolved in dry toluene (35 mL). Under N_2, the product obtained in the previous step (3.44g, 15.7 mmol) and ethyl formate (4.14 mL, 54.4 mmol) were added. The reaction was stirred for 3 h while a white solid precipitated. After this time, H_2O (100 ml) was added and the mixture was washed with Et_2O (2 x 50 mL). The aqueous phase was separated and treated with HCl until pH = 5 before organics were

extracted with Et_2O (2 x 80 mL). After drying with $MgSO_4$, the mixture was filtered and evaporated giving the desired product as a white solid (3.4 g, 86% yield).

VIII:

The product obtained in the previous step (3.75 g, 14.1 mmol) was placed to a 250 mL one-neck flask and dissolved in 75 mL of MeOH. Hydrazine monohydrate (197 µL, 14.1 mmol) was added and the mixture heated to reflux (ca 90 °C) for 12 h. The resulting yellow solution was evaporated affording a yellow solid that was crystallized from MeOH solutions at -30 °C. The pyrazole was obtained as a light yellow solid with a yield of 85%. (3 g).

Analysis calculated for $C_{17}H_{16}N_2$ (3-(3,5-dimethyl-[1,1'-biphenyl]-4-yl)-pyrazole)): C, 81.89; H, 6.87; N, 11.24 %. Found: C, 81.41; H, 6.27; N, 11.10 %.

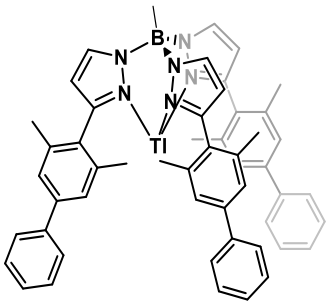


^{1}H NMR (500 MHz, $CDCl_3$) δ 2.14 (s, 6H, CH_{3Me}), 6.23 (s, 1H, CH_{pz}), 7.28 (s, 2H, CH_{arom}), 7.34 (m, 1H, CH_{arom}), 7.42 (t, 2H, $J_{H\text{-}H}$ = 8 Hz CH_{arom}), 7.56 (d, 2H, $J_{H\text{-}H}$ = 8 Hz CH_{arom}), 7.61 (s, 1H, CH_{pz}). ^{13}C{^{1}H} (125 MHz, $CDCl_3$) δ 20.6 (CH_{3Me}), 105.8 (CH_{pz}), 126.1 (CH_{arom}), 127.1 (CH_{arom}), 127.3 (CH_{arom}), 128.7 (CH_{arom}), 130.2 (C_{qarom}), 135.9 (CH_{pz}), 138.4 (C_{qarom}), 140.7 (C_{qarom}), 141.2 (C_{qarom}), 144.3 (C_{qpz}).

Step B: Synthesis of Tl(Me-Tp$^{Me2\text{-}biphen}$)

In a Schlenk tube and under nitrogen atmosphere, 3-(3,5-dimethyl-[1,1'-biphenyl]-4-yl)-pyrazole (2.5 g, 10.01 mmol) and $MeBH_3Li$ (109.2 mg, 3.06 mmol) were placed along with 10 mL of mesitylene, and the mixture was stirred for 5 h at room temperature. Since H_2 is released, the tube was connected to the gas line to release over-pressures. After that time, the mixture was heated at 180 °C for 60 h, before being cooled at 50 °C. Volatiles were removed at that temperature under reduced pressure and the residue dissolved in dry THF (20 mL). Tl(OAc) (805 mg, 3.06 mmol) was then added and the mixture stirred for 24 h at room temperature. Solid was removed by filtration, volatiles removed under reduced pressure and the resulting white solid was washed with MeOH (4 x 30 mL) to remove excess of pyrazole. Tl(Me-Tp$^{Me2\text{-}biphen}$) was obtained as a white solid in 90% yield.

Analysis calculated for $C_{17}H_{16}BrN_2$: C, 64.24; H, 4.98; N, 8.64 %. Found: C, 64.15; H, 5.01; N, 8.54 %.

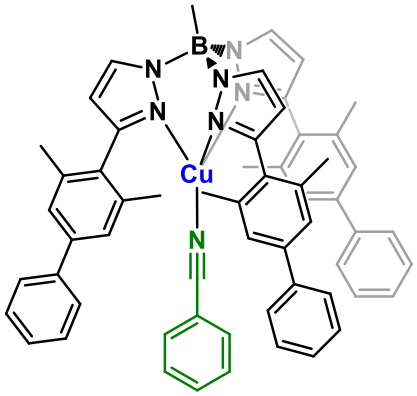


^{1}H NMR (500 MHz, $CDCl_3$) δ 1.20 (s, 3H, C*H*$_{3BMe}$), 2.01 (s, 18H, C*H*$_{3Me}$), 6.12 (d, 3H, $J_{H\text{-}H}$ = 2 Hz C*H*$_{pz}$), 7.25 (s, 6H, C*H*$_{arom}$), 7.29 (t, 3H, t, 3H, $J_{H\text{-}H}$ = 8 Hz C*H*$_{arom}$), 7.38 (t, 6H, $J_{H\text{-}H}$ = 8 Hz C*H*$_{arom}$), 7.57 (d, 6H, $J_{H\text{-}H}$ = 8 Hz C*H*$_{arom}$), 7.90 (d, 3H, $J_{H\text{-}H}$ = 2 Hz C*H*$_{pz}$). ^{13}C{^{1}H} (125 MHz, $CDCl_3$) δ 20.8 (*C*H$_{3Me}$), 104.6 (*C*H$_{pz}$), 125.9 (*C*H$_{arom}$), 126.9 (*C*H$_{arom}$), 127.2 (*C*H$_{arom}$), 128.6 (*C*H$_{arom}$), 132.9 (*C*$_{qarom}$), 133.4 (*C*H$_{pz}$), 137.9 (*C*$_{qarom}$), 140.4 (*C*$_{qarom}$), 140.7 (*C*$_{qarom}$), 149.75 (*C*$_{qpz}$). ^{11}B{^{1}H} (160 MHz, $CDCl_3$) δ 0.05 (*B*-Me).

Step C: Synthesis of Me-Tp$^{Me2\text{-}biphen}$Cu(NCPh) (4).

In a Schlenk tube, Tl(Me-Tp$^{Me2\text{-}biphen}$) (0.49 g, 0.5 mmol) was dissolved in 15 mL of dichloromethane, then four equivalents of benzonitrile (206 µL, 2 mmol) were added. CuCl (0.049 g, 0.5 mmol) was added to the mixture which was stirred for 12 h at room temperature. The yellow solution was filtered through celite, under nitrogen, and the volatiles were removed. The resulting solid was washed with hexane (2 x 5 mL) to give complex **4** as a yellow solid with in 92% yield.

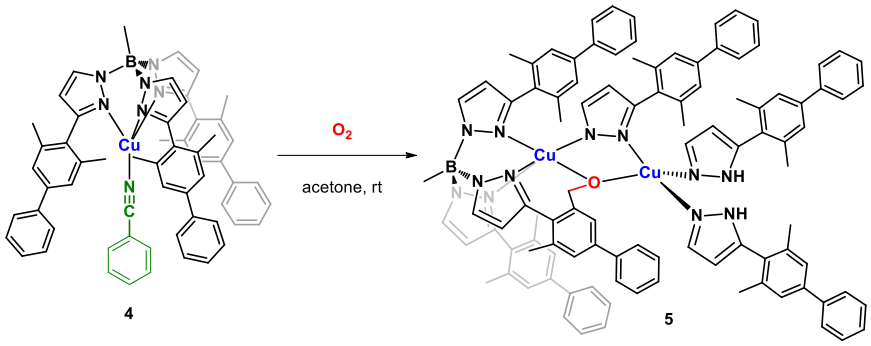
Analysis calculated for $C_{59}H_{53}BCuN_7$ (**4**): C, 75.83; H, 5.75; N, 10.49 %. Found: C, 75.60; H, 5.64; N, 40.42 %.



4

^{1}H NMR (500 MHz, $CDCl_3$) δ 1.05 (s, 3H, C*H*$_{3BMe}$), 2.28 (s, 18H, C*H*$_{3Me}$), 6.10 (m, 3H, C*H*$_{pz}$), 6.26 (t, 2H, *J* = 7 Hz, C*H*$_{bznit}$), 6.53 (d, 2H, *J* = 7 Hz , C*H*$_{bznit}$), 6.62 (t, 1H, *J* = 7 Hz, C*H*$_{bznit}$), 7.05 (m, 6H, C*H*$_{arom}$), 7.16 (m, 9H, C*H*$_{arom}$), 7.17 (s, 6H, C*H*$_{arom}$), 7.70 (m, 3H, C*H*$_{pz}$). ^{13}C{^{1}H} (125 MHz, $CDCl_3$) δ 21.9 (*C*H$_{3Me}$), 104.0 (*C*H$_{pz}$), 125.2 (*C*H$_{arom}$), 126.7 (*C*H$_{arom}$), 127.0 (*C*H$_{arom}$), 128.3 (*C*H$_{arom}$), 131.1 (*C*H$_{bznit}$), 131.6 (*C*H$_{bznit}$), 131.9 (*C*H$_{bznit}$), 132.2 (*C*$_{qarom}$), 134.4 (*C*H$_{pz}$), 138.7 (*C*$_{qarom}$), 139.6 (*C*$_{qarom}$), 140.9 (*C*$_{qarom}$), 149.5 (*C*$_{qpz}$).^{11}B{^{1}H} (160 MHz, $CDCl_3$) δ -0.927 (*B*-Me).

4. Generation of complex 5.

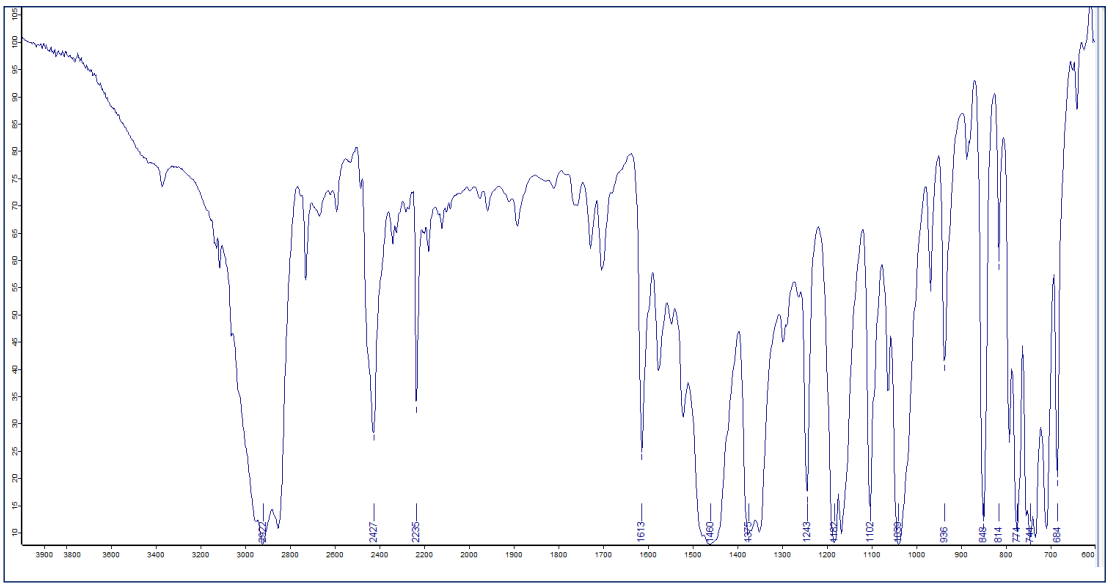


4 5

Complex **4** (0.1 g, 0.107 mmol) was dissolved in oxygenated acetone (upon bubbling O_2 for one hour through 5 mL, and maintaining volume constant). The mixture was left undisturbed, and after two weeks green crystals deposited, some of them suitable for X-Ray studies. Yield = 13%.

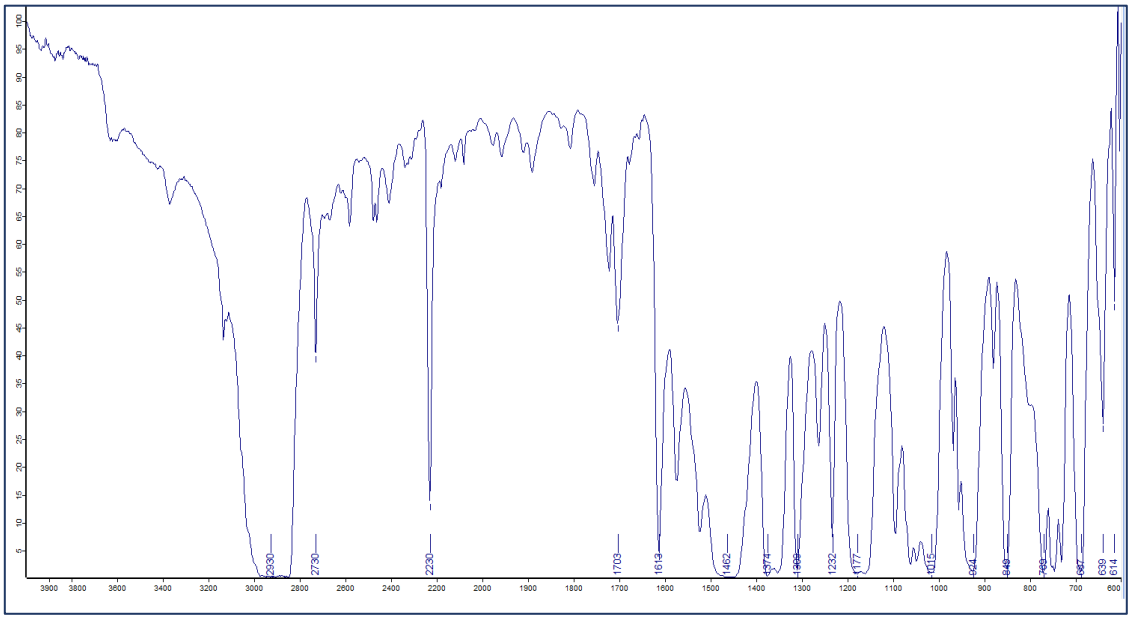
5. IR Spectra.

1a (nujol)



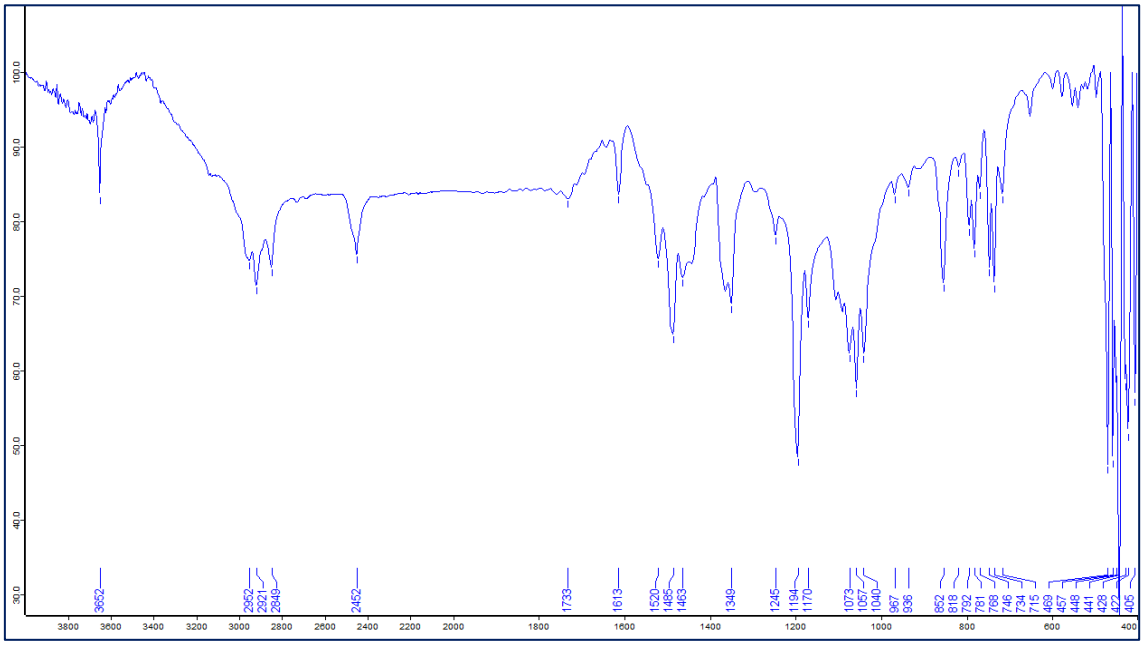
$\nu(CN)$ =2235 cm^{-1}.

1b (nujol)



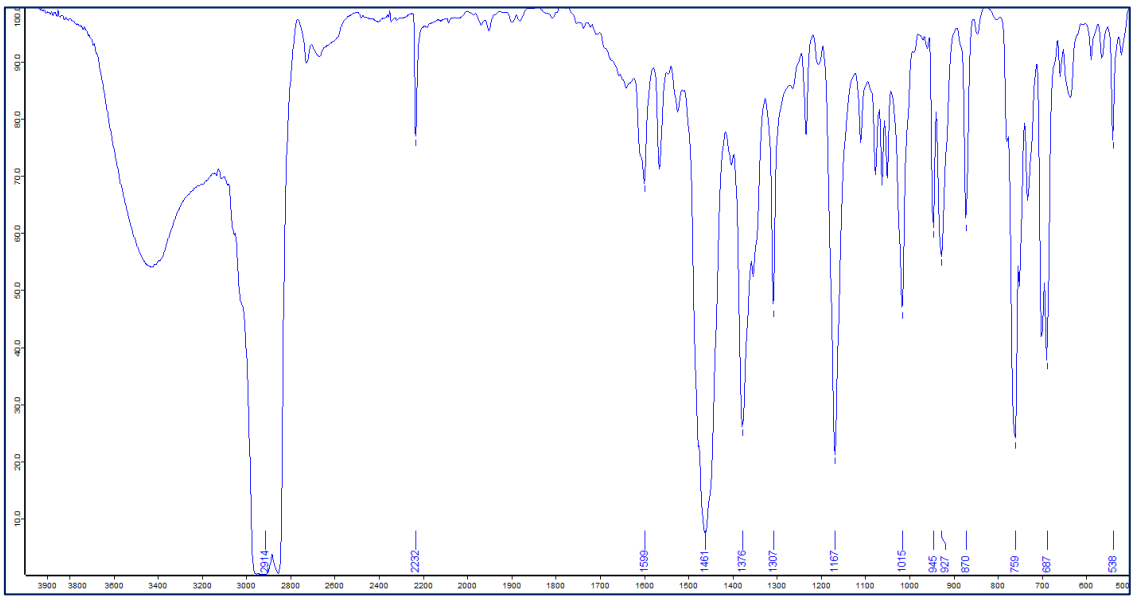
$\nu(CN)$ =2230 cm^{-1}

2a (KBr)



$\nu(BH)$ =2452 cm^{-1} ; $\nu(OH)$ =3652 cm^{-1}

4 (nujol)

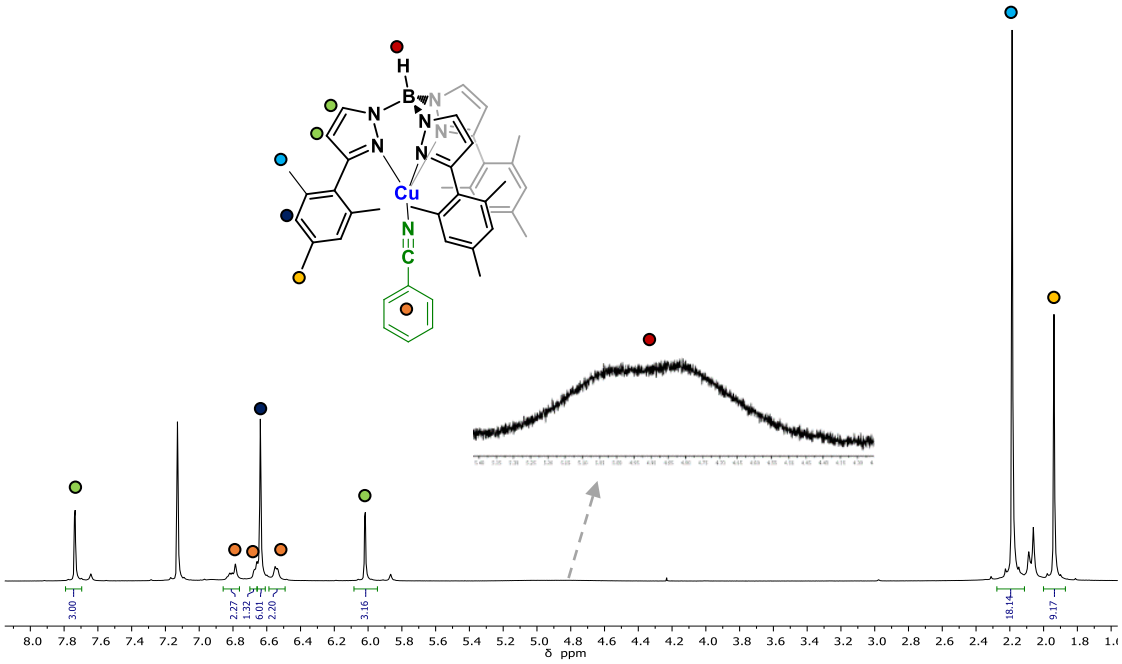


$\nu(CN)$ = 2232 cm^{-1}.

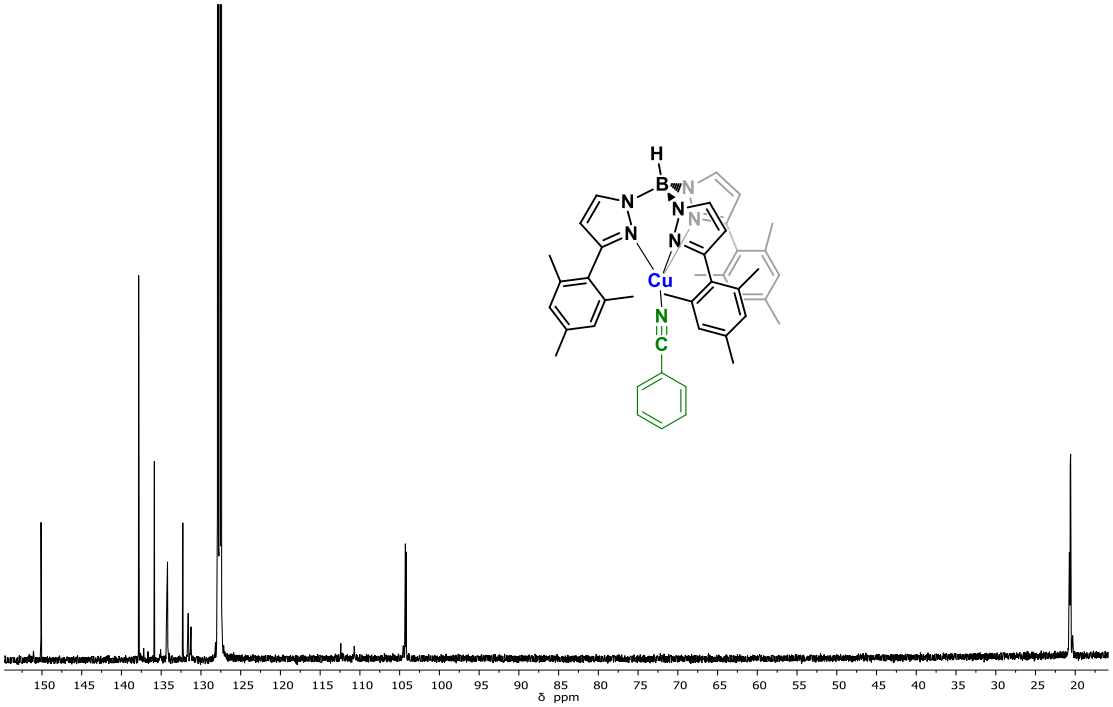
6. NMR Spectra for Product Characterization.

Complex $Tp^{Ms}Cu(NCPh)$ (1a)

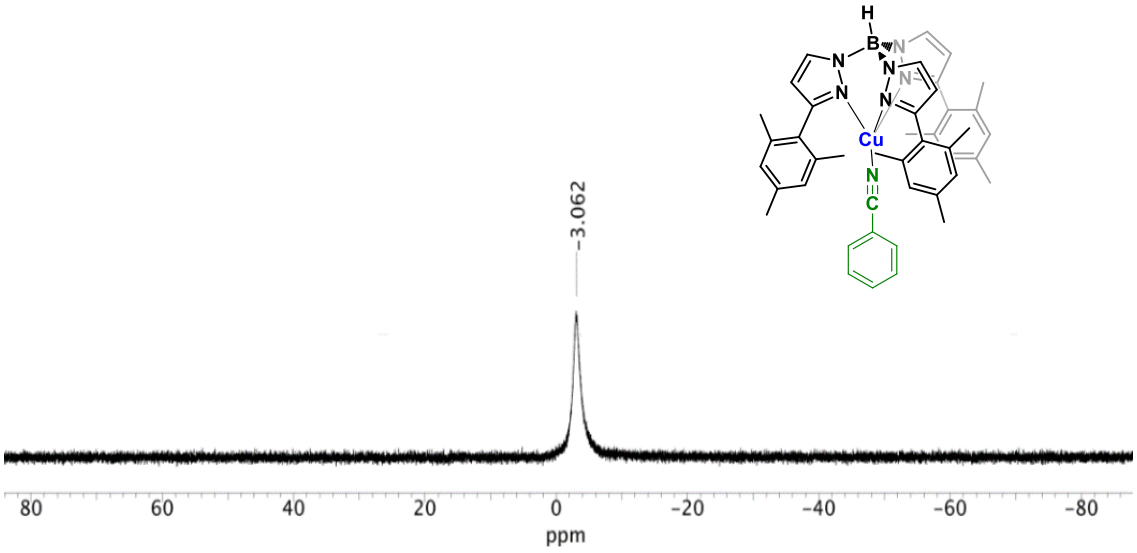
^{1}H NMR (500 MHz, C_6D_6)



$^{13}C\{^{1}H\}$ NMR (125 MHz, C_6D_6)

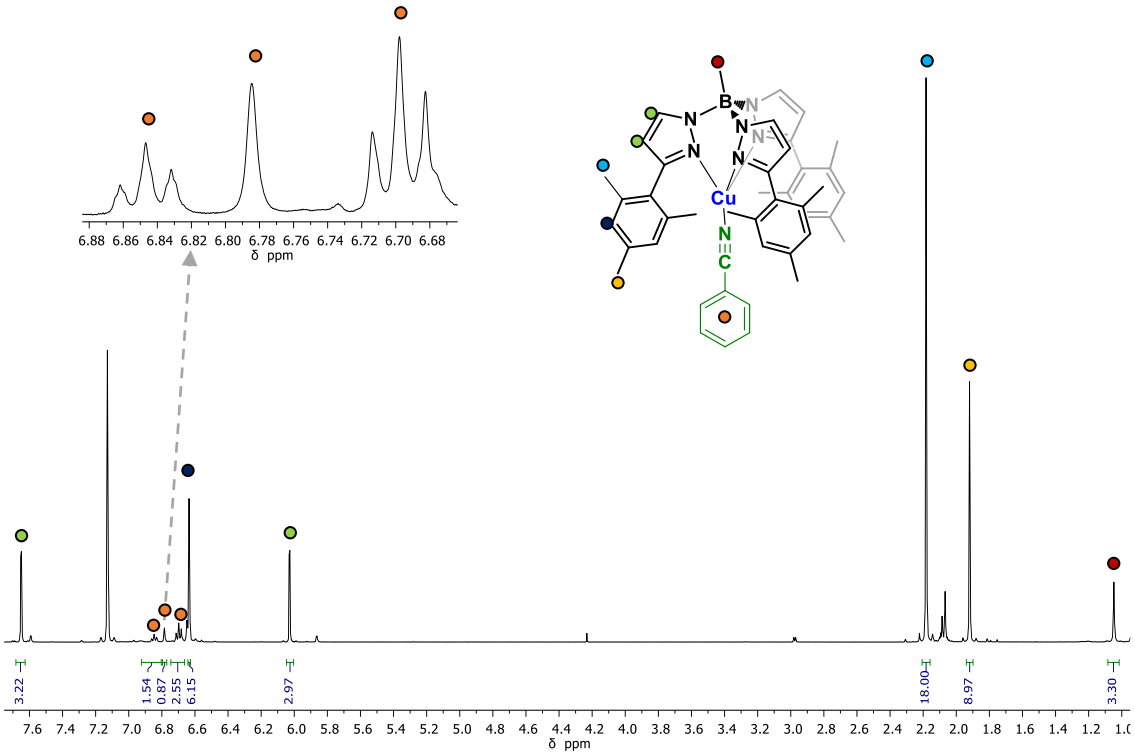


$^{11}B\{^{1}H\}$ NMR (160 MHz, C_6D_6)

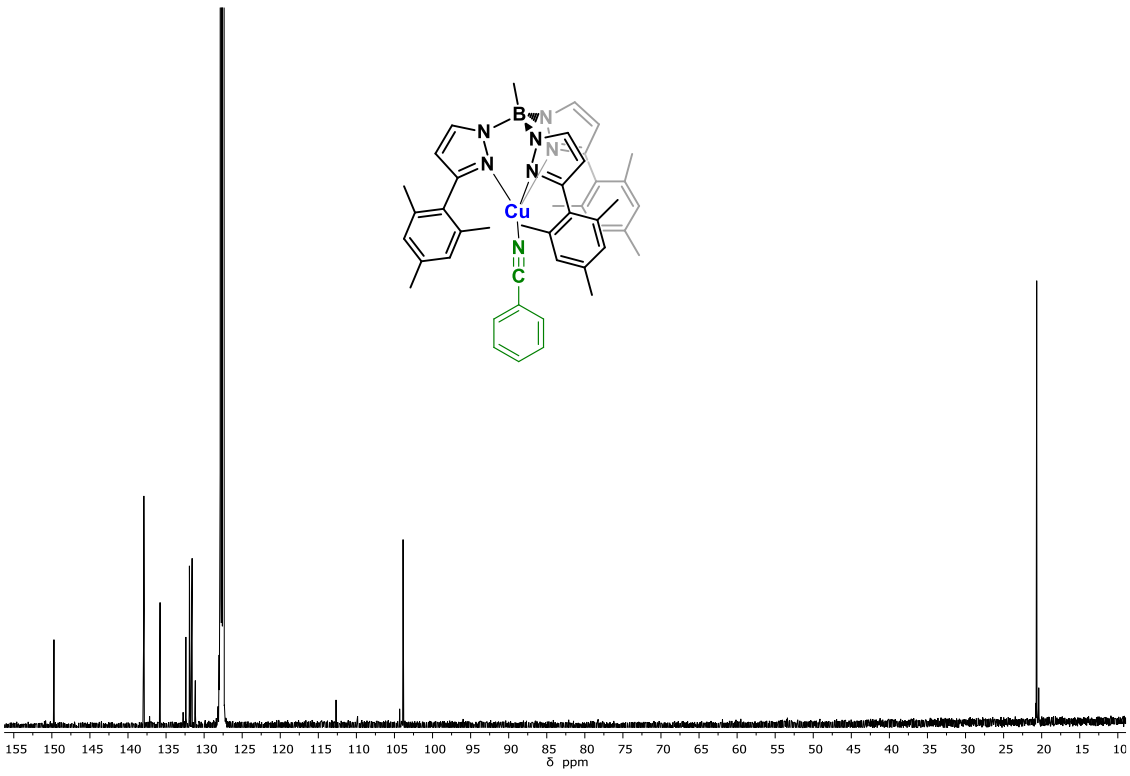


Complex Me-Tp^{Ms}Cu(NCPh) (1b)

^{1}H NMR (500 MHz, C_6D_6)

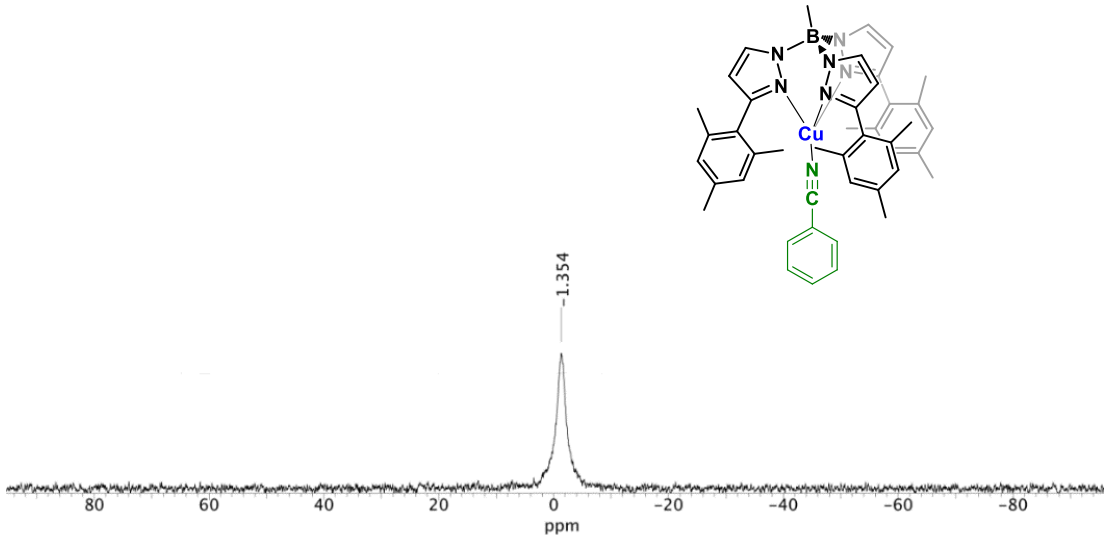


$^{13}C\{^{1}H\}$ NMR (125 MHz, C_6D_6)



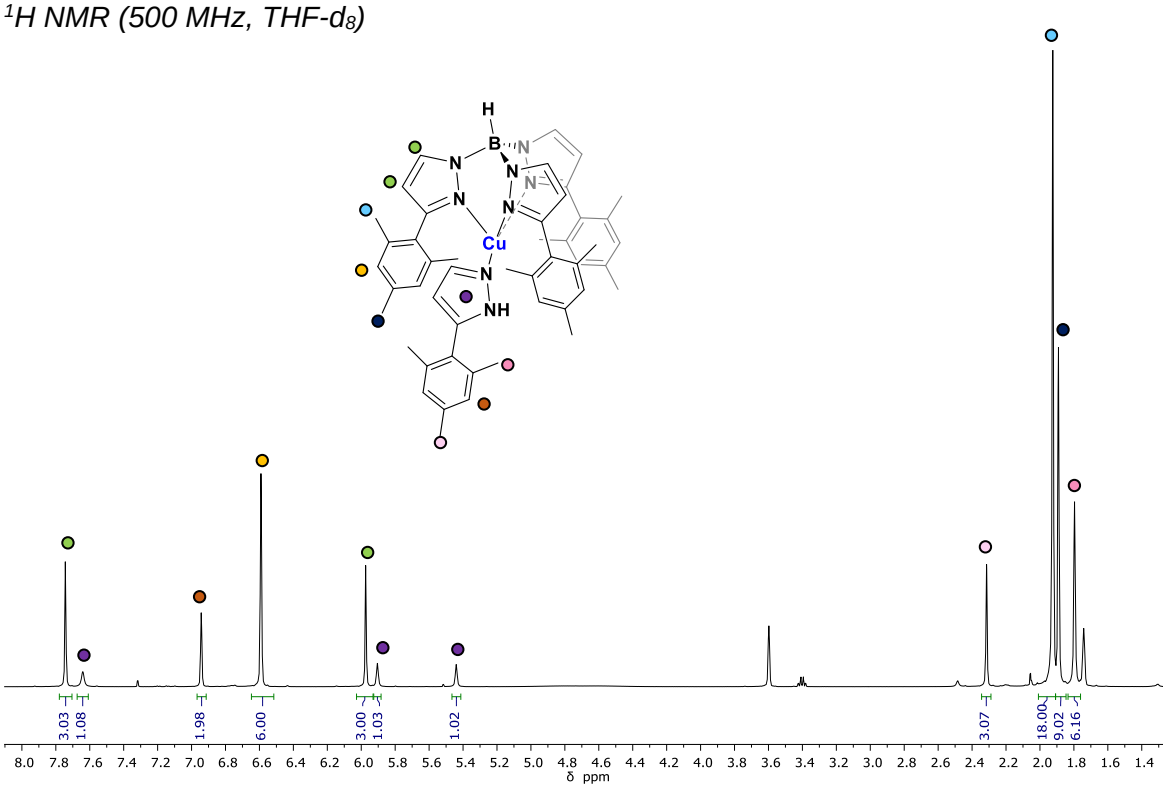
δ ppm

$^{11}B\{^{1}H\}$ NMR (160 MHz, C_6D_6)

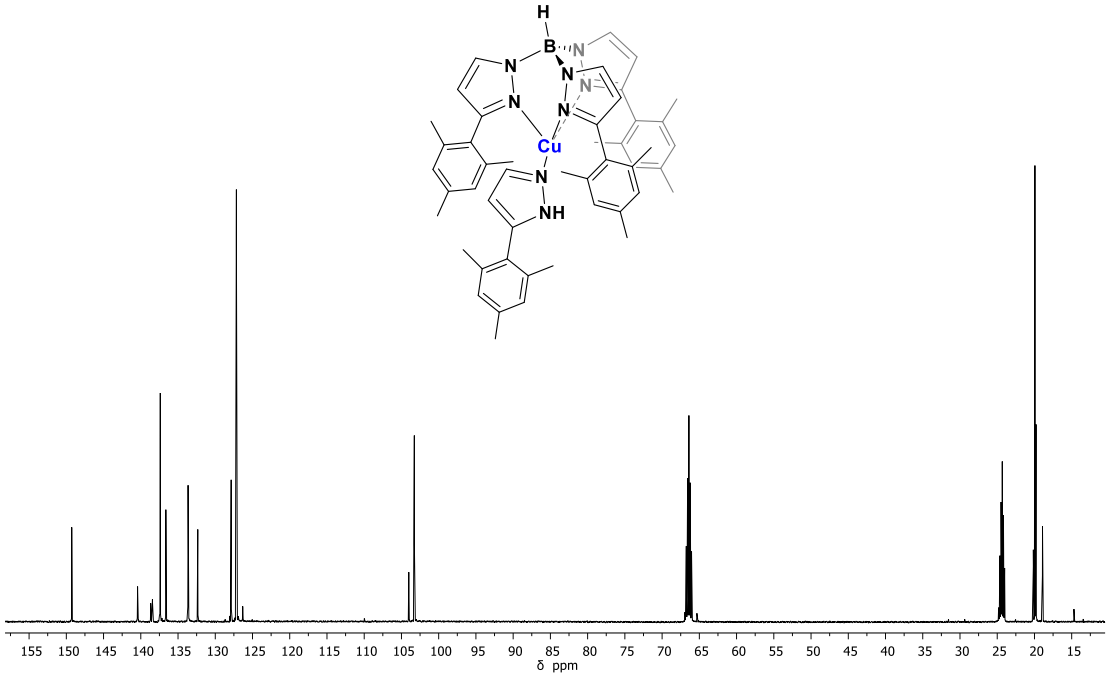


Complex $Tp^{Ms}Cu(Hpz^{Ms})$ (3a)

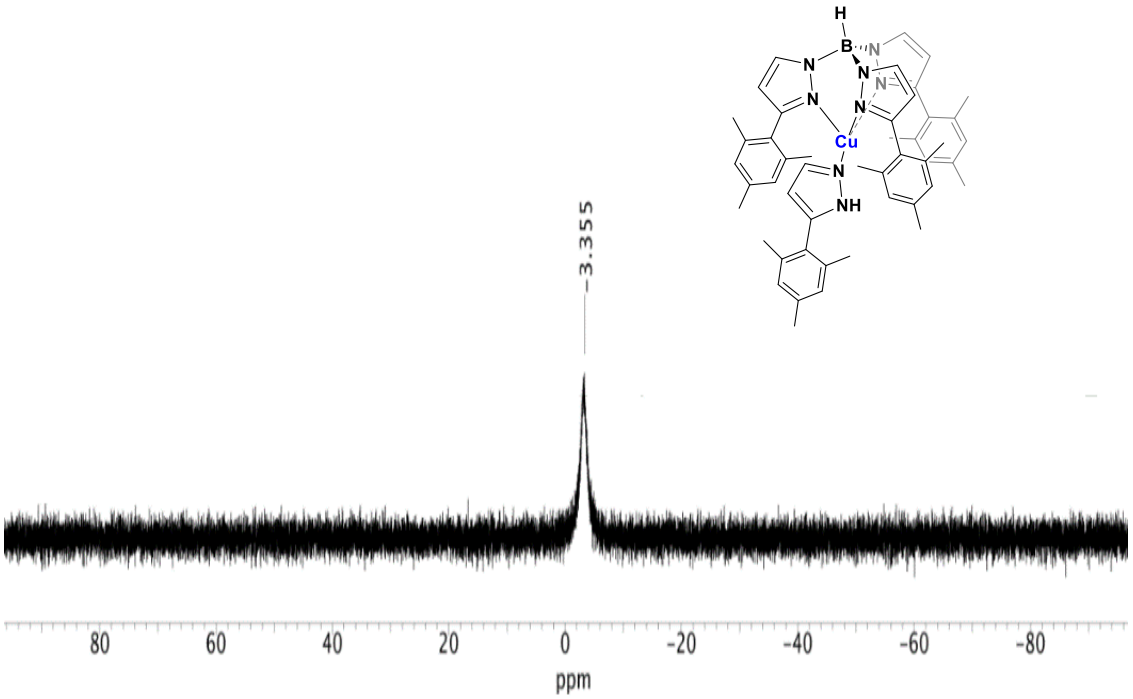
^{1}H NMR (500 MHz, THF-d_8)



$^{13}C\{^{1}H\}$ NMR (125 MHz, THF-d_8)

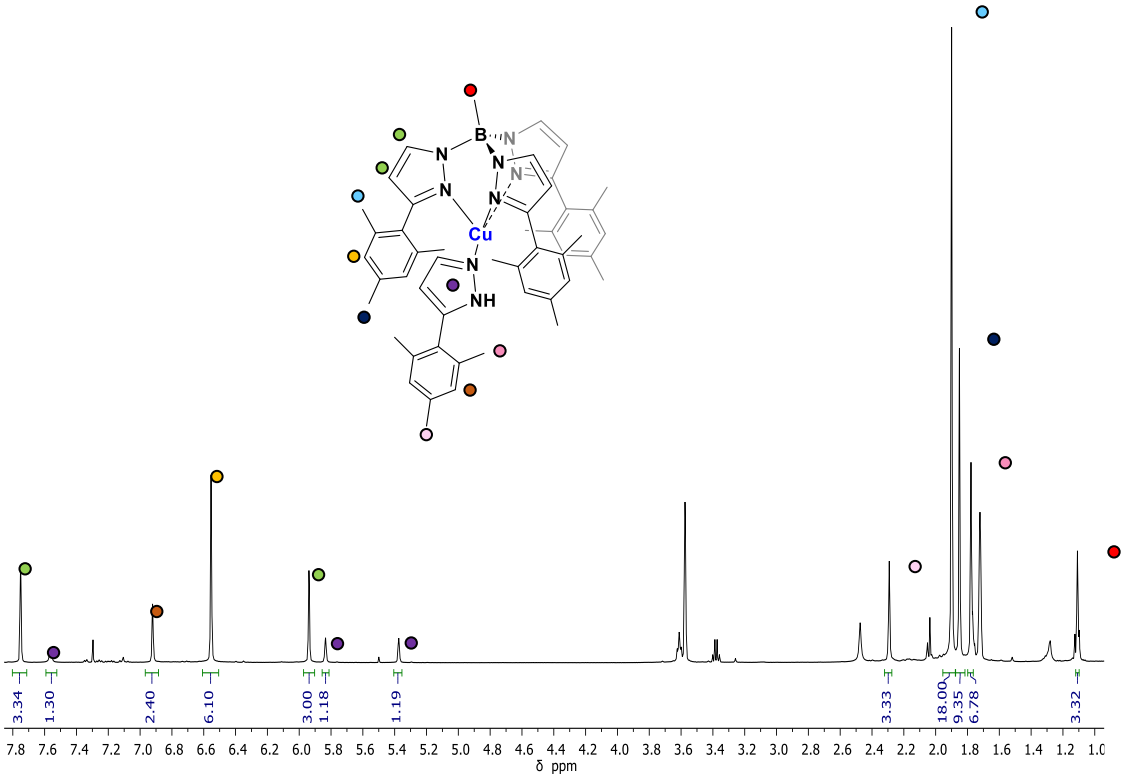


$^{11}B\{^{1}H\}$ NMR (160 MHz, THF-d_8)

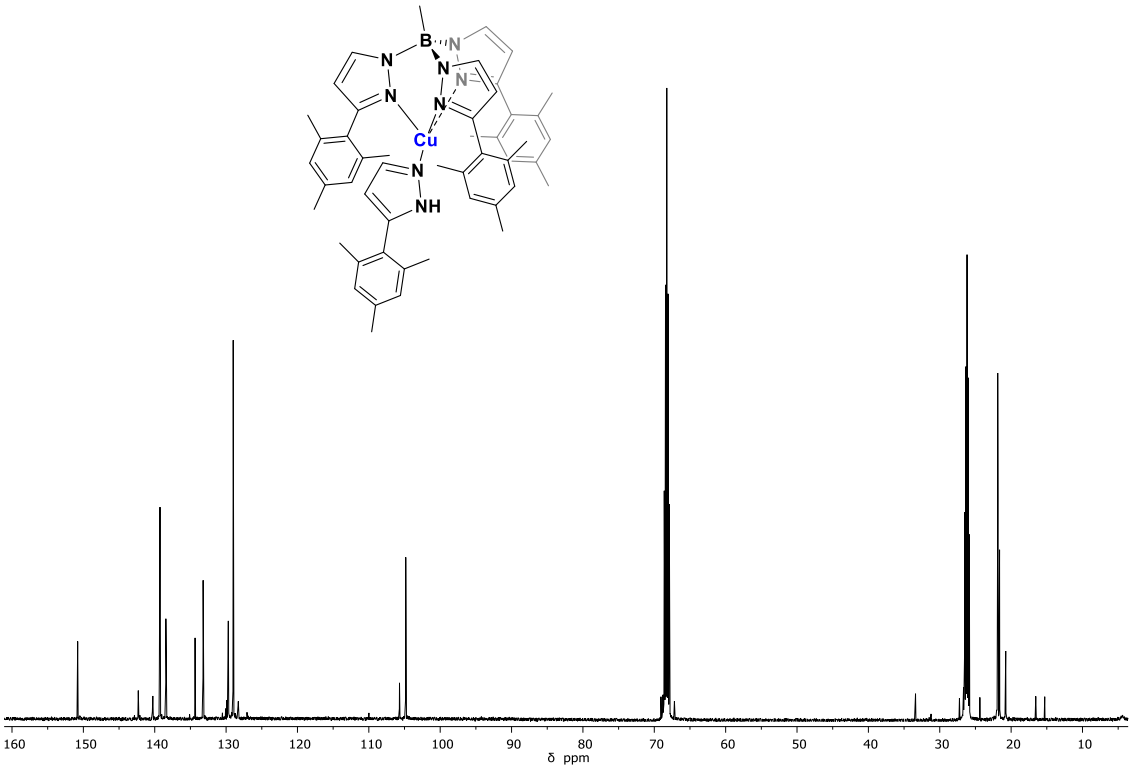


Complex Me-Tp^{Ms}Cu(Hpz^{Ms}) (3b)

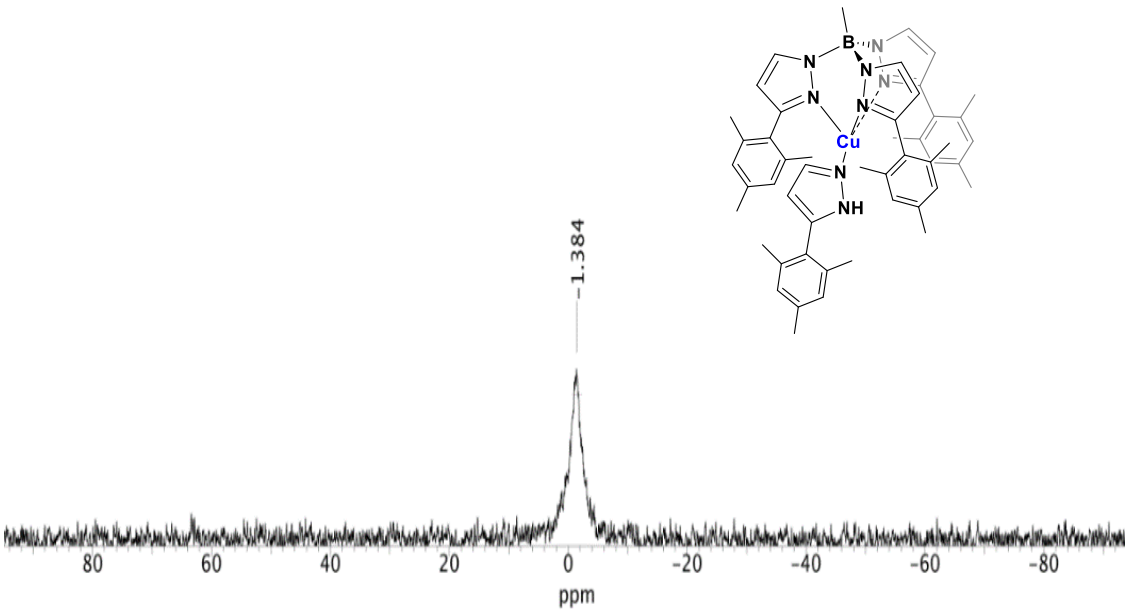
^{1}H NMR (500 MHz, THF-d_8)



^{13}C{^{1}H} NMR (125 MHz, THF-d_8)

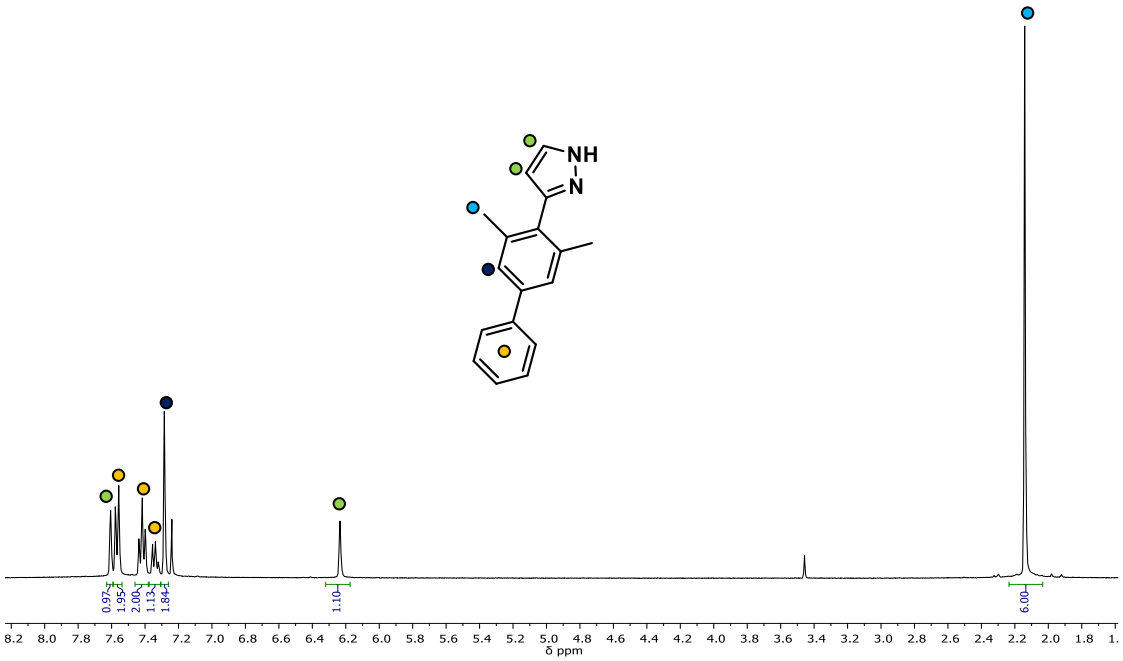


$^{11}B\{^{1}H\}$ NMR (160 MHz, THF-d_8)

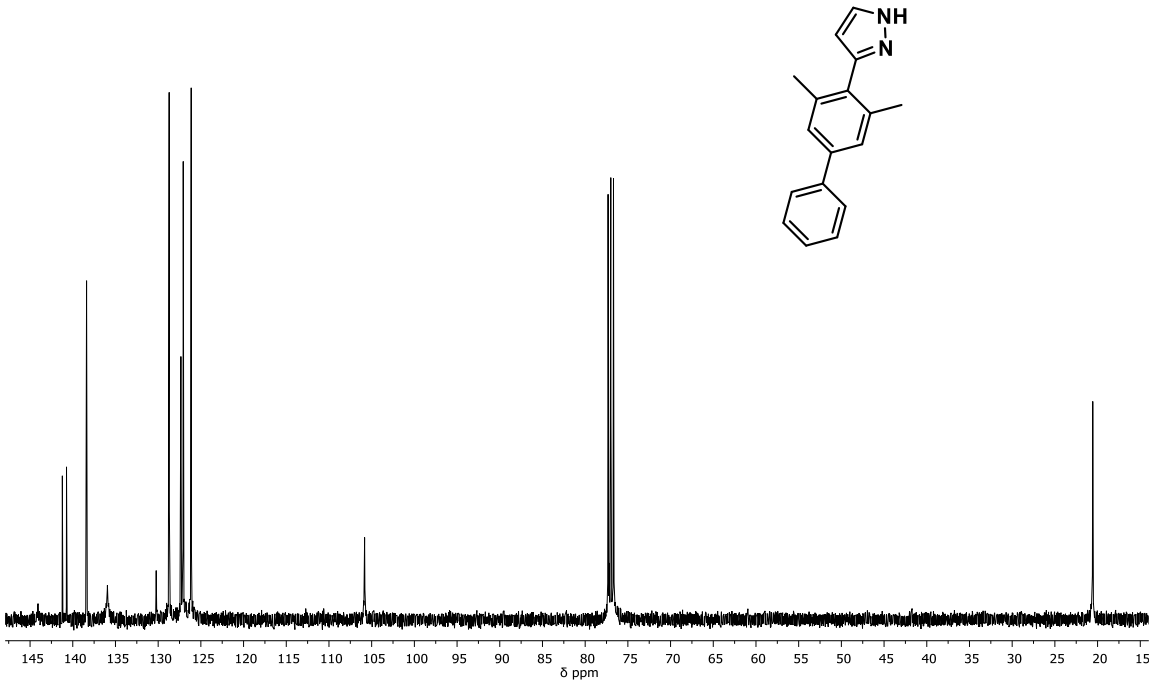


3-(3,5-dimethyl-[1,1'-biphenyl]-4-yl)-pyrazole)

^{1}H NMR (500 MHz, $CDCl_3$)

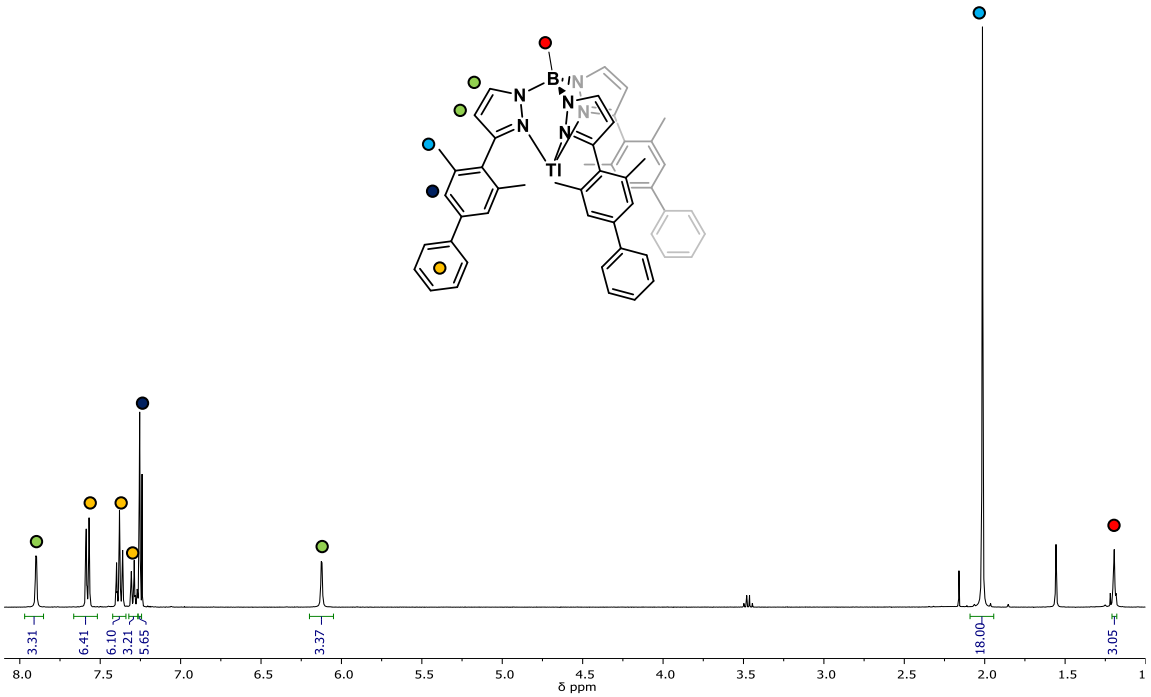


$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$)

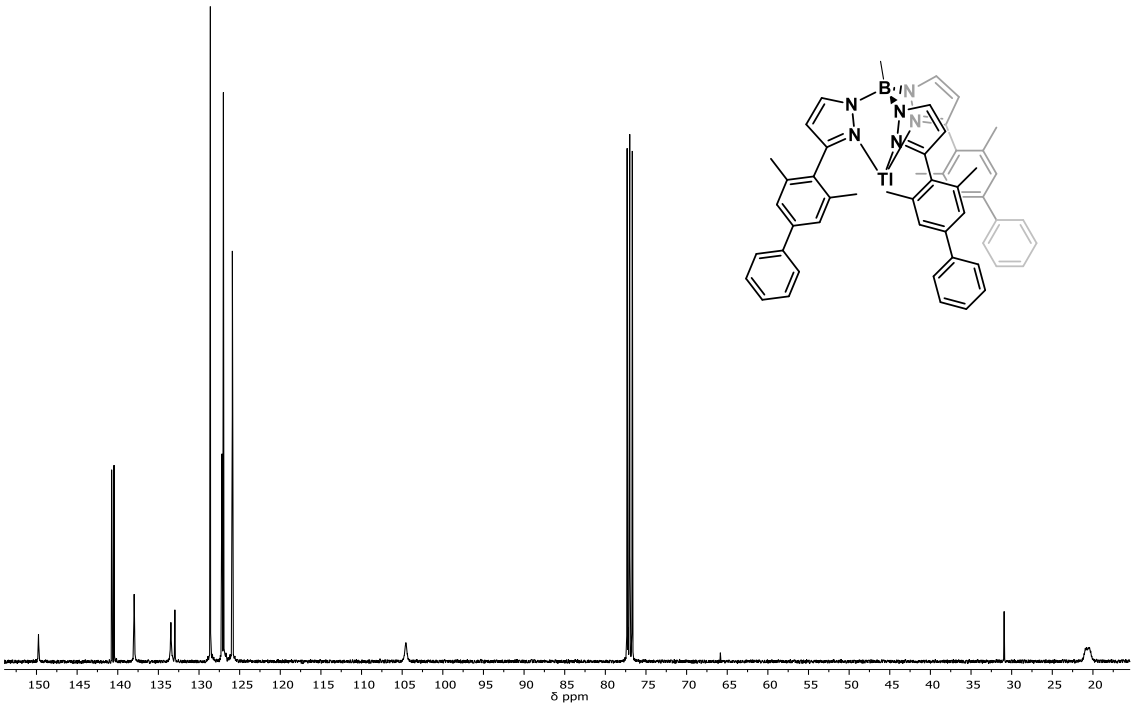


Complex Tl(Me-Tp$^{Me2\text{-}biphen}$)

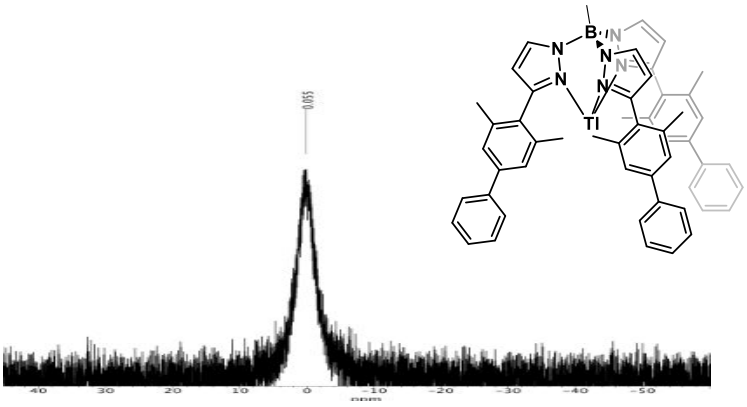
^{1}H NMR (500 MHz, $CDCl_3$)



^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$)

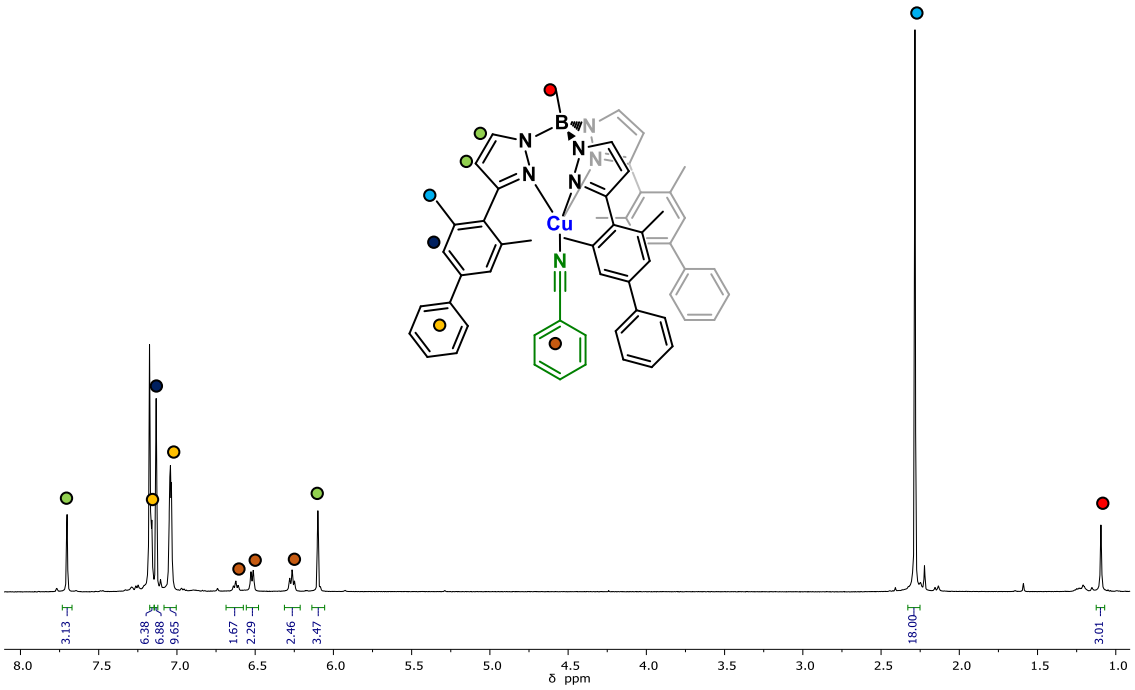


$^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$)

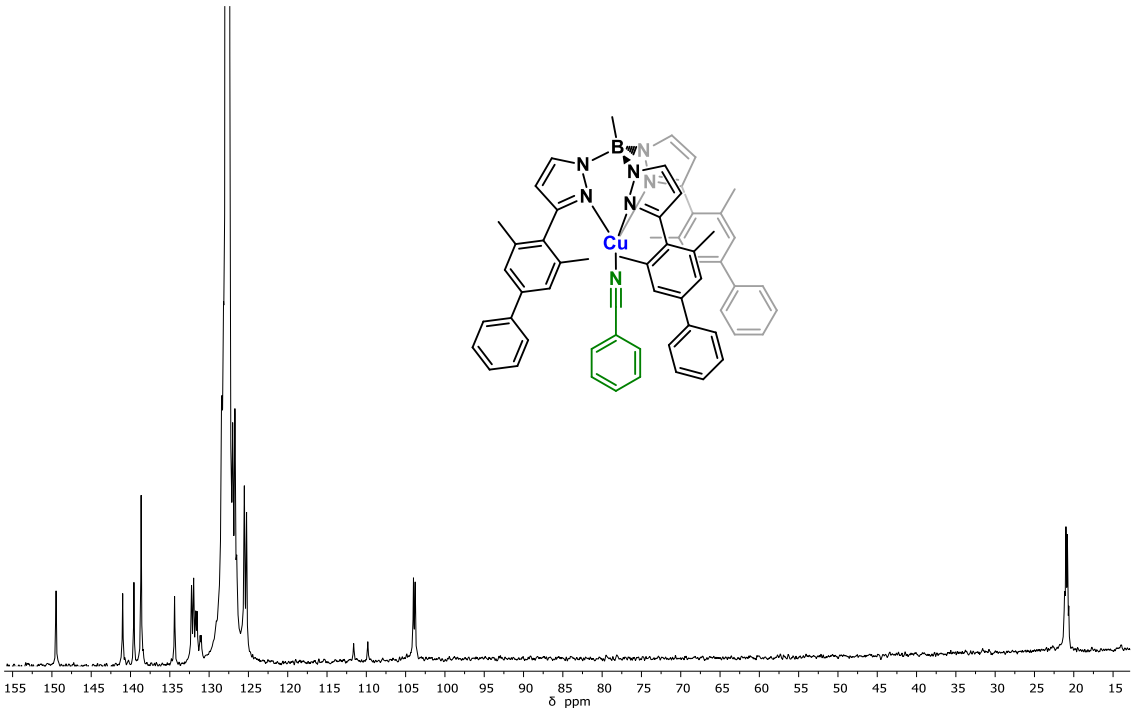


Complex Me-Tp$^{Me2\text{-}biphen}$Cu(NCPh) (4)

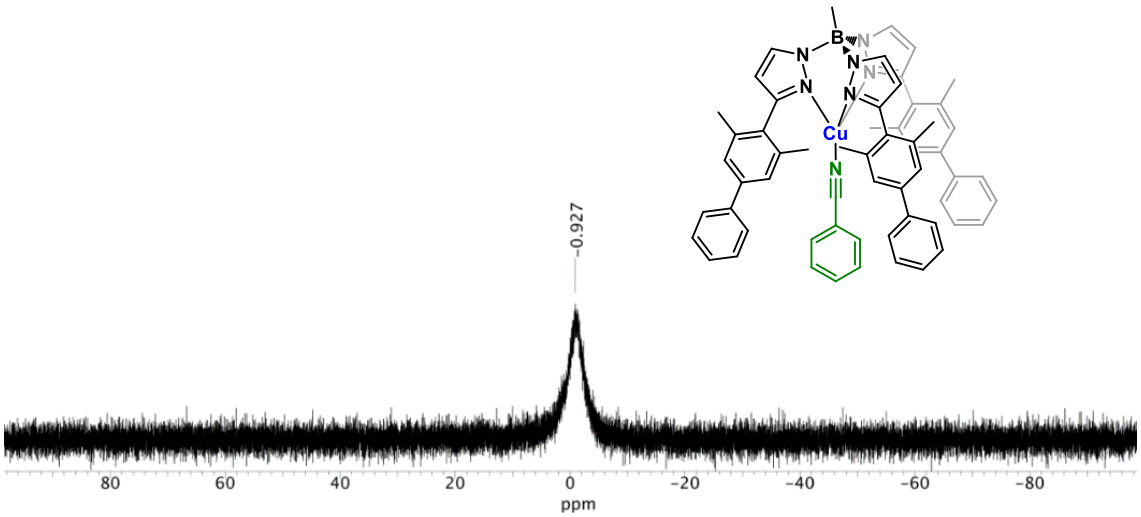
^{1}H NMR (500 MHz, C_6D_6)



^{13}C{^{1}H} NMR (125 MHz, C_6D_6)



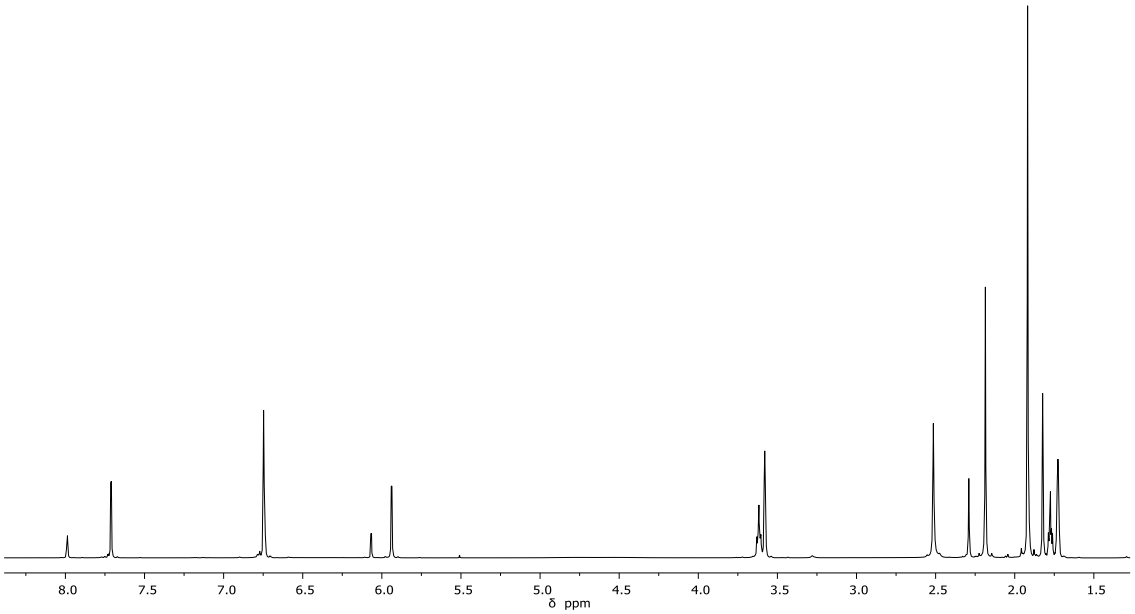
$^{11}B\{^{1}H\}$ NMR (160 MHz, C_6D_6)



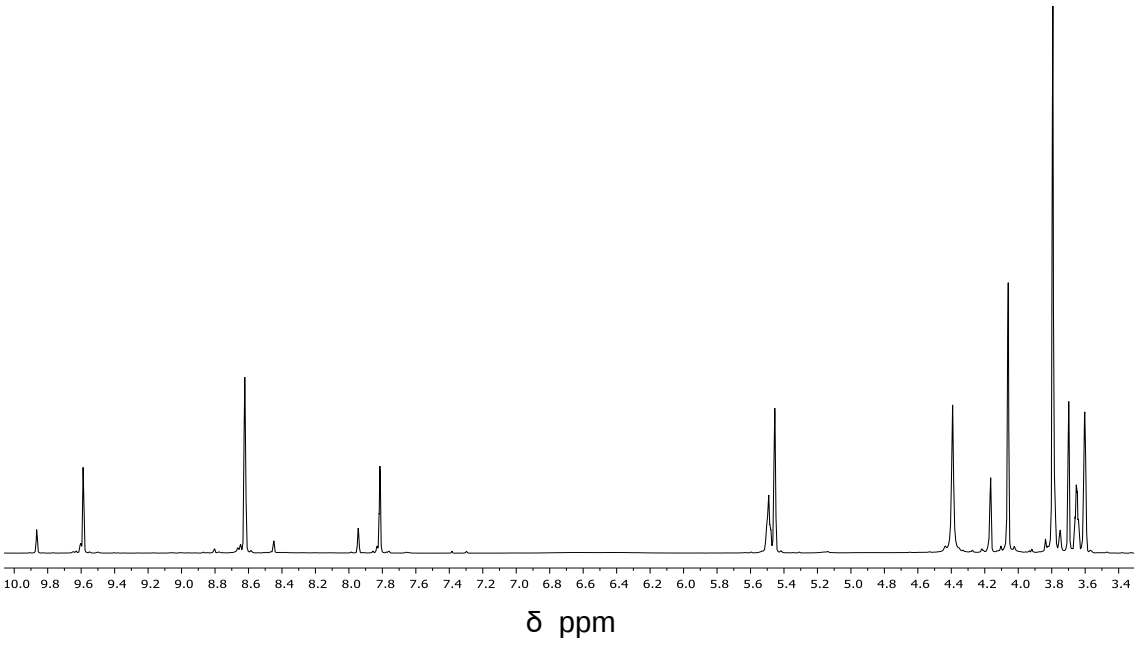
7. NMR monitoring of the reactions leading to complexes 2a and 2b.

$Tp^{Ms}Cu(THF)$ (15 mg, 0.021 mmol) was dissolved in 0.6 mL de THF-d_8 (oxygenated), and the sample was monitored for one week by ^1H NMR spectroscopy.

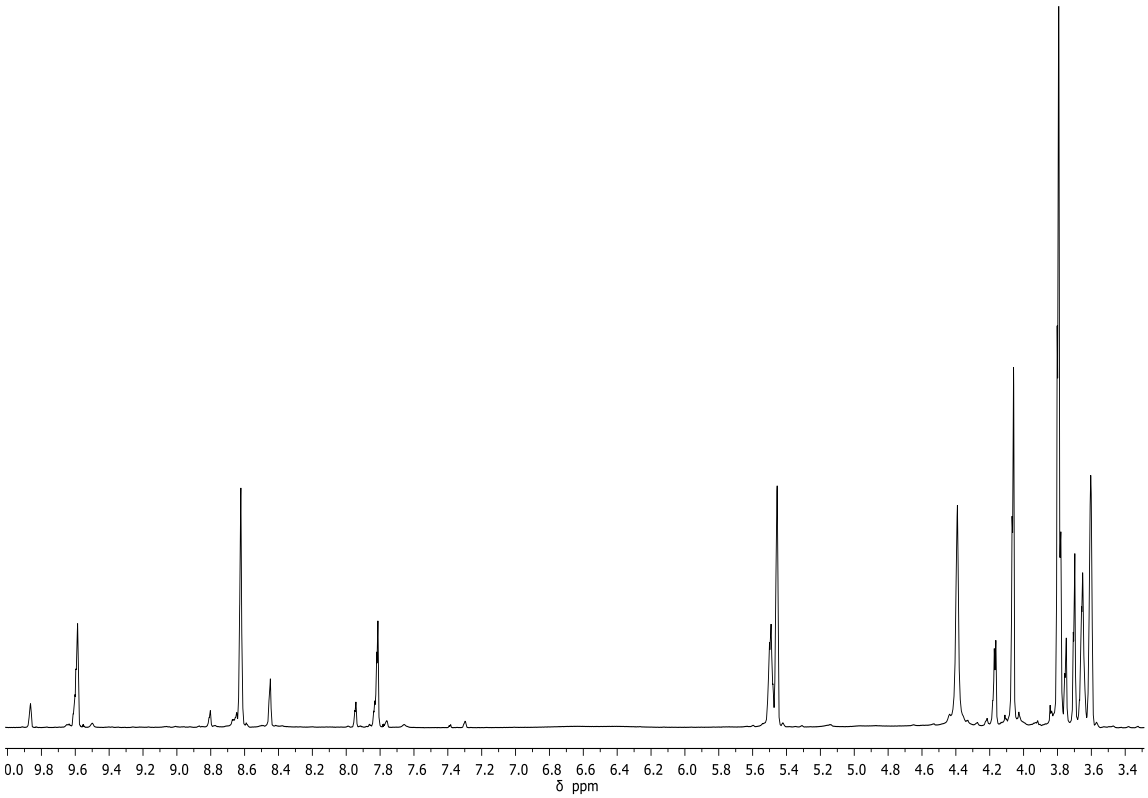
t = 5 min (500 MHz,THF-d_8).



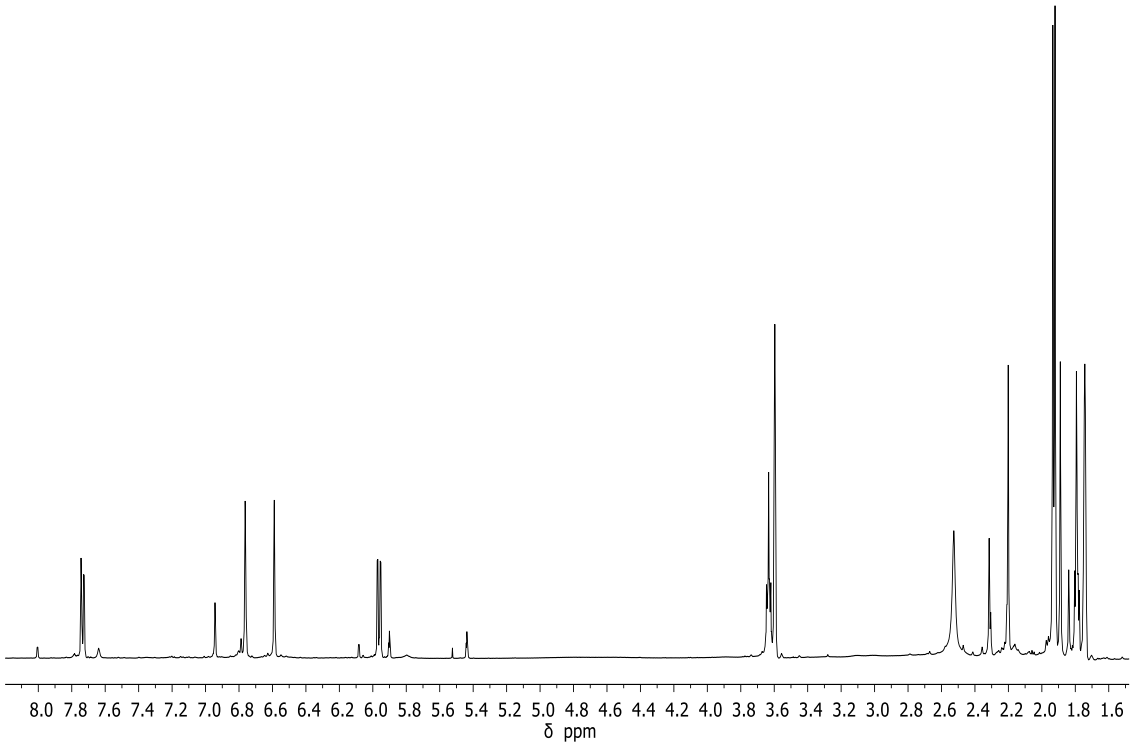
t = 32 h (500 MHz,THF-d_8)



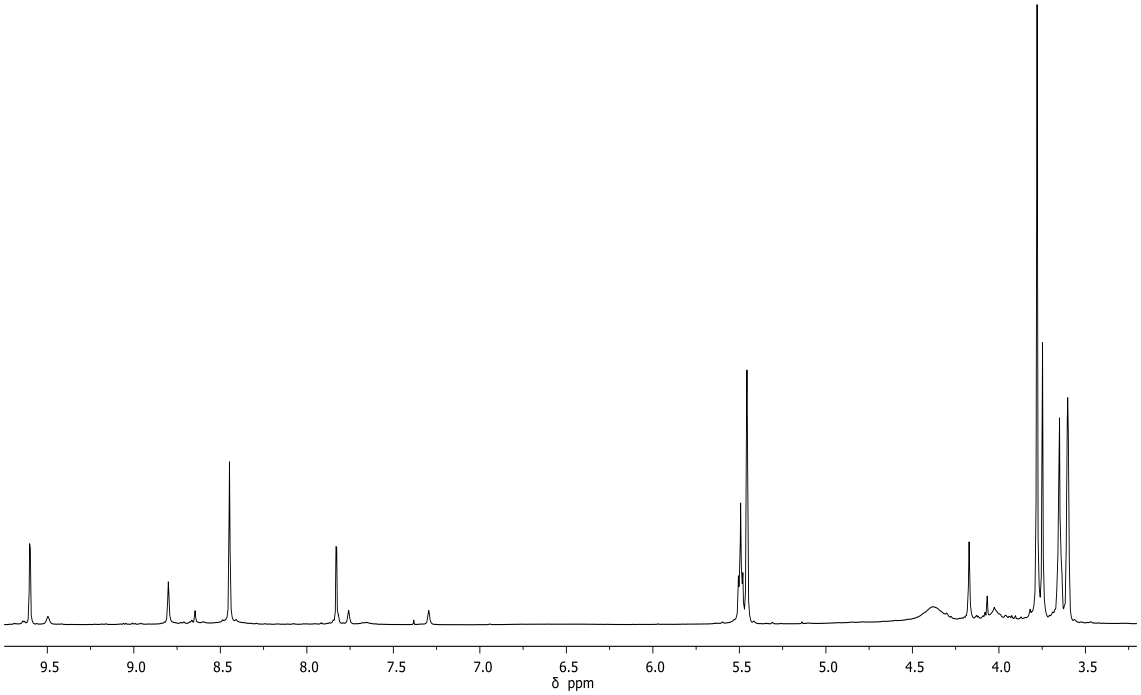
t = 72 h (500 MHz,THF-d_8).



t = 96 h (500 MHz,THF-d_8).

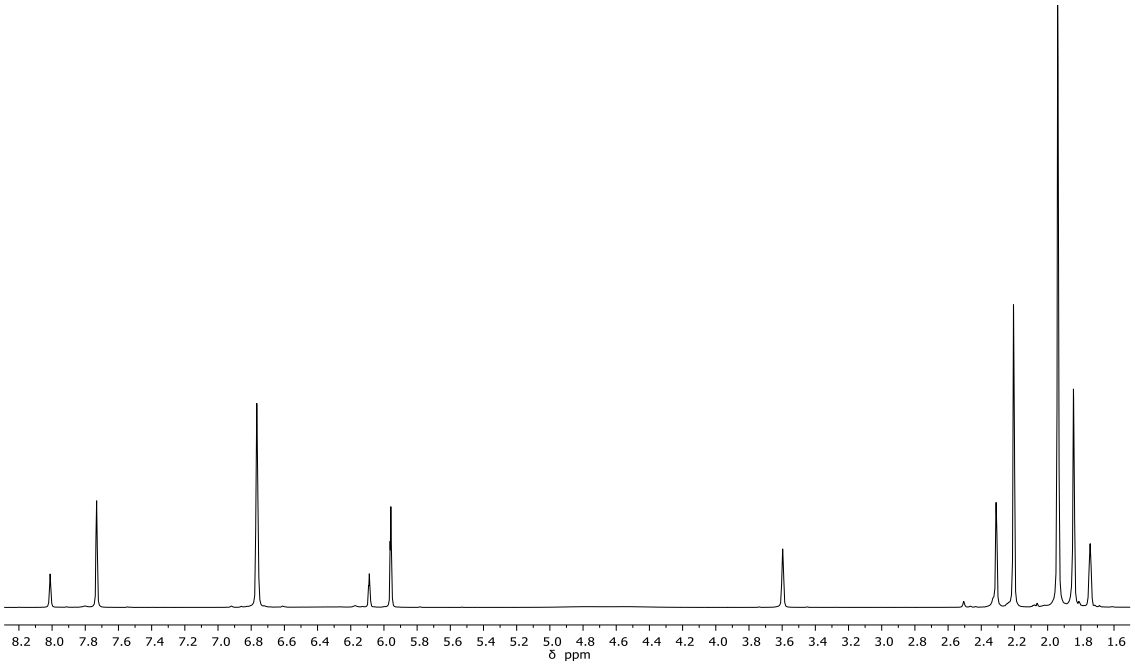


t = 6 days (500 MHz,THF-d_8).

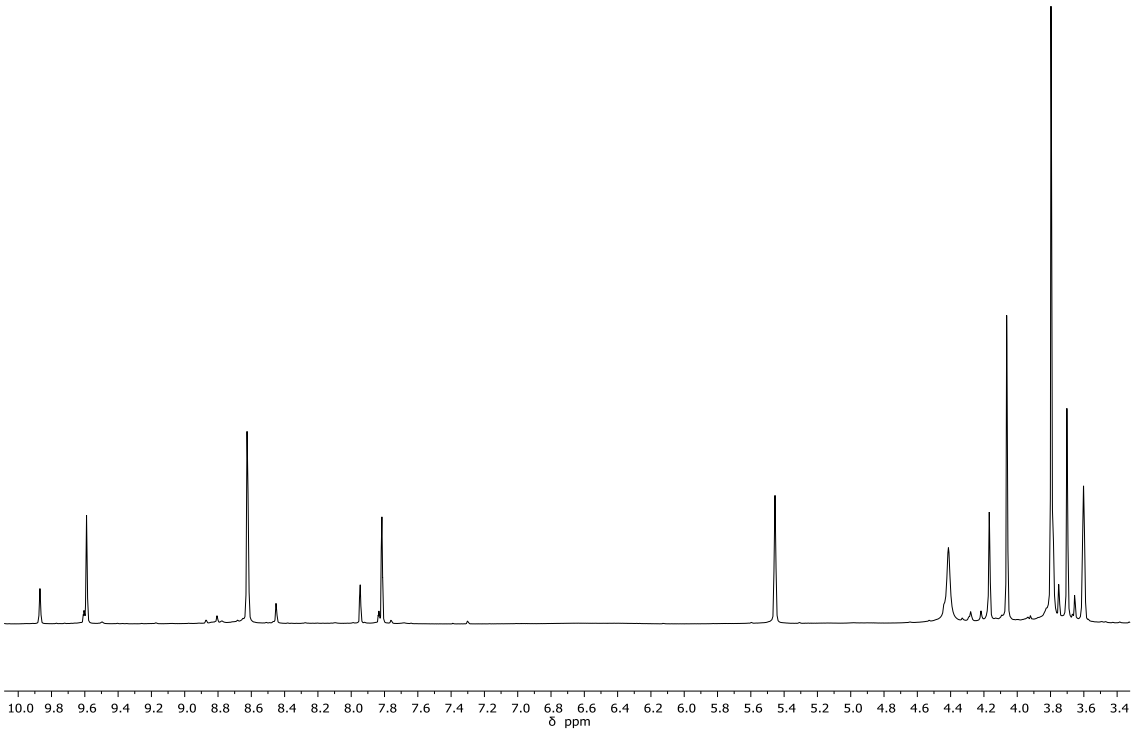


A second experiment was carried out starting from the dinuclear complex $[Tp^{Ms}Cu]_2$ (15 mg, 0.012 mmol) in 0.6 mL of THF-d_8.

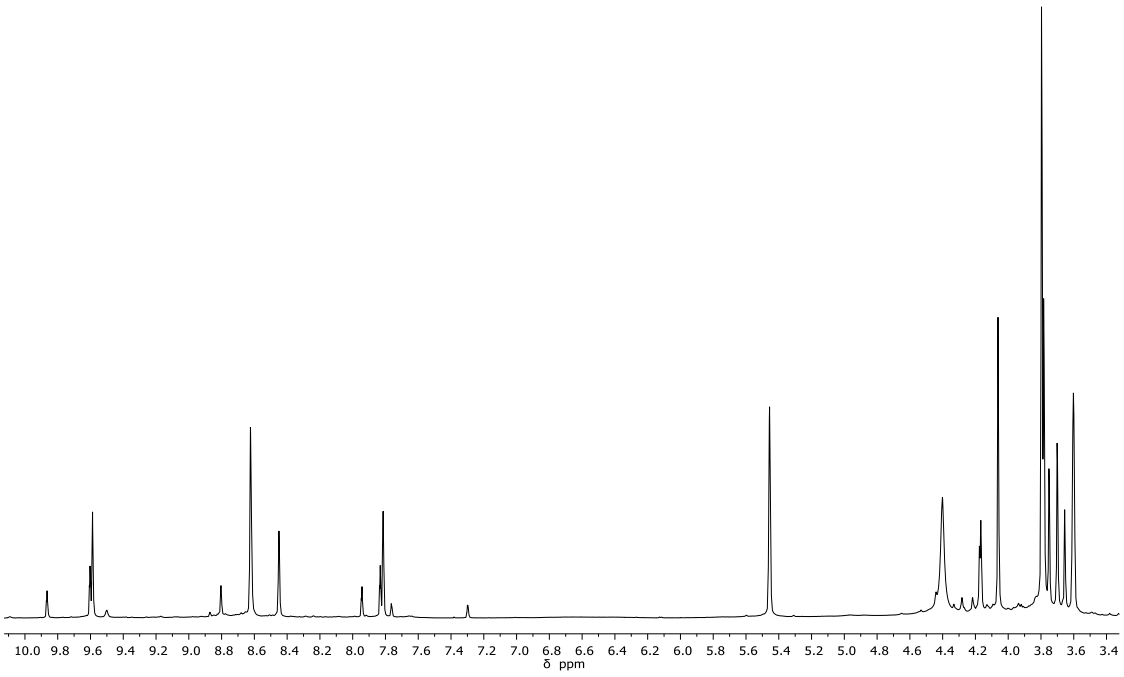
t = 5 min (500 MHz,THF-d_8).



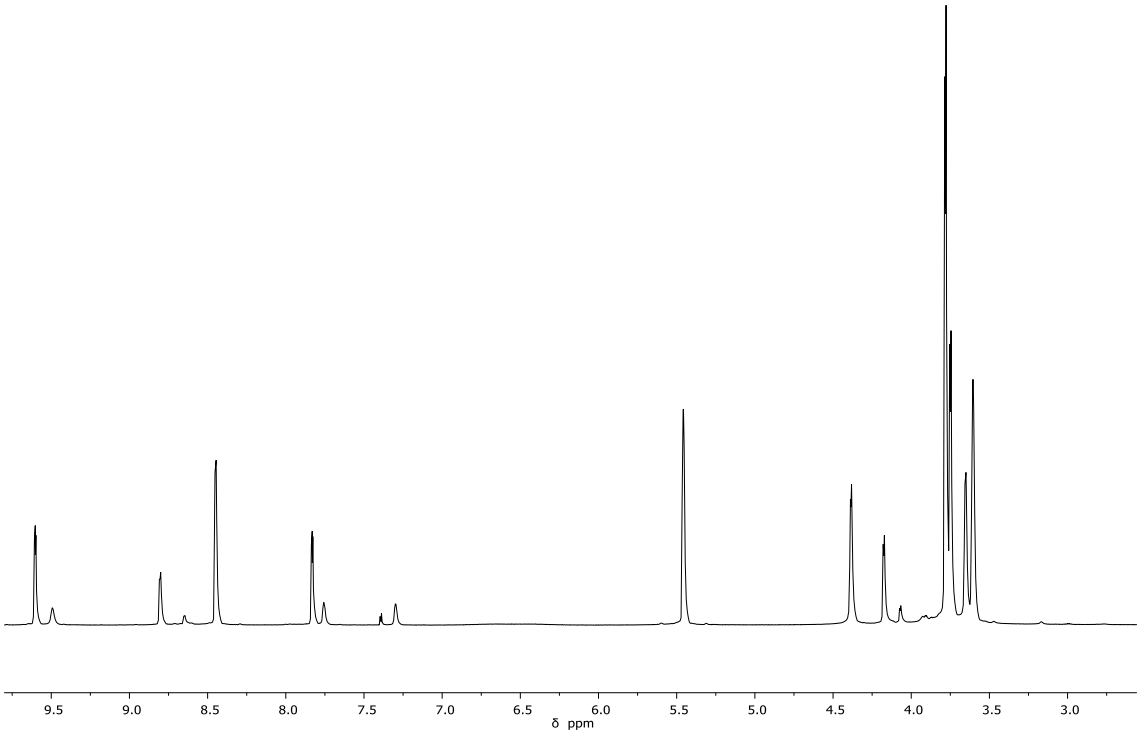
t = 72 h (500 MHz, THF-d_8).



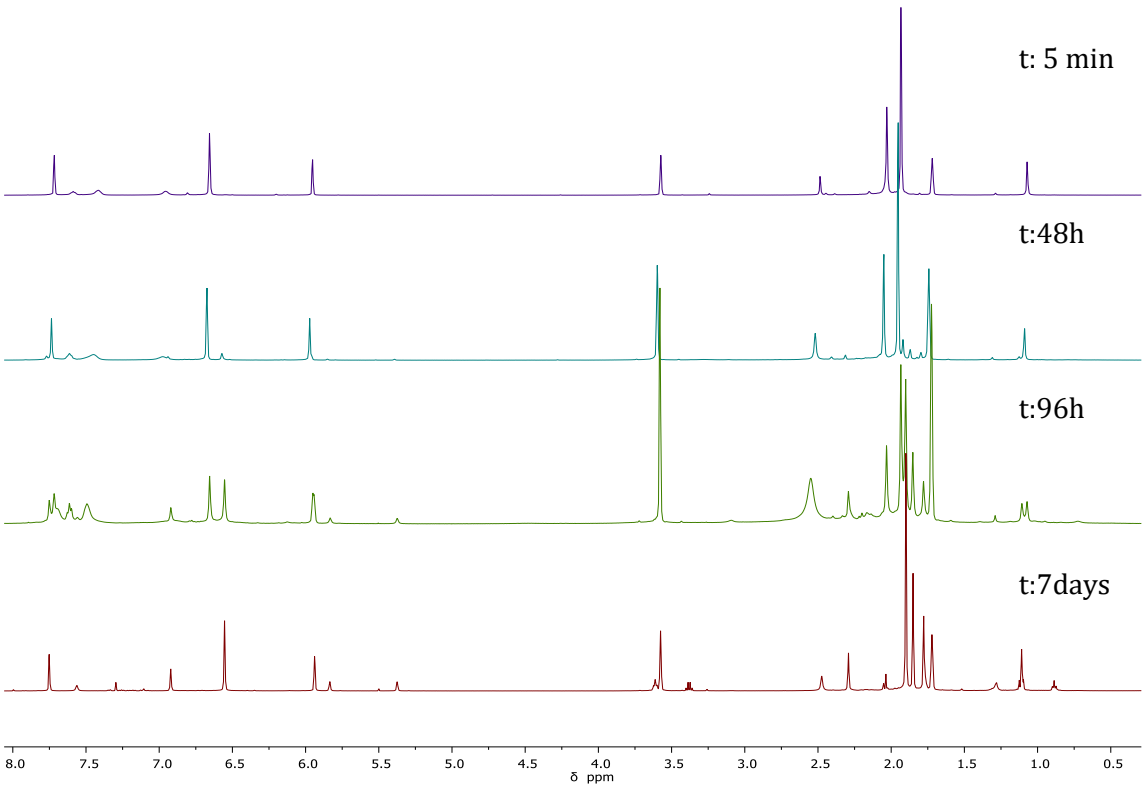
t = 120 h (500 MHz,THF-d_8).



t = 7 days (500 MHz,THF-d_8).



In a third experiment, a sample of complex **1b** (15 mg, 0.012 mmol) in 0.6 mL of THF-d_8 was used.



8. Determination of the magnetic susceptibility of complex 2a.

The determination of the magnetic susceptibility of complex **2a** was carried out using an Evans balance. The empty sample tube was first introduced to obtain R_o. Subsequently, the tube was filled with compacted complex **2a**, finely divided after crushing crystalline material in a mortar. The sample mass was then weighed and calculated by difference from the weight of the empty tube. The height of the sample in the tube was also measured, in cm (L). Finally, the tube was introduced in the balance and the value of the measurement R was noted:

m = 47 mg

R_o = -25

R = 111

L = 0.85cm

χ_g was obtained with the following equation::

$$\chi_g = \frac{LC_{bal}(R - R_o)}{10^9 m}$$

C_{bal} was obtained from:

$$C_{bal} = \frac{C_{std}}{(R - R_o)}$$

C_{std} = 1112

R = 853

R_o = -32

From χ_g, the molar magnetic susceptibility (χ_M) was calculated by multiplying χ_g by the molecular weight of complex **2a**. In addition, a correction was made for the existence of additional diamagnetic effects of the metal center and the ligands:

$$\chi_{M\ corrected} = \chi_M + 10^{-6} \square\square Z_{corrections}$$

The summation factor of the corrections is obtained from the following Table, with the approcah of the pyridine values for the pyrazole ligands (this affect t o the third decimal integer).

***Table**. Correction values for calculating magnetic susceptibility.*

Cations		Anions		Molecules	
Li^+	1.0	F^-	9.1	H_2O	13
Na^+	6.8	Cl^-	23.4	NH_3	16
K^+	14.9	Br^-	34.6	en	47
Rb^+	22.5	I^-	50.6	py	49
Cs^+	35	$CH_3CO_2^-$	29	PPh_3	167
Tl^+	35.7	$C_6H_5CO_{2-}$	71		
NH^{4+}	13.3	CN^-	13		
Hg^{2+}	38	CON^-	23		
Mg^{2+}	5	CNS^-	34		
Zn^{2+}	15	ClO^{4-}	34		
Pb^{2+}	32	CO_3^{2-}	28		
Ca^{2+}	10.4	$C_2O_4^{2-}$	28		
Sr^{2+}	16	HCO^{2-}	17		
Ba^{2+}	26	NO^{3-}	19		
Fe^{2+}	12.8	O^{2-}	6		
Cu^{2+}	12.8	OH^-	11		
Cu^{1+}	15	S^{2-}	28		
Ag^{1+}	27	SO_4^{2-}	38		
Cd^{2+}	20	$S_2O_3^{2-}$	46		
Other metals	13	$acac^-$	55		

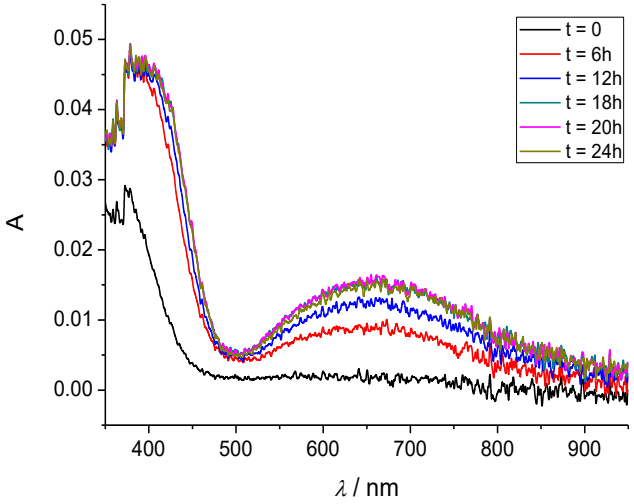
From all the previous data, and considering a temperature of 25 °C (298 K), the following value of μ_{ef} was obtained:

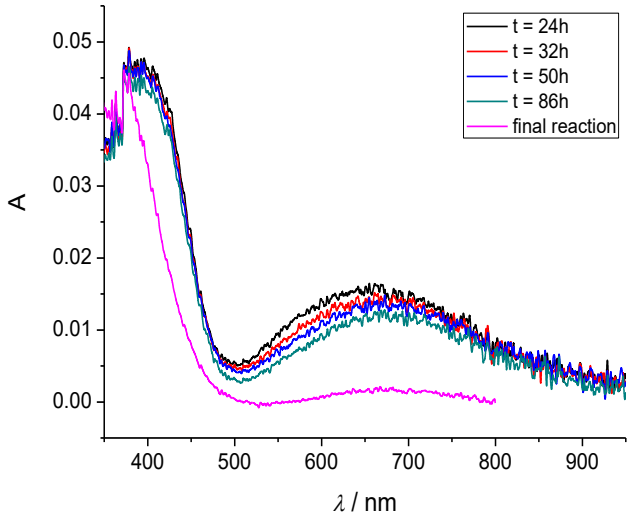
$$\mu_{ef} = 2.828\sqrt{\chi_M T}$$

μ_{ef}= 3.329 MB

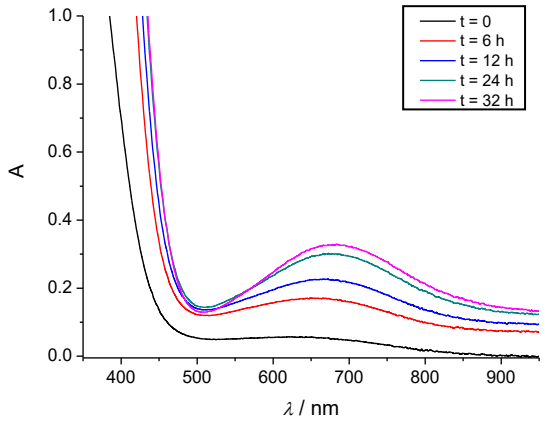
9. UV-visible studies.

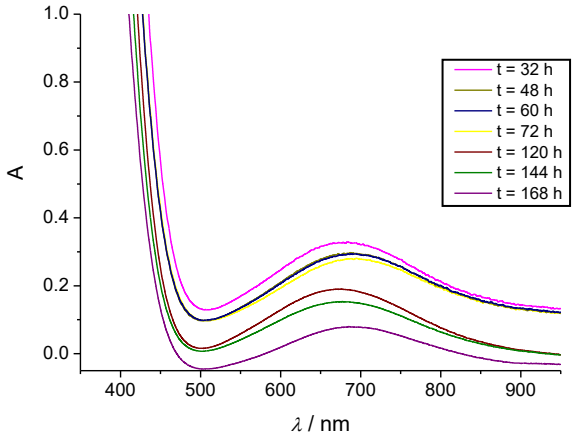
In a quartz cuvette, 15 mg of $Tp^{Ms}Cu(THF)$ were dissolved in 0.6 mL of THF previously oxygenated for one hour, the mixture being monitored by UV-Visible for several days. The spectra obtained were the following:





In a second experiment, metallic copper powder (150 mg) was added, using the same conditions, obtaining the following spectra:


t = 0
t = 6 h
t = 12 h
t = 24 h
t = 32 h
A
λ / nm


t = 32 h
t = 48 h
t = 60 h
t = 72 h
t = 120 h
t = 144 h
t = 168 h
A
λ / nm

10. DFT Calculations.

I Computational Details

I.I ***Potential Energy Surface exploration***

Theoretical calculations were performed at the DFT level of theory using Gaussian09 software.[5] All the energies reported in the main text have been obtained with the hybrid meta-GGA TPSSh functional[6] supplemented with the Grimme's dispersion correction D3.[7] This 10% exchange functional accurately reproduce the relative energies of spin states of first-row transition metal complexes[8] and predicts reactivity at CuIII.[9] We have already employed this methodology in recent studies of copper reactivity involving different spin states of the metal[10] and O_2 activation in transition metal systems.[11] Additional calibration calculations employing a set of functionals as well as highly-correlated methods were carried out for certain structures (see section VI in the Supporting Information). The geometries of all the intermediates and transition states were optimized in tetrahydrofuran solvent (ε= 7.4257) with the SMD continuum model[12] using the TPSSh-D3 functional. Basis set BS1 was used for the optimizations. BS1 includes the 6-31G(d,p) basis set for the main group elements,[13] and the scalar relativistic Stuttgart-Dresden SDD pseudopotential and its associated double-ζ basis set,[14] complemented with a set of *f* polarization functions,[15] for the copper atoms. Frequency calculations were carried out for all the optimized geometries in order to characterize the stationary points as either minima or transition states.

Gibbs energies in tetrahydrofuran (ΔG_{THF}) were calculated at 298.15 K adding to the potential energies in tetrahydrofuran, obtained with single point calculations using an extended basis set (BS2) at the BS1 optimized geometries, the thermal and entropic corrections obtained with BS1. In BS2 the main group element atoms are described with a 6-311++G(d,p) basis set.[16]

A correction of 1.9 kcal mol^{-1} was applied to all Gibbs values to change the standard state from the gas phase (1 atm) to solution (1 M) at 298.15 K.[17] In this way, all the energy values in the energy profiles are Gibbs energies calculated using the formula:

$$G_{THF} = E_{THF}(BS2) + G_{THF}(BS1) - E_{THF}(BS1) + \Delta G^{1atm\rightarrow 1M}$$

where $\Delta G^{1atm\rightarrow 1M}$ = 1.9 kcal mol^{-1} is the Gibbs energy change for compression of 1 mol of an ideal gas from 1 atm to the 1 M solution phase standard state.

Unrestricted open-shell singlet calculations (OSS) have been performed with the broken-symmetry formalism. It is important to note that, in open-singlet biradicals, the

unrestricted wavefunction is often contaminated by higher spin states, especially by the triplet state. In order to take into account this spin contamination the energy of all stationary points with an open-shell singlet spin state was further corrected with the Yamaguchi approach.[18]

I.II Calculation of electronic spectra

Simulations of the electronic spectra of the mononuclear copper complex **C**, the dinuclear **C-Cu** and trinuclear **2a** in THF solvent have been carried out with the TD-DFT approach at the B3LYP/BS1[19] level of theory, using the TPSSh-D3/BS1 geometries optimized in THF solvent. For all systems we have run calculations asking for 10 roots, except for **C** in the triplet state, for which the simulation was done for 18 roots. This way we could cover up to 500 nm and thus, analyze the wavelength range where the experimental band was observed. Simulated spectra for the three compounds are shown in Figure S8-S10. In addition, for **2a** we have also performed calculations with CAM-B3LYP[20] and with the BS2 basis set, to assess the influence of i) considering a range separated functional, which has been shown to provide better results for charge transfer excitations, and ii) further enlarging the basis set. Results are given in Figure S10 and Figure S11.

II. Comparison of triplet and open-shell singlet Gibbs energy profiles.

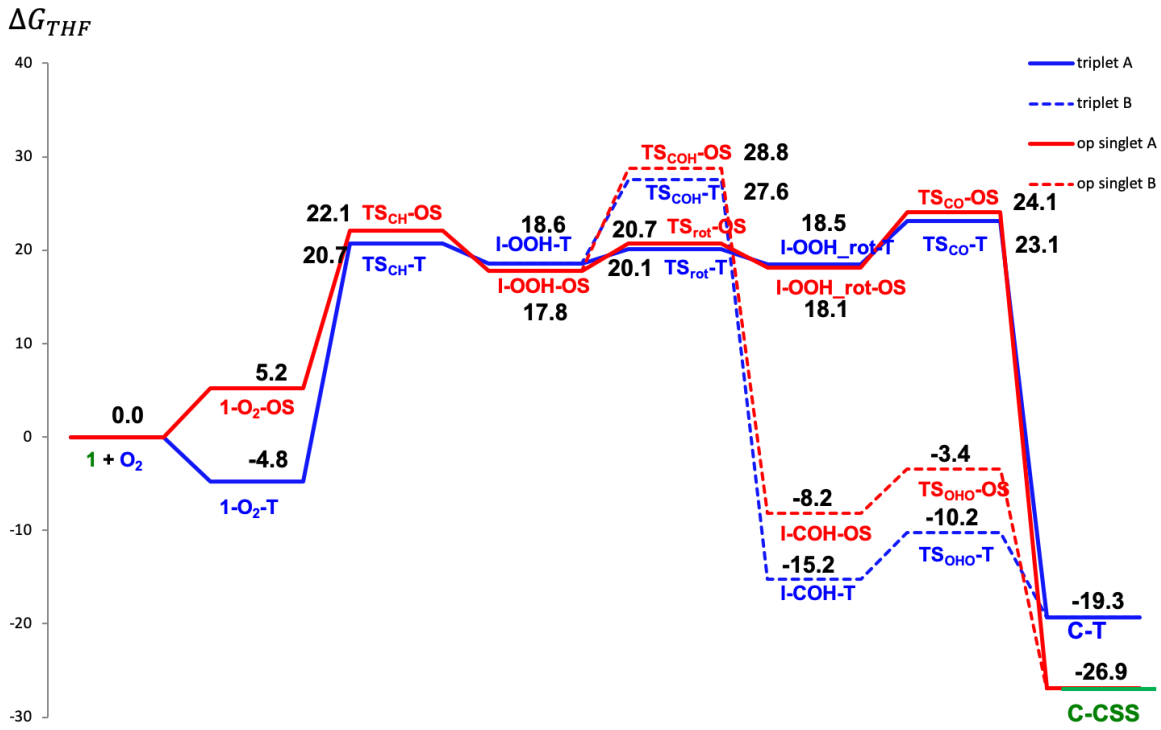
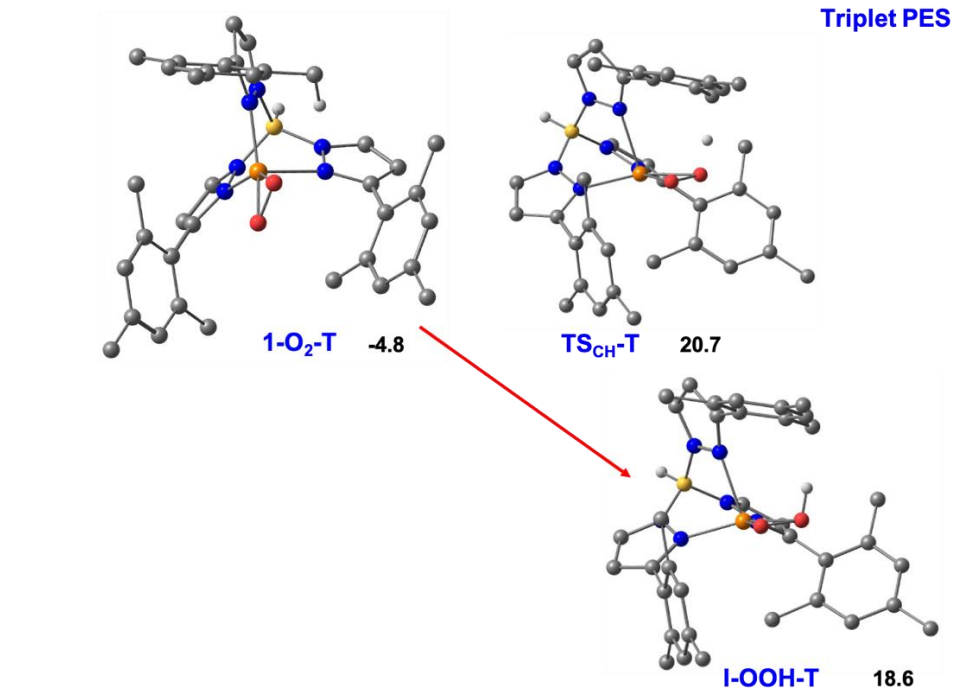


Figure S1. DFT-computed (TPSSh-D3/BS2) Gibbs energy profile for the reaction of **1** with O_2 in tetrahydrofuran, in the triplet (blue lines) and open-shell singlet (red lines) spin states. Solid lines: pathway A; dotted lines: pathway B. Relative ΔG_{THF} values are given in kcal mol^{-1} and are reported with respect to separated **1** and O_2

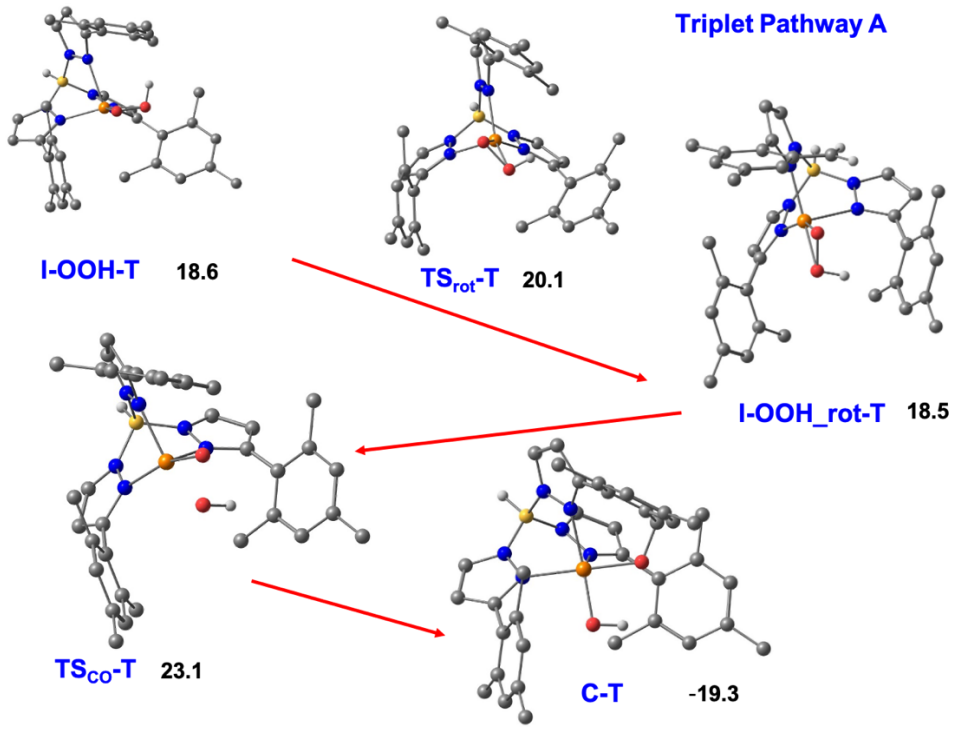
.

III. Optimized structures of all the intermediates and transition states in the pathway for the formation of C from 1 and O_2 in the triplet state (Gibbs energy profile in Figure 4 of the main text)

a)



b)



c)

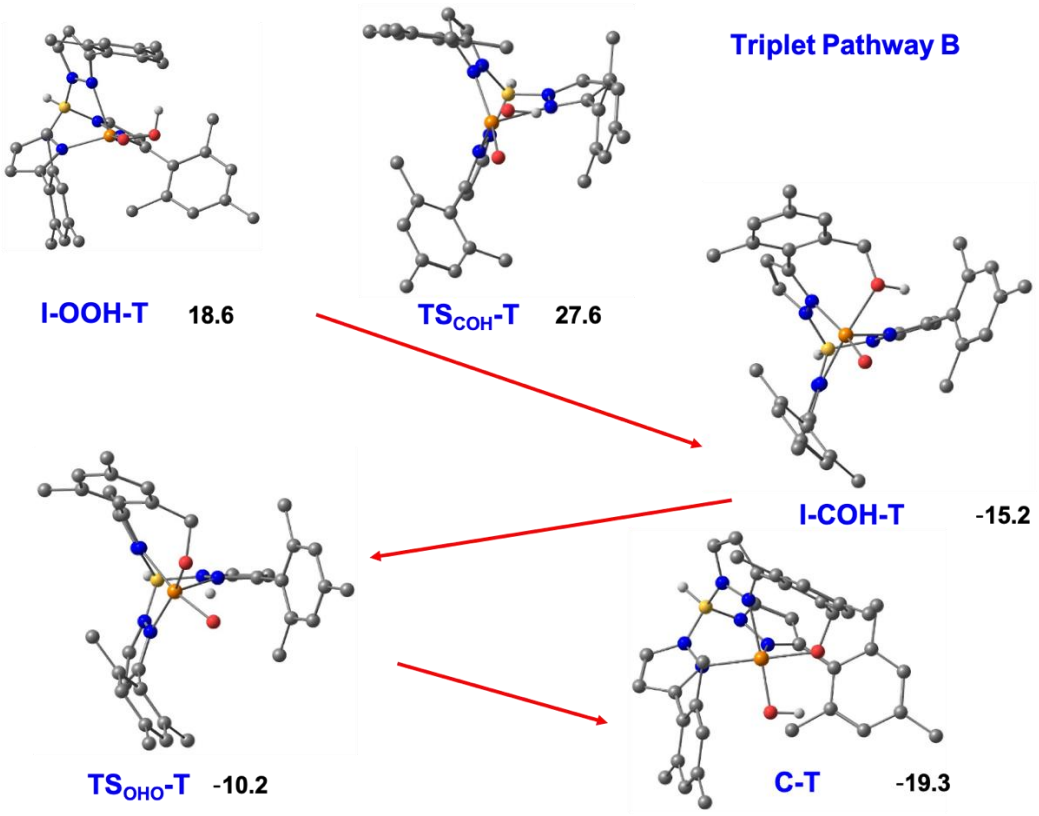


Figure S2. Optimized structures of all the intermediates and transition states in the pathway for the formation of **C** from **1** and O_2 in the triplet state (Gibbs energy profile in Figure 4 of the main text): a) formation of hydroperoxo intermediate; b) pathway A; c) pathway B. Geometries of the corresponding species in the open-shell singlet state are very similar.

IV. Closed-shell singlet Gibbs energy profile

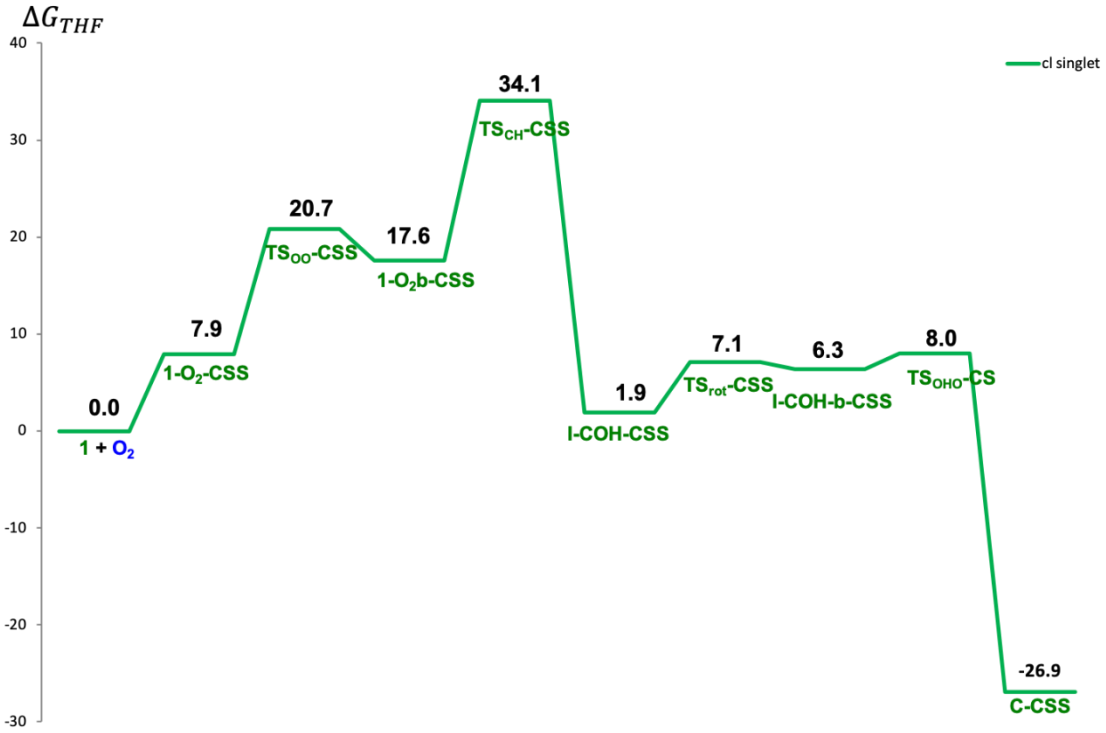
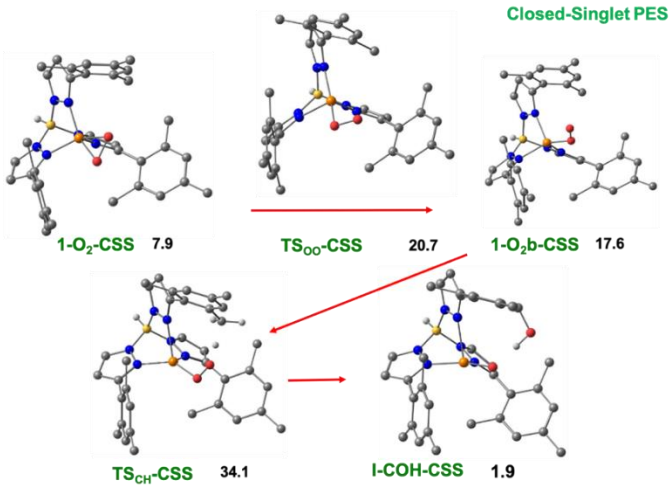


Figure S3. DFT-computed (TPSSh-D3/BS2) Gibbs energy profile for the reaction of **1** with O_2 in tetrahydrofuran, in the closed-shell singlet spin state. Relative ΔG_{THF} values are given in kcal mol^{-1} and are reported with respect to separated **1** and O_2.

V. Optimized structures of all the intermediates and transition states in the pathway for the formation of C from 1 and O_2 in the closed-shell singlet state (Gibbs energy profile in Figure S3)

a)



b)

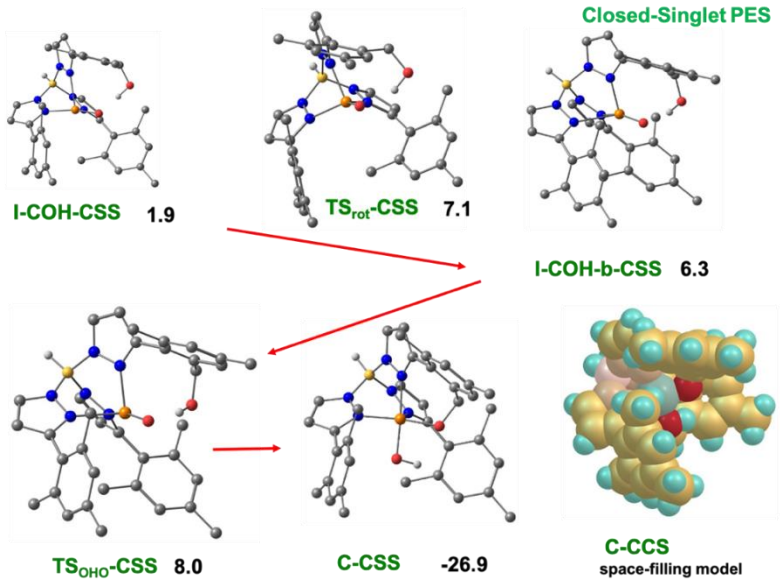


Figure S4. Optimized structures of all the intermediates and transition states in the pathway for the formation of **C** from **1** and O_2 in the closed-shell singlet state (Gibbs energy profile in Figure S3). In this spin state hydrogen abstraction and O-O bond splitting (a) takes place in a concerted way (**TS_{CH}-CSS**) yielding the copper-oxo/alcohol intermediate **I-COH-CSS**. From this intermediate, proton transfer to the oxo group, with concomitant formation of a Cu-O bond with the alkoxy group (**TS_{OHO}-CSS**) leads to intermediate **C-CSS** (b).

VI. DFT benchmark study for the nature of intermediate C and relative stabilities of Cu^{I}, Cu^{II} and Cu^{III} species

The transformation of **1** + O_2 in **2a** involves four different oxidation states of copper (0, I, II and III) and takes place in different spin states. To computationally deal with both issues is challenging. Accurate calculations of the energy splitting between low-spin and high-spin states[21] and between compounds including copper centers in different oxidation states[22] is difficult due to the strong functional dependence it displays. Thus, in order to determine the correct ground state of intermediate **C**, as well as to benchmark the relative energies of copper species in different oxidation states, we performed Coupled Cluster calculations including single, double, and perturbatively estimated triple excitations [CCSD(T)] within a domain-based local pair natural orbital (DLPNO) formulation[23] of species **1** (Cu^{I}, closed-shell singlet) + O_2 (triplet), **C-T** (Cu^{II}, triplet) and **C-CSS** (Cu^{III}, closed-shell singlet). The obtained values were benchmarked against several density functional-based methods (Table S1). DLPNO-CCSD(T) has been devised to obtain accurate electronic energies for large molecules and already employed to benchmark singlet-triplet gaps in copper complexes.[22b,24]

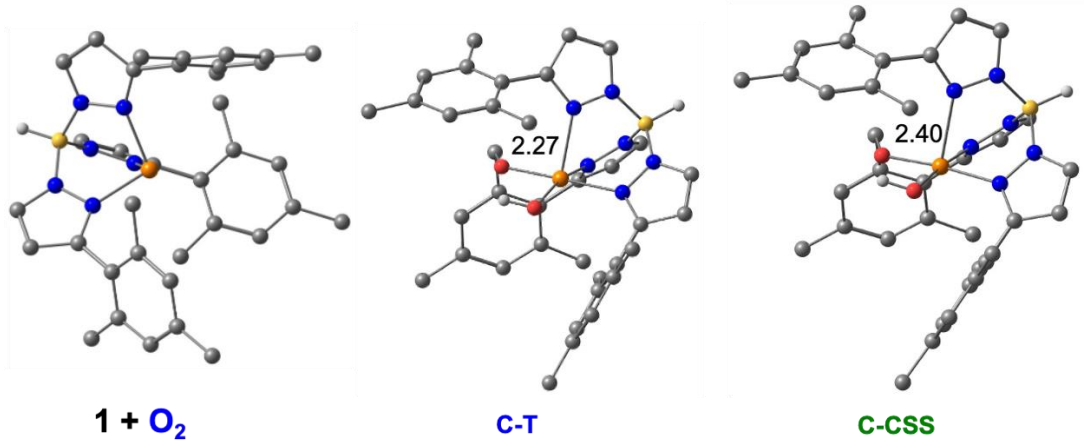


Figure S5. TPSSh-D3 optimized geometries of **1**, **C-T** and **C-CSS** used for the benchmarking calculations.

All these benchmarking calculations have been performed at the TPSSh-D3/BS1 optimized geometries of the complexes using a further extended basis ser (BS3). BS3 consists in the def2-TZVP basis set for the main group elements, and the quadruple-ζ def2-QZVP basis set for Cu.[25] Data collected in Table 1 enable us to assign a singlet-Cu^{III} nature to the mononuclear species **C** resulting from the hydroxylation of **1**, though highlighting the difficulties of DFT methods in accurately estimate in a balanced way the relative energies of these three copper complexes. The results also show that the level

of calculation used to build up the energy profiles (single point TPSSh-D3/BS2 calculations over TPSSh-D3/BS1 optimized geometries) is giving a good estimation of **1** + $O_2 \rightarrow$ **C-CSS** reaction, although overestimates the stability of **C-T**. Overall, the lower absolute deviations with respect the DLPNO-CCSD(T) values are obtained with PBE-D3 and TPSSh-D3 functionals.

Table S1. Relative energies of copper species in different oxidation states and Cu(III)/Cu(II) singlet-triplet energy gap, in kcal mol^{-1}, computed for **1** and **C** using various density functionals compared against DLPNO-CCSD(T) reference values. All single-point calculations are done using BS3 on TPSSh/BS1 singlet and triplet optimized geometries.

Method	%HF exchange	1 (Cu^{I}) + O2	C-T (Cu^{II})	C-CSS (Cu^{III})	ΔE (Cu(II)-Cu(III))	Absolute deviation[a]
DLPNO-CCSD(T)/BS3 (gp)	*/*	0.0	-22.9	-42.7	*19.8*	*0.0*
TPSSh-D3/BS1 (opt)	10	0.0	-35.3	-44.1	*8.8*	*13.8*
TPSSh-D3/BS2	10	0.0	-33.8	-42.7	*8.9*	*10.9*
TPSSh-D3/BS3	10	0.0	-26.1	-35.5	*9.4*	*10.4*
PBE-D3/BS3	0	0.0	-28.2	-39.6	*11.4*	*8.4*
M11-L/BS3	0	0.0	-44.5	-50.0	*5.5*	*28.9*
B3LYP-D3/BS3	20	0.0	-15.7	-31.1	*15.4*	*18.8*
PBE0-D3/BS3	25	0.0	-10.7	-26.5	*15.8*	*28.4*
M06/BS3	27	0.0	-19.0	-27.7	*8.7*	*18.9*
MN15/BS3	44	0.0	7.4	-8.7	*16.1*	*64.3*
CAM-B3LYP-D3	19(SR)65(LR)	0.0	-22.2	-28.0	*5.8*	*15.4*
wB97XD	22(SR)/100(LR)	0.0	-14.9	-20.3	*5.4*	*30.4*
M11/BS3	42.8(SR)/100(LR)	0.0	-16.2	-13.9	*-2.2*	*35.5*

[a)] Computed as the sum of the absolute values of the differences of the relative energies of the Cu^{II} and Cu^{III} species with respect the corresponding DLPNO-CCSD(T)/BS3 relative energy values.

VII. Minimum Energy Crossing Point (MECP) of the triplet and closed-shell singlet potential energy surfaces

Optimization of the triplet hydroperoxide intermediate **I-OOH-T** in the closed-shell singlet state leads to intermediate **I-COH-CSS** with a copper(III)-oxo/C-OH nature. We have explored this alternative route to enter into the Cu(III) PES, by locating the minimum energy crossing point (MECP) between the triplet and singlet surfaces that connects both intermediates. To locate the MECP between potential energy surfaces of different spin, the program developed by the group of Harvey was employed.[26] To confirm that the MECP connects the two intermediates located in the two energy surfaces, the MECP structure was optimized in the different spin states involved in the crossing. The Gibbs energies in solution of the MECP was estimated by adding to the calculated potential energy of the MECP thermal and entropic corrections calculated with the option freq = projected of the Gaussian 09 program.[27] The structure of the MECP is depicted in Figure S6.

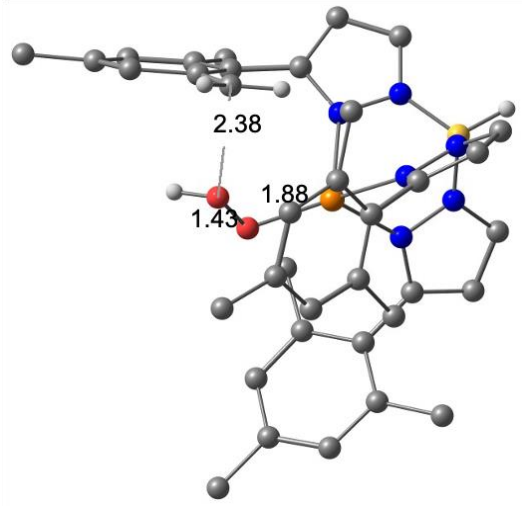
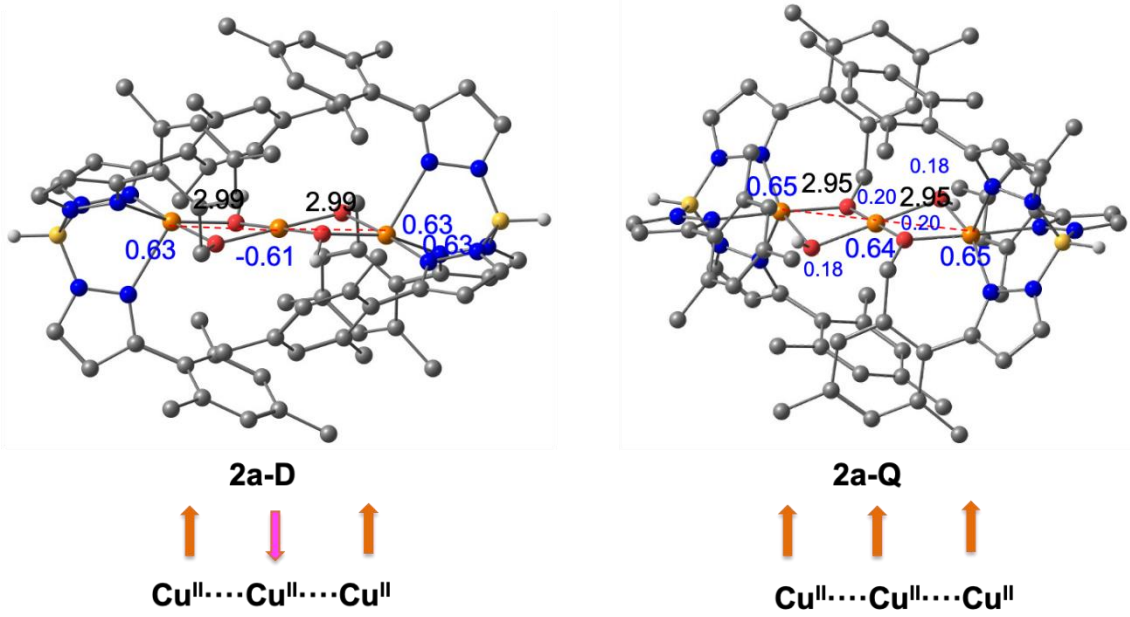


Figure S6. TPSSh-D3/BS1 optimized structure of MECP connecting **I-OOH-T** and **I-COH-CSS** intermediates. Selected distances in Å.

The MECP is found at 31.0 kcal mol^{-1}, much higher than **TS$_{rot}$-T** (20.1 kcal mol^{-1}) and **TS$_{Co}$-T** (23.1 kcal mol^{-1}). Consequently, this alternative route to reach **C** can be discarded.

VIII. Structural and electronic analysis of the trinuclear complex 2a.



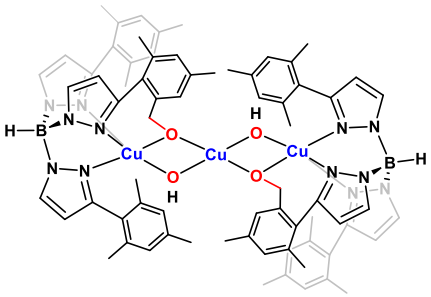
2 C-CSS + **Cu(0)** ⟶ **2a-D** **ΔG = -148.4 kcal mol^{-1}**

Energy difference D-Q
(ΔG in THF, kcal mol^{-1})

	2a-D	2a-Q
TPSSh/BS1	0.	0.9
TPSSh/BS2	0.	0.9
TPSSh/BS3	0.	1.2

Figure S7. TPSSh-D3/BS1 optimized structures of the trinuclear complex **2a** optimized in the doublet (**2a-D**) and quadruplet (**2a-Q**) spin states. In black Cu···Cu distances (in Å) and in blue Mulliken atomic spin populations, displaying the presence of three equivalent copper(II) centers. There is a huge thermodynamic driving force directing the formation of the trimetallic copper(II) complex from two monuclear copper(III) complexes **C-CSS** and one copper atom.

Table S2. Comparison of the X-ray determined and DFT-optimized main geometrical parameters of **2a**. Distances in Å, angles in degrees.



	X-ray	**2a-D**[a]	**2a-Q**[a]
Cu_L-O_C	1.916	1.928	1.929
Cu_L-O_H	1.945	1.984	1.975
Cu_C-O_C	1.930	1.934	1.943
Cu_C-O_H	1.906	1.940	1.945
Cu_L-N	2.01/2.026/2.026	2.033/2.069/2.218	2.048/2.061/2.323
$Cu_L \cdots Cu_C$	3.0067	2.992	2.948
O_C-Cu_L-O_H	76.65	77.3	78.7
O_C-Cu_C-O_H	77.25	78.3	79.1
N-Cu_L-N	85.27/91.47/87.08	90.4/85.9/86.6	89.9/85.4/86.6

[a] TPSSh-D3/BS1 optimized geometry in THF

IX. TD-DFT calculation of the UV-Vis spectra

UV-Vis simulated spectra in THF for the mononuclear (**C**), dinuclear (**C-Cu**) and trinuclear (**2a**) complexes are shown in Figures S8-S10. Results for **C** in the singlet state (**C-CSS**) indicate that the wavelength of the most intense band is 500 nm. This band mainly corresponds to $O_p \rightarrow Cu_d$ excitation. However, in the triplet state (**C-T**) simulations indicate that there is an intense band at 1498 nm corresponding mainly to the $O1_p \rightarrow O2_p$ excitation and a less intense band at 644 nm corresponding to a L→ O transition. For the dinuclear complex **C-Cu** we have run simulations both for the doublet and quartet spin states and found intense bands at 394 and 565 nm, respectively. Former band mainly corresponds to a $Cu1_{3d} \rightarrow$ L transition whereas that of the quartet state corresponds to a $Cu1_{4s} \rightarrow$ L transition. Finally, for the trinuclear complex **2a**, both in the doublet and quartet state, most intense band shows contributions from $O_p \rightarrow Cu_d$ and $Cu_d \rightarrow Cu_d$ transitions among the different copper sites. In addition, for **2a** we have also performed calculations with CAM-B3LYP[20] (Figure S10) and with the BS2 basis set (Figure S11), to assess the influence of i) considering a range separated functional, which has been shown to provide better results for charge transfer excitations, and ii) further enlarging the basis set. Results show that neither changing the functional to CAM-B3LYP nor enlarging the basis set has a major influence on the computed spectrum, the wavelength of the band maximum differing by less that 1 nm. Overall, and because the ground state of complex **C** is the singlet state, observed bands at 675 nm are assigned to d → d transitions of the trinuclear complex **2a**.

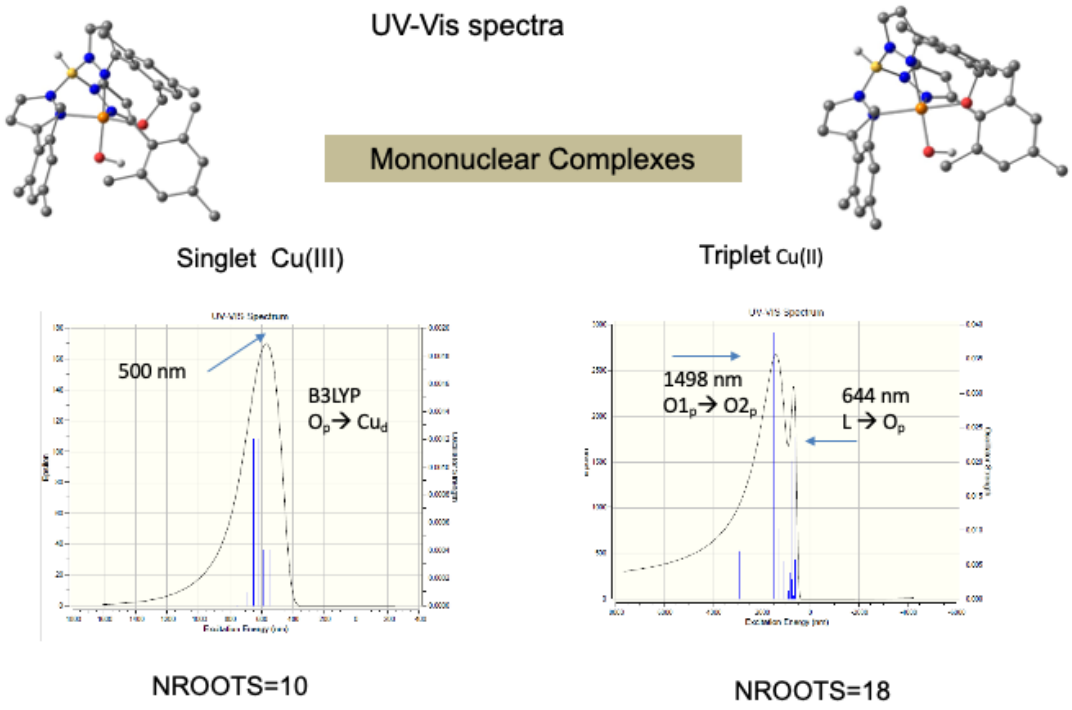


Figure S8. UV-Vis Absorption spectrum for complex **C**, both for the singlet and triplet spin states, at the TD-DFT B3LYP/BS1 level of theory.

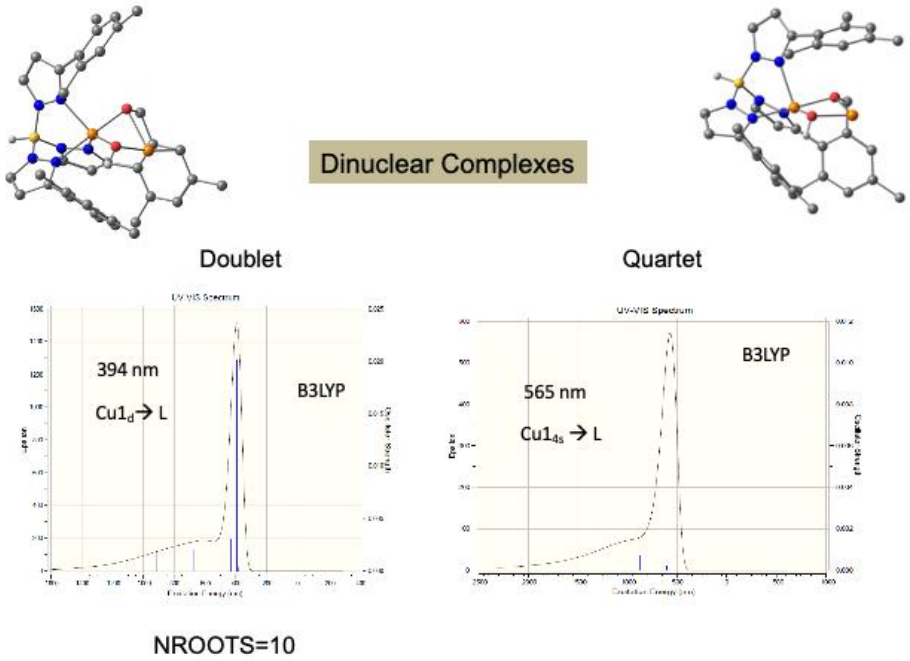


Figure S9. UV-Vis Absorption spectrum for complex **C-Cu**, both for the doublet and quartet spin states, at the TD-DFT B3LYP/BS1 level of theory.

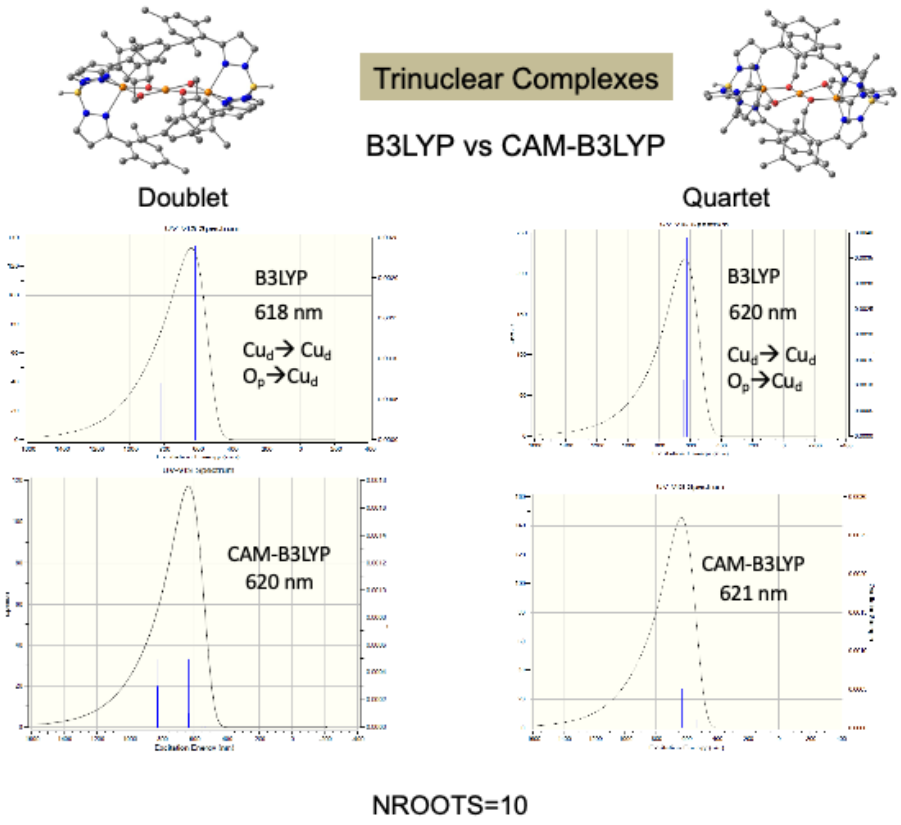


Figure S10. UV-Vis absorption spectrum for trinuclear complex **2a** both at the TD-DFT B3LYP/BS1 and CAM-B3LYP/BS1 levels of theory.

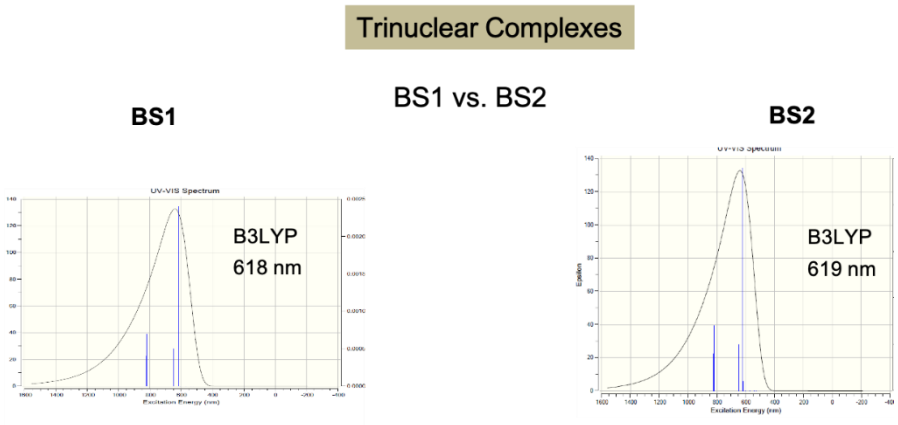


Figure S11. UV-Vis absorption spectrum for trinuclear complex **2a** both at the TDDFT B3LYP/BS1 and B3LYP/BS2 levels of theory.

11. References

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12. Cartesian coordinates and absolute E and G energies in tetrahydrofuran of the optimized structures.

Cartesian coordinates, BS1 and BS2 TPSSh-D3 energies (hartrees) in THF solvent and uncorrected Gibbs energies (298.15 K) of all the optimized structures.

1

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-1947.024309
Thermal and entropic correction, BS1 (a.u.)	0.610311
Electronic Energy, BS2 (a.u.)	-1947.392129
Gibbs Energy, BS2 (a.u)	-1946.781818
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

C	1.271194	-2.248975	-3.498724
H	1.260194	-2.230970	-4.579175
C	1.846515	-3.136667	0.031595
C	0.804204	-3.485037	0.925888
C	1.134753	-3.916975	2.215946
H	0.332480	-4.190608	2.899318
C	2.465304	-4.008713	2.648817
C	3.478381	-3.651956	1.750930
H	4.517139	-3.703446	2.072125
C	3.194098	-3.219203	0.448448
C	-0.652158	-3.393897	0.524110
H	-1.275689	-3.997141	1.191157
H	-0.810539	-3.732339	-0.505101
H	-1.013418	-2.357835	0.570420
C	2.790163	-4.492443	4.042536
H	2.184341	-3.974714	4.795070
H	3.845481	-4.333226	4.284745
H	2.581463	-5.564978	4.144232
C	4.328609	-2.828486	-0.472076
H	4.109612	-1.900145	-1.009396
H	4.515639	-3.599745	-1.229128
H	5.254579	-2.690286	0.094321
C	-3.160810	-0.001028	-1.225948
C	-3.795330	-0.041995	-2.488419
H	-4.856259	-0.044002	-2.690703
C	-2.760201	-0.056179	-3.411867
H	-2.770833	-0.078229	-4.492210
C	-3.725568	0.053316	0.141329
C	-3.433565	1.150966	0.983056
C	-3.963861	1.168996	2.282106
H	-3.747307	2.020095	2.925371

C	-4.767810	0.132455	2.768007
C	-5.041329	-0.948234	1.916517
H	-5.659342	-1.767988	2.278656
C	-4.534856	-1.007643	0.614068
C	-2.571261	2.306012	0.521743
H	-1.503328	2.067652	0.610854
H	-2.764111	3.197226	1.126857
H	-2.749178	2.550037	-0.530047
C	-5.320997	0.160907	4.173386
H	-4.852597	-0.611587	4.795940
H	-6.399677	-0.032774	4.179184
H	-5.145958	1.128758	4.652748
C	-4.836354	-2.208164	-0.254552
H	-5.310566	-2.999548	0.333322
H	-3.922873	-2.612753	-0.704635
H	-5.512612	-1.952983	-1.078361
B	-0.132023	-0.026123	-3.289073
H	-0.162785	-0.028753	-4.487919
H	2.419860	0.169177	0.344445

1-THF

Charge	0
Spin State	Singlet
Electronic Energy, BS1 (a.u.)	-2179.545872
Thermal and entropic correction, BS1 (a.u.)	0.722537
Electronic Energy, BS2 (a.u.)	-2179.966942
Gibbs Energy, BS2 (a.u)	-2179.244405
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-0.035142	0.155130	-0.574247
N	0.584336	1.863059	-1.570722
N	0.381049	1.820502	-2.915842
N	0.981951	-1.058381	-1.946192
N	0.851141	-0.647178	-3.236077
N	-1.759495	0.051002	-1.720835
N	-1.530538	0.173933	-3.057422
C	1.002464	3.106850	-1.274681
C	1.060211	3.885018	-2.452074
H	1.366405	4.917016	-2.543676
C	0.660442	3.026655	-3.467322
H	0.561158	3.180137	-4.532563
C	1.352950	3.439244	0.125354
C	2.459343	2.796184	0.729686
C	2.768910	3.089936	2.062749
H	3.622182	2.597435	2.526011
C	2.009107	4.000049	2.813620
C	0.919689	4.622177	2.194780
H	0.314885	5.325882	2.763983
C	0.577554	4.359686	0.860015
C	3.295791	1.801222	-0.044439
H	3.644992	2.228271	-0.991644
H	4.168276	1.487479	0.536295
C	2.356742	4.289525	4.255018
H	2.127858	3.430843	4.898386
H	1.795041	5.148692	4.634032
H	3.425803	4.503037	4.369818

C	-0.609452	5.056542	0.235117
H	-1.262654	5.477214	1.005646
H	-1.198272	4.371137	-0.381865
H	-0.290288	5.879988	-0.415732
C	1.854515	-2.082531	-1.945803
C	2.299921	-2.331240	-3.263895
H	2.992434	-3.092957	-3.591278
C	1.633798	-1.399632	-4.047843
H	1.652025	-1.222380	-5.113795
C	2.179063	-2.772441	-0.676348
C	1.155291	-3.427836	0.047649
C	1.477540	-4.058083	1.256166
H	0.690448	-4.571406	1.805424
C	2.777553	-4.040429	1.778892
C	3.772268	-3.373999	1.052256
H	4.785716	-3.335736	1.447130
C	3.498074	-2.746031	-0.170677
C	-0.274506	-3.441890	-0.442836
H	-0.881059	-4.135674	0.146678
H	-0.334280	-3.733811	-1.497036
H	-0.720983	-2.443021	-0.368089
C	3.097269	-4.734769	3.081541
H	2.251548	-4.690951	3.775651
H	3.967244	-4.285185	3.570582
H	3.326385	-5.795104	2.914455
C	4.604693	-2.025541	-0.907026
H	4.282121	-1.034461	-1.243030
H	4.920998	-2.578403	-1.799341
H	5.480828	-1.903932	-0.263077
C	-3.061464	-0.256195	-1.572984
C	-3.680475	-0.342150	-2.839696
H	-4.716976	-0.561044	-3.050823
C	-2.671884	-0.058746	-3.749667
H	-2.681468	0.001139	-4.828679
C	-3.632377	-0.418322	-0.216827
C	-3.666184	0.687402	0.662136
C	-4.198338	0.515838	1.947159
H	-4.226798	1.369180	2.622199
C	-4.673418	-0.723510	2.391445
C	-4.623873	-1.808727	1.504886
H	-4.984119	-2.781856	1.833943
C	-4.119752	-1.676675	0.205147
C	-3.106954	2.031440	0.255804
H	-2.010433	2.004662	0.242157
H	-3.420537	2.812026	0.955507
H	-3.426856	2.314780	-0.752685
C	-5.188796	-0.901698	3.800095
H	-4.458971	-1.443756	4.415030
H	-6.119082	-1.479991	3.817546
H	-5.375710	0.063057	4.281239
C	-4.084994	-2.876690	-0.714053
H	-4.210974	-3.803450	-0.146104
H	-3.141179	-2.933757	-1.264904
H	-4.887857	-2.832510	-1.460052
B	-0.113761	0.514983	-3.590530
H	-0.153924	0.663177	-4.780821
H	2.710836	0.910063	-0.299646
C	-0.976143	-0.659039	2.258482
O	0.124807	-0.199888	1.422478
C	1.398847	-0.438979	2.091709
C	1.031710	-0.845024	3.516211

C	-0.325526	-1.537118	3.318406
H	1.974228	0.485724	2.035892
H	1.787593	-1.498557	3.959653
H	0.918965	0.042012	4.149594
H	-0.179645	-2.550079	2.930999
H	-0.923368	-1.589623	4.232327
H	-1.686908	-1.178543	1.614375
H	-1.461192	0.220807	2.693719
H	1.918299	-1.235560	1.553284

02

Charge	0
Spin State	Triplet
Electronic Energy, BS1 (a.u.)	-150.327093
Thermal and entropic correction, BS1 (a.u.)	-0.016258
Electronic Energy, BS2 (a.u.)	-150.377867
Gibbs Enegy, BS2 (a.u.)	-150.394125
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

O	0.000000	0.000000	0.608944
O	0.000000	0.000000	-0.608944

Mononuclear complexes

Triplet Potential Energy Surface

1-O_2-T

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.380953
Thermal and entropic correction, BS1 (a.u.)	0.613080
Electronic Energy, BS2 (a.u.)	-2097.793749
Gibbs Energy, BS2 (a.u.)	-2097.180669
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	0.112351	-0.030869	-0.361583
O	-0.391564	-0.622594	1.488002
O	-0.141884	0.658925	1.533480
N	0.687708	-1.570403	-1.533170
N	0.558333	-1.382460	-2.874353
N	-1.735330	0.129711	-1.517302
N	-1.530677	0.022660	-2.858644
N	0.956753	1.311789	-1.585889
N	0.739328	1.124171	-2.916087
C	1.260477	-2.774289	-1.343067
C	1.506806	-3.373059	-2.594467
H	1.951229	-4.339878	-2.778292
C	1.044716	-2.458302	-3.532429
H	1.021353	-2.495149	-4.612016

C	1.516384	-3.265758	0.030135
C	0.428044	-3.653429	0.840680
C	0.682882	-4.092014	2.146808
H	-0.154224	-4.391951	2.773890
C	1.982747	-4.147116	2.664705
C	3.046380	-3.751796	1.840397
H	4.062254	-3.780669	2.230111
C	2.836982	-3.314773	0.527613
C	-0.987528	-3.601526	0.312608
H	-1.089518	-4.194663	-0.603984
H	-1.695441	-3.985650	1.052183
C	2.243912	-4.631257	4.071420
H	2.791637	-5.581644	4.064286
H	1.310511	-4.785970	4.620499
H	2.853960	-3.913018	4.630857
C	4.008724	-2.903105	-0.334370
H	4.900046	-2.733105	0.276514
H	3.793986	-1.988445	-0.895436
H	4.251646	-3.679630	-1.069956
C	-3.065112	0.181584	-1.324706
C	-3.730233	0.100373	-2.568630
H	-4.795237	0.127713	-2.746086
C	-2.717246	0.002787	-3.511670
H	-2.750263	-0.073010	-4.589170
C	-3.613568	0.349463	0.041170
C	-3.336834	1.534877	0.759885
C	-3.848449	1.674806	2.055720
H	-3.635112	2.587200	2.609579
C	-4.624558	0.674373	2.656008
C	-4.882426	-0.492611	1.925637
H	-5.473713	-1.285577	2.379929
C	-4.391403	-0.673110	0.626076
C	-2.503177	2.641633	0.154192
H	-2.543639	3.542093	0.774005
H	-2.850317	2.898259	-0.853024
H	-1.454999	2.340383	0.060902
C	-5.193154	0.863708	4.042418
H	-4.523551	1.460215	4.670333
H	-5.365426	-0.096780	4.538292
H	-6.156006	1.389311	4.001187
C	-4.682804	-1.956223	-0.118810
H	-3.773334	-2.378761	-0.559149
H	-5.389812	-1.792460	-0.940518
H	-5.117903	-2.702775	0.552120
C	1.697786	2.427948	-1.443492
C	1.959147	2.971517	-2.718195
H	2.535293	3.856527	-2.943009
C	1.337355	2.114469	-3.615918
H	1.279151	2.132389	-4.694576
C	2.117336	2.893696	-0.102431
C	2.950638	2.079896	0.699317
C	3.324378	2.539346	1.968374
H	3.970054	1.915356	2.583459
C	2.888363	3.773614	2.466302
C	2.063589	4.562269	1.653595
H	1.709346	5.521491	2.026234
C	1.669403	4.145737	0.376106
C	3.436893	0.730559	0.220514
H	2.642700	-0.024151	0.277438
H	4.269887	0.376925	0.834705
H	3.761958	0.765991	-0.824270

C	3.304696	4.244660	3.839719
H	3.492684	3.397405	4.506355
H	2.532635	4.873808	4.294116
H	4.227478	4.837475	3.794471
C	0.762823	5.027561	-0.453326
H	0.318383	5.812512	0.165563
H	-0.047009	4.452708	-0.914411
H	1.312666	5.516589	-1.266149
B	-0.094180	-0.084835	-3.421194
H	-0.111077	-0.103241	-4.617874
H	-1.278597	-2.576442	0.061709

TS_{CH}-T

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.338729
Thermal and entropic correction, BS1 (a.u.)	0.612191
Electronic Energy, BS2 (a.u.)	-2097.752197
Gibbs Energy, BS2 (a.u.)	-2097.140006
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-1408.3i

Molecular Geometry in Cartesian Coordinates

Cu	-0.274439	-0.102727	-0.324656
O	0.593329	0.102128	1.387222
O	-0.396401	-0.891956	1.559421
N	0.119389	1.315921	-1.719103
N	0.030821	0.918371	-3.018497
N	1.196421	-1.371890	-1.427584
N	0.974995	-1.398213	-2.768109
N	-1.756308	-0.841288	-1.431492
N	-1.530062	-1.034224	-2.756311
C	0.380534	2.635819	-1.712181
C	0.455291	3.101379	-3.041095
H	0.658987	4.109860	-3.368962
C	0.231968	1.981179	-3.830996
H	0.209583	1.859747	-4.904376
C	0.587947	3.337163	-0.424615
C	1.727019	3.021195	0.348161
C	1.904501	3.665466	1.579572
H	2.781727	3.425236	2.177095
C	0.982359	4.601393	2.062472
C	-0.139133	4.899380	1.275226
H	-0.867874	5.622458	1.637484
C	-0.351849	4.285505	0.035456
C	2.744312	2.012041	-0.134300
H	3.051034	2.219739	-1.165730
H	3.635039	2.024964	0.500454
C	1.180958	5.276246	3.399199
H	0.350183	5.053526	4.079347
H	1.224091	6.366529	3.290663
H	2.107138	4.945722	3.878284
C	-1.569262	4.641203	-0.787446
H	-2.329939	5.124229	-0.167100
H	-2.014488	3.757428	-1.254259
H	-1.311220	5.335629	-1.596625
C	2.374500	-1.989154	-1.212412
C	2.908966	-2.436072	-2.444414

H	3.827628	-2.980825	-2.602854
C	1.990753	-2.035326	-3.401145
H	1.983794	-2.151620	-4.475443
C	2.954239	-2.080707	0.143522
C	2.208597	-2.646874	1.227181
C	2.806728	-2.702120	2.514865
H	2.228952	-3.129193	3.331579
C	4.090199	-2.229668	2.751267
C	4.798388	-1.671567	1.669369
H	5.796351	-1.273726	1.841774
C	4.258741	-1.593232	0.378429
C	0.856898	-3.119317	1.080550
H	0.466374	-3.761511	1.870064
H	0.468201	-3.312412	0.083133
H	0.141975	-1.894089	1.405774
C	4.718283	-2.291755	4.122183
H	4.036123	-2.733512	4.853985
H	4.991335	-1.289463	4.472338
H	5.637585	-2.889098	4.107525
C	5.083040	-0.948996	-0.714344
H	4.470862	-0.312690	-1.359875
H	5.559009	-1.699030	-1.356519
H	5.878537	-0.337772	-0.278197
C	-2.995521	-1.290192	-1.153661
C	-3.575216	-1.794701	-2.336254
H	-4.563393	-2.214436	-2.450985
C	-2.615404	-1.608090	-3.322598
H	-2.626442	-1.832999	-4.379231
C	-3.538627	-1.164902	0.217486
C	-3.700057	0.117594	0.787418
C	-4.185438	0.218177	2.098282
H	-4.314352	1.206178	2.535784
C	-4.506395	-0.913780	2.855659
C	-4.339808	-2.175478	2.267192
H	-4.582225	-3.067049	2.842423
C	-3.862263	-2.322653	0.960571
C	-3.357870	1.376449	0.021316
H	-2.273392	1.542642	-0.006833
H	-3.814742	2.251284	0.492881
H	-3.696256	1.322305	-1.018708
C	-4.994170	-0.787790	4.279304
H	-4.186487	-1.011761	4.987727
H	-5.809741	-1.489360	4.485227
H	-5.349116	0.225167	4.491741
C	-3.670432	-3.704894	0.378538
H	-3.846504	-4.472150	1.138063
H	-2.653825	-3.834801	-0.009737
H	-4.356633	-3.893560	-0.454593
B	-0.188838	-0.578739	-3.380849
H	-0.216179	-0.716243	-4.569837
H	2.332347	0.997790	-0.116237

I-OOH-T

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.342765
Thermal and entropic correction, BS1 (a.u.)	0.614355
Electronic Energy, BS2 (a.u.)	-2097.757690
Gibbs Energy, BS2 (a.u.)	-2097.143335
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-0.276520	-0.096694	-0.315806
O	0.569035	0.225713	1.361333
O	-0.406039	-0.824713	1.630805
N	0.120066	1.316410	-1.718484
N	0.037760	0.917841	-3.017808
N	1.207726	-1.383227	-1.424004
N	0.990128	-1.396382	-2.766248
N	-1.741773	-0.852880	-1.432053
N	-1.513960	-1.041159	-2.757259
C	0.381216	2.636506	-1.711220
C	0.461677	3.100692	-3.040305
H	0.666507	4.109056	-3.367881
C	0.242339	1.979867	-3.830365
H	0.225339	1.857285	-4.903725
C	0.584427	3.341442	-0.424905
C	1.724284	3.032640	0.349283
C	1.897664	3.680436	1.579259
H	2.775133	3.445229	2.178450
C	0.969563	4.611338	2.060276
C	-0.152384	4.902809	1.271235
H	-0.885290	5.622629	1.631648
C	-0.360176	4.286282	0.031927
C	2.745639	2.025982	-0.129586
H	3.057047	2.235362	-1.159348
H	3.633217	2.040289	0.509531
C	1.161820	5.287301	3.397431
H	0.332234	5.057814	4.076689
H	1.196640	6.377918	3.289691
H	2.089951	4.963661	3.877299
C	-1.577663	4.635329	-0.793767
H	-2.340544	5.118597	-0.176249
H	-2.019933	3.748416	-1.257567
H	-1.320727	5.327240	-1.605528
C	2.386969	-2.002302	-1.215189
C	2.925230	-2.434247	-2.450028
H	3.846345	-2.974290	-2.610999
C	2.008321	-2.024367	-3.404171
H	2.003378	-2.128301	-4.479779
C	2.966211	-2.106604	0.140003
C	2.229703	-2.730966	1.207853
C	2.815589	-2.767164	2.509901
H	2.249074	-3.231483	3.314111
C	4.069838	-2.235015	2.765559
C	4.771700	-1.642439	1.695687
H	5.750747	-1.207112	1.884547
C	4.244670	-1.573906	0.396283
C	0.953998	-3.311077	1.015760
H	0.477349	-3.849524	1.831437
H	0.494355	-3.367732	0.034985
H	0.143361	-1.659248	1.575495
C	4.682179	-2.273570	4.144654
H	4.008520	-2.741303	4.868003
H	4.912604	-1.261966	4.498036
H	5.623318	-2.835855	4.141331
C	5.061806	-0.897771	-0.682625
H	4.437444	-0.287010	-1.340717
H	5.576705	-1.631684	-1.313687
H	5.825785	-0.255749	-0.234648
C	-2.984015	-1.298002	-1.159034

C	-3.562265	-1.796406	-2.344553
H	-4.551559	-2.212507	-2.462621
C	-2.599716	-1.609018	-3.328026
H	-2.608958	-1.829457	-4.385601
C	-3.534294	-1.174374	0.209399
C	-3.706802	0.107861	0.776261
C	-4.200826	0.207595	2.083894
H	-4.337582	1.195383	2.519435
C	-4.518994	-0.925321	2.840971
C	-4.342408	-2.186854	2.254962
H	-4.583834	-3.078993	2.829774
C	-3.856874	-2.333084	0.951187
C	-3.366691	1.366612	0.009322
H	-2.282546	1.533611	-0.019731
H	-3.823642	2.241410	0.480730
H	-3.706176	1.311379	-1.030371
C	-5.013840	-0.800628	4.262263
H	-4.208030	-1.019382	4.974318
H	-5.826320	-1.506524	4.465356
H	-5.375332	0.210460	4.472163
C	-3.656750	-3.714608	0.370193
H	-3.837187	-4.482848	1.127710
H	-2.636729	-3.841981	-0.010020
H	-4.335638	-3.904229	-0.468681
B	-0.174384	-0.580011	-3.379599
H	-0.199683	-0.717430	-4.568666
H	2.335198	1.011006	-0.113412

Triplet PES, pathway A

TS_{rot}-T

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.338443
Thermal and entropic correction, BS1 (a.u.)	0.613692
Electronic Energy, BS2 (a.u.)	-2097.754648
Gibbs Energy, BS2 (a.u.)	-2097.140956
Number of Imaginary Frequencies	2
Imaginary frequencies (cm-1)	-71.8i, -1.0i

Molecular Geometry in Cartesian Coordinates

Cu	-0.033496	0.100886	-0.368166
O	-0.133298	-0.758848	1.313893
O	0.174816	0.617075	1.703498
N	1.644642	-0.732804	-1.489815
N	1.522542	-0.617734	-2.840408
N	-1.294939	-0.921360	-1.629881
N	-0.987092	-0.890780	-2.952419
N	-0.028527	1.647278	-1.622643
N	0.037052	1.403583	-2.956367
C	2.858672	-1.256358	-1.245834
C	3.535997	-1.475223	-2.466312
H	4.522630	-1.893277	-2.602068
C	2.649523	-1.058430	-3.449188
H	2.731187	-1.049448	-4.526745
C	3.266470	-1.565984	0.144150
C	2.567593	-2.565076	0.857433
C	2.948937	-2.844713	2.175924
H	2.412890	-3.616185	2.725460

C	3.995747	-2.158463	2.803635
C	4.677545	-1.175216	2.073511
H	5.495581	-0.632494	2.544265
C	4.333368	-0.868540	0.751442
C	1.435996	-3.334360	0.216170
H	1.725745	-3.723017	-0.766670
H	1.132422	-4.176470	0.845279
C	4.372642	-2.452600	4.236758
H	3.991889	-1.673356	4.909935
H	5.460228	-2.486777	4.364621
H	3.958141	-3.409094	4.570651
C	5.104369	0.192174	-0.001602
H	5.698347	0.800940	0.685868
H	4.438444	0.855411	-0.561727
H	5.793174	-0.256178	-0.727644
C	-2.408244	-1.666157	-1.483475
C	-2.816469	-2.135972	-2.752470
H	-3.677252	-2.747714	-2.977117
C	-1.893520	-1.617126	-3.648583
H	-1.816143	-1.705576	-4.722620
C	-3.025739	-1.857144	-0.156657
C	-3.341686	-0.714177	0.662324
C	-3.932046	-0.946282	1.940640
H	-4.172787	-0.083062	2.558118
C	-4.210799	-2.223822	2.404899
C	-3.877381	-3.320086	1.583687
H	-4.066917	-4.328909	1.945124
C	-3.289913	-3.155861	0.319645
C	-3.109078	0.618412	0.254217
H	-3.356894	1.437658	0.922791
H	-2.743811	0.867396	-0.734293
H	-0.706759	0.987410	1.922263
C	-4.848738	-2.455321	3.753596
H	-5.036278	-1.512071	4.275259
H	-4.207496	-3.075860	4.390881
H	-5.804836	-2.982258	3.649417
C	-2.930696	-4.387708	-0.482834
H	-1.950341	-4.287049	-0.958600
H	-3.658846	-4.579098	-1.279393
H	-2.910027	-5.269967	0.162823
C	-0.144782	2.978109	-1.448196
C	-0.158772	3.605809	-2.709189
H	-0.234294	4.663660	-2.911915
C	-0.037606	2.572273	-3.631577
H	0.005350	2.583572	-4.711081
C	-0.224755	3.508890	-0.067762
C	0.900990	3.395130	0.779097
C	0.784347	3.801528	2.113798
H	1.648537	3.708954	2.768121
C	-0.415269	4.310172	2.628725
C	-1.511039	4.433817	1.763374
H	-2.448556	4.834836	2.143802
C	-1.436276	4.046237	0.418891
C	2.208514	2.832602	0.270476
H	2.120612	1.762996	0.053033
H	3.000314	2.958037	1.013834
H	2.520634	3.325120	-0.657231
C	-0.533505	4.681794	4.087806
H	-0.893302	3.828064	4.677223
H	-1.241986	5.503182	4.236711
H	0.434578	4.979778	4.502874

C	-2.639563	4.204398	-0.481799
H	-3.542904	4.394135	0.105042
H	-2.806295	3.313444	-1.094642
H	-2.507434	5.046662	-1.171394
B	0.221412	-0.056288	-3.458286
H	0.274330	-0.082278	-4.653857
H	0.565561	-2.688825	0.065128

I-OOH_rot-T

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.341826
Thermal and entropic correction, BS1 (a.u.)	0.614301
Electronic Energy, BS2 (a.u.)	-2097.757792
Gibbs Energy, BS2 (a.u.)	-2097.143491
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	0.092252	-0.014763	-0.344536
O	-0.838707	0.192813	1.588282
O	0.213365	-0.803970	1.364691
N	-0.254700	1.458817	-1.662687
N	-0.287293	1.136384	-2.982981
N	1.611986	-0.712709	-1.516146
N	1.386028	-0.723690	-2.857974
N	-1.345867	-1.214854	-1.516278
N	-1.090744	-1.242345	-2.850372
C	-0.554076	2.767797	-1.551062
C	-0.788087	3.297075	-2.836797
H	-1.039025	4.317033	-3.086551
C	-0.605564	2.231717	-3.708769
H	-0.672942	2.173096	-4.785505
C	-0.587001	3.409457	-0.218431
C	0.583854	3.444784	0.574006
C	0.517737	4.017183	1.850292
H	1.418786	4.045102	2.459852
C	-0.672893	4.548314	2.362175
C	-1.818954	4.504060	1.557316
H	-2.754999	4.906086	1.940643
C	-1.798097	3.946441	0.273232
C	1.898284	2.885974	0.073942
H	2.071315	3.143006	-0.976224
H	2.732417	3.269088	0.668791
C	-0.712566	5.184417	3.731279
H	-1.700549	5.080089	4.191106
H	-0.492060	6.258054	3.669635
H	0.028050	4.736013	4.400864
C	-3.064221	3.923358	-0.553679
H	-3.939958	4.100870	0.077433
H	-3.196652	2.966379	-1.067426
H	-3.049238	4.702419	-1.325651
C	2.898108	-1.063351	-1.318854
C	3.511112	-1.302798	-2.566173
H	4.530771	-1.611369	-2.741971
C	2.517726	-1.078005	-3.508721
H	2.528281	-1.149072	-4.586785
C	3.455255	-1.161965	0.045681
C	2.937152	-2.150187	0.951705
C	3.495538	-2.210676	2.263203

H	3.105026	-2.954008	2.954866
C	4.507476	-1.353002	2.672945
C	4.989827	-0.394341	1.757849
H	5.772789	0.293206	2.071776
C	4.479458	-0.290043	0.454196
C	1.920938	-3.056185	0.581959
H	1.545126	-3.773895	1.303993
H	1.467094	-3.040801	-0.401669
C	5.088416	-1.428337	4.064982
H	4.967065	-0.475595	4.593860
H	6.163239	-1.643405	4.031612
H	4.604032	-2.209822	4.657434
C	5.034035	0.764052	-0.478189
H	4.243938	1.238000	-1.068097
H	5.750304	0.331388	-1.187067
H	5.555925	1.541653	0.087084
C	-2.340919	-2.086809	-1.285681
C	-2.732061	-2.697335	-2.497778
H	-3.510219	-3.432081	-2.643688
C	-1.912831	-2.128080	-3.463720
H	-1.858292	-2.282086	-4.532039
C	-2.854289	-2.229739	0.096666
C	-3.497973	-1.125628	0.709233
C	-3.900599	-1.233794	2.048693
H	-4.389624	-0.384164	2.521324
C	-3.693980	-2.408800	2.788038
C	-3.073862	-3.490368	2.152954
H	-2.899468	-4.406216	2.713968
C	-2.646209	-3.421796	0.819336
C	-3.757130	0.153508	-0.059707
H	-2.823138	0.628659	-0.376409
H	-4.315654	0.865717	0.553446
H	-4.333130	-0.047978	-0.970141
C	-4.144426	-2.497459	4.226193
H	-3.773465	-3.408349	4.704662
H	-5.239245	-2.502823	4.294627
H	-3.789631	-1.637256	4.804564
C	-1.939599	-4.597450	0.186297
H	-1.761878	-5.387560	0.921325
H	-0.974292	-4.292837	-0.232274
H	-2.526322	-5.024638	-0.634503
B	0.003965	-0.319656	-3.436370
H	0.021469	-0.390274	-4.631299
H	1.921288	1.791340	0.140638
H	-1.652868	-0.360471	1.570830

TS_{CO}-T

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.334876
Thermal and entropic correction, BS1 (a.u.)	0.615017
Electronic Energy, BS2 (a.u.)	-2097.751092
Gibbs Energy, BS2 (a.u.)	-2097.136075
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-524.0i

Molecular Geometry in Cartesian Coordinates

Cu	0.107027	0.042143	-0.319440
O	-0.848891	0.191250	1.508026

O	0.389473	-0.850700	1.316092
N	-0.359288	1.479246	-1.636240
N	-0.375029	1.159071	-2.958033
N	1.624196	-0.578377	-1.511568
N	1.394760	-0.616724	-2.850682
N	-1.295715	-1.259745	-1.526477
N	-1.041247	-1.265232	-2.859899
C	-0.713713	2.773705	-1.522768
C	-0.971169	3.295192	-2.807416
H	-1.266071	4.303787	-3.055178
C	-0.741113	2.241365	-3.681337
H	-0.805106	2.182282	-4.758234
C	-0.758529	3.418562	-0.192341
C	0.417801	3.506238	0.585227
C	0.343563	4.089178	1.857656
H	1.249519	4.157053	2.456733
C	-0.858603	4.584552	2.374969
C	-2.011247	4.491248	1.582003
H	-2.956146	4.867516	1.969920
C	-1.983555	3.918722	0.306014
C	1.748299	2.991641	0.080756
H	1.873257	3.171720	-0.991598
H	2.574238	3.471757	0.614008
C	-0.914930	5.234375	3.736972
H	-1.814175	4.931519	4.284117
H	-0.943079	6.327961	3.646869
H	-0.040976	4.973954	4.341657
C	-3.254587	3.839441	-0.509376
H	-4.129397	4.019112	0.122292
H	-3.368910	2.861549	-0.987606
H	-3.262023	4.590960	-1.308048
C	2.904737	-0.952517	-1.304917
C	3.506539	-1.234957	-2.550163
H	4.517927	-1.569793	-2.723791
C	2.515731	-1.013188	-3.494822
H	2.521506	-1.112678	-4.570551
C	3.480217	-1.031741	0.052168
C	2.845295	-1.832022	1.060693
C	3.441756	-1.892068	2.351339
H	2.954694	-2.495492	3.114017
C	4.607938	-1.203419	2.656608
C	5.200409	-0.415309	1.649610
H	6.101298	0.149714	1.880293
C	4.656768	-0.319141	0.360190
C	1.635113	-2.540844	0.831841
H	1.242456	-3.187195	1.608011
H	1.217361	-2.647976	-0.161298
C	5.230474	-1.274046	4.030396
H	5.307250	-0.276284	4.478177
H	6.246483	-1.683697	3.982082
H	4.641320	-1.903808	4.703053
C	5.330723	0.579019	-0.653599
H	4.599417	1.173192	-1.211231
H	5.907226	0.003520	-1.386842
H	6.021877	1.264237	-0.154435
C	-2.215366	-2.211484	-1.298108
C	-2.553777	-2.852975	-2.511116
H	-3.269891	-3.648149	-2.658353
C	-1.785076	-2.216163	-3.476401
H	-1.717474	-2.363534	-4.544983
C	-2.730969	-2.391126	0.078749

C	-3.461020	-1.335972	0.681999
C	-3.883260	-1.478068	2.010979
H	-4.437293	-0.665020	2.476164
C	-3.612536	-2.639124	2.751347
C	-2.906830	-3.672843	2.126381
H	-2.683626	-4.578118	2.687389
C	-2.457866	-3.569671	0.801797
C	-3.787334	-0.070476	-0.084442
H	-2.881506	0.491220	-0.334739
H	-4.441026	0.578377	0.504914
H	-4.288033	-0.302177	-1.031254
C	-4.077055	-2.760055	4.182904
H	-3.739491	-3.698193	4.632944
H	-5.171466	-2.728272	4.246463
H	-3.694769	-1.932825	4.792081
C	-1.677806	-4.703308	0.177374
H	-1.341716	-5.410481	0.941254
H	-0.800359	-4.333242	-0.362225
H	-2.289339	-5.257169	-0.545023
B	-0.004835	-0.271003	-3.429552
H	0.023134	-0.323033	-4.625334
H	1.842486	1.909790	0.235414
H	-1.591693	-0.447615	1.464721

C-T

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.407686
Thermal and entropic correction, BS1 (a.u.)	0.620126
Electronic Energy, BS2 (a.u.)	-2097.823876
Gibbs Energy, BS2 (a.u.)	-2097.203750
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-0.006553	-0.256263	-0.202087
O	-0.527387	-1.019080	1.440992
O	1.310240	0.730816	0.842617
N	-1.411917	-1.281199	-1.286266
N	-1.076513	-1.669029	-2.547998
N	0.126691	0.981630	-1.827051
N	0.127688	0.450297	-3.073101
N	1.598036	-1.463833	-1.253431
N	1.464065	-1.615668	-2.593727
C	-2.621426	-1.804011	-1.006731
C	-3.064155	-2.559462	-2.115217
H	-4.000271	-3.088749	-2.210259
C	-2.062167	-2.438970	-3.064760
H	-1.980205	-2.829355	-4.068868
C	-3.336941	-1.507491	0.253635
C	-3.614233	-0.170791	0.615498
C	-4.321121	0.076994	1.800893
H	-4.537675	1.108030	2.074999
C	-4.750540	-0.957232	2.638366
C	-4.461478	-2.276021	2.260052
H	-4.777416	-3.095892	2.902832
C	-3.765249	-2.569715	1.083415
C	-3.165805	1.005434	-0.222405
H	-3.202413	0.787725	-1.293775
H	-3.789786	1.881712	-0.021312

C	-5.514713	-0.672261	3.909723
H	-5.063566	-1.186220	4.766180
H	-6.551721	-1.022762	3.834879
H	-5.538252	0.399128	4.130175
C	-3.460755	-4.010998	0.740357
H	-3.635697	-4.655852	1.606696
H	-2.419873	-4.135033	0.423117
H	-4.092570	-4.377581	-0.077172
C	0.031475	2.322963	-1.950668
C	-0.025050	2.653929	-3.322306
H	-0.082287	3.639565	-3.757822
C	0.039303	1.439926	-3.990968
H	0.037071	1.208048	-5.046104
C	0.011602	3.179764	-0.751370
C	0.945580	2.971690	0.293546
C	0.909404	3.769668	1.443682
H	1.628553	3.579615	2.236895
C	-0.021645	4.802218	1.582112
C	-0.945429	4.994241	0.543724
H	-1.700276	5.771307	0.647461
C	-0.948562	4.212482	-0.617660
C	1.955809	1.833786	0.251889
H	2.838417	2.091878	0.848495
H	2.256674	1.602845	-0.777618
C	-0.032543	5.692198	2.800613
H	-1.055976	5.943557	3.097246
H	0.489065	6.636142	2.597635
H	0.466027	5.213205	3.648306
C	-2.003455	4.467247	-1.670121
H	-2.392975	3.532657	-2.084923
H	-1.605316	5.053481	-2.506633
H	-2.837588	5.030545	-1.242166
C	2.887825	-1.697319	-0.955763
C	3.598074	-2.021286	-2.137220
H	4.641387	-2.285744	-2.227023
C	2.655105	-1.951856	-3.151851
H	2.739787	-2.116714	-4.216669
C	3.340921	-1.554928	0.444118
C	2.704909	-2.296616	1.474708
C	3.110738	-2.098407	2.799672
H	2.624096	-2.670440	3.587717
C	4.126678	-1.195554	3.136928
C	4.756478	-0.489559	2.102205
H	5.551407	0.212816	2.345559
C	4.387525	-0.654662	0.763067
C	1.598316	-3.275933	1.184487
H	0.634329	-2.739832	1.152760
H	1.538958	-4.032166	1.974012
H	1.731175	-3.776858	0.221355
C	4.522777	-0.985705	4.578430
H	5.449536	-0.409931	4.659618
H	4.665485	-1.941693	5.094397
H	3.740808	-0.441087	5.122379
C	5.102840	0.142381	-0.303546
H	5.649985	0.977820	0.143342
H	4.406826	0.542035	-1.047470
H	5.829261	-0.475704	-0.844868
B	0.173759	-1.097840	-3.260518
H	0.152820	-1.370052	-4.426538
H	-2.129656	1.279596	0.013206
H	0.163373	-0.685386	2.042035

Triplet PES, pathway B

TS_{COH}-T

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.325232
Thermal and entropic correction, BS1 (a.u.)	0.612756
Electronic Energy, BS2 (a.u.)	-2097.741711
Gibbs Energy, BS2 (a.u.)	-2097.128955
Number of Imaginary Frequencies	1
Imaginary frequency (cm-1)	-692.6i

Molecular Geometry in Cartesian Coordinates

Cu	-0.229880	0.044123	-0.298418
O	-0.611721	-0.547338	1.445278
O	1.015659	-0.046711	1.295922
N	-1.815784	-0.215735	-1.486222
N	-1.588314	-0.403060	-2.815154
N	0.628725	1.298312	-1.639015
N	0.494139	1.008785	-2.959352
N	0.843455	-1.602175	-1.505047
N	0.699008	-1.483197	-2.849607
C	-3.132649	-0.388001	-1.266540
C	-3.767135	-0.697343	-2.487444
H	-4.819636	-0.877029	-2.647678
C	-2.754127	-0.694474	-3.435900
H	-2.774749	-0.872647	-4.501295
C	-3.704065	-0.212594	0.087149
C	-3.653335	1.054417	0.708424
C	-4.197125	1.198518	1.991134
H	-4.161010	2.174405	2.471443
C	-4.780828	0.122594	2.670664
C	-4.812871	-1.126217	2.035576
H	-5.250225	-1.976973	2.554540
C	-4.286970	-1.313817	0.752347
C	-3.016982	2.243453	0.024793
H	-3.282964	2.290862	-1.036472
H	-3.326544	3.177018	0.503699
C	-5.381702	0.304801	4.044126
H	-4.919671	1.144102	4.573820
H	-5.258881	-0.596723	4.653574
H	-6.458556	0.509488	3.977528
C	-4.323633	-2.683255	0.112840
H	-4.610062	-3.443541	0.845026
H	-3.347370	-2.956116	-0.301868
H	-5.045920	-2.723807	-0.710961
C	1.311619	2.459224	-1.543029
C	1.621381	2.918732	-2.840931
H	2.168048	3.811826	-3.103029
C	1.090011	1.969422	-3.701368
H	1.095419	1.902575	-4.779576
C	1.627502	3.073673	-0.235623
C	2.357897	2.348684	0.758983
C	2.649545	2.984078	1.993126
H	3.198764	2.422013	2.744937
C	2.252176	4.288783	2.260813
C	1.531263	4.977265	1.267757
H	1.195648	5.993092	1.466877

C	1.213547	4.396273	0.032067
C	2.779067	0.997020	0.574673
H	3.431369	0.543268	1.312851
H	2.717769	0.521337	-0.396941
C	2.567700	4.957375	3.576785
H	3.132709	4.292815	4.236572
H	1.648711	5.252531	4.096448
H	3.158049	5.868250	3.422747
C	0.413332	5.199521	-0.968926
H	-0.353814	4.588604	-1.454829
H	1.052118	5.608920	-1.760173
H	-0.079135	6.041285	-0.473881
C	1.759290	-2.562816	-1.293988
C	2.213236	-3.075279	-2.531182
H	2.934908	-3.862418	-2.692966
C	1.512724	-2.358368	-3.491067
H	1.530662	-2.405367	-4.570714
C	2.139265	-2.897892	0.098366
C	1.161059	-3.393366	0.993489
C	1.524325	-3.626517	2.328821
H	0.771743	-4.004625	3.017607
C	2.820586	-3.386620	2.796706
C	3.777486	-2.910743	1.888095
H	4.791848	-2.720837	2.234004
C	3.463419	-2.665843	0.546760
C	-0.260043	-3.648434	0.548342
H	-0.820456	-2.707267	0.563662
H	-0.753662	-4.351798	1.226138
H	-0.300124	-4.051849	-0.468055
C	3.183817	-3.615151	4.244662
H	3.322654	-2.660704	4.767570
H	4.122348	-4.173012	4.335698
H	2.401230	-4.171188	4.769151
C	4.532687	-2.151461	-0.390013
H	5.385741	-1.762989	0.173861
H	4.154808	-1.356365	-1.040012
H	4.902842	-2.949489	-1.044641
B	-0.160310	-0.327820	-3.411276
H	-0.209051	-0.377928	-4.606617
H	-1.922668	2.188361	0.075642
H	1.396268	-0.950518	1.225074

I-COH-T

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.401090
Thermal and entropic correction, BS1 (a.u.)	0.619841
Electronic Energy, BS2 (a.u.)	-2097.817051
Gibbs Energy, BS2 (a.u.)	-2097.197210
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-0.130768	-0.084332	-0.232820
O	-0.574490	-1.022454	1.264093
O	1.389689	0.853746	0.941924
N	-1.393961	-1.108871	-1.458987
N	-1.053010	-1.267519	-2.765385
N	-0.014206	1.347129	-1.674388
N	0.033731	0.978058	-2.979890

N	1.630453	-1.060719	-1.416537
N	1.469334	-1.067534	-2.763885
C	-2.487486	-1.856885	-1.224768
C	-2.853932	-2.520770	-2.415188
H	-3.697147	-3.178972	-2.561764
C	-1.922551	-2.115965	-3.360588
H	-1.818114	-2.358966	-4.408182
C	-3.152075	-1.843718	0.096451
C	-3.671746	-0.632607	0.606457
C	-4.326384	-0.647734	1.845527
H	-4.732797	0.283390	2.235525
C	-4.471975	-1.822725	2.590306
C	-3.943348	-3.011382	2.065781
H	-4.039877	-3.933990	2.635326
C	-3.287147	-3.044183	0.832033
C	-3.541421	0.671666	-0.148084
H	-3.712699	0.540800	-1.221555
H	-4.253207	1.410957	0.231515
C	-5.172943	-1.819683	3.928330
H	-4.471895	-2.049028	4.740085
H	-5.963787	-2.577820	3.963081
H	-5.624455	-0.845944	4.140248
C	-2.717865	-4.346647	0.317021
H	-2.712990	-5.103099	1.107365
H	-1.691801	-4.217370	-0.043108
H	-3.305277	-4.743407	-0.519304
C	-0.129460	2.690509	-1.633774
C	-0.151026	3.192511	-2.952072
H	-0.218459	4.225142	-3.258764
C	-0.043809	2.074646	-3.767090
H	-0.012757	1.978550	-4.842649
C	-0.193532	3.397347	-0.338691
C	0.776476	3.149301	0.658600
C	0.705705	3.824598	1.883879
H	1.461340	3.620482	2.639230
C	-0.307709	4.748600	2.151795
C	-1.267325	4.976838	1.154122
H	-2.075129	5.679451	1.349791
C	-1.233261	4.325474	-0.082849
C	1.879063	2.140791	0.464689
H	2.752076	2.412094	1.065953
H	2.175612	2.051394	-0.584447
C	-0.388610	5.468961	3.475574
H	0.464412	5.225009	4.115201
H	-1.303850	5.195568	4.013998
H	-0.409755	6.555502	3.333063
C	-2.321297	4.601928	-1.095621
H	-2.681921	3.678479	-1.560341
H	-1.966800	5.253333	-1.902623
H	-3.168907	5.100975	-0.617235
C	2.893734	-1.452636	-1.174846
C	3.558797	-1.718599	-2.393739
H	4.573562	-2.063256	-2.528171
C	2.613745	-1.460590	-3.376488
H	2.667446	-1.527934	-4.453812
C	3.370539	-1.528376	0.226312
C	2.751074	-2.425753	1.132584
C	3.181982	-2.440040	2.465061
H	2.708225	-3.129592	3.160970
C	4.199665	-1.594775	2.926652
C	4.804297	-0.722726	2.012933

H	5.598247	-0.060468	2.352035
C	4.413734	-0.676761	0.667700
C	1.627660	-3.336489	0.697484
H	0.678092	-2.785348	0.730765
H	1.550473	-4.196736	1.370235
H	1.773837	-3.701325	-0.323781
C	4.611175	-1.606335	4.379448
H	3.941692	-0.975352	4.977831
H	5.628579	-1.225080	4.510588
H	4.563829	-2.616883	4.797599
C	5.105730	0.278574	-0.278850
H	5.621911	1.066767	0.277009
H	4.400368	0.746970	-0.972052
H	5.853647	-0.242133	-0.888829
B	0.160422	-0.520622	-3.371412
H	0.167948	-0.635753	-4.563559
H	-2.534346	1.091269	-0.036572
H	2.126026	0.208724	0.896988

TS_{OHO}-T

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.387451
Thermal and entropic correction, BS1 (a.u.)	0.612350
Electronic Energy, BS2 (a.u.)	-2097.801507
Gibbs Energy, BS2 (a.u.)	-2097.189157
Number of Imaginary Frequencies	1
Imaginary frequency (cm-1)	-1074.6i

Molecular Geometry in Cartesian Coordinates

Cu	0.013181	-0.146372	-0.303286
O	1.304720	0.311445	1.075921
O	-0.979629	0.498857	1.291268
N	1.010946	-1.435428	-1.482419
N	0.896192	-1.290222	-2.828223
N	-1.636872	-0.286905	-1.498039
N	-1.391432	-0.224204	-2.837946
N	0.681796	1.482866	-1.635551
N	0.659122	1.208415	-2.964973
C	1.854084	-2.457431	-1.245050
C	2.298691	-2.978300	-2.478893
H	2.970167	-3.809636	-2.632142
C	1.666928	-2.212282	-3.449116
H	1.706663	-2.254528	-4.527995
C	2.147242	-2.877119	0.143137
C	1.098235	-3.315619	0.983281
C	1.397946	-3.680804	2.303329
H	0.590857	-4.023805	2.947788
C	2.700468	-3.621334	2.810348
C	3.725699	-3.193780	1.954536
H	4.745678	-3.140961	2.330712
C	3.474058	-2.820528	0.630520
C	-0.332843	-3.413175	0.500391
H	-0.389754	-3.675297	-0.560164
H	-0.880270	-4.166045	1.076014
C	2.995393	-3.979729	4.247463
H	3.060602	-3.075891	4.867309
H	3.951395	-4.506085	4.340023
H	2.210379	-4.614530	4.670822

C	4.612845	-2.349630	-0.245529
H	5.506171	-2.155649	0.355275
H	4.351638	-1.430314	-0.780052
H	4.875830	-3.098365	-1.002004
C	-2.979071	-0.215864	-1.330294
C	-3.591776	-0.098038	-2.597850
H	-4.647994	-0.014030	-2.802148
C	-2.555105	-0.106167	-3.514319
H	-2.555249	-0.036257	-4.592282
C	-3.676578	-0.262496	-0.023036
C	-3.315851	0.587351	1.052112
C	-4.068425	0.579115	2.229796
H	-3.770225	1.235768	3.044699
C	-5.176823	-0.260563	2.391710
C	-5.498411	-1.122145	1.338071
H	-6.333159	-1.810734	1.454219
C	-4.777145	-1.141947	0.135833
C	-2.050856	1.411081	1.019639
H	-2.073537	2.185731	1.794535
H	-1.905332	1.896681	0.046646
C	-5.995713	-0.235084	3.659212
H	-5.368144	-0.040390	4.534537
H	-6.520070	-1.182948	3.813643
H	-6.753508	0.557561	3.618625
C	-5.197650	-2.132675	-0.928776
H	-4.343460	-2.513877	-1.495012
H	-5.892788	-1.684259	-1.648644
H	-5.712368	-2.981491	-0.468249
C	1.361709	2.630460	-1.478081
C	1.775329	3.114341	-2.737654
H	2.331639	4.017385	-2.942951
C	1.311631	2.175558	-3.652000
H	1.396769	2.125488	-4.728311
C	1.584435	3.147781	-0.107482
C	2.709599	2.699964	0.622415
C	2.884920	3.155223	1.936274
H	3.748140	2.809611	2.501396
C	1.971048	4.025531	2.541432
C	0.864835	4.458398	1.794533
H	0.147263	5.138159	2.250271
C	0.657823	4.037509	0.475357
C	3.725393	1.780244	-0.013737
H	3.231519	0.984619	-0.577890
H	4.360443	1.317815	0.747642
H	4.372900	2.332934	-0.707706
C	2.153797	4.461679	3.975949
H	1.695636	3.738390	4.663505
H	1.685525	5.433659	4.161574
H	3.214523	4.533126	4.238965
C	-0.523291	4.552515	-0.314368
H	-1.292623	4.958564	0.348624
H	-0.972910	3.766151	-0.927358
H	-0.215498	5.353782	-0.997907
B	0.045120	-0.136501	-3.418607
H	0.013671	-0.212446	-4.612713
H	-0.862299	-2.460207	0.623784
H	0.179535	0.713302	1.478864

Open-shell singlet Potential Energy Surface

1-O_2-OS

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.369734
Thermal and entropic correction, BS1 (a.u.)	0.613778
Electronic Energy, BS2 (a.u.)	-2097.782520
Gibbs Energy, BS2 (a.u.)	-2097.168742
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	0.169361	-0.013114	-0.368400
O	-0.249717	-0.579859	1.430168
O	-0.126939	0.738620	1.378724
N	0.684357	-1.513274	-1.560704
N	0.562596	-1.304336	-2.899397
N	-1.736015	0.147480	-1.525516
N	-1.547633	0.061361	-2.869997
N	0.938480	1.349986	-1.583015
N	0.699035	1.201949	-2.913014
C	1.262390	-2.717301	-1.381141
C	1.519973	-3.293937	-2.639959
H	1.968699	-4.256572	-2.834407
C	1.059269	-2.368283	-3.567690
H	1.041745	-2.390139	-4.647748
C	1.499548	-3.238169	-0.016518
C	0.395249	-3.618798	0.777947
C	0.631309	-4.099831	2.070968
H	-0.216968	-4.397690	2.684021
C	1.927094	-4.204159	2.594292
C	3.005051	-3.819415	1.786070
H	4.017938	-3.892471	2.177425
C	2.814889	-3.340004	0.483800
C	-1.016673	-3.515678	0.247360
H	-1.118479	-4.030936	-0.714803
H	-1.729891	-3.953531	0.951137
C	2.154907	-4.692234	4.005356
H	3.100470	-5.237081	4.092134
H	1.345405	-5.351017	4.334739
H	2.197835	-3.849166	4.706691
C	4.005403	-2.945878	-0.360713
H	4.889284	-2.788309	0.264291
H	3.813467	-2.028591	-0.925575
H	4.249815	-3.726903	-1.091257
C	-3.063407	0.184447	-1.317667
C	-3.743436	0.114023	-2.554789
H	-4.810818	0.131908	-2.719175
C	-2.740974	0.038596	-3.511205
H	-2.785744	-0.023545	-4.589203
C	-3.591397	0.324544	0.059438
C	-3.332108	1.510125	0.782146
C	-3.809049	1.620034	2.094690
H	-3.607036	2.532337	2.652846
C	-4.531022	0.588077	2.706729
C	-4.777407	-0.577991	1.969088
H	-5.329221	-1.394399	2.431646
C	-4.322153	-0.727369	0.653418
C	-2.554250	2.648127	0.161666

H	-2.568593	3.528498	0.810854
H	-2.968791	2.929855	-0.813221
H	-1.511496	2.362583	-0.003960
C	-5.051952	0.730322	4.117449
H	-4.548343	1.543550	4.648855
H	-4.908555	-0.193203	4.688710
H	-6.127680	0.948198	4.118704
C	-4.609121	-2.004633	-0.103581
H	-3.732384	-2.349813	-0.660383
H	-5.416247	-1.862205	-0.832772
H	-4.918561	-2.799889	0.581183
C	1.649523	2.482054	-1.410658
C	1.863715	3.079513	-2.669013
H	2.407608	3.989677	-2.872426
C	1.249577	2.236605	-3.585843
H	1.167783	2.293000	-4.661577
C	2.085867	2.898773	-0.059911
C	2.954392	2.069652	0.686319
C	3.328196	2.471187	1.974696
H	3.998823	1.834911	2.549139
C	2.859937	3.662325	2.543128
C	2.005362	4.469972	1.781254
H	1.629235	5.397650	2.208140
C	1.609795	4.111513	0.487345
C	3.479728	0.763328	0.132846
H	2.748942	-0.046281	0.254351
H	4.390896	0.461166	0.657593
H	3.700066	0.834354	-0.936796
C	3.281723	4.075383	3.933189
H	3.448646	3.202632	4.572417
H	2.524046	4.708054	4.405927
H	4.218343	4.647218	3.907962
C	0.673569	5.010284	-0.288133
H	0.223908	5.758866	0.370636
H	-0.132052	4.440133	-0.761727
H	1.201516	5.544081	-1.087129
B	-0.113956	-0.013555	-3.437221
H	-0.126196	-0.020225	-4.633667
H	-1.302705	-2.472106	0.082253

TS_{CH}-OS

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.337040
Thermal and entropic correction, BS1 (a.u.)	0.611195
Electronic Energy, BS2 (a.u.)	-2097.750489
Gibbs Energy, BS2 (a.u.)	-2097.139294
Number of Imaginary Frequencies	1
Imaginary frequency (cm-1)	-1547.5i

Molecular Geometry in Cartesian Coordinates

Cu	-0.281577	-0.095757	-0.323675
O	0.593208	0.097766	1.387354
O	-0.421569	-0.872074	1.555157
N	0.149551	1.297670	-1.727226
N	0.056328	0.891299	-3.023633
N	1.165215	-1.408608	-1.414626
N	0.941298	-1.446736	-2.754334
N	-1.776756	-0.811717	-1.426580

N	-1.553457	-1.019460	-2.749689
C	0.445115	2.610274	-1.729972
C	0.538375	3.062138	-3.062452
H	0.770160	4.062109	-3.397630
C	0.289385	1.941486	-3.843909
H	0.268734	1.811515	-4.916321
C	0.666318	3.318440	-0.448439
C	1.797167	2.984801	0.329066
C	1.989705	3.640042	1.552393
H	2.861174	3.386675	2.152923
C	1.089846	4.603244	2.023412
C	-0.024237	4.917734	1.232043
H	-0.736254	5.661592	1.585327
C	-0.250954	4.294167	-0.000357
C	2.788756	1.943808	-0.139038
H	3.095302	2.125294	-1.175430
H	3.682393	1.947530	0.491805
C	1.302190	5.286883	3.353502
H	0.475964	5.071704	4.041685
H	1.348478	6.376149	3.237405
H	2.230523	4.955533	3.827765
C	-1.460377	4.667424	-0.827274
H	-2.208914	5.176289	-0.212803
H	-1.927054	3.788083	-1.281455
H	-1.187452	5.344842	-1.645909
C	2.325885	-2.055577	-1.192587
C	2.845286	-2.535097	-2.418719
H	3.748191	-3.107292	-2.570806
C	1.937129	-2.121851	-3.379814
H	1.925015	-2.253083	-4.452360
C	2.908505	-2.137192	0.163051
C	2.155781	-2.668505	1.258592
C	2.754934	-2.709954	2.545803
H	2.170981	-3.109617	3.371894
C	4.047892	-2.257530	2.770456
C	4.764176	-1.735005	1.676338
H	5.770209	-1.353668	1.838786
C	4.222771	-1.670648	0.385235
C	0.793445	-3.118447	1.122883
H	0.399576	-3.746545	1.922264
H	0.408082	-3.334541	0.128558
H	0.103063	-1.901692	1.411673
C	4.676877	-2.303047	4.141658
H	3.993548	-2.732352	4.879771
H	4.952980	-1.296766	4.478012
H	5.594410	-2.903184	4.134957
C	5.055981	-1.062659	-0.721516
H	4.454284	-0.425448	-1.375896
H	5.514172	-1.833177	-1.352147
H	5.865255	-0.460075	-0.299026
C	-3.022461	-1.240429	-1.144817
C	-3.609444	-1.746096	-2.323331
H	-4.603936	-2.151559	-2.434714
C	-2.647037	-1.582163	-3.311119
H	-2.661130	-1.816254	-4.365715
C	-3.565696	-1.097929	0.224701
C	-3.708401	0.190301	0.786728
C	-4.198507	0.306765	2.094391
H	-4.313605	1.299450	2.525166
C	-4.541360	-0.815288	2.857105
C	-4.391982	-2.082975	2.277174

H	-4.650667	-2.967183	2.856659
C	-3.910988	-2.245665	0.973485
C	-3.340378	1.438055	0.015010
H	-2.253028	1.583223	-0.008115
H	-3.783067	2.324214	0.478873
H	-3.674191	1.383649	-1.026455
C	-5.033285	-0.672242	4.277686
H	-4.227172	-0.886114	4.990929
H	-5.848477	-1.372163	4.490099
H	-5.389947	0.342856	4.476591
C	-3.739260	-3.634300	0.400485
H	-3.919115	-4.393787	1.166896
H	-2.727108	-3.778881	0.005928
H	-4.433542	-3.821194	-0.426428
B	-0.200266	-0.602326	-3.375508
H	-0.229121	-0.747923	-4.563450
H	2.353065	0.939902	-0.099771

I-OOH-OS

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.342590
Thermal and entropic correction, BS1 (a.u.)	0.612889
Electronic Energy, BS2 (a.u.)	-2097.757677
Gibbs Energy, BS2 (a.u.)	-2097.144788
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-0.211600	0.009260	-0.341289
O	0.656692	0.129278	1.347341
O	-0.376939	-0.885027	1.542499
N	0.197696	1.587728	-1.567471
N	0.114405	1.344295	-2.904466
N	1.221445	-1.178891	-1.566574
N	1.078470	-0.978817	-2.902883
N	-1.665209	-0.610624	-1.543465
N	-1.422190	-0.643271	-2.879577
C	0.422373	2.904783	-1.407060
C	0.479305	3.524414	-2.672722
H	0.655429	4.569397	-2.880219
C	0.283753	2.498981	-3.588055
H	0.260836	2.502598	-4.668347
C	0.607093	3.474115	-0.053397
C	1.749747	3.117523	0.694726
C	1.912108	3.661474	1.975884
H	2.793491	3.390521	2.553605
C	0.970519	4.535638	2.531504
C	-0.159592	4.868662	1.770632
H	-0.905660	5.541564	2.189643
C	-0.357385	4.354742	0.484313
C	2.785309	2.168571	0.135431
H	3.090183	2.461538	-0.875829
H	3.675063	2.146002	0.771448
C	1.159044	5.112473	3.915010
H	0.318325	4.852332	4.568925
H	1.213968	6.207337	3.882591
H	2.076807	4.741421	4.380542
C	-1.587544	4.739872	-0.306005

H	-2.338985	5.197418	0.344180
H	-2.039262	3.872101	-0.796981
H	-1.344049	5.462473	-1.094355
C	2.381859	-1.839741	-1.390086
C	2.992744	-2.071398	-2.644861
H	3.917734	-2.594101	-2.837876
C	2.131637	-1.507179	-3.573050
H	2.186436	-1.443805	-4.650441
C	2.842919	-2.213049	-0.038055
C	1.994496	-2.991754	0.829152
C	2.476950	-3.322734	2.132940
H	1.831647	-3.907309	2.785035
C	3.726411	-2.920412	2.578183
C	4.531135	-2.158125	1.706090
H	5.506522	-1.820136	2.049600
C	4.111554	-1.803328	0.414142
C	0.708569	-3.437833	0.446312
H	0.132236	-4.066620	1.120137
H	0.304342	-3.246566	-0.540945
H	0.115915	-1.735304	1.398354
C	4.225696	-3.272343	3.958529
H	3.496941	-3.878882	4.503686
H	4.422964	-2.367692	4.545505
H	5.165936	-3.833495	3.904982
C	5.033460	-0.968997	-0.447514
H	4.484685	-0.205911	-1.006879
H	5.563986	-1.588574	-1.180110
H	5.786839	-0.471526	0.170194
C	-2.885015	-1.142203	-1.331014
C	-3.435889	-1.530431	-2.569996
H	-4.405361	-1.973386	-2.741837
C	-2.479260	-1.193102	-3.518281
H	-2.474724	-1.296746	-4.593607
C	-3.445467	-1.212622	0.036819
C	-3.658969	-0.024553	0.770596
C	-4.182970	-0.116377	2.067137
H	-4.354851	0.799455	2.629373
C	-4.483973	-1.348551	2.657587
C	-4.258533	-2.514521	1.911819
H	-4.482901	-3.482715	2.355880
C	-3.745886	-2.469433	0.611081
C	-3.324747	1.336302	0.202075
H	-2.254809	1.555679	0.312807
H	-3.876361	2.121358	0.727593
H	-3.554052	1.400774	-0.866000
C	-5.008420	-1.428378	4.071465
H	-4.203529	-1.692181	4.769283
H	-5.785146	-2.194576	4.167242
H	-5.426507	-0.471145	4.397311
C	-3.498485	-3.755950	-0.144011
H	-3.620709	-4.619214	0.516414
H	-2.486342	-3.784193	-0.562293
H	-4.193591	-3.875861	-0.982685
B	-0.081868	-0.102007	-3.435833
H	-0.094574	-0.104522	-4.632926
H	2.389269	1.149821	0.071961

Open-shell singlet PES, pathway A

TS_{rot}-OS

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.340637
Thermal and entropic correction, BS1 (a.u.)	0.616093
Electronic Energy, BS2 (a.u.)	-2097.756304
Gibbs Energy, BS2 (a.u.)	-2097.140211
Number of Imaginary Frequencies	1
Imaginary frequency (cm-1)	-38.5i

Molecular Geometry in Cartesian Coordinates

Cu	0.090982	0.011975	-0.358247
O	0.049504	-0.840100	1.322001
O	-0.211325	0.534036	1.736110
N	1.724487	-0.767564	-1.440813
N	1.563316	-0.785142	-2.792413
N	-1.241259	-1.137251	-1.547290
N	-0.936875	-1.186777	-2.869199
N	-0.090766	1.482353	-1.698145
N	-0.027792	1.146648	-3.013943
C	2.980145	-1.175872	-1.182897
C	3.641831	-1.459887	-2.396839
H	4.654177	-1.815371	-2.520858
C	2.706028	-1.199876	-3.388246
H	2.764398	-1.282455	-4.464148
C	3.460555	-1.288087	0.213979
C	2.938607	-2.303351	1.045940
C	3.394293	-2.393430	2.365673
H	2.995935	-3.177097	3.007454
C	4.340923	-1.498276	2.883499
C	4.844495	-0.501711	2.038375
H	5.580261	0.202396	2.422663
C	4.422629	-0.382447	0.706980
C	1.915779	-3.283741	0.520925
H	2.271145	-3.774286	-0.393438
H	1.700789	-4.056847	1.264605
C	4.778660	-1.589586	4.326504
H	4.065531	-1.073545	4.982230
H	5.759564	-1.128134	4.478650
H	4.831866	-2.630814	4.661865
C	5.000857	0.700630	-0.175154
H	5.508041	1.461087	0.426028
H	4.225641	1.192921	-0.770820
H	5.733762	0.289636	-0.880467
C	-2.322269	-1.916692	-1.350025
C	-2.714386	-2.485978	-2.585091
H	-3.548287	-3.146762	-2.767773
C	-1.813116	-1.992891	-3.516028
H	-1.731787	-2.150877	-4.581995
C	-2.926531	-2.047638	-0.009956
C	-3.218307	-0.870078	0.772653
C	-3.771964	-1.045434	2.077879
H	-3.983716	-0.155290	2.666886
C	-4.048643	-2.298972	2.601435
C	-3.767665	-3.427752	1.805674

H	-3.967814	-4.419431	2.206346
C	-3.215862	-3.321056	0.518566
C	-3.009682	0.447798	0.308926
H	-3.293786	1.289660	0.935067
H	-2.647082	0.663322	-0.688284
H	-1.194555	0.558726	1.761004
C	-4.629338	-2.469870	3.984145
H	-4.774294	-1.505090	4.479199
H	-3.969653	-3.079834	4.612713
H	-5.598457	-2.981530	3.943137
C	-2.929977	-4.593546	-0.248725
H	-1.985547	-4.534177	-0.798118
H	-3.719045	-4.805921	-0.980409
H	-2.879046	-5.446353	0.434267
C	-0.393948	2.793464	-1.620748
C	-0.526394	3.311797	-2.924847
H	-0.753037	4.330590	-3.201514
C	-0.286287	2.236550	-3.771114
H	-0.276895	2.167262	-4.849331
C	-0.541993	3.430850	-0.293849
C	0.564897	3.476288	0.584444
C	0.388997	4.016249	1.863664
H	1.240290	4.051448	2.540541
C	-0.851188	4.503917	2.296112
C	-1.928817	4.463997	1.402028
H	-2.897700	4.845809	1.718831
C	-1.797154	3.938902	0.109736
C	1.923759	2.960517	0.166010
H	1.958482	1.864831	0.171785
H	2.699952	3.318514	0.848482
H	2.177292	3.280176	-0.850375
C	-1.029559	5.026394	3.701905
H	-1.260742	4.205311	4.393949
H	-1.852189	5.746843	3.759648
H	-0.117752	5.511730	4.065957
C	-2.993184	3.921632	-0.815632
H	-3.920818	4.053074	-0.250656
H	-3.061424	2.984090	-1.375634
H	-2.937740	4.731287	-1.553707
B	0.229307	-0.329284	-3.428681
H	0.281642	-0.422600	-4.620967
H	0.977252	-2.777376	0.272084

I-OOH_rot-OS

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.341750
Thermal and entropic correction, BS1 (a.u.)	0.613709
Electronic Energy, BS2 (a.u.)	-2097.757798
Gibbs Energy, BS2 (a.u.)	-2097.144089
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	0.087735	-0.076596	-0.329716
O	-0.891187	0.199372	1.607838
O	0.084462	-0.867875	1.376660
N	-0.108511	1.367953	-1.701880
N	-0.167053	0.991377	-3.006941

N	1.587348	-0.923505	-1.449699
N	1.369158	-0.972449	-2.792240
N	-1.437915	-1.179164	-1.468647
N	-1.140114	-1.317649	-2.786954
C	-0.290580	2.702439	-1.649254
C	-0.474649	3.192114	-2.958948
H	-0.633860	4.218152	-3.254721
C	-0.385071	2.077483	-3.782031
H	-0.454027	1.977445	-4.855571
C	-0.271064	3.405378	-0.347837
C	0.879543	3.340069	0.472099
C	0.857060	3.977240	1.719694
H	1.742359	3.924668	2.350389
C	-0.268755	4.672258	2.175840
C	-1.395556	4.727382	1.343881
H	-2.283576	5.256380	1.684917
C	-1.417281	4.110626	0.087975
C	2.126244	2.597249	0.045188
H	2.299116	2.677349	-1.031914
H	3.003914	2.984522	0.570975
C	-0.267016	5.364467	3.517960
H	-1.235951	5.262873	4.018403
H	-0.071459	6.438553	3.404560
H	0.504548	4.955275	4.177356
C	-2.664493	4.200061	-0.762603
H	-3.533118	4.449556	-0.145778
H	-2.869461	3.261155	-1.285139
H	-2.569990	4.979707	-1.528714
C	2.857034	-1.322112	-1.233208
C	3.464683	-1.632759	-2.467461
H	4.470563	-1.992119	-2.625126
C	2.486987	-1.398541	-3.423487
H	2.499350	-1.507622	-4.498347
C	3.412404	-1.392802	0.133706
C	2.849222	-2.315511	1.081182
C	3.410446	-2.352136	2.392091
H	2.986178	-3.046867	3.113844
C	4.467789	-1.532749	2.763888
C	4.995619	-0.640051	1.808440
H	5.816590	0.016234	2.090503
C	4.484676	-0.561958	0.503117
C	1.788655	-3.184298	0.750307
H	1.382545	-3.856121	1.499700
H	1.333028	-3.185163	-0.232387
C	5.047555	-1.578681	4.157533
H	4.939657	-0.609997	4.659993
H	6.118985	-1.809880	4.131123
H	4.550849	-2.335694	4.771048
C	5.094126	0.420914	-0.472339
H	4.334556	0.886064	-1.106976
H	5.812511	-0.073185	-1.137833
H	5.629381	1.211443	0.061816
C	-2.490390	-1.974219	-1.214913
C	-2.873975	-2.649219	-2.395274
H	-3.691958	-3.343531	-2.519647
C	-1.990980	-2.198168	-3.367141
H	-1.910977	-2.429728	-4.419729
C	-3.087286	-1.969361	0.140367
C	-3.662716	-0.770619	0.633048
C	-4.176477	-0.752909	1.938022
H	-4.614151	0.168447	2.317141

C	-4.147070	-1.890230	2.759532
C	-3.584797	-3.063675	2.244194
H	-3.544983	-3.953055	2.869578
C	-3.049489	-3.123345	0.949861
C	-3.726818	0.480439	-0.219055
H	-2.731212	0.910716	-0.372087
H	-4.355928	1.237833	0.256582
H	-4.132815	0.261167	-1.212544
C	-4.713730	-1.837332	4.158222
H	-4.588764	-2.792420	4.676884
H	-5.784069	-1.598979	4.139529
H	-4.221073	-1.059426	4.753178
C	-2.408484	-4.397514	0.451458
H	-2.364949	-5.147109	1.246684
H	-1.388594	-4.207704	0.098557
H	-2.965597	-4.827489	-0.388473
B	0.021642	-0.499931	-3.398062
H	0.042854	-0.620394	-4.589017
H	2.053748	1.527345	0.278201
H	-1.745505	-0.284967	1.549333

TS_{CO}-OS

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.334316
Thermal and entropic correction, BS1 (a.u.)	0.615508
Electronic Energy, BS2 (a.u.)	-2097.750404
Gibbs Energy, BS2 (a.u.)	-2097.134896
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-523.0i

Molecular Geometry in Cartesian Coordinates

Cu	0.115239	0.025668	-0.312112
O	-0.857813	0.217879	1.471612
O	0.388722	-0.836086	1.352877
N	-0.348155	1.469286	-1.636485
N	-0.366496	1.148423	-2.958119
N	1.629556	-0.591705	-1.512898
N	1.404745	-0.621481	-2.852546
N	-1.282899	-1.273209	-1.525450
N	-1.030438	-1.276348	-2.859421
C	-0.702153	2.764355	-1.524520
C	-0.960596	3.284687	-2.809464
H	-1.254884	4.293350	-3.057606
C	-0.732489	2.229887	-3.682424
H	-0.797669	2.169353	-4.759169
C	-0.749199	3.415435	-0.197214
C	0.424234	3.504965	0.584261
C	0.346914	4.097381	1.852085
H	1.250606	4.166603	2.454340
C	-0.856105	4.598228	2.362167
C	-2.005752	4.503028	1.565416
H	-2.951160	4.883862	1.947564
C	-1.974644	3.922825	0.293006
C	1.754820	2.981686	0.089330
H	1.885761	3.154205	-0.983466
H	2.580336	3.461528	0.623596
C	-0.916817	5.254973	3.720622

H	-1.820719	4.959366	4.263809
H	-0.938759	6.348222	3.625497
H	-0.047987	4.992732	4.331557
C	-3.243207	3.843029	-0.526138
H	-4.119840	4.022776	0.103092
H	-3.356203	2.865176	-1.004820
H	-3.248622	4.594694	-1.324745
C	2.915007	-0.947247	-1.306060
C	3.525258	-1.209905	-2.551643
H	4.541801	-1.528539	-2.725778
C	2.533644	-0.994636	-3.496988
H	2.543575	-1.085359	-4.573454
C	3.479113	-1.033775	0.054795
C	2.824784	-1.829863	1.055104
C	3.404430	-1.895229	2.353341
H	2.902810	-2.494785	3.109583
C	4.573104	-1.217151	2.673007
C	5.184688	-0.434154	1.673632
H	6.087778	0.122527	1.915569
C	4.657512	-0.331670	0.377417
C	1.613423	-2.530860	0.810453
H	1.207424	-3.174593	1.581889
H	1.206105	-2.636296	-0.187013
C	5.179052	-1.294250	4.053986
H	5.258357	-0.297609	4.503960
H	6.192421	-1.711705	4.016816
H	4.577499	-1.920284	4.718968
C	5.351227	0.562920	-0.626413
H	4.631217	1.162784	-1.192809
H	5.933850	-0.015722	-1.352555
H	6.040395	1.242844	-0.117289
C	-2.216407	-2.212410	-1.300299
C	-2.565684	-2.843683	-2.515540
H	-3.293072	-3.628256	-2.665206
C	-1.789362	-2.213367	-3.479076
H	-1.726089	-2.356303	-4.548555
C	-2.734230	-2.388006	0.076455
C	-3.459709	-1.327987	0.676449
C	-3.881438	-1.463842	2.006236
H	-4.431673	-0.646996	2.469302
C	-3.614807	-2.623696	2.750148
C	-2.914099	-3.662545	2.128101
H	-2.694382	-4.566987	2.691863
C	-2.465747	-3.565390	0.802795
C	-3.780930	-0.064209	-0.094918
H	-2.871927	0.486580	-0.357573
H	-4.422804	0.594865	0.496221
H	-4.293100	-0.297519	-1.035328
C	-4.080536	-2.738612	4.181803
H	-3.731681	-3.668140	4.640707
H	-5.175381	-2.721387	4.242559
H	-3.711462	-1.900980	4.784449
C	-1.691613	-4.704122	0.180287
H	-1.359317	-5.412140	0.945103
H	-0.812252	-4.339546	-0.359919
H	-2.306146	-5.255609	-0.541429
B	0.004439	-0.281215	-3.430263
H	0.030574	-0.332972	-4.626113
H	1.843657	1.900468	0.251344
H	-1.594751	-0.428359	1.454939

C-CSS

Charge	0
Spin State	Closed-shell singlet
Electronic Energy, BS1 (a.u.)	-2097.421713
Thermal and entropic correction, BS1 (a.u.)	0.622276
Electronic Energy, BS2 (a.u.)	-2097.838041
Gibbs Energy, BS2 (a.u.)	-2097.215765
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	0.039495	0.119828	-0.256110
O	-0.137067	1.359710	1.048253
O	-0.600545	-1.048318	1.001299
N	0.786336	1.482614	-1.421810
N	0.336802	1.573623	-2.700634
N	0.441171	-1.189405	-1.641142
N	0.173032	-0.880227	-2.937348
N	-2.060090	0.400063	-1.383912
N	-1.942492	0.466590	-2.734393
C	1.621852	2.515417	-1.184697
C	1.698413	3.295625	-2.355994
H	2.297938	4.181092	-2.502788
C	0.880812	2.664369	-3.281968
H	0.655849	2.897686	-4.312395
C	2.347116	2.680197	0.092418
C	3.212995	1.663017	0.550569
C	3.896207	1.852366	1.758923
H	4.568352	1.070884	2.108727
C	3.737939	3.013212	2.524530
C	2.877533	4.010214	2.045169
H	2.739998	4.919581	2.627256
C	2.179366	3.866124	0.841352
C	3.411848	0.373273	-0.213504
H	3.403143	0.528746	-1.296827
H	4.358292	-0.099086	0.065588
C	4.451518	3.174989	3.845541
H	3.829664	2.803878	4.670322
H	4.675538	4.226180	4.053765
H	5.389842	2.611410	3.864542
C	1.246815	4.963479	0.381986
H	1.056875	5.671372	1.193989
H	0.286240	4.557236	0.049484
H	1.668174	5.527920	-0.458002
C	1.130995	-2.355800	-1.618757
C	1.288266	-2.802617	-2.945973
H	1.767558	-3.712917	-3.271108
C	0.673141	-1.844607	-3.737290
H	0.543849	-1.780503	-4.807693
C	1.553627	-2.997784	-0.362051
C	0.636564	-3.096675	0.710297
C	1.010144	-3.757907	1.881964
H	0.293261	-3.825623	2.698005
C	2.282279	-4.327799	2.027685
C	3.187245	-4.191755	0.968499
H	4.190877	-4.598758	1.074897
C	2.853400	-3.538661	-0.226462
C	-0.710179	-2.412829	0.643479
H	-1.385599	-2.849670	1.393837

H	-1.190961	-2.540526	-0.335803
C	2.657173	-5.063361	3.291257
H	2.394335	-4.480522	4.180788
H	3.728998	-5.278933	3.325757
H	2.119777	-6.017476	3.359554
C	3.902981	-3.410396	-1.306855
H	3.834531	-2.450733	-1.827609
H	3.805004	-4.198952	-2.062723
H	4.903985	-3.497468	-0.874076
C	-3.372962	0.313468	-1.115944
C	-4.113819	0.324244	-2.323182
H	-5.187698	0.283512	-2.434506
C	-3.162235	0.422143	-3.327572
H	-3.258134	0.465727	-4.403335
C	-3.847626	0.246503	0.287830
C	-3.712701	1.376414	1.123102
C	-4.126267	1.284279	2.459071
H	-4.019040	2.154903	3.103759
C	-4.670855	0.105819	2.984552
C	-4.802284	-1.000232	2.133792
H	-5.217623	-1.927361	2.525041
C	-4.403503	-0.948988	0.792340
C	-3.109128	2.660011	0.603577
H	-2.020559	2.550979	0.527152
H	-3.331471	3.494570	1.276287
H	-3.490396	2.906434	-0.393467
C	-5.136028	0.037565	4.420509
H	-4.605070	0.761151	5.047038
H	-4.982896	-0.960881	4.843231
H	-6.208050	0.261459	4.496691
C	-4.560595	-2.168163	-0.087901
H	-4.771090	-3.057772	0.513482
H	-3.658018	-2.355742	-0.678130
H	-5.386287	-2.044257	-0.799185
B	-0.532794	0.450949	-3.330906
H	-0.557729	0.562443	-4.521542
H	2.611751	-0.341728	0.014823
H	-0.637294	0.837107	1.703390

Open-shell singlet PES, pathway B

TS_{COH}-OS

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.323577
Thermal and entropic correction, BS1 (a.u.)	0.611638
Electronic Energy, BS2 (a.u.)	-2097.740084
Gibbs Energy, BS2 (a.u.)	-2097.128446
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-684.2i

Molecular Geometry in Cartesian Coordinates

Cu	-0.204921	0.036122	-0.296456
O	-0.535561	-0.623633	1.416849
O	1.025247	0.105228	1.311710
N	-1.744785	-0.440569	-1.495216
N	-1.493622	-0.609501	-2.821658

N	0.466505	1.375158	-1.644532
N	0.375478	1.070860	-2.964615
N	1.070916	-1.468895	-1.499030
N	0.917761	-1.371225	-2.844684
C	-3.025276	-0.788886	-1.270919
C	-3.611199	-1.195741	-2.488246
H	-4.629862	-1.516439	-2.646147
C	-2.608495	-1.064237	-3.438210
H	-2.605011	-1.254528	-4.501753
C	-3.620237	-0.673341	0.078637
C	-3.689987	0.588646	0.710074
C	-4.277684	0.676678	1.978134
H	-4.339375	1.649719	2.461567
C	-4.791265	-0.447498	2.634829
C	-4.702761	-1.689401	1.992288
H	-5.087219	-2.576362	2.491880
C	-4.124736	-1.824154	0.725237
C	-3.138768	1.836150	0.056940
H	-3.322500	1.848338	-1.022551
H	-3.582381	2.734462	0.497848
C	-5.397250	-0.332054	4.013123
H	-4.646482	-0.534456	4.787936
H	-6.211535	-1.050966	4.153366
H	-5.790916	0.673347	4.192250
C	-4.024970	-3.190317	0.085133
H	-4.255764	-3.974208	0.812083
H	-3.018434	-3.371410	-0.306335
H	-4.721118	-3.298959	-0.754760
C	0.962119	2.625722	-1.545478
C	1.196612	3.131472	-2.841830
H	1.599409	4.098279	-3.102820
C	0.815054	2.114036	-3.704259
H	0.828954	2.052359	-4.782722
C	1.180426	3.267106	-0.231676
C	2.004666	2.647358	0.759606
C	2.202927	3.311196	1.997035
H	2.828042	2.830235	2.745624
C	1.618624	4.542019	2.273162
C	0.798604	5.120585	1.287018
H	0.312157	6.071068	1.495976
C	0.571252	4.509367	0.046447
C	2.602902	1.362111	0.573888
H	3.318768	1.007390	1.307764
H	2.615260	0.887508	-0.400472
C	1.840740	5.245744	3.590105
H	2.452290	4.642051	4.266365
H	0.887699	5.457312	4.088385
H	2.347160	6.206905	3.440723
C	-0.349138	5.182475	-0.946445
H	-1.040305	4.465126	-1.401096
H	0.210303	5.654857	-1.762029
H	-0.935573	5.962182	-0.451954
C	2.093442	-2.312943	-1.282879
C	2.609463	-2.770306	-2.517341
H	3.420029	-3.466415	-2.674535
C	1.832136	-2.144040	-3.481314
H	1.858159	-2.192044	-4.560741
C	2.503423	-2.611132	0.109448
C	1.594336	-3.242202	0.991210
C	1.986161	-3.461237	2.321379
H	1.286056	-3.943412	3.000337

C	3.245394	-3.078856	2.795845
C	4.133763	-2.463798	1.901198
H	5.117686	-2.158577	2.252966
C	3.788320	-2.225517	0.566321
C	0.213396	-3.656966	0.539708
H	-0.454963	-2.789356	0.578887
H	-0.190087	-4.431137	1.199670
H	0.218121	-4.036016	-0.486890
C	3.641871	-3.305309	4.235819
H	3.724814	-2.352489	4.773491
H	4.616514	-3.801431	4.305755
H	2.905845	-3.921950	4.760118
C	4.780338	-1.555811	-0.357422
H	5.584632	-1.083702	0.215266
H	4.301934	-0.791422	-0.978249
H	5.238449	-2.280519	-1.041282
B	-0.086484	-0.343887	-3.414708
H	-0.122471	-0.404421	-4.610035
H	-2.052036	1.897490	0.196692
H	1.520411	-0.741599	1.250466

I-COH-OS

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.395777
Thermal and entropic correction, BS1 (a.u.)	0.620842
Electronic Energy, BS2 (a.u.)	-2097.811940
Gibbs Energy, BS2 (a.u.)	-2097.191098
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-0.141058	-0.077885	-0.230365
O	-0.590016	-1.004110	1.276235
O	1.388657	0.843587	0.936509
N	-1.404028	-1.095019	-1.459808
N	-1.057433	-1.266892	-2.763211
N	0.005718	1.334893	-1.675535
N	0.059298	0.961333	-2.979634
N	1.624621	-1.090515	-1.412110
N	1.467738	-1.102493	-2.759672
C	-2.503443	-1.834412	-1.224239
C	-2.868407	-2.504943	-2.411151
H	-3.715476	-3.158462	-2.556190
C	-1.929801	-2.114294	-3.355307
H	-1.821899	-2.366511	-4.400359
C	-3.172764	-1.812932	0.094363
C	-3.691807	-0.599200	0.597898
C	-4.352252	-0.608803	1.833712
H	-4.757973	0.324560	2.219158
C	-4.502542	-1.780884	2.582393
C	-3.973042	-2.972091	2.064850
H	-4.072498	-3.892223	2.637876
C	-3.311162	-3.010294	0.834214
C	-3.549784	0.702783	-0.157981
H	-3.712546	0.571466	-1.232733
H	-4.260714	1.446466	0.214583
C	-5.209180	-1.771825	3.917342
H	-4.512308	-2.001625	4.732549

H	-6.002973	-2.526970	3.950802
H	-5.658091	-0.795894	4.124846
C	-2.738811	-4.314727	0.327406
H	-2.739312	-5.068462	1.120334
H	-1.710059	-4.186494	-0.025645
H	-3.320459	-4.714247	-0.511654
C	-0.092225	2.680204	-1.638990
C	-0.096518	3.178098	-2.958628
H	-0.147681	4.210783	-3.268230
C	0.002342	2.056690	-3.769739
H	0.040824	1.956983	-4.844701
C	-0.156055	3.395364	-0.348500
C	0.809185	3.146746	0.653095
C	0.741848	3.832696	1.872465
H	1.493345	3.627777	2.631656
C	-0.263426	4.768821	2.129420
C	-1.218464	4.997483	1.127487
H	-2.019904	5.709583	1.314916
C	-1.187708	4.335104	-0.103755
C	1.900848	2.125357	0.467800
H	2.771327	2.382579	1.078745
H	2.206765	2.034772	-0.578609
C	-0.340710	5.501349	3.446693
H	0.507782	5.253850	4.090938
H	-1.260416	5.242402	3.984647
H	-0.349971	6.586778	3.294887
C	-2.269800	4.613370	-1.122326
H	-2.634275	3.690001	-1.584050
H	-1.907739	5.258712	-1.930875
H	-3.116233	5.119994	-0.649945
C	2.883245	-1.492853	-1.164663
C	3.549681	-1.771560	-2.380270
H	4.561491	-2.126688	-2.509885
C	2.610237	-1.509415	-3.367323
H	2.666617	-1.582591	-4.444174
C	3.355010	-1.562350	0.238721
C	2.722407	-2.443967	1.151450
C	3.148604	-2.450021	2.485609
H	2.664334	-3.127237	3.186447
C	4.173287	-1.611136	2.943095
C	4.790831	-0.754772	2.023086
H	5.590440	-0.097461	2.358622
C	4.406022	-0.718174	0.675934
C	1.587463	-3.343427	0.723762
H	0.646204	-2.777777	0.761325
H	1.502942	-4.200374	1.399817
H	1.724019	-3.713105	-0.297075
C	4.578101	-1.612111	4.397807
H	3.907656	-0.974455	4.987945
H	5.596074	-1.233186	4.530945
H	4.525625	-2.619167	4.824011
C	5.111548	0.220800	-0.276853
H	5.638834	1.005361	0.273759
H	4.412973	0.694485	-0.973360
H	5.852210	-0.314090	-0.883504
B	0.167579	-0.539431	-3.369490
H	0.174050	-0.655433	-4.561443
H	-2.541328	1.116914	-0.037609
H	2.114070	0.185768	0.893844

TS_{OHO}-OS

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.382568
Thermal and entropic correction, BS1 (a.u.)	0.613832
Electronic Energy, BS2 (a.u.)	-2097.796776
Gibbs Energy, BS2 (a.u.)	-2097.182944
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-907.2i

Molecular Geometry in Cartesian Coordinates

Cu	0.034363	-0.146878	-0.307307
O	1.339693	0.242671	1.114130
O	-0.946128	0.512378	1.289522
N	0.977438	-1.449812	-1.504569
N	0.908119	-1.264697	-2.847479
N	-1.598882	-0.191511	-1.516518
N	-1.337277	-0.116882	-2.853042
N	0.789055	1.492363	-1.605225
N	0.761408	1.246578	-2.940097
C	1.749919	-2.526204	-1.270001
C	2.199905	-3.040818	-2.504517
H	2.826212	-3.906036	-2.661978
C	1.641594	-2.214829	-3.471229
H	1.708134	-2.234363	-4.549376
C	1.964289	-2.994264	0.116761
C	0.858112	-3.384456	0.906118
C	1.082794	-3.795896	2.227544
H	0.231261	-4.102285	2.832191
C	2.365425	-3.826801	2.784616
C	3.447326	-3.443026	1.979235
H	4.452822	-3.460677	2.395239
C	3.271507	-3.027559	0.655709
C	-0.558480	-3.381028	0.371763
H	-0.593119	-3.587114	-0.702015
H	-1.164119	-4.130381	0.890867
C	2.581137	-4.238878	4.221313
H	2.643773	-3.358032	4.873415
H	3.515489	-4.798007	4.340249
H	1.757843	-4.860961	4.586306
C	4.469276	-2.603655	-0.163326
H	5.352531	-2.497617	0.473477
H	4.291153	-1.646768	-0.665820
H	4.705574	-3.337677	-0.942557
C	-2.938879	-0.067648	-1.359184
C	-3.533458	0.095940	-2.630031
H	-4.583403	0.227277	-2.842004
C	-2.489038	0.060122	-3.537063
H	-2.475782	0.148214	-4.613600
C	-3.652348	-0.106244	-0.060199
C	-3.271135	0.712357	1.032146
C	-4.038727	0.719272	2.200428
H	-3.723544	1.351476	3.028497
C	-5.182898	-0.075568	2.336097
C	-5.525526	-0.909166	1.265627
H	-6.389171	-1.564624	1.361389
C	-4.789778	-0.942784	0.072501
C	-1.971868	1.480552	1.028626
H	-1.966125	2.237784	1.820546

H	-1.791570	1.979158	0.068251
C	-6.018671	-0.032896	3.592314
H	-5.402637	0.172323	4.473493
H	-6.546491	-0.978445	3.751609
H	-6.775835	0.759652	3.530893
C	-5.235368	-1.901476	-1.011973
H	-4.388228	-2.313910	-1.567283
H	-5.896539	-1.413098	-1.738672
H	-5.795498	-2.732457	-0.571435
C	1.487258	2.624926	-1.425189
C	1.908572	3.128580	-2.674755
H	2.480654	4.025668	-2.861862
C	1.428730	2.217042	-3.608041
H	1.511769	2.188060	-4.685247
C	1.728574	3.103581	-0.043569
C	2.835920	2.592526	0.673204
C	3.035957	3.014718	1.994138
H	3.886331	2.623047	2.548908
C	2.162057	3.912066	2.619573
C	1.072246	4.405057	1.886777
H	0.386009	5.105795	2.358838
C	0.842260	4.019013	0.560162
C	3.807723	1.643032	0.012330
H	3.275229	0.852063	-0.522644
H	4.460607	1.175815	0.755526
H	4.439456	2.172617	-0.712987
C	2.374001	4.316669	4.059413
H	1.952495	3.566540	4.741503
H	1.890173	5.273139	4.282298
H	3.439834	4.406234	4.294866
C	-0.320735	4.597628	-0.212783
H	-1.070164	5.020501	0.463004
H	-0.805092	3.842788	-0.839552
H	0.015523	5.400431	-0.881474
B	0.107594	-0.068028	-3.422908
H	0.080818	-0.120299	-4.618404
H	-1.040702	-2.407458	0.528445
H	0.196235	0.689262	1.495641

Closed-shell singlet Potential Energy Surface

1-O_2-CSS

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.364719
Thermal and entropic correction, BS1 (a.u.)	0.617014
Electronic Energy, BS2 (a.u.)	-2097.777346
Gibbs Energy, BS2 (a.u.)	-2097.160332
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-0.209345	0.160854	-0.363119
O	0.511941	0.349981	1.330307
O	-0.502235	-0.556480	1.311267
N	0.435945	1.544653	-1.577518
N	0.404922	1.285694	-2.912530
N	1.182528	-1.281947	-1.509196

N	1.094638	-1.125196	-2.857757
N	-1.623539	-0.416498	-1.564889
N	-1.342835	-0.509832	-2.891739
C	0.859696	2.813878	-1.406113
C	1.099121	3.383794	-2.670296
H	1.449824	4.384584	-2.872688
C	0.803692	2.384030	-3.588523
H	0.855566	2.368966	-4.667457
C	1.042147	3.384117	-0.052682
C	2.134367	2.951624	0.733346
C	2.300234	3.498532	2.009437
H	3.138933	3.167305	2.618566
C	1.409052	4.450665	2.526026
C	0.332322	4.857126	1.728878
H	-0.373145	5.589002	2.117432
C	0.134271	4.342714	0.440086
C	3.100548	1.911819	0.213440
H	3.504722	2.197499	-0.764624
H	3.935735	1.776096	0.906115
C	1.624581	5.036055	3.901371
H	2.421908	5.790072	3.884155
H	1.924124	4.264831	4.618795
H	0.718131	5.521011	4.275944
C	-1.031414	4.818809	-0.396387
H	-1.792425	5.291917	0.230942
H	-1.500080	3.995152	-0.943376
H	-0.707999	5.556970	-1.140839
C	2.180053	-2.154590	-1.284595
C	2.746842	-2.563134	-2.514734
H	3.555371	-3.263837	-2.663245
C	2.025665	-1.884743	-3.485629
H	2.099650	-1.887246	-4.563935
C	2.519410	-2.569466	0.096814
C	1.568738	-3.279697	0.865850
C	1.899236	-3.652008	2.173459
H	1.169021	-4.203032	2.763477
C	3.142218	-3.337948	2.740581
C	4.069105	-2.639052	1.958581
H	5.039713	-2.385621	2.381147
C	3.780002	-2.249065	0.643424
C	0.218434	-3.645506	0.293942
H	-0.314570	-4.327323	0.963295
H	0.316408	-4.127367	-0.685743
H	-0.394739	-2.750718	0.158002
C	3.457403	-3.724538	4.166557
H	4.536203	-3.728233	4.351134
H	3.064039	-4.718369	4.405570
H	3.002792	-3.017615	4.872374
C	4.816151	-1.495226	-0.159861
H	4.364658	-0.687074	-0.743036
H	5.328320	-2.155830	-0.870263
H	5.577043	-1.063794	0.497577
C	-2.890318	-0.839819	-1.370585
C	-3.430813	-1.219945	-2.613992
H	-4.427982	-1.589311	-2.799782
C	-2.422715	-0.993617	-3.541827
H	-2.393842	-1.136361	-4.612160
C	-3.507434	-0.832744	-0.027357
C	-3.709862	0.391267	0.646172
C	-4.302523	0.372362	1.915470
H	-4.463618	1.315437	2.433634

C	-4.687443	-0.822790	2.532821
C	-4.466206	-2.026399	1.847752
H	-4.749698	-2.966244	2.317925
C	-3.884957	-2.054574	0.575877
C	-3.290095	1.710632	0.038980
H	-2.216636	1.884089	0.182662
H	-3.820603	2.542048	0.511950
H	-3.478947	1.744294	-1.038730
C	-5.329334	-0.825955	3.900074
H	-5.390676	0.184578	4.314408
H	-4.760365	-1.447198	4.601338
H	-6.345415	-1.236592	3.857270
C	-3.660934	-3.379173	-0.118516
H	-3.685058	-4.199843	0.604370
H	-2.698298	-3.406283	-0.637883
H	-4.437635	-3.575126	-0.868050
B	0.062934	-0.137346	-3.433977
H	0.065796	-0.152937	-4.629688
H	2.605395	0.943337	0.089527

TS_{CO}-CSS

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.341379
Thermal and entropic correction, BS1 (a.u.)	0.616458
Electronic Energy, BS2 (a.u.)	-2097.756323
Gibbs Energy, BS2 (a.u.)	-2097.139865
Number of Imaginary Frequencies	1
Imaginary frequency (cm-1)	-130.9i

Molecular Geometry in Cartesian Coordinates

Cu	-0.039950	0.012168	-0.385575
O	0.907084	-0.509741	1.908177
O	-0.074251	-0.943750	1.174860
N	1.670006	-0.532951	-1.501088
N	1.446362	-0.493740	-2.846205
N	-1.279454	-1.184965	-1.523277
N	-0.996558	-1.169498	-2.853133
N	-0.359060	1.528912	-1.621138
N	-0.344862	1.255026	-2.949671
C	2.986546	-0.752554	-1.325272
C	3.621541	-0.854224	-2.581449
H	4.668192	-1.042020	-2.769716
C	2.608482	-0.684708	-3.512926
H	2.623329	-0.692787	-4.593369
C	3.571138	-0.894064	0.028328
C	3.232307	-2.018524	0.816755
C	3.818629	-2.157657	2.079548
H	3.558141	-3.022214	2.687008
C	4.718512	-1.210540	2.584525
C	5.034188	-0.102738	1.787582
H	5.725931	0.647160	2.166777
C	4.481342	0.069487	0.511487
C	2.267641	-3.061561	0.306651
H	2.547308	-3.405433	-0.695949
H	2.243638	-3.927698	0.974425
C	5.346094	-1.395259	3.946198

H	6.125097	-2.167768	3.917332
H	4.603586	-1.714055	4.685636
H	5.809331	-0.469995	4.302004
C	4.871269	1.269911	-0.321382
H	5.290591	2.059321	0.309526
H	4.016982	1.680117	-0.867430
H	5.631198	1.004031	-1.066688
C	-2.233917	-2.109519	-1.315746
C	-2.568363	-2.711049	-2.549180
H	-3.308505	-3.477630	-2.723533
C	-1.765578	-2.083153	-3.490927
H	-1.690122	-2.211396	-4.561182
C	-2.785652	-2.315470	0.041770
C	-3.369498	-1.229010	0.733008
C	-3.869257	-1.440797	2.025418
H	-4.324745	-0.605361	2.553853
C	-3.803026	-2.691078	2.649655
C	-3.222876	-3.753785	1.943005
H	-3.159309	-4.733579	2.412674
C	-2.714260	-3.590073	0.650225
C	-3.475609	0.150997	0.122191
H	-4.264726	0.728132	0.613381
H	-3.689147	0.107193	-0.949987
H	-2.538656	0.711152	0.236792
C	-4.318056	-2.889943	4.055409
H	-4.834289	-3.850276	4.159293
H	-5.011312	-2.093634	4.343067
H	-3.491833	-2.886522	4.777719
C	-2.078114	-4.765368	-0.057196
H	-1.114305	-4.491221	-0.499612
H	-2.710521	-5.139584	-0.870612
H	-1.913422	-5.590774	0.641530
C	-0.749844	2.807778	-1.461053
C	-0.988650	3.371350	-2.731844
H	-1.299759	4.381955	-2.949731
C	-0.719324	2.355301	-3.640435
H	-0.760423	2.336193	-4.719847
C	-0.864472	3.376237	-0.100044
C	0.264733	3.396419	0.755296
C	0.119409	3.899860	2.053096
H	0.988242	3.917476	2.708455
C	-1.107315	4.382326	2.527966
C	-2.208341	4.355848	1.663715
H	-3.171179	4.719157	2.017435
C	-2.110654	3.863473	0.355856
C	1.618656	2.887761	0.310382
H	1.715445	1.809419	0.488571
H	2.416898	3.381099	0.872904
H	1.786019	3.056058	-0.757151
C	-1.226331	4.922155	3.933195
H	-0.633592	5.837324	4.052855
H	-0.853156	4.198740	4.666875
H	-2.264512	5.158540	4.184074
C	-3.337990	3.844673	-0.527194
H	-4.244730	3.968130	0.072040
H	-3.418816	2.907677	-1.086469
H	-3.314566	4.656702	-1.263913
B	0.045107	-0.171502	-3.422302
H	0.065222	-0.227703	-4.617339
H	1.251631	-2.657849	0.239104

1-O_2b-CSS

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-2097.342363
Thermal and entropic correction, BS1 (a.u.)	0.613401
Electronic Energy, BS2 (a.u.)	-2097.758244
Gibbs Energy, BS2 (a.u.)	-2097.144843
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	0.050538	0.068896	-0.408352
O	0.840843	-0.545871	2.147103
O	-0.140939	-0.555942	1.319427
N	1.478963	-0.810442	-1.582401
N	1.272989	-0.695532	-2.922834
N	-1.487489	-0.882453	-1.567460
N	-1.249647	-0.866917	-2.906987
N	-0.054398	1.622626	-1.629557
N	-0.128027	1.382923	-2.962151
C	2.709226	-1.327232	-1.403599
C	3.308351	-1.551053	-2.660714
H	4.284459	-1.970158	-2.854252
C	2.363843	-1.138154	-3.590148
H	2.381598	-1.136157	-4.670507
C	3.207414	-1.588301	-0.035775
C	2.513782	-2.497870	0.797034
C	2.983816	-2.711990	2.101904
H	2.448595	-3.409854	2.741974
C	4.116530	-2.056731	2.597602
C	4.791951	-1.170209	1.749029
H	5.674666	-0.650000	2.116277
C	4.358192	-0.922710	0.439770
C	1.301315	-3.255002	0.311867
H	1.416961	-3.584156	-0.725679
H	1.118536	-4.131264	0.940545
C	4.578474	-2.273440	4.018778
H	5.667188	-2.194824	4.102643
H	4.273440	-3.256193	4.391620
H	4.143611	-1.519597	4.687499
C	5.120170	0.052955	-0.428160
H	5.763921	0.691469	0.183899
H	4.444814	0.693793	-1.003275
H	5.760653	-0.468704	-1.149804
C	-2.602203	-1.606968	-1.367469
C	-3.089178	-2.075323	-2.608777
H	-3.971766	-2.672590	-2.784090
C	-2.203130	-1.579173	-3.554242
H	-2.182740	-1.672962	-4.630622
C	-3.139450	-1.772892	0.002187
C	-3.519144	-0.633621	0.748222
C	-4.006868	-0.808004	2.049739
H	-4.306639	0.069626	2.619491
C	-4.120484	-2.075718	2.633637
C	-3.737387	-3.189952	1.875803
H	-3.814966	-4.183658	2.313115
C	-3.248518	-3.062118	0.569976
C	-3.413714	0.762127	0.174570
H	-4.006539	1.467556	0.764138
H	-3.757453	0.798264	-0.864456

H	-2.375670	1.115277	0.176274
C	-4.617407	-2.236831	4.050816
H	-5.157297	-3.180570	4.179598
H	-5.284161	-1.416720	4.335508
H	-3.780104	-2.240000	4.760449
C	-2.830319	-4.295833	-0.197990
H	-1.847838	-4.162956	-0.663842
H	-3.537913	-4.529427	-1.002052
H	-2.780895	-5.164525	0.465094
C	-0.173747	2.949517	-1.433975
C	-0.333958	3.580114	-2.685264
H	-0.444508	4.637168	-2.875310
C	-0.295860	2.552303	-3.620411
H	-0.370493	2.567807	-4.698128
C	-0.122776	3.477197	-0.051882
C	1.035261	3.260463	0.733938
C	1.037576	3.691235	2.065238
H	1.928049	3.526114	2.668998
C	-0.072524	4.325796	2.639557
C	-1.201534	4.538353	1.839865
H	-2.073539	5.027784	2.269207
C	-1.247763	4.127746	0.500653
C	2.263884	2.580084	0.170476
H	2.155387	1.488934	0.179909
H	3.147597	2.826423	0.766294
H	2.447539	2.873248	-0.867847
C	-0.035438	4.783412	4.078184
H	0.672837	5.610896	4.209050
H	0.287998	3.974314	4.742496
H	-1.018302	5.127786	4.413164
C	-2.493796	4.381238	-0.316998
H	-3.343343	4.606720	0.334187
H	-2.753967	3.519334	-0.938638
H	-2.357971	5.235413	-0.991625
B	-0.041880	-0.082005	-3.474131
H	-0.043218	-0.109426	-4.670599
H	0.401783	-2.629559	0.348979

TS_{CH}-CSS

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-2097.309766
Thermal and entropic correction, BS1 (a.u.)	0.607810
Electronic Energy, BS2 (a.u.)	-2097.726454
Gibbs Energy, BS2 (a.u.)	-2097.118644
Number of Imaginary Frequencies	1
Imaginary frequency (cm-1)	-440.1i

Molecular Geometry in Cartesian Coordinates

Cu	-0.297881	0.143542	-0.297161
O	0.681937	-0.934045	2.065508
O	-0.453323	-0.453387	1.466489
N	1.585886	-0.057726	-1.517631
N	1.323336	0.087057	-2.845802
N	-1.171530	-1.184090	-1.613988
N	-0.973316	-0.943563	-2.937444
N	-0.751790	1.719573	-1.435959
N	-0.707742	1.566513	-2.784723

C	2.926900	-0.179118	-1.405913
C	3.525704	-0.106083	-2.684907
H	4.575914	-0.188840	-2.920975
C	2.470501	0.057545	-3.565161
H	2.446677	0.153439	-4.641116
C	3.624243	-0.404848	-0.124871
C	3.289270	-1.524658	0.708803
C	4.059517	-1.771299	1.878351
H	3.786314	-2.617338	2.504351
C	5.128999	-0.962069	2.235707
C	5.417312	0.145717	1.416362
H	6.228215	0.812674	1.701610
C	4.692434	0.435543	0.250407
C	2.141741	-2.342558	0.474462
H	1.601999	-2.279452	-0.466296
H	2.046425	-3.272601	1.029994
C	5.963574	-1.249272	3.458922
H	6.897903	-1.753018	3.180783
H	5.429919	-1.896858	4.159614
H	6.234691	-0.324405	3.979243
C	5.068618	1.659010	-0.554528
H	5.615879	2.369836	0.071162
H	4.185625	2.161219	-0.959886
H	5.714479	1.400125	-1.401218
C	-1.854270	-2.340191	-1.511017
C	-2.095086	-2.855254	-2.804009
H	-2.632507	-3.757037	-3.057425
C	-1.521188	-1.939054	-3.673759
H	-1.463635	-1.918580	-4.752622
C	-2.258922	-2.863403	-0.187005
C	-3.133165	-2.108286	0.630392
C	-3.503508	-2.619854	1.877840
H	-4.179440	-2.039735	2.503494
C	-3.021664	-3.850057	2.346168
C	-2.152959	-4.576439	1.524058
H	-1.763663	-5.531222	1.872535
C	-1.764381	-4.106880	0.261830
C	-3.660198	-0.761918	0.189960
H	-4.524698	-0.466702	0.791994
H	-3.953023	-0.763464	-0.864966
H	-2.891232	0.010857	0.305873
C	-3.423480	-4.363950	3.708445
H	-3.030293	-5.368933	3.888432
H	-4.513968	-4.400827	3.813597
H	-3.046116	-3.707465	4.501761
C	-0.818872	-4.931325	-0.582775
H	-0.037158	-4.312389	-1.035185
H	-1.345284	-5.432241	-1.404190
H	-0.337966	-5.705835	0.022266
C	-1.239034	2.947728	-1.178470
C	-1.516678	3.600061	-2.398284
H	-1.907708	4.597613	-2.532262
C	-1.161010	2.690789	-3.386038
H	-1.190560	2.762007	-4.463721
C	-1.376364	3.397055	0.225329
C	-0.221694	3.517545	1.032314
C	-0.372157	3.893088	2.373339
H	0.516037	3.985507	2.995380
C	-1.630515	4.146960	2.933325
C	-2.759727	4.021983	2.112916
H	-3.746448	4.205384	2.533986

C	-2.656002	3.650874	0.767069
C	1.159936	3.243284	0.480224
H	1.334015	2.166505	0.364150
H	1.929631	3.637794	1.149911
H	1.294857	3.691715	-0.509827
C	-1.766230	4.573495	4.375649
H	-1.737095	5.667373	4.464393
H	-0.952321	4.172958	4.988140
H	-2.716627	4.236841	4.802484
C	-3.903228	3.500464	-0.074233
H	-4.800836	3.584765	0.545102
H	-3.926747	2.529846	-0.581998
H	-3.958502	4.270455	-0.852143
B	-0.122390	0.267250	-3.386232
H	-0.101737	0.335871	-4.582028
H	1.256164	-1.477437	1.311837

I-COH-CSS

	Value
Charge	0
Electronic Energy, BS1 (a.u.)	-2097.370683
Thermal and entropic correction, BS1 (a.u.)	0.618558
Electronic Energy, BS2 (a.u.)	-2097.788449
Gibbs Energy, BS2 (a.u.)	-2097.169891
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-0.134322	0.076937	-0.378184
O	-0.146260	-0.894728	1.014613
O	1.126168	-3.166126	1.165631
N	-0.223936	1.606559	-1.571760
N	-0.030314	1.465934	-2.903433
N	1.861193	-0.367134	-1.469340
N	1.743622	-0.296023	-2.823337
N	-1.068606	-1.022729	-1.655187
N	-0.700106	-0.933214	-2.962562
C	-0.573724	2.882734	-1.317305
C	-0.599335	3.585837	-2.537759
H	-0.832615	4.629602	-2.683646
C	-0.249384	2.653765	-3.508880
H	-0.134647	2.749902	-4.578666
C	-0.863287	3.278400	0.078295
C	0.136314	3.138499	1.068772
C	-0.189153	3.436189	2.399458
H	0.580231	3.332422	3.161722
C	-1.468826	3.862621	2.770344
C	-2.438536	4.007531	1.766938
H	-3.438953	4.339972	2.037268
C	-2.160868	3.724057	0.426492
C	1.543384	2.689105	0.735573
H	1.849164	3.018975	-0.261121
H	2.254356	3.082253	1.468247
C	-1.810778	4.141621	4.214135
H	-2.407732	3.323189	4.635562
H	-2.401812	5.058490	4.313212
H	-0.909414	4.244057	4.825365
C	-3.243939	3.883919	-0.616038
H	-4.225386	3.968646	-0.141131

H	-3.267371	3.036632	-1.308672
H	-3.086927	4.787121	-1.217659
C	3.153833	-0.621477	-1.202741
C	3.883319	-0.708048	-2.410351
H	4.937585	-0.913052	-2.525145
C	2.947869	-0.496613	-3.412138
H	3.044883	-0.476528	-4.488347
C	3.609064	-0.768392	0.200536
C	3.186434	-1.863836	0.975599
C	3.572730	-1.943214	2.322080
H	3.218120	-2.784070	2.913920
C	4.381389	-0.969496	2.911182
C	4.809483	0.106869	2.115409
H	5.437438	0.878149	2.558341
C	4.440287	0.225884	0.773256
C	2.318001	-2.980715	0.415907
H	2.873907	-3.925434	0.475253
H	2.099077	-2.797262	-0.644047
H	0.626430	-2.293463	1.128703
C	4.789693	-1.055892	4.362729
H	4.396686	-1.961429	4.834015
H	4.419049	-0.192195	4.927633
H	5.881143	-1.063784	4.467505
C	4.911944	1.410736	-0.038662
H	4.094049	1.852784	-0.616404
H	5.688718	1.119330	-0.755976
H	5.331876	2.183911	0.611394
C	-2.059891	-1.928927	-1.537351
C	-2.330934	-2.441612	-2.821162
H	-3.084210	-3.172223	-3.074274
C	-1.458645	-1.788312	-3.681775
H	-1.323914	-1.862635	-4.751022
C	-2.727847	-2.189605	-0.247369
C	-3.524440	-1.174465	0.330187
C	-4.164329	-1.433798	1.546040
H	-4.778536	-0.655813	1.994999
C	-4.030878	-2.666801	2.200560
C	-3.231383	-3.653075	1.608855
H	-3.107166	-4.609994	2.111730
C	-2.574640	-3.440195	0.391535
C	-3.670410	0.181242	-0.323586
H	-2.775698	0.793925	-0.158600
H	-4.522501	0.724149	0.094673
H	-3.807748	0.098989	-1.407097
C	-4.756867	-2.937744	3.496142
H	-4.185290	-3.615956	4.137567
H	-5.729911	-3.409519	3.306570
H	-4.942779	-2.012735	4.050734
C	-1.652887	-4.500548	-0.159070
H	-1.866305	-5.473158	0.294619
H	-0.613544	-4.234242	0.080288
H	-1.733812	-4.601534	-1.245197
B	0.386722	0.072993	-3.447542
H	0.440572	0.076338	-4.640991
H	1.635919	1.595666	0.756109

TS_{rot}-CSS

Charge	0

Electronic Energy, BS1 (a.u.)	-2097.360062
Thermal and entropic correction, BS1 (a.u.)	0.615061
Electronic Energy, BS2 (a.u.)	-2097.776626
Gibbs Energy, BS2 (a.u.)	-2097.161565
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-142.4i

Molecular Geometry in Cartesian Coordinates

Cu	0.220791	-0.192024	-0.387206
O	0.670775	-0.359235	1.279910
O	1.213743	-2.960047	1.547701
N	-0.444054	1.393439	-1.705252
N	-0.324723	1.165705	-3.040359
N	1.699056	-0.399982	-1.590868
N	1.525336	-0.512569	-2.925916
N	-1.029572	-1.361826	-1.631436
N	-0.873526	-1.279225	-2.978320
C	-0.889656	2.653796	-1.547332
C	-1.061185	3.249807	-2.816996
H	-1.400087	4.252847	-3.029773
C	-0.689520	2.272947	-3.730165
H	-0.660491	2.281451	-4.810455
C	-1.160060	3.156927	-0.181163
C	-0.124445	3.214256	0.777450
C	-0.442534	3.576354	2.095949
H	0.355540	3.610359	2.835383
C	-1.750059	3.880370	2.485449
C	-2.755403	3.855001	1.507167
H	-3.777813	4.101804	1.787453
C	-2.484731	3.504510	0.181038
C	1.312537	2.883729	0.441678
H	1.518690	2.982298	-0.626305
H	1.994224	3.541347	0.991104
C	-2.085921	4.195384	3.923851
H	-2.524459	3.318213	4.417492
H	-2.817007	5.007782	3.996426
H	-1.194270	4.480895	4.490637
C	-3.609881	3.483708	-0.828882
H	-4.579111	3.544139	-0.325544
H	-3.592351	2.574594	-1.438414
H	-3.541651	4.332301	-1.520402
C	3.007762	-0.563259	-1.297776
C	3.697022	-0.770030	-2.508714
H	4.755353	-0.946337	-2.627002
C	2.726088	-0.737317	-3.504386
H	2.803863	-0.844658	-4.576443
C	3.463823	-0.474582	0.100009
C	3.033249	-1.435203	1.050459
C	3.400966	-1.279288	2.400379
H	3.049991	-2.018268	3.114826
C	4.179018	-0.207437	2.819665
C	4.607438	0.728299	1.852710
H	5.207151	1.577927	2.172931
C	4.269166	0.616869	0.503484
C	2.287537	-2.701181	0.660130
H	2.975432	-3.554351	0.718713
H	1.940865	-2.631429	-0.380552
H	0.765854	-2.072108	1.600952
C	4.554447	-0.020733	4.268559

H	4.273597	-0.890067	4.869548
H	4.046788	0.857217	4.686603
H	5.631689	0.145555	4.381461
C	4.719048	1.664877	-0.486548
H	3.886511	2.003456	-1.111512
H	5.489376	1.272972	-1.160822
H	5.135379	2.532813	0.032111
C	-2.050451	-2.199964	-1.386979
C	-2.560324	-2.680479	-2.613672
H	-3.380096	-3.369147	-2.756815
C	-1.788213	-2.067505	-3.592893
H	-1.825611	-2.129038	-4.671240
C	-2.486276	-2.394696	0.018366
C	-3.137875	-1.320540	0.670641
C	-3.458931	-1.444520	2.026083
H	-3.947744	-0.612415	2.529604
C	-3.156463	-2.607019	2.750863
C	-2.527268	-3.661409	2.080321
H	-2.275077	-4.566586	2.629531
C	-2.177618	-3.573733	0.724029
C	-3.460115	-0.043601	-0.070566
H	-2.546495	0.508017	-0.320717
H	-4.092418	0.608842	0.537488
H	-3.976535	-0.248941	-1.015536
C	-3.510664	-2.709461	4.216393
H	-3.000669	-3.552270	4.692485
H	-4.590580	-2.850296	4.355010
H	-3.232730	-1.795129	4.753028
C	-1.389687	-4.689726	0.081460
H	-1.558287	-5.638665	0.599866
H	-0.320525	-4.455025	0.151523
H	-1.641134	-4.820711	-0.974726
B	0.116587	-0.233022	-3.541535
H	0.168764	-0.273957	-4.734887
H	1.541512	1.852938	0.737424

I-COH-b-CSS

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.365798
Thermal and entropic correction, BS1 (a.u.)	0.619955
Electronic Energy, BS2 (a.u.)	-2097.782755
Gibbs Energy, BS2 (a.u.)	-2097.162800
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	0.084472	-0.508679	-0.346069
O	0.797918	-0.175339	1.172426
O	1.508317	-2.780377	1.451802
N	-0.669147	1.494671	-1.550601
N	-0.640238	1.294946	-2.896897
N	1.517387	-0.436956	-1.634535
N	1.218624	-0.402277	-2.959038
N	-1.204951	-1.326395	-1.548685
N	-1.173775	-1.146419	-2.888851
C	-1.163183	2.730334	-1.357179
C	-1.452997	3.337452	-2.603526
H	-1.846516	4.328575	-2.775312

C	-1.104690	2.389714	-3.552194
H	-1.149292	2.408404	-4.631989
C	-1.329477	3.266170	0.013786
C	-0.207200	3.392485	0.865167
C	-0.395104	3.881317	2.165201
H	0.470726	3.982159	2.817264
C	-1.658974	4.245278	2.644651
C	-2.755110	4.120392	1.781141
H	-3.746300	4.398354	2.135137
C	-2.613847	3.637858	0.474198
C	1.178428	3.002547	0.410169
H	1.341840	3.247823	-0.643389
H	1.939982	3.510239	1.010937
C	-1.840359	4.731592	4.063147
H	-2.022692	3.889467	4.743145
H	-2.695016	5.410548	4.147099
H	-0.948017	5.253620	4.423137
C	-3.836042	3.509843	-0.407589
H	-4.750253	3.549587	0.192326
H	-3.831526	2.569562	-0.967841
H	-3.887158	4.321080	-1.143823
C	2.864086	-0.473518	-1.492760
C	3.434665	-0.462675	-2.780063
H	4.487632	-0.498016	-3.013963
C	2.369030	-0.417544	-3.666830
H	2.341054	-0.376429	-4.745873
C	3.538231	-0.431509	-0.182291
C	3.425297	-1.488476	0.746876
C	4.081889	-1.390838	1.980959
H	3.970981	-2.203573	2.694469
C	4.853962	-0.277579	2.312282
C	4.960156	0.763853	1.370644
H	5.548465	1.644450	1.620722
C	4.326724	0.709442	0.130425
C	2.570053	-2.716222	0.502615
H	3.173244	-3.621964	0.634658
H	2.186440	-2.724344	-0.527940
H	1.167259	-1.846582	1.501244
C	5.566310	-0.176620	3.637652
H	5.347193	-1.036925	4.275957
H	5.267217	0.732119	4.172702
H	6.652524	-0.124026	3.495583
C	4.473136	1.861598	-0.836358
H	3.522591	2.110612	-1.316532
H	5.185468	1.622971	-1.635215
H	4.840666	2.751224	-0.317469
C	-2.204162	-2.180661	-1.251981
C	-2.832518	-2.562589	-2.452926
H	-3.668709	-3.236432	-2.563086
C	-2.153306	-1.882679	-3.457896
H	-2.299408	-1.862299	-4.527991
C	-2.467560	-2.527520	0.162951
C	-2.948391	-1.527542	1.039832
C	-3.133467	-1.851258	2.388997
H	-3.501686	-1.084594	3.067799
C	-2.856393	-3.132330	2.885088
C	-2.387407	-4.105824	1.993287
H	-2.158738	-5.102455	2.365060
C	-2.185916	-3.825990	0.636736
C	-3.261108	-0.134146	0.541992
H	-2.347214	0.428846	0.318156

H	-3.821545	0.429758	1.292558
H	-3.847537	-0.164909	-0.382801
C	-3.087075	-3.460351	4.340730
H	-2.510193	-4.337675	4.648576
H	-4.146443	-3.677903	4.528567
H	-2.809096	-2.620787	4.986180
C	-1.635495	-4.887431	-0.287393
H	-1.423837	-5.808873	0.262013
H	-0.704995	-4.551818	-0.759869
H	-2.338203	-5.125820	-1.093443
B	-0.218863	-0.074379	-3.464577
H	-0.239880	-0.077927	-4.659662
H	1.317306	1.920847	0.530975

TS_{OHO}-CSS

Charge	0
Electronic Energy, BS1 (a.u.)	-2097.365071
Thermal and entropic correction, BS1 (a.u.)	0.620752
Electronic Energy, BS2 (a.u.)	-2097,780983
Gibss Energy, BS2 (a.u.)	-2097.160231
Number of Imaginary Frequencies	1
Imaginary frequency (cm-1)	-52.3i

Molecular Geometry in Cartesian Coordinates

Cu	0.043156	-0.340151	-0.352022
O	0.809326	0.193782	1.081245
O	1.212574	-2.419125	1.114377
N	-0.721996	1.508431	-1.532926
N	-0.708438	1.291647	-2.876653
N	1.569666	-0.334464	-1.576124
N	1.288655	-0.245848	-2.904876
N	-1.117246	-1.337905	-1.540832
N	-1.031762	-1.186826	-2.883445
C	-1.305786	2.703814	-1.336727
C	-1.677542	3.264882	-2.581021
H	-2.152141	4.219908	-2.752239
C	-1.276724	2.336070	-3.528878
H	-1.345612	2.339864	-4.607451
C	-1.444166	3.262878	0.027914
C	-0.283122	3.558312	0.779935
C	-0.430119	4.081380	2.070702
H	0.463446	4.311770	2.648114
C	-1.690177	4.314630	2.636816
C	-2.824985	4.023982	1.869678
H	-3.812988	4.200521	2.291207
C	-2.724824	3.505745	0.571507
C	1.098454	3.307905	0.225280
H	1.166118	3.581206	-0.832906
H	1.848567	3.878606	0.782083
C	-1.819725	4.838315	4.047539
H	-1.801370	4.014299	4.772423
H	-2.761455	5.378214	4.188583
H	-0.994518	5.511911	4.300647
C	-3.984066	3.220820	-0.216081
H	-4.844390	3.122870	0.452820
H	-3.896326	2.302243	-0.803104
H	-4.205959	4.032064	-0.920697

C	2.912820	-0.337108	-1.421320
C	3.501518	-0.258786	-2.698627
H	4.557980	-0.265817	-2.919265
C	2.447137	-0.203418	-3.597382
H	2.431128	-0.129540	-4.674893
C	3.581183	-0.393884	-0.107508
C	3.422045	-1.507746	0.743828
C	4.091819	-1.536637	1.973290
H	3.952593	-2.395844	2.625618
C	4.922569	-0.488669	2.377944
C	5.064697	0.613379	1.517969
H	5.693839	1.446124	1.826031
C	4.417797	0.682301	0.282380
C	2.453016	-2.623039	0.427324
H	2.860006	-3.583441	0.764484
H	2.275140	-2.698587	-0.653994
H	1.133958	-1.435198	1.294156
C	5.649468	-0.524113	3.699679
H	5.403477	-1.425587	4.268033
H	5.390475	0.347129	4.312401
H	6.735797	-0.501307	3.551450
C	4.599443	1.903547	-0.589547
H	3.653750	2.222130	-1.037721
H	5.298372	1.710216	-1.412149
H	5.000424	2.735132	-0.003241
C	-2.019766	-2.303677	-1.274992
C	-2.521941	-2.789441	-2.498371
H	-3.264975	-3.560805	-2.633482
C	-1.874627	-2.054173	-3.484335
H	-1.958328	-2.076100	-4.561056
C	-2.359352	-2.650184	0.123178
C	-2.993252	-1.688365	0.939534
C	-3.294917	-2.026069	2.266562
H	-3.786514	-1.288103	2.897236
C	-2.983715	-3.282857	2.796190
C	-2.351076	-4.218751	1.964221
H	-2.090913	-5.196595	2.364907
C	-2.028516	-3.924004	0.636744
C	-3.342483	-0.313611	0.414712
H	-2.453523	0.326366	0.349486
H	-4.057693	0.183162	1.075865
H	-3.771079	-0.363581	-0.591691
C	-3.300500	-3.626952	4.232024
H	-2.380309	-3.752539	4.815364
H	-3.856714	-4.568833	4.301388
H	-3.895690	-2.842821	4.708957
C	-1.296270	-4.935473	-0.212726
H	-1.036212	-5.820088	0.375462
H	-0.370227	-4.505839	-0.610604
H	-1.897404	-5.263260	-1.068250
B	-0.159014	-0.035886	-3.437208
H	-0.157692	-0.036261	-4.632282
H	1.337292	2.241690	0.317399

MECP

Charge	0
Spin State	Singlet/Triplet
Electronic Energy, BS1 (a.u.)	-2097.321569

Thermal and entropic correction, BS1 (a.u.)	0.61500024
Electronic Energy, BS2 (a.u.)	-2097.738502
Gibbs Energy, BS2 (a.u.)	-2097.123502

Molecular Geometry in Cartesian Coordinates

Cu	0.018245	0.011256	-0.329890
O	-0.366766	-0.139879	1.504723
O	-0.879758	1.113850	1.953272
N	1.002991	-1.497933	-1.464852
N	0.887810	-1.361931	-2.813096
N	-1.657748	-0.227544	-1.519718
N	-1.401423	-0.280094	-2.854963
N	0.812664	1.400507	-1.632450
N	0.673316	1.138647	-2.958300
C	1.869404	-2.502182	-1.239717
C	2.323052	-3.022484	-2.473287
H	3.014100	-3.838194	-2.627413
C	1.673602	-2.270362	-3.441385
H	1.709357	-2.313549	-4.520709
C	2.202378	-2.891745	0.149791
C	1.181481	-3.332566	1.022252
C	1.514624	-3.658012	2.345106
H	0.728143	-4.002974	3.013661
C	2.823710	-3.551202	2.826966
C	3.820881	-3.115544	1.942429
H	4.844572	-3.020645	2.300503
C	3.535560	-2.787432	0.612795
C	-0.254410	-3.456523	0.563905
H	-0.320003	-3.863289	-0.450499
H	-0.818543	-4.108333	1.238479
C	3.165670	-3.888680	4.259322
H	3.591711	-3.020516	4.776150
H	3.911697	-4.690613	4.310777
H	2.281760	-4.212077	4.816835
C	4.648873	-2.318852	-0.297067
H	5.522445	-2.011966	0.286094
H	4.334083	-1.474971	-0.918185
H	4.969264	-3.116052	-0.978926
C	-2.999200	-0.315823	-1.371875
C	-3.603971	-0.422717	-2.644378
H	-4.659895	-0.489090	-2.859133
C	-2.557001	-0.391557	-3.550169
H	-2.547266	-0.441901	-4.629357
C	-3.691182	-0.291906	-0.070324
C	-3.581247	0.837085	0.813906
C	-4.392858	0.872742	1.989269
H	-4.312655	1.740288	2.640892
C	-5.264164	-0.155622	2.308750
C	-5.317141	-1.270316	1.444640
H	-5.973583	-2.099943	1.698561
C	-4.557915	-1.351999	0.269452
C	-2.672975	1.887601	0.592617
H	-2.680788	2.760257	1.236626
H	-2.038701	1.923766	-0.285375
H	-1.542139	0.825998	2.612785
C	-6.139900	-0.107524	3.537075
H	-5.957562	0.797117	4.124181
H	-5.962078	-0.976306	4.181006
H	-7.199944	-0.124409	3.257381
C	-4.683450	-2.585897	-0.596949

H	-3.715605	-2.886728	-1.008041
H	-5.358152	-2.415826	-1.443523
H	-5.087835	-3.419052	-0.015237
C	1.413245	2.601328	-1.521975
C	1.656469	3.124634	-2.810231
H	2.132093	4.061659	-3.059013
C	1.174482	2.162532	-3.687935
H	1.155742	2.127771	-4.767917
C	1.728381	3.130492	-0.175789
C	2.620566	2.417051	0.655589
C	2.841414	2.874633	1.961617
H	3.525530	2.321748	2.602457
C	2.198528	4.011444	2.463741
C	1.338320	4.718376	1.611579
H	0.836396	5.610283	1.982740
C	1.094750	4.301393	0.298333
C	3.313437	1.161383	0.175384
H	2.638536	0.298028	0.226012
H	4.187248	0.938746	0.795014
H	3.634781	1.251611	-0.867181
C	2.394783	4.453022	3.894488
H	1.532793	4.164402	4.509542
H	2.493592	5.541381	3.968319
H	3.284340	3.995548	4.337738
C	0.152601	5.091025	-0.581880
H	-0.373248	5.854612	-0.001134
H	-0.594082	4.443821	-1.054907
H	0.691208	5.599829	-1.390029
B	0.047671	-0.206291	-3.407202
H	0.028007	-0.275418	-4.603255
H	-0.748636	-2.478089	0.550333

Dinuclear complexes

Cu

Charge	0
Spin State	Doublet
Electronic Energy, BS1 (a.u.)	-197.215307
Thermal and entropic correction, BS1 (a.u.)	-0.016509
Electronic Energy, BS2 (a.u.)	-197.215307
Gibs Energy, BS2 (a.u.)	-197.231816
Number of Imaginary Frequencies	N/A

Molecular Geometry in Cartesian Coordinates

Cu	0.000000	0.000000	0.000000

C-Cu-D

Charge	0
Spin State	Doublet
Electronic Energy, BS1 (a.u.)	-2294.781275
Thermal and entropic correction, BS1 (a.u.)	0.617984
Electronic Energy, BS2 (a.u.)	-2295.195061

Gibbs Energy, BS2 (a.u.)	-2294.577077
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-1.035248	0.358071	-1.962632
N	2.182518	0.422306	1.384359
N	2.107410	0.940741	2.637875
C	0.504025	2.518877	-1.363612
H	0.809045	3.143019	-0.512441
H	0.953851	2.950729	-2.271080
C	3.486253	0.364981	1.056725
C	4.263226	0.861368	2.129737
H	5.339791	0.928222	2.181535
C	3.347921	1.211594	3.109665
H	3.482211	1.622547	4.100068
C	3.939841	-0.192084	-0.236667
C	3.578453	-1.504873	-0.618735
C	4.045589	-2.007432	-1.840895
H	3.768470	-3.019790	-2.130071
C	4.852779	-1.249355	-2.696550
C	5.187882	0.052955	-2.304010
H	5.799995	0.666372	-2.962950
C	4.747890	0.594377	-1.090862
C	2.682871	-2.377847	0.231811
H	2.875878	-3.436272	0.028154
H	2.822349	-2.195175	1.301061
H	1.630184	-2.177878	-0.003693
C	5.370191	-1.827884	-3.992154
H	4.655719	-2.533740	-4.427946
H	5.570510	-1.042420	-4.727863
H	6.309807	-2.372562	-3.830941
C	5.118886	2.018389	-0.739583
H	4.258606	2.568973	-0.345020
H	5.905249	2.058724	0.023248
H	5.489460	2.546115	-1.623618
H	-0.164784	-5.572691	1.150244
H	-0.650307	-4.793370	2.664865
Cu	0.324794	0.194255	0.319842
O	0.946939	1.182006	-1.243093
O	-0.339298	-1.162538	-1.043626
H	-1.006393	-1.742273	-0.640945
N	-0.453003	1.923632	1.290921
N	-0.124196	2.149389	2.582950
N	-0.391842	-0.784026	2.016663
N	-0.017152	-0.262629	3.220606
C	-1.340458	2.869059	0.922809
C	-1.581696	3.730286	2.016907
H	-2.228661	4.594049	2.046612
C	-0.790709	3.234700	3.045675
H	-0.656612	3.570738	4.063855
C	-1.900106	2.777958	-0.439621
C	-1.014572	2.528814	-1.523280
C	-1.546390	2.198409	-2.804355
H	-0.876804	2.168609	-3.665800
C	-2.947137	2.121798	-3.008210
C	-3.788367	2.422568	-1.930446
C	-3.297616	2.760846	-0.659503
C	-3.507132	1.819452	-4.374913
H	-3.670742	2.748807	-4.935367
H	-2.820272	1.198449	-4.957133

H	-4.469590	1.304075	-4.303758
C	-1.175951	-1.850393	2.276997
C	-1.284821	-2.029870	3.670821
H	-1.848256	-2.793486	4.186088
C	-0.542329	-0.998664	4.225908
H	-0.357112	-0.726675	5.255090
C	-1.881372	-2.589613	1.203706
C	-2.934079	-1.945030	0.512241
C	-3.606915	-2.645676	-0.498986
H	-4.413948	-2.149336	-1.034049
C	-3.264833	-3.960790	-0.836849
C	-2.223438	-4.580944	-0.131032
H	-1.942081	-5.600899	-0.385759
C	-1.526553	-3.920491	0.887061
C	-3.304805	-0.514494	0.823461
H	-2.500077	0.168086	0.522339
H	-3.462338	-0.366172	1.897470
C	-3.980000	-4.692377	-1.947435
H	-3.319091	-4.831195	-2.811707
H	-4.862653	-4.141026	-2.284555
C	-0.396832	-4.610012	1.614373
H	0.509895	-3.995766	1.605874
B	0.739347	1.092417	3.324510
H	0.874378	1.400795	4.474232
H	-4.301158	-5.688711	-1.624008
H	-4.865252	2.378331	-2.077400
C	-4.275822	3.029752	0.458309
H	-4.282687	4.091218	0.731926
H	-5.290940	2.755583	0.158466
H	-4.015496	2.468209	1.361396
H	-4.214216	-0.223490	0.291027

C-Cu-Q

Charge	0
Spin State	Quadruplet
Electronic Energy, BS1 (a.u.)	-2294.714860
Thermal and entropic correction, BS1 (a.u.)	0.619262
Electronic Energy, BS2 (a.u.)	-2295.28948
Gibbs Energy, BS2 (a.u.)	-2294.509686
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	0.465782	0.250407	-2.389891
N	1.945216	0.070323	1.711234
N	1.798408	0.228936	3.050733
C	0.322302	2.676237	-0.725100
H	0.654966	3.084611	0.236919
H	0.845819	3.214427	-1.524752
C	3.234770	0.304824	1.420270
C	3.937421	0.620599	2.606596
H	4.990410	0.839011	2.709110
C	2.985435	0.561836	3.615820
H	3.063491	0.726875	4.681150
C	3.676600	0.196443	0.010196
C	3.575732	-1.043600	-0.655984
C	3.891940	-1.105804	-2.020064
H	3.808531	-2.060711	-2.535793

C	4.300034	0.025733	-2.737382
C	4.411977	1.241505	-2.049302
H	4.730059	2.131851	-2.588903
C	4.102621	1.346656	-0.687873
C	3.094065	-2.285308	0.056888
H	3.389965	-3.185456	-0.491807
H	3.490168	-2.352044	1.075435
H	2.000759	-2.268053	0.118745
C	4.561527	-0.054704	-4.222576
H	3.621448	0.050863	-4.780590
H	5.235135	0.740838	-4.556534
H	4.999528	-1.018720	-4.501588
C	4.180535	2.689335	0.000858
H	3.241401	2.919520	0.515482
H	4.974544	2.714699	0.756021
H	4.379751	3.486462	-0.721667
H	0.185157	-5.779303	-0.049402
H	-0.654594	-5.492843	1.482321
Cu	0.079041	0.010026	0.520835
O	0.741701	1.312177	-0.773785
O	0.273541	-1.174864	-1.067105
H	-0.537920	-1.693267	-1.214067
N	-0.719436	1.419293	1.754099
N	-0.466974	1.341014	3.084442
N	-0.597112	-1.355152	1.849507
N	-0.314961	-1.149221	3.164892
C	-1.566874	2.448565	1.550563
C	-1.851784	3.055586	2.793359
H	-2.482050	3.912917	2.974525
C	-1.137971	2.321835	3.730862
H	-1.058314	2.424253	4.803438
C	-2.069690	2.737777	0.190792
C	-1.172475	2.845187	-0.896925
C	-1.667408	3.071960	-2.187128
H	-0.959282	3.151392	-3.009973
C	-3.038858	3.192155	-2.437110
C	-3.914679	3.071873	-1.349727
C	-3.462586	2.850917	-0.042590
C	-3.554905	3.460892	-3.829830
H	-3.559466	4.537564	-4.042877
H	-2.924985	2.981251	-4.585781
H	-4.579947	3.097737	-3.952647
C	-1.273213	-2.515326	1.750334
C	-1.417157	-3.077086	3.035314
H	-1.918162	-3.998349	3.292174
C	-0.802584	-2.177641	3.895841
H	-0.681277	-2.189401	4.969296
C	-1.763083	-2.981496	0.433610
C	-2.705177	-2.201493	-0.276320
C	-3.108794	-2.625778	-1.551954
H	-3.829896	-2.023870	-2.100876
C	-2.609525	-3.797687	-2.132540
C	-1.683559	-4.558703	-1.403273
H	-1.279920	-5.468535	-1.842895
C	-1.249544	-4.172641	-0.131054
C	-3.255969	-0.913830	0.292917
H	-2.528811	-0.098022	0.195472
H	-3.484456	-1.010171	1.358945
C	-3.043227	-4.234452	-3.511380
H	-2.198712	-4.220151	-4.210615
H	-3.822606	-3.579413	-3.911121

C	-0.222034	-5.001824	0.603112
H	0.607831	-4.380811	0.957535
B	0.379094	0.158216	3.644939
H	0.406282	0.201415	4.841069
H	-3.431782	-5.259164	-3.496850
H	-4.986694	3.141256	-1.524361
C	-4.477216	2.697864	1.067689
H	-4.535494	3.598129	1.690536
H	-5.473005	2.521687	0.650793
H	-4.227129	1.863221	1.730283
H	-4.163916	-0.612659	-0.236915

4a

Charge	0
Spin State	Doublet
Electronic Energy, BS1 (a.u.)	-5134.351687

Molecular Geometry in Cartesian Coordinates

29	-4.490350	0.144280	0.044910
29	-1.121519	0.608072	0.152592
8	-2.984642	0.880384	1.023890
7	-5.968390	-0.950915	-0.948870
7	-5.800395	2.063580	0.094441
7	-5.573966	-0.349057	1.722069
7	-7.253685	-0.530956	-0.784911
7	-7.136548	1.830393	0.214928
7	-6.926538	-0.215367	1.675097
6	-2.979471	-4.225567	-1.515858
7	0.312614	1.847449	0.850771
6	-5.983461	-1.952239	-1.856229
7	1.184277	-1.242503	0.811114
7	-2.052780	0.394963	-1.597920
6	-5.260298	-0.930622	2.899625
7	1.558895	1.821171	0.306049
6	-1.804834	5.378226	0.196141
6	-2.614141	-4.452338	-2.851019
6	-4.454939	-2.998169	-3.553493
7	-3.406568	0.314611	-1.623785
6	-3.758545	4.524305	1.40004 0
6	-7.307570	-2.151514	-2.304694
6	-1.236503	-1.631476	4.293870
6	-3.866683	-1.202768	3.305172
7	-0.150527	-1.212034	0.628238
6	-5.633419	3.395328	0.191077
6	-1.593534	-0.422539	3.676050
6	0.461509	-0.723586	-3.663078
6	-8.073546	-1.241527	-1.597183
6	6.815473	0.370683	-4.708225
6	-2.710202	0.389375	-3.752970
6	-4.298730	4.046518	0.186135
6	1.824475	-0.703101	-3.978459
6	-6.885559	4.030488	0.358149
6	-4.052788	-3.398258	-1.170837
6	4.048308	0.442988	-4.146536
6	1.970531	1.614114	-3.331319
6	-3.372325	-3.831557	-3.854176
6	-6.447953	-1.167825	3.627027

6	-0.158590	0.452771	-3.186706
6	-4.794383	-2.763899	-2.198770
6	-2.874987	-0.201272	3.167688
6	-3.516663	-2.449177	3.880431
6	-3.818791	0.317646	-2.909181
6	-0.282747	-5.251606	-2.388003
6	0.834960	-6.026178	-2.703175
6	0.816636	-6.866093	-3.822249
6	-0.328957	-6.921209	-4.623236
6	-1.447603	-6.146075	-4.308254
6	-1.442958	-5.298789	-3.184762
6	0.603069	1.632318	-3.022274
6	-7.809547	2.999255	0.372787
6	-3.604745	4.252866	-1.024828
6	6.170784	1.469662	1.050252
6	4.047026	-2.050289	0.245191
6	0.482206	2.401858	2.061622
6	3.941997	2.379396	0.763941
6	-2.375702	4.917972	-1.001717
6	-2.211115	-2.642125	4.346032
6	-7.469787	-0.700445	2.817619
6	-2.515999	5.169577	1.388299
6	-0.525987	-2.499162	0.640769
6	2.600243	0.455984	-3.822132
6	3.139333	-2.697390	1.120522
6	1.831677	2.726286	2.288397
5	-7.664704	0.383616	0.420536
6	5.915319	-0.351373	-5.499384
6	-1.609993	0.433055	-2.877366
6	6.333660	1.132523	-3.638516
6	-0.093372	6.874365	-0.888473
6	1.142158	7.524891	-0.886909
6	2.010680	7.388733	0.201433
6	1.633365	6.586700	1.283643
6	0.399085	5.934486	1.280404
6	-0.489824	6.067525	0.196223
6	1.689060	-2.501228	0.933799
6	3.628273	-3.465245	2.206262
6	0.581833	-3.346654	0.838009
6	4.832291	1.509296	1.441326
6	6.659295	2.277494	0.008523
6	4.965574	1.167975	-3.363391
6	0.297538	-2.723120	5.960851
6	0.109924	-1.827881	4.888251
6	1.231498	-1.109814	4.426385
6	2.484251	-1.278066	5.019578
6	2.654215	-2.175885	6.077903
6	1.553451	-2.901105	6.543328
6	4.546675	-0.316332	-5.222372
6	5.770116	3.163756	-0.615492
6	4.415967	3.231021	-0.256430
6	2.509720	2.353175	1.132826
6	8.777657	3.293746	-0.901015
6	10.100114	3.177578	-1.334449
6	10.745484	1.936824	-1.305199
6	10.056340	0.812430	-0.838841
6	8.733775	0.926450	-0.407802
6	8.072562	2.169898	-0.430489
6	5.006079	-3.494636	2.446212
6	5.417305	-2.121094	0.511882
6	5.918395	-2.810510	1.624839

6	8.330139	-2.819161	0.901071
6	9.694525	-2.766981	1.195738
6	10.126662	-2.680761	2.523541
6	9.182875	-2.651155	3.555399
6	7.818506	-2.705173	3.262490
6	7.369791	-2.788778	1.930852
6	-4.186278	3.773959	-2.330525
1	-3.506303	3.975035	-3.163001
1	-4.376719	2.698820	-2.297258
1	-5.142918	4.268688	-2.540389
6	-4.511108	4.393263	2.705174
1	-5.210906	5.228450	2.836610
1	-5.098694	3.472889	2.747504
1	-3.821692	4.405290	3.554969
6	-3.145564	1.081645	2.411759
1	-4.155185	1.453734	2.629220
1	-2.434921	1.852484	2.742879
6	-4.498907	-3.593559	4.002451
1	-3.967596	-4.550379	3.990940
1	-5.056714	-3.542538	4.945685
1	-5.231011	-3.593900	3.191038
6	3.527417	4.232186	-0.958447
1	3.686718	4.200635	-2.041019
1	2.466820	4.074056	-0.757457
1	3.773055	5.247174	-0.627290
6	4.361750	0.630930	2.574737
1	3.482159	0.044316	2.293989
1	5.148123	-0.065680	2.874202
1	4.083933	1.232011	3.447675
6	-4.397399	-3.242132	0.290972
1	-5.477940	-3.201152	0.455104
1	-3.983864	-4.073068	0.870068
1	-3.983055	-2.314182	0.699709
6	-5.219797	-2.377336	-4.701129
1	-4.555488	-2.211555	-5.554827
1	-6.027563	-3.038481	-5.039742
1	-5.675110	-1.423208	-4.428066
6	-0.058300	2.904411	-2.550262
1	-0.892193	3.168212	-3.209693
1	-0.479206	2.784979	-1.546401
1	0.648736	3.738540	-2.533798
6	-0.326738	-2.001822	-3.795779
1	0.331741	-2.850688	-3.996027
1	-0.891210	-2.203613	-2.880807
1	-1.060043	-1.939304	-4.606893
1	1.421033	8.148504	-1.731983
1	2.970098	7.898228	0.204474
1	2.306063	6.456686	2.127034
1	0.130525	5.294952	2.114836
1	-0.768636	7.014065	-1.727928
1	8.294222	4.266639	-0.906548
1	10.629112	4.058698	-1.686896
1	11.774434	1.847778	-1.641818
1	10.545176	-0.157463	-0.816152
1	8.204776	0.040139	-0.069574
1	10.420490	-2.803597	0.388128
1	8.005199	-2.905290	-0.132154
1	7.091226	-2.656655	4.068536
1	9.508138	-2.577005	4.589417
1	11.187827	-2.638075	2.751536
1	-0.244448	-4.572050	-1.541918

1	1.724221	-5.962221	-2.081591
1	1.686480	-7.468159	-4.069525
1	-0.355110	-7.574204	-5.491429
1	-2.339084	-6.210945	-4.926496
1	4.608203	1.735697	-2.510621
1	7.022746	1.687428	-3.008378
1	7.880280	0.339323	-4.921309
1	6.277670	-0.939723	-6.338067
1	3.855800	-0.867139	-5.854760
1	-0.552743	-3.265932	6.362857
1	1.667140	-3.596554	7.370358
1	3.632058	-2.308021	6.532295
1	3.334845	-0.718319	4.646761
1	1.127187	-0.432638	3.584183
1	-9.138194	-1.063896	-1.603608
1	-7.649032	-2.883956	-3.020700
1	-8.536915	-0.675144	2.978058
1	-6.537122	-1.599893	4.612114
1	6.121796	3.792717	-1.429401
1	6.847670	0.801274	1.574916
1	6.101425	-1.592732	-0.147005
1	5.376402	-4.075463	3.287312
1	-1.568096	-2.743874	0.506122
1	0.587332	-4.425087	0.887767
1	-1.951273	-3.616938	4.750886
1	-0.867264	0.380942	3.596026
1	-7.073993	5.090038	0.454780
1	-8.883159	3.015862	0.487260
1	-1.842250	5.057938	-1.937007
1	-2.113653	5.544408	2.326556
1	2.263633	3.184309	3.165361
1	-0.373567	2.542866	2.704473
1	-4.873860	0.270768	-3.136191
1	-2.694029	0.403635	-4.833961
1	1.667295	1.521934	-0.660032
1	1.691833	-0.368267	0.858803
1	2.298524	-1.621833	-4.314924
1	2.542012	2.533845	-3.237723
1	-2.435752	-4.732270	-0.722393
1	-3.092478	-3.967868	-4.895848
6	-9.258684	0.370916	0.630788
1	-9.782574	0.795382	-0.234589
1	-9.645921	-0.644384	0.776283
1	-9.559860	0.959939	1.505196
6	3.595625	-1.275614	-0.971710
1	4.383511	-1.274771	-1.728591
1	2.690783	-1.696818	-1.415976
1	3.388610	-0.225386	-0.732302
6	2.701292	-4.252206	3.102136
1	2.341783	-5.153844	2.591554
1	3.219996	-4.568921	4.010432
1	1.821966	-3.669491	3.390571

Trinuclear complexes

2a-D

Charge 0 S111

Spin State	Doublet
Electronic Energy, BS1 (a.u.)	-4392.354178
Thermal and entropic correction, BS1 (a.u.)	1.279815
Electronic Energy, BS2 (a.u.)	-4393.179673
Gibbs Energy, BS2 (a.u.)	-4391.899858
Number of Imaginary Frequencies	1
Imaginary frequencies (cm-1)	-5.4i

Molecular Geometry in Cartesian Coordinates

Cu	2.991833	0.147128	-0.074872
Cu	0.004198	-0.004159	0.002602
O	1.475021	1.007966	0.747440
O	1.519605	-1.136143	-0.426593
H	1.514618	-1.546495	-1.306298
N	4.090458	1.900526	-0.107284
N	5.429253	1.795470	0.109016
N	4.482206	-0.820100	-1.063180
N	5.758480	-0.560495	-0.665941
C	3.819621	3.214182	-0.290966
C	5.021946	3.950746	-0.185440
H	5.137168	5.020916	-0.260520
C	6.008024	3.014914	0.069653
H	7.070304	3.121206	0.234895
C	2.471015	3.789328	-0.471418
C	1.403289	3.426026	0.384622
C	0.210576	4.156585	0.349674
H	-0.594691	3.872533	1.021311
C	0.041920	5.252051	-0.504663
C	1.072908	5.541441	-1.406283
H	0.940088	6.350930	-2.122072
C	2.279891	4.830882	-1.414473
C	-1.197040	6.111137	-0.444096
H	-1.002724	7.023218	0.135661
H	-2.023280	5.584878	0.039464
H	-1.518907	6.426850	-1.442086
C	3.326675	5.211438	-2.440325
H	2.842446	5.605211	-3.339318
H	3.946919	4.358630	-2.729356
H	3.998868	5.993514	-2.067056
C	4.552236	-1.735598	-2.055134
C	5.903138	-2.058024	-2.295929
H	6.285322	-2.745612	-3.035040
C	6.627626	-1.292124	-1.397029
H	7.690546	-1.209984	-1.222345
C	3.349515	-2.274278	-2.725837
C	2.449689	-1.414819	-3.395386
C	1.298308	-1.963971	-3.984903
H	0.594374	-1.294398	-4.472975
C	1.029987	-3.335563	-3.943846
C	1.952726	-4.172792	-3.298554
H	1.755512	-5.241836	-3.250583
C	3.104490	-3.670604	-2.687189
C	2.669862	0.078142	-3.478683
H	2.146604	0.597417	-2.666036
H	2.271853	0.464002	-4.419905
H	3.728125	0.342867	-3.409721
C	-0.229354	-3.912332	-4.543020
H	-0.820557	-4.427962	-3.776865
H	-0.855035	-3.133196	-4.984832

C	4.041998	-4.620096	-1.976429
H	4.286692	-4.263896	-0.970216
B	6.076689	0.440041	0.470092
H	7.263293	0.572545	0.573220
N	-4.158560	0.376092	-1.852063
N	-5.477550	0.057532	-1.775510
C	-1.517359	-2.289755	-1.358208
H	-2.463636	-2.360059	-1.913046
H	-0.699534	-2.350444	-2.084806
C	-3.923025	0.735817	-3.127459
C	-5.116170	0.633181	-3.883437
H	-5.252868	0.873140	-4.927713
C	-6.076602	0.200926	-2.983168
H	-7.130157	-0.007864	-3.104552
C	-2.608524	1.262818	-3.560095
C	-2.088216	2.423336	-2.940770
C	-0.873770	2.949455	-3.397735
H	-0.475975	3.840264	-2.916977
C	-0.167327	2.370198	-4.458413
C	-0.697842	1.219634	-5.055613
H	-0.163265	0.751141	-5.880257
C	-1.905497	0.654499	-4.623330
C	-2.806944	3.111200	-1.804933
H	-2.540384	4.170129	-1.778241
H	-3.893634	3.027781	-1.897335
H	-2.512618	2.651584	-0.854141
C	1.125927	2.985782	-4.938394
H	1.893208	2.948425	-4.157315
H	1.513215	2.467833	-5.821026
H	0.983854	4.040813	-5.200874
C	-2.425831	-0.597036	-5.293652
H	-2.694591	-1.359683	-4.554846
H	-3.323903	-0.398408	-5.889635
H	-1.671520	-1.016468	-5.965977
H	0.003589	-4.648560	-5.321305
H	-3.581592	5.630084	1.879526
H	-4.977683	4.751285	2.507185
N	4.155213	-0.381699	1.858645
N	5.474248	-0.061494	1.794508
C	1.521533	2.281392	1.367325
H	2.467212	2.350336	1.923139
H	0.702360	2.339758	2.092799
C	3.906413	-0.738786	3.132046
C	5.091176	-0.632039	3.900389
H	5.217800	-0.870324	4.946374
C	6.060497	-0.200439	3.008967
H	7.112367	0.010345	3.141226
Cu	-2.984672	-0.151458	0.082548
O	-1.469118	-1.014713	-0.741621
O	-1.510718	1.128675	0.429318
H	-1.505885	1.550001	1.303734
N	-4.081488	-1.903411	0.124328
N	-5.421171	-1.797705	-0.086749
N	-4.469536	0.826041	1.071030
N	-5.747847	0.560871	0.684193
C	-3.810997	-3.216889	0.310550
C	-5.014526	-3.952431	0.212252
H	-5.130466	-5.022226	0.290657
C	-6.000815	-3.016444	-0.041229
H	-7.063926	-3.122321	-0.201405
C	-2.462680	-3.794708	0.485781

C	-1.397669	-3.433258	-0.374560
C	-0.206733	-4.167050	-0.345834
H	0.596634	-3.883290	-1.019907
C	-0.037530	-5.264761	0.505329
C	-1.065729	-5.553380	1.410491
C	-2.270258	-4.838786	1.426222
C	1.200136	-6.125377	0.438731
H	1.002899	-7.036094	-0.142187
H	2.025421	-5.599002	-0.046658
H	1.525240	-6.443508	1.434924
C	-4.535434	1.750484	2.055082
C	-5.885443	2.072804	2.300906
H	-6.264355	2.765639	3.036779
C	-6.613983	1.297677	1.413433
H	-7.677744	1.212247	1.245585
C	-3.332602	2.295183	2.720767
C	-2.433226	1.440385	3.397530
C	-1.290346	1.995774	3.996699
H	-0.589439	1.330841	4.495041
C	-1.028186	3.368970	3.957572
C	-1.948116	4.200537	3.301641
H	-1.757268	5.270756	3.255509
C	-3.092886	3.692036	2.681353
C	-2.649337	-0.053004	3.481066
H	-2.129127	-0.569665	2.664853
H	-3.707312	-0.320253	3.417120
C	0.228293	3.948022	4.560348
H	0.926966	4.254373	3.771323
H	0.739927	3.220613	5.195735
C	-4.031539	4.637465	1.966658
H	-4.276242	4.277082	0.961964
B	-6.070829	-0.443143	-0.446904
H	-7.257882	-0.577040	-0.543050
H	3.590715	-5.612432	-1.893145
H	4.988206	-4.732682	-2.517083
H	0.008371	4.838133	5.160220
H	-0.932126	-6.364671	2.124082
C	-3.313374	-5.219713	2.455659
H	-3.984237	-6.004431	2.085422
H	-2.825699	-5.610421	3.354135
H	-3.935160	-4.368236	2.745045
C	2.588342	-1.272403	3.545399
C	1.857786	-0.662649	4.589112
C	2.090043	-2.440197	2.922078
C	0.644330	-1.233475	4.997462
C	0.869103	-2.971270	3.354331
C	0.133615	-2.389511	4.393437
H	0.088533	-0.763600	5.807247
H	0.487132	-3.866218	2.869097
H	-2.245493	-0.439432	4.419307
C	2.351119	0.600385	5.258418
H	1.595944	0.991763	5.946509
H	3.266413	0.428192	5.835642
H	2.579853	1.376212	4.519350
C	2.835211	-3.127021	1.802662
H	2.558282	-2.668441	0.846282
H	3.919558	-3.040224	1.917425
H	2.572581	-4.186852	1.770589
C	-1.172652	-3.005472	4.836058
H	-1.041587	-4.063965	5.090608

H	-1.581057	-2.495064	5.713658
H	-1.918855	-2.956860	4.035150

2a-Q

Charge	0
Spin State	Quadruplet
Electronic Energy, BS1 (a.u.)	-4392.350813
Thermal and entropic correction, BS1 (a.u.)	1.277817
Electronic Energy, BS2 (a.u.)	-4393.176164
Gibbs Energy, BS2 (a.u.)	-4391.898347
Number of Imaginary Frequencies	0

Molecular Geometry in Cartesian Coordinates

Cu	-2.940426	-0.198497	-0.075555
Cu	0.000030	-0.000085	-0.000040
O	-1.435575	-1.059207	0.770388
O	-1.528079	1.160791	-0.319871
H	-1.533213	1.597911	-1.186613
N	-3.989415	-1.958675	-0.295688
N	-5.334563	-1.919498	-0.101881
N	-4.467600	0.822270	-0.981986
N	-5.735855	0.495725	-0.609630
C	-3.671897	-3.229247	-0.636039
C	-4.852648	-4.007342	-0.657320
H	-4.930982	-5.062382	-0.868729
C	-5.873343	-3.140037	-0.311192
H	-6.935124	-3.297108	-0.188309
C	-2.298866	-3.737761	-0.828564
C	-1.272993	-3.428427	0.099161
C	-0.059240	-4.120342	0.040500
H	0.710489	-3.883403	0.769583
C	0.173765	-5.126672	-0.904152
C	-0.816047	-5.359413	-1.865159
H	-0.635654	-6.096524	-2.645942
C	-2.042974	-4.682580	-1.854361
C	1.436826	-5.951080	-0.869157
H	1.298727	-6.836312	-0.234224
H	2.272179	-5.380777	-0.457716
H	1.714220	-6.306278	-1.866759
C	-3.040027	-5.003174	-2.948244
H	-2.510531	-5.272634	-3.867349
H	-3.699739	-4.159515	-3.166295
H	-3.675931	-5.856711	-2.682708
C	-4.564567	1.831090	-1.877267
C	-5.924137	2.146364	-2.078206
H	-6.326411	2.894157	-2.744490
C	-6.625777	1.277405	-1.259051
H	-7.685582	1.152643	-1.090781
C	-3.384050	2.457352	-2.510276
C	-2.461163	1.678578	-3.247084
C	-1.344345	2.309545	-3.818877
H	-0.627228	1.701482	-4.364983
C	-1.130442	3.687383	-3.698921
C	-2.071673	4.442436	-2.985606
H	-1.919876	5.514436	-2.877082
C	-3.191888	3.856308	-2.387184

C	-2.628428	0.187457	-3.435329
H	-2.064337	-0.370937	-2.677506
H	-2.240892	-0.110416	-4.411982
H	-3.673242	-0.123913	-3.360376
C	0.102028	4.341652	-4.273288
H	0.900112	4.382257	-3.520885
H	0.487517	3.785821	-5.132350
C	-4.155110	4.728050	-1.614051
H	-4.413916	4.284113	-0.647176
B	-6.027839	-0.634124	0.404404
H	-7.209916	-0.816272	0.482846
N	4.146569	-0.113504	-1.885285
N	5.447168	0.264722	-1.779515
C	1.461448	2.408119	-1.203435
H	2.421905	2.573762	-1.711357
H	0.663494	2.535587	-1.943988
C	3.906473	-0.304419	-3.196537
C	5.078803	-0.031736	-3.943251
H	5.210884	-0.117987	-5.011829
C	6.030699	0.325078	-3.001865
H	7.069434	0.605928	-3.104276
C	2.610232	-0.831640	-3.679225
C	2.133770	-2.067337	-3.180735
C	0.931446	-2.582585	-3.679299
H	0.567238	-3.529848	-3.288584
C	0.193309	-1.921317	-4.667423
C	0.681889	-0.700300	-5.148394
H	0.123842	-0.167924	-5.916802
C	1.875835	-0.142226	-4.670319
C	2.882084	-2.851923	-2.130010
H	2.651245	-3.915606	-2.224034
H	3.964837	-2.721600	-2.211033
H	2.577081	-2.515144	-1.132419
C	-1.089391	-2.524000	-5.190023
H	-1.842655	-2.590071	-4.397207
H	-1.508474	-1.930582	-6.008423
H	-0.922309	-3.541933	-5.561624
C	2.344026	1.186600	-5.220162
H	2.615364	1.878908	-4.416220
H	3.227034	1.074749	-5.859576
H	1.558161	1.650523	-5.823717
H	-0.103578	5.369916	-4.587293
H	3.719548	-5.715744	1.438706
H	5.092481	-4.875091	2.161767
N	-4.146362	0.113738	1.885603
N	-5.446995	-0.264410	1.779903
C	-1.461249	-2.408415	1.203220
H	-2.421609	-2.574112	1.711307
H	-0.663154	-2.535985	1.943600
C	-3.906211	0.304675	3.196844
C	-5.078529	0.032090	3.943614
H	-5.210563	0.118406	5.012192
C	-6.030484	-0.324688	3.002279
H	-7.069241	-0.605441	3.104733
Cu	2.940491	0.198387	0.075677
O	1.435701	1.058983	-0.770432
O	1.528118	-1.160957	0.319823
H	1.533172	-1.598126	1.186540
N	3.989352	1.958715	0.296039
N	5.334541	1.919556	0.102460
N	4.467629	-0.822296	0.982160

N	5.735909	-0.495733	0.609913
C	3.671736	3.229341	0.636103
C	4.852460	4.007481	0.657456
H	4.930735	5.062557	0.868699
C	5.873238	3.140157	0.311634
H	6.935035	3.297245	0.188902
C	2.298654	3.737843	0.828296
C	1.272954	3.428279	-0.099550
C	0.059157	4.120122	-0.041232
H	-0.710431	3.883011	-0.770403
C	-0.174087	5.126616	0.903189
C	0.815532	5.359595	1.864322
C	2.042520	4.682845	1.853860
C	-1.437169	5.950967	0.867669
H	-1.299334	6.835344	0.231489
H	-2.272695	5.380130	0.457327
H	-1.714152	6.307466	1.864916
C	4.564517	-1.831266	1.877278
C	5.924066	-2.146642	2.078203
H	6.326290	-2.894565	2.744371
C	6.625773	-1.277552	1.259244
H	7.685592	-1.152781	1.091058
C	3.383946	-2.457495	2.510208
C	2.461042	-1.678693	3.246957
C	1.344167	-2.309630	3.818686
H	0.627059	-1.701548	4.364779
C	1.130196	-3.687446	3.698680
C	2.071421	-4.442526	2.985376
H	1.919570	-5.514514	2.876809
C	3.191704	-3.856443	2.387052
C	2.628256	-0.187564	3.435197
H	2.063814	0.370783	2.677600
H	3.673000	0.123930	3.359875
C	-0.102322	-4.341686	4.272977
H	-0.900217	-4.382691	3.520396
H	-0.488103	-3.785596	5.131738
C	4.154918	-4.728210	1.613938
H	4.413881	-4.284210	0.647135
B	6.027920	0.634271	-0.403931
H	7.209993	0.816488	-0.482277
H	-3.719822	5.715642	-1.438956
H	-5.092747	4.874779	-2.161791
H	0.103358	-5.369806	4.587410
H	0.634967	6.096859	2.644919
C	3.039367	5.003820	2.947817
H	3.675284	5.857293	2.682105
H	2.509696	5.273572	3.866735
H	3.699082	4.160265	3.166266
C	-2.609932	0.831795	3.679539
C	-1.875573	0.142269	4.670590
C	-2.133387	2.067486	3.181131
C	-0.681610	0.700251	5.148714
C	-0.931046	2.582654	3.679753
C	-0.192959	1.921285	4.667841
H	-0.123575	0.167785	5.917068
H	-0.566801	3.529930	3.289100
H	2.241052	0.110247	4.412005
C	-2.343794	-1.186609	5.220280
H	-1.557940	-1.650602	5.823797
H	-3.226811	-1.074825	5.859693
H	-2.615110	-1.878825	4.416252

C	-2.881611	2.852151	2.130392
H	-2.576560	2.515422	1.132795
H	-3.964372	2.721843	2.211332
H	-2.650760	3.915823	2.224518
C	1.089785	2.523817	5.190507
H	0.922753	3.541634	5.562447
H	1.508948	1.930140	6.008677
H	1.842969	2.590131	4.397636