Electronic Supporting Information for

New copper(I) complexes of bulky 5-substituted-2-iminopyrrolyl ligands as catalysts for azide-alkyne cycloaddition

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Synthesis and characterization of the potassium salt KLd and its precursors

2-[2,6-$(MeO)_2C_6H_3$]-*1H*-pyrrole: This compound was prepared by adapting a reported procedure.[1] A Schlenk flask was charged with a solid mixture of pyrrolyl sodium (2.67 g, 30 mmol) and $ZnCl_2$ (4.09 g, 30 mmol) and THF (ca. 20 mL) was added, and the resulting suspension was stirred for 15 minutes at room temperature. Subsequently, $Pd(OAc)_2$ (0.034 g, 0.05 mmol), 2-(di-*tert*-butylphosphino)biphenyl (0.015 g, 0.05 mmol) and 2-bromo-1,3-dimethoxybenzene (2.17 g, 10 mmol) were added, and the mixture stirred for 24 h at 100 ºC. After cooling to room temperature, water and Et_2O (1:1 in volume) were added to the stirred reaction mixture. The residue was extracted with Et_2O, the combined extracts evaporated under reduced pressure and the residue dried under vacuum. The residue was extracted with hot *n*-hexane and the resulting colorless solution cooled to -20 ºC, yielding the product as an off-white solid. Yield: 1.5 g (74%).

Anal. Calc. for $C_{12}H_{13}NO_2$, obtained (calculated): 70.91 (70.92) H 6.40 (6.45) N 6.90 (6.89). ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.87 (br, 1H, N*H*), 7.14 (t, 1H, 5-Ph-H$_{para}$, $^3J_{HH}$ = 8.3 Hz), 6.95 (m, 1H, H3), 6.88 (m, 1H, H5), 6.72 (d, 2H, 5-Ph-H$_{meta}$, $^3J_{HH}$ = 8.3 Hz), 6.32 (m, 1H, H4), 3.92 (s, 6H, OC*H*$_3$). ^{13}C{^{1}H} NMR (75 MHz, $CDCl_3$): δ 157.0 (5-Ph-C$_{ortho}$), 126.5 (5-Ph-C$_{para}$), 125.0 (C2), 116.9 (C5), 111.6 (C3), 111.0 (5-Ph-C$_{ipso}$), 108.4 (C4), 105.0 (5-Ph-C$_{meta}$), 56.1 (O*C*H$_3$).

5-[2,6-$(MeO)_2C_6H_3$]-*1H*-pyrrole-2-carbaldehyde: A toluene solution of $POCl_3$ (0.7 mL, 7.5 mmol) was added dropwise and under dinitrogen to an ice-cooled toluene solution of *N*,*N*-dimethylformamide (0.67 mL, 7.5 mmol). The mixture was stirred for 30 minutes at room temperature and ice-cooled again. Then, a solution of 2-[2,6-$(MeO)_2$-C_6H_3]-*1H*-pyrrole (1.5 g, 7.4 mmol) in toluene was added dropwise. The yellow-orange mixture was stirred overnight. A water-ice mixture and $NaHCO_3$ powder were slowly added until pH = 7. Subsequently, NaOH was added until pH = 12. The organic phase was extracted with CH_2Cl_2, dried with $MgSO_4$ and all the volatile materials removed under reduced pressure. The resulting solid was washed with *n*-hexane and dried under vacuum to give the title compound as a beige solid. Yield: 1.4 g (82%).

Anal. Calc. for $C_{13}H_{13}NO_3$, obtained (calculated): C 67.46 (67.52) H 5.62 (5.67) N 6.02 (6.06). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.56 (br, 1H, N*H*), 9.48 (s, 1H, O=C*H*), 7.29 (t, 1H, 5-Ph-H$_{para}$, $^3J_{HH}$ = 8.4 Hz), 7.00 (m, 2H, H3 + H4), 6.72 (d, 2H, 5-Ph-H$_{meta}$, $^3J_{HH}$ = 8.4 Hz), 3.94 (s, 6H, OC*H*$_3$). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 178.5 (O=*C*H), 158.3 (5-Ph-C$_{ortho}$), 133.9

(C5), 131.7 (C2), 129.7 (5-Ph-C_{para}), 120.6 (C3), 114.8 (C4), 108.6 (5-Ph-C_{ipso}), 105.0 (5-Ph-C_{meta}), 56.4 (O*C*H_3).

5-[2,6-$(MeO)_2C_6H_3$]-2-[*N*-(2,6-*i*$Pr_2C_6H_3$)formimino]-1*H*-pyrrole: A mixture of 5-[2,6-$(MeO)_2C_6H_3$]-*1H*-pyrrole-2-carbaldehyde (1.4 g, 5.9 mmol) and 2,6-diisopropylaniline (1.11 g, 5.9 mmol), with a catalytic amount of *p*-toluenesulfonic acid, was dissolved in *ca.* 50 mL of toluene and refluxed for 45 h, in a flask equipped with a Soxhlet apparatus charged with pre-dried 4 Å molecular sieves and a $CaCl_2$ guard tube. The mixture was filtered, and the resulting solution evaporated under reduced pressure. The crude product was washed with *n*-hexane, to yield the product as a green powder. Yield: 1.49 g (64%).

Anal. Calc. for $C_{25}H_{30}N_2O_2$, obtained (calculated): C 75.45 (76.89) H 7.45 (7.74) N 6.81(7.17). ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.68 (br, 1H, N*H*), 7.94 (s, 1H, N=C*H*), 7.23-7.06 (m, 4H, 5-Ph-H_{para} + N-Ph-H_{meta} + N-Ph-H_{para}), 6.99 (d, 1H, H3, $^3J_{HH}$ = 3.9 Hz), 6.61-6.68 (m, 3H, 5-Ph-H_{meta} + H4), 3.95 (s, 6H, OCH_3), 3.09 (sept, 2H, C*H*$(CH_3)_2$, $^3J_{HH}$ = 6.8 Hz), 1.19 (d, 12H, CH(C$H_3)_2$, $^3J_{HH}$ = 6.9 Hz). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 157.7 (5-Ph-C_{ortho}), 151.4 (N=*C*H), 149.4 (N-Ph-C_{ipso}), 138.4 (N-Ph-C_{ortho}), 136.1 (C5), 129.7 (C2), 128.5 (5-Ph-C_{para}), 123.8 (N-Ph-C_{para}), 123.1 (N-Ph-C_{meta}), 115.5 (C3), 113.6 (C4), 109.7 (5-Ph-C_{ipso}) 104.8 (5-Ph-C_{meta}), 56.2 (O*C*H_3), 28.1 (*C*H$(CH_3)_2$), 23.7 (CH(*C*$H_3)_2$).

5-[2,6-$(MeO)_2C_6H_3$]-2-[N-(2,6-*i*$Pr_2C_6H_3$)formimino]pyrrolyl potassium (KLd): Toluene solutions of K[$N(SiMe_3)_2$] (0.30 g, 1.50 mmol) and 5-(2,6-$(MeO)_2C_6H_3$)-2-[*N*-(2,6-*i*$Pr_2C_6H_3$)formimino]-1*H*-pyrrole (0.48 g, 1.23 mmol) were combined, immediately giving rise to a suspension. The resulting suspension was stirred for two hours, the supernatant filtered off, the pale-yellow solid washed three times with *n*-hexane and dried under vacuum. Yield: 0.36 g (69%).

^{1}H NMR (300 MHz, THF-d_8): δ 7.71 (s, 1H, N=C*H*), 7.02 (d, 2H, N-Ph-H_{meta}, $^3J_{HH}$ = 7.8 Hz), 6.97 (t, 1H, 5-Ph-H_{para}, $^3J_{HH}$ = 8.1 Hz), 6.88 (t, 1H, N-Ph-H_{para}, $^3J_{HH}$ = 7.8 Hz), 6.62 (d, 2H, 5-Ph-H_{meta}, $^3J_{HH}$ = 8.1 Hz), 6.48 (d, 1H, H3, $^3J_{HH}$ = 3.3 Hz), 6.31 (d, 1H, H4, $^3J_{HH}$ = 3.3 Hz), 3.61 (s, 6H, OCH_3), 3.27 (sept, 2H, C*H*$(CH_3)_2$, $^3J_{HH}$ = 6.6 Hz), 1.13 (d, 12H, CH(C$H_3)_2$, $^3J_{HH}$ = 6.9 Hz). ^{13}C{^{1}H} NMR (75 MHz, THF-d_8): δ 159.7 (5-Ph-C_{ortho}), 159.5 (N=*C*H), 154.0 (N-Ph-C_{ipso}), 140.4 (N-Ph-C_{ortho}), 140.2 (C5), 139.4 (C2), 125.8 (5-Ph-C_{para}), 123.2 (N-Ph-C_{meta}), 122.7 (N-Ph-C_{para}), 120.1 (C3), 113.8 (C4), 108.2 (5-Ph-C_{meta}), 56.9 (O*C*H_3), 28.5 (*C*H$(CH_3)_2$), 24.6 (CH(*C*$H_3)_2$).

NMR data of the potassium salt KLd and its precursors

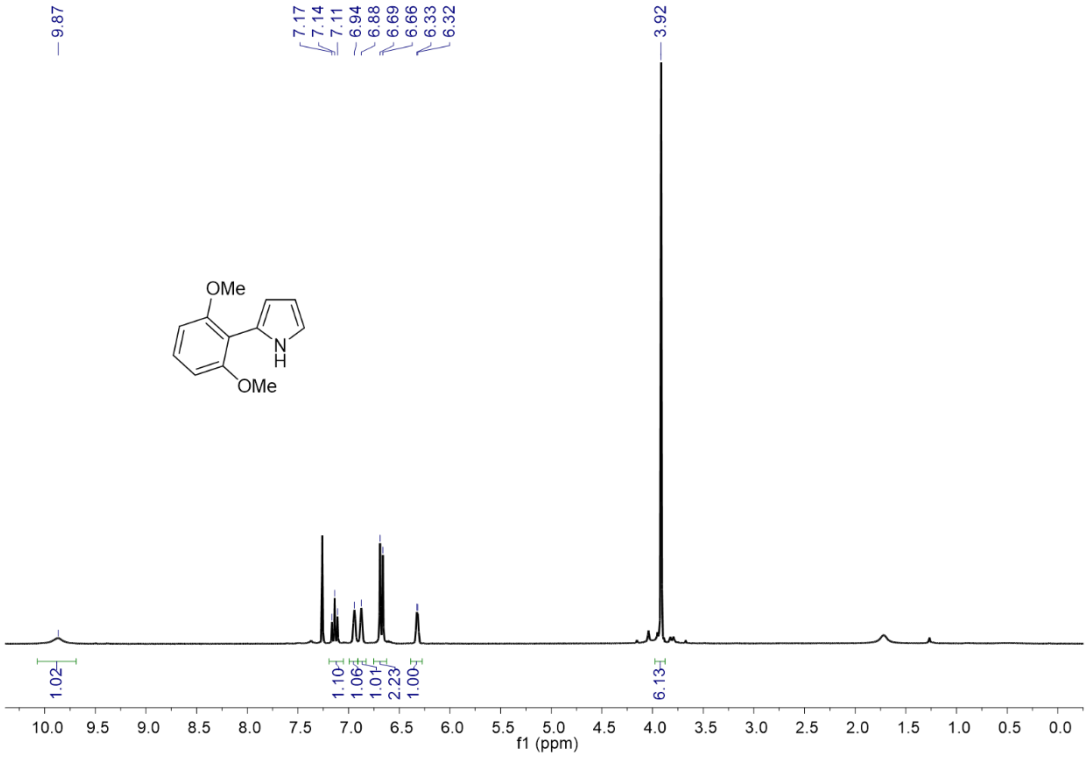

Figure S1 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 2-[2,6-$(MeO)_2C_6H_3$]-*1H*-pyrrole.

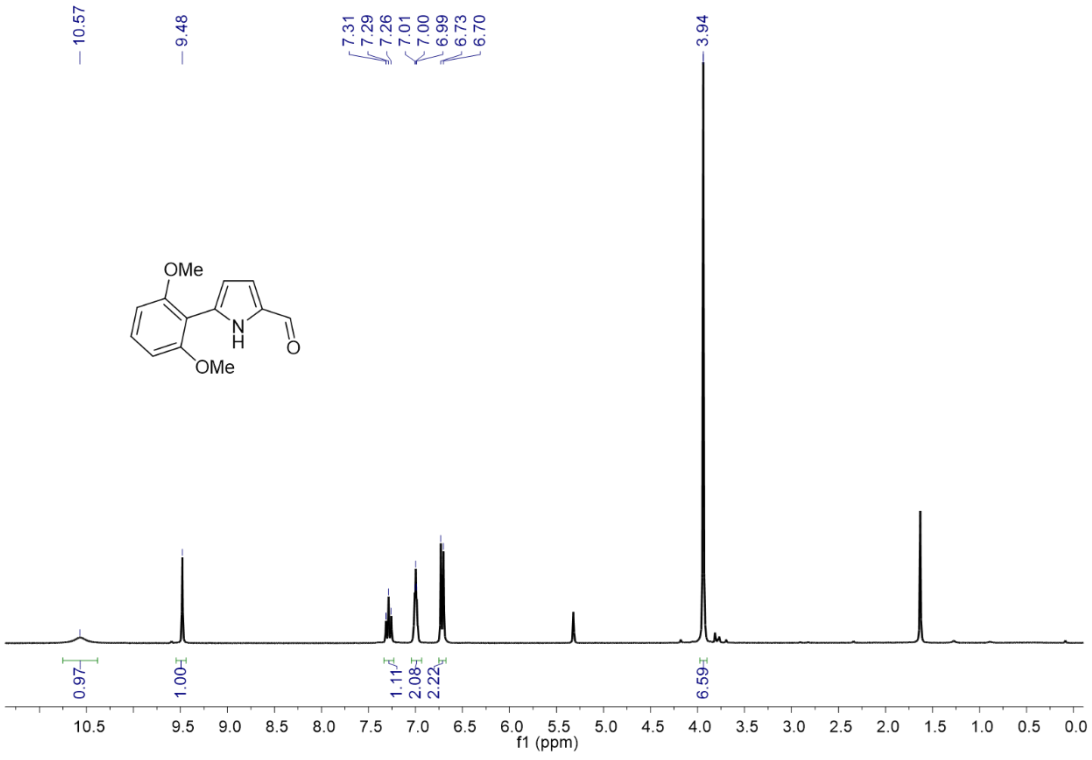

Figure S2 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 5-[2,6-$(MeO)_2C_6H_3$]-1H-pyrrole-2-carbaldehyde.

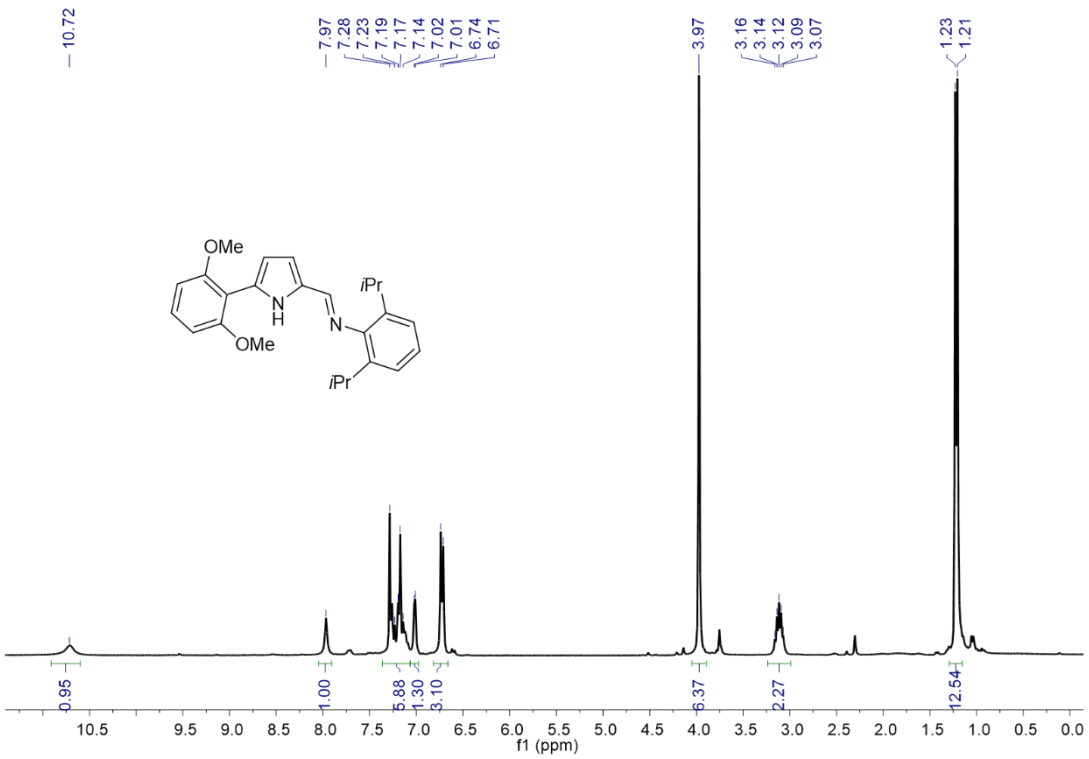

Figure S3 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of 5-[2,6-$(MeO)_2C_6H_3$]-2-[*N*-(2,6-diisopropylphenyl)formimino]-1*H*-pyrrole.

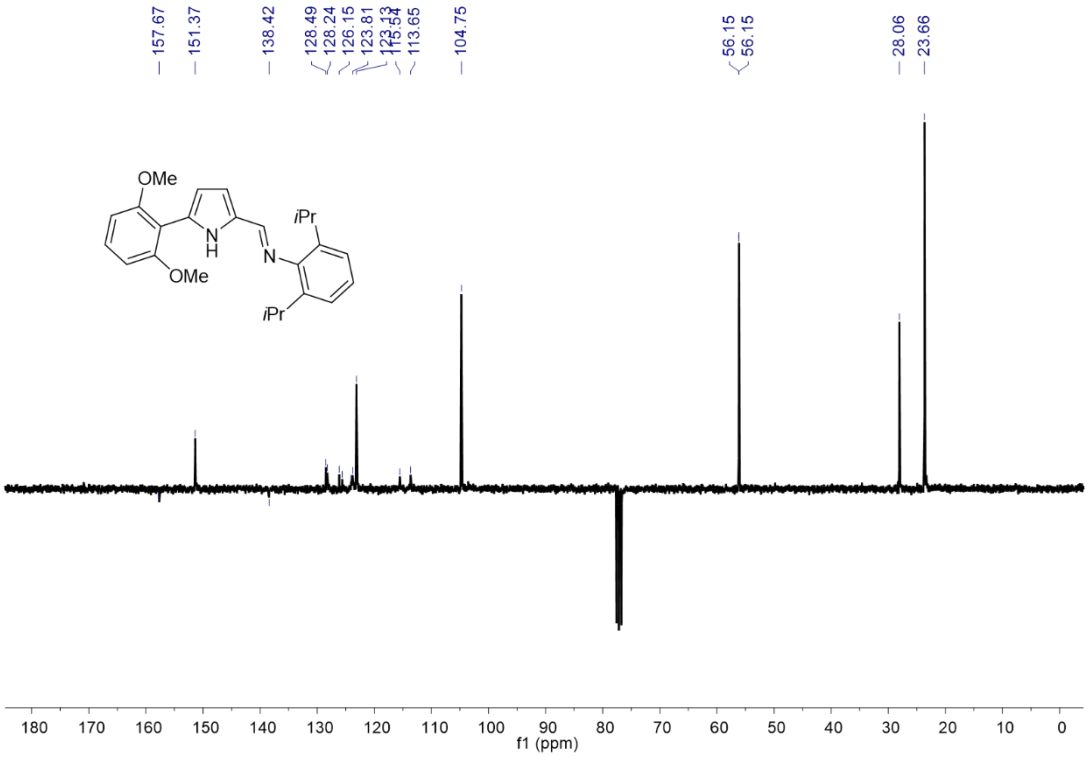

Figure S4 ^{13}C APT NMR spectrum (75 MHz, $CDCl_3$) of 5-[2,6-$(MeO)_2C_6H_3$]-2-[*N*-(2,6-diisopropylphenyl)formimino]-1*H*-pyrrole.

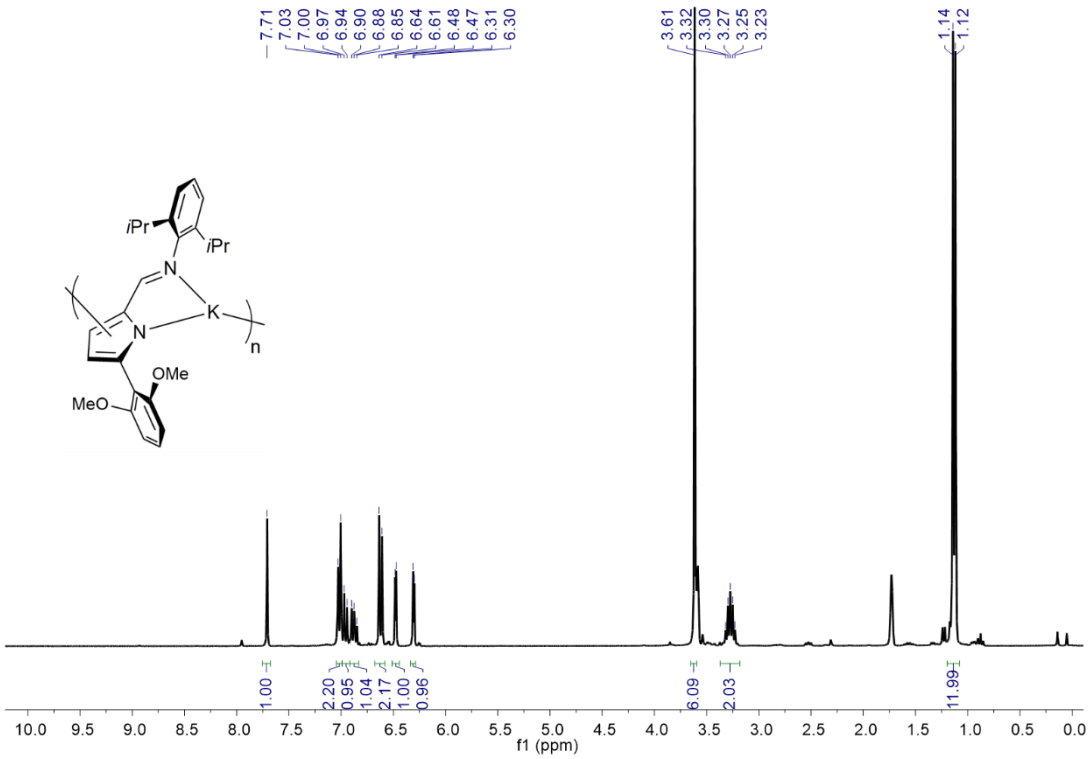

Figure S5 ^{1}H NMR spectrum (300 MHz, THF-d_8) of the potassium salt **KLd**.

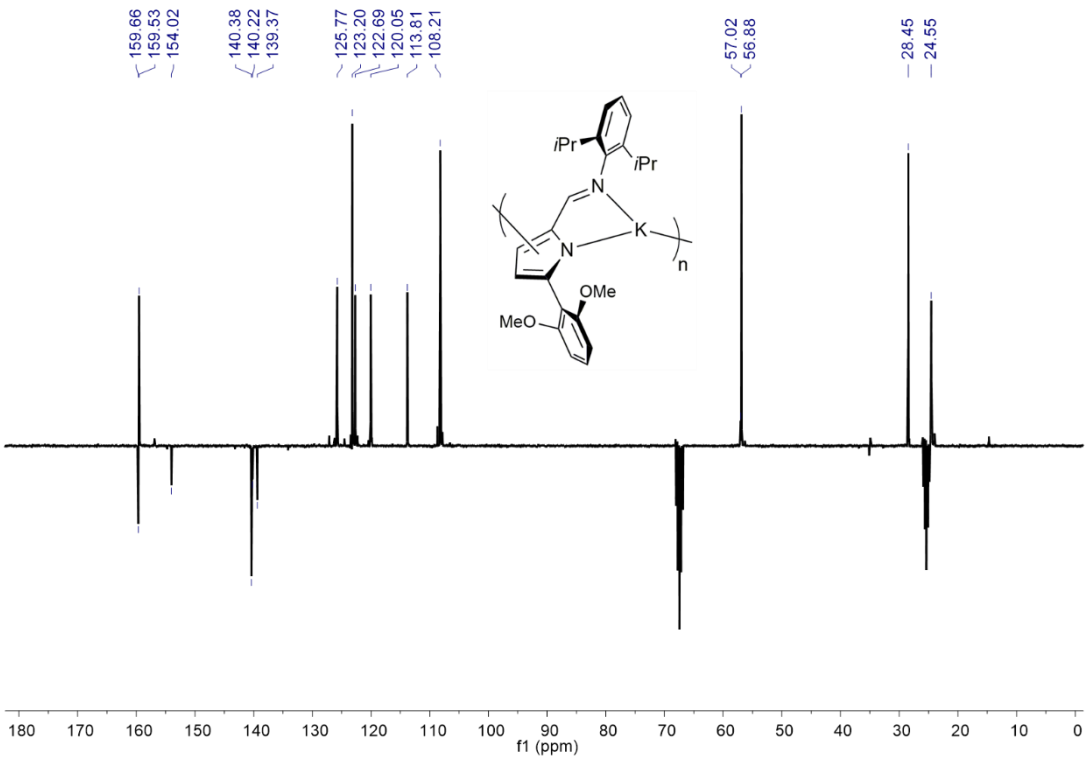

Figure S6 ^{13}C APT NMR spectrum (75 MHz, THF-d_8) of the potassium salt **KLd**.

NMR spectra of the complexes

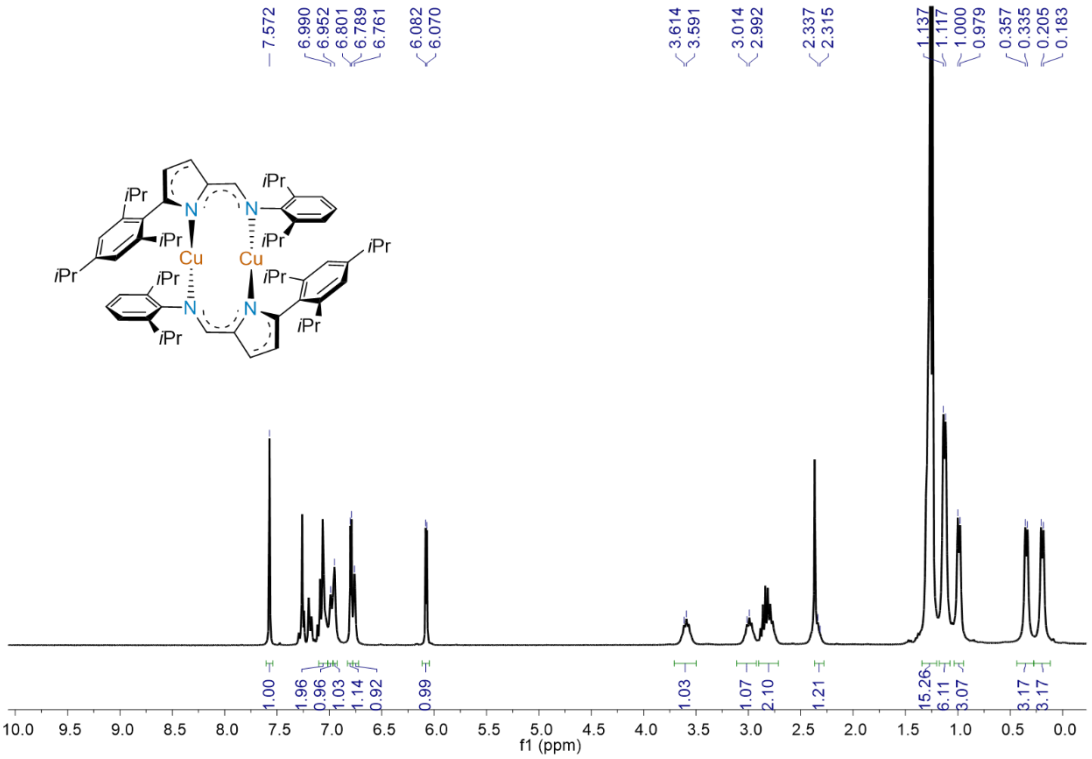

Figure S7 ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) of complex **1a**.

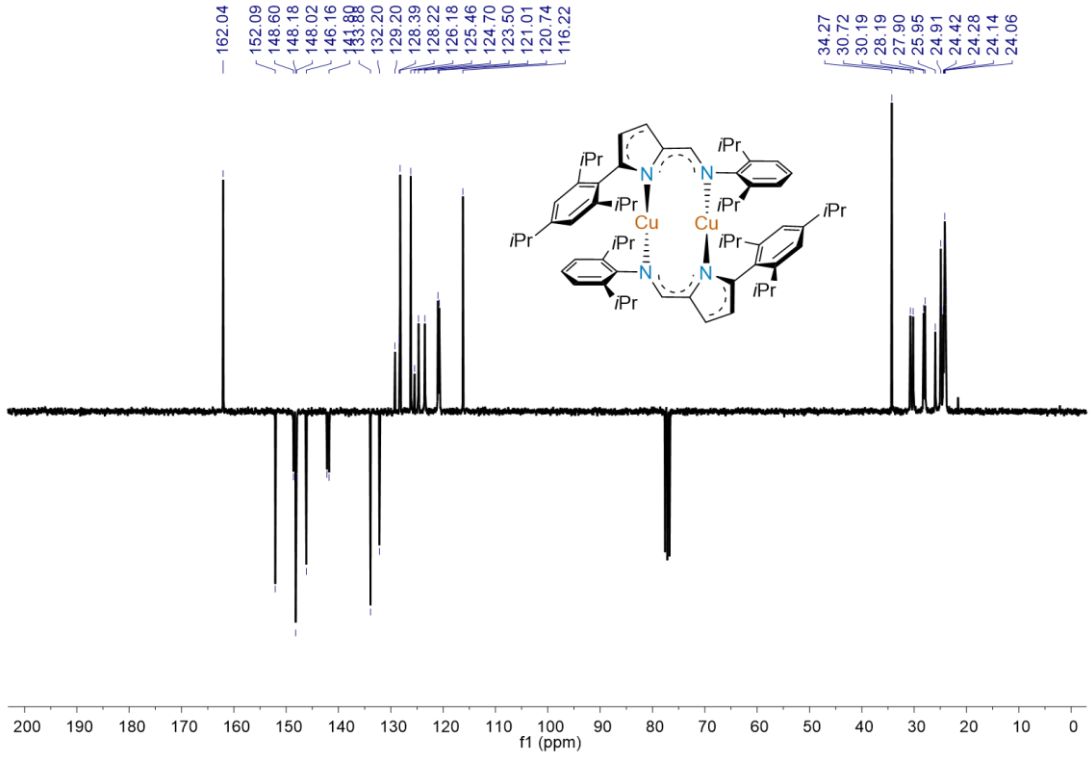

Figure S8 ^{13}C APT NMR spectrum (75 MHz, $CDCl_3$, 298 K) of complex **1a**.

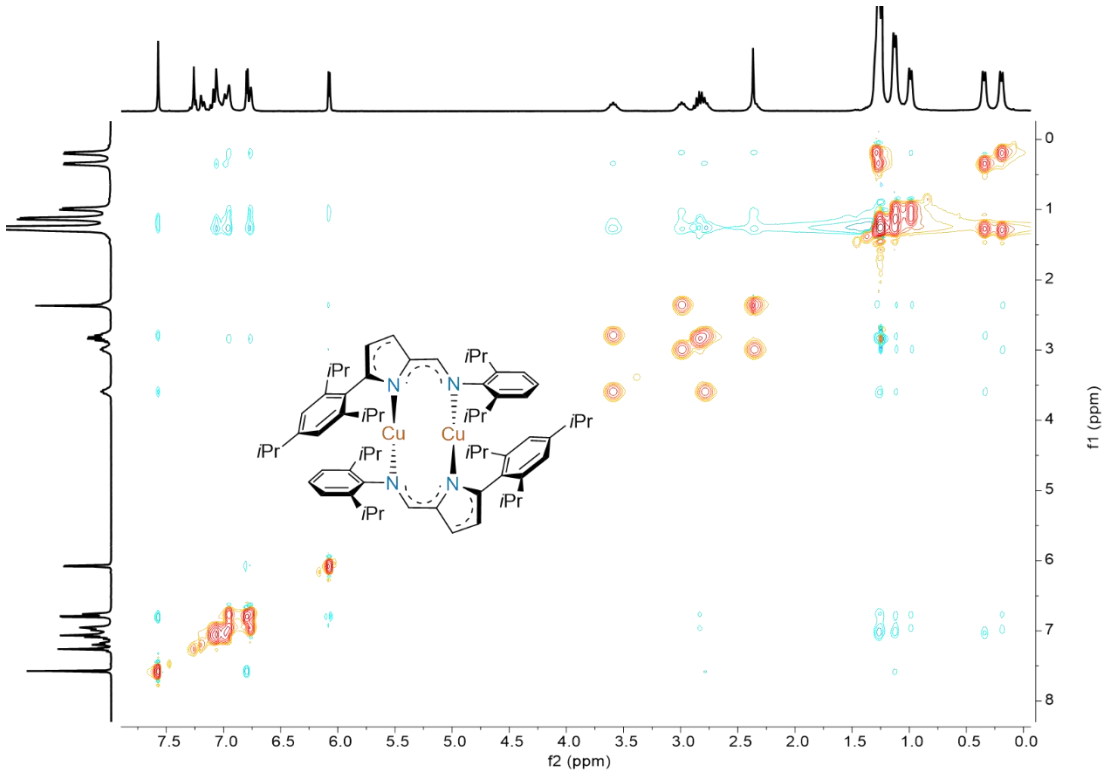

Figure S9 ^{1}H-^{1}H NOESY NMR (300 MHz, $CDCl_3$, 298 K) of complex **1a**. The off-diagonal cross peaks presented in blue and orange-red correspond to NOE (through-space dipolar interactions) and chemical exchange resonances, respectively.

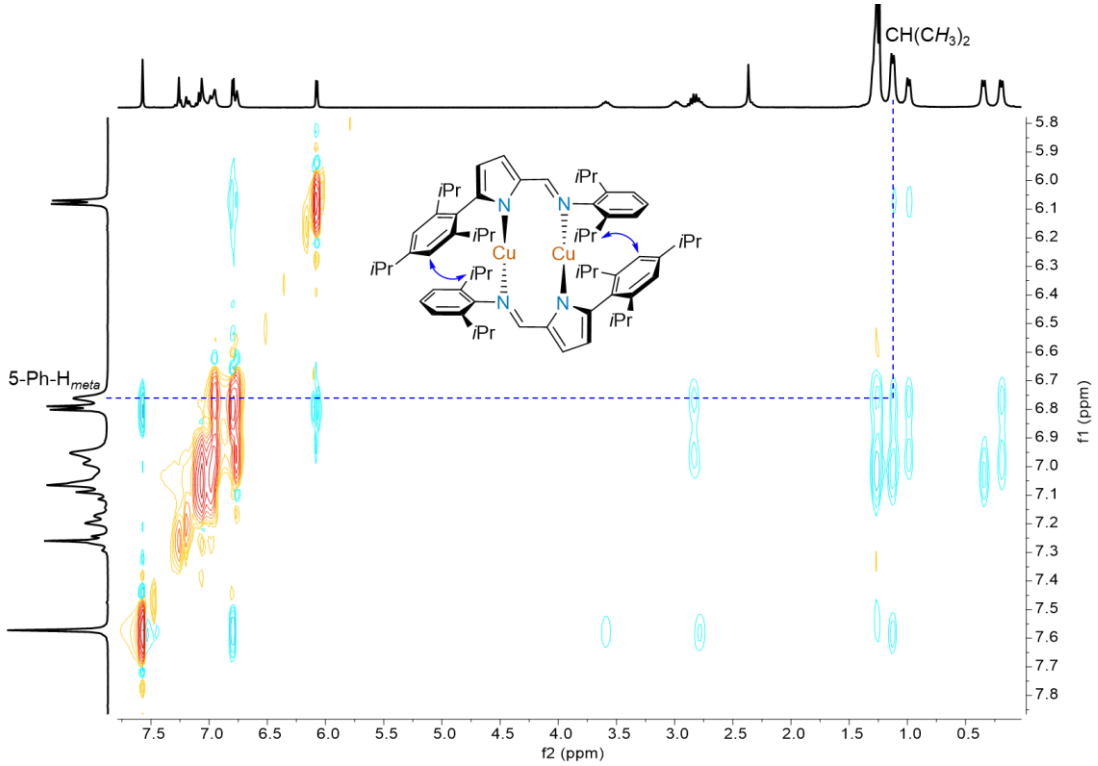

Figure S10 Magnification of the ^{1}H-^{1}H NOESY NMR spectrum (300 MHz, $CDCl_3$, 298 K) of complex **1a**, showing the NOE off-diagonal cross peaks between the H_{meta} protons of the 5-aryl ring and the methyl protons of the isopropyl groups of the *N*-aryl ring. The off-diagonal cross peaks presented in blue and orange-red correspond to NOE (through-space dipolar interactions) and chemical exchange resonances, respectively.

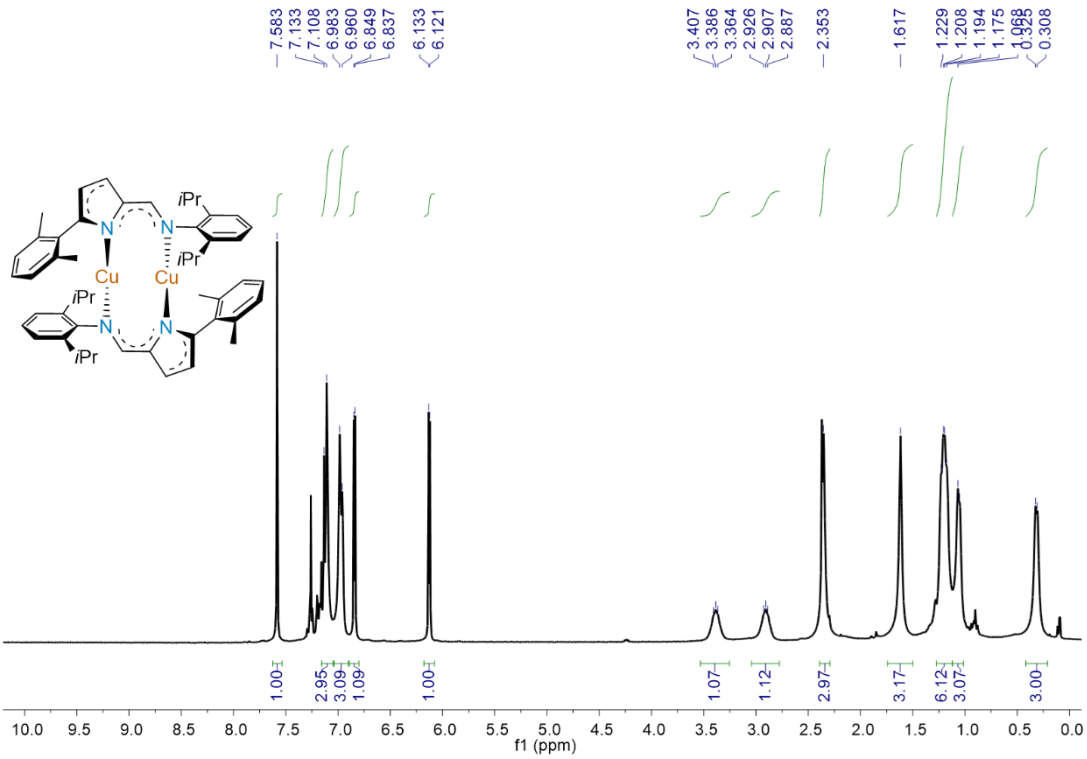

Figure S11 ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) of complex **1b**.

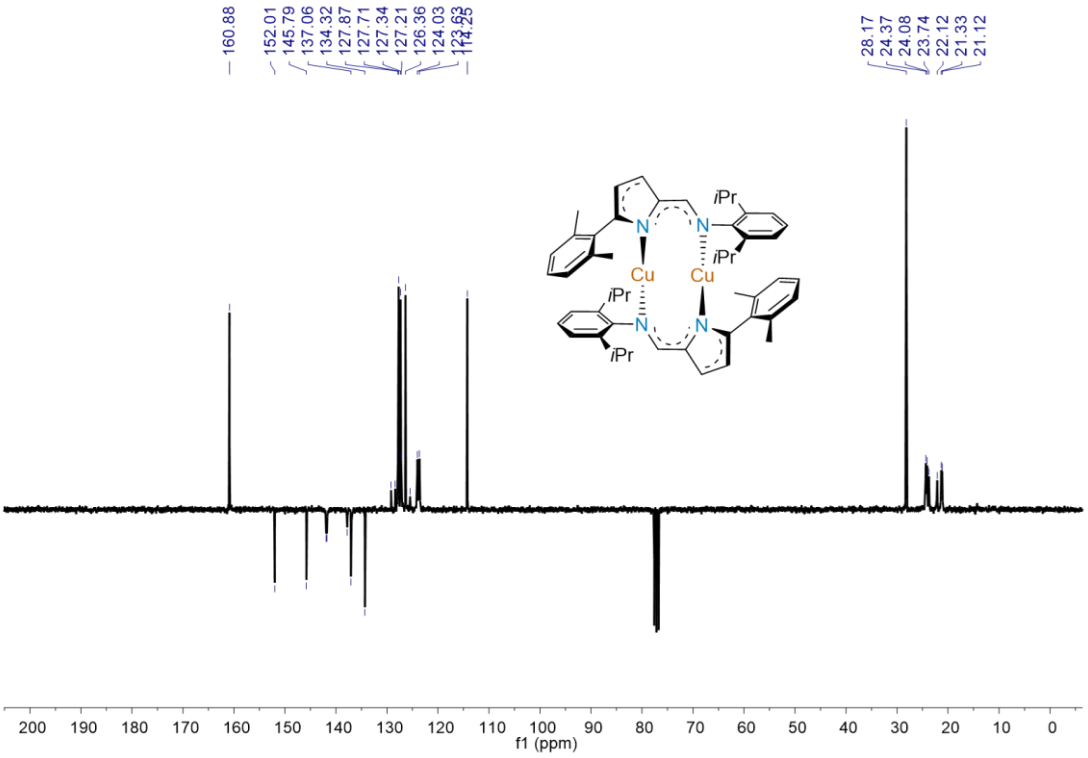

Figure S12 ^{13}C APT NMR spectrum (75 MHz, $CDCl_3$, 298 K) of complex **1b**.

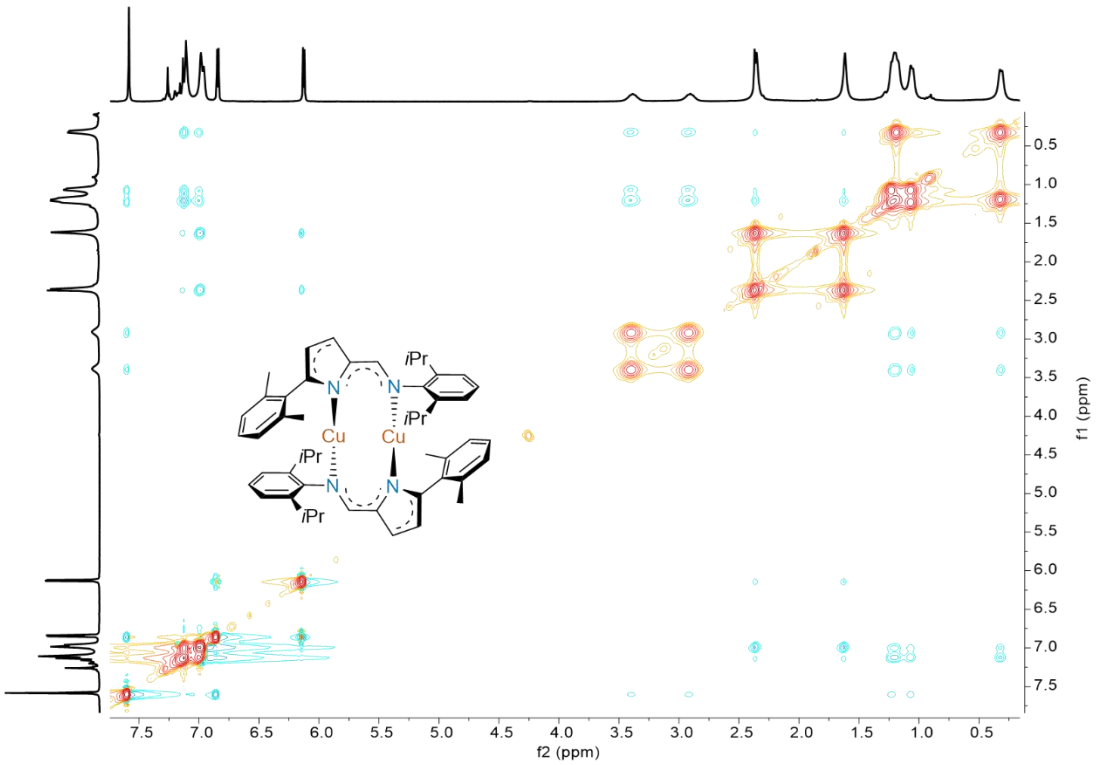

Figure S13 ^{1}H-^{1}H NOESY NMR (300 MHz, $CDCl_3$, 298 K) of complex **1b**. The off-diagonal cross peaks presented in blue and orange-red correspond to NOE (through-space dipolar interactions) and chemical exchange resonances, respectively.

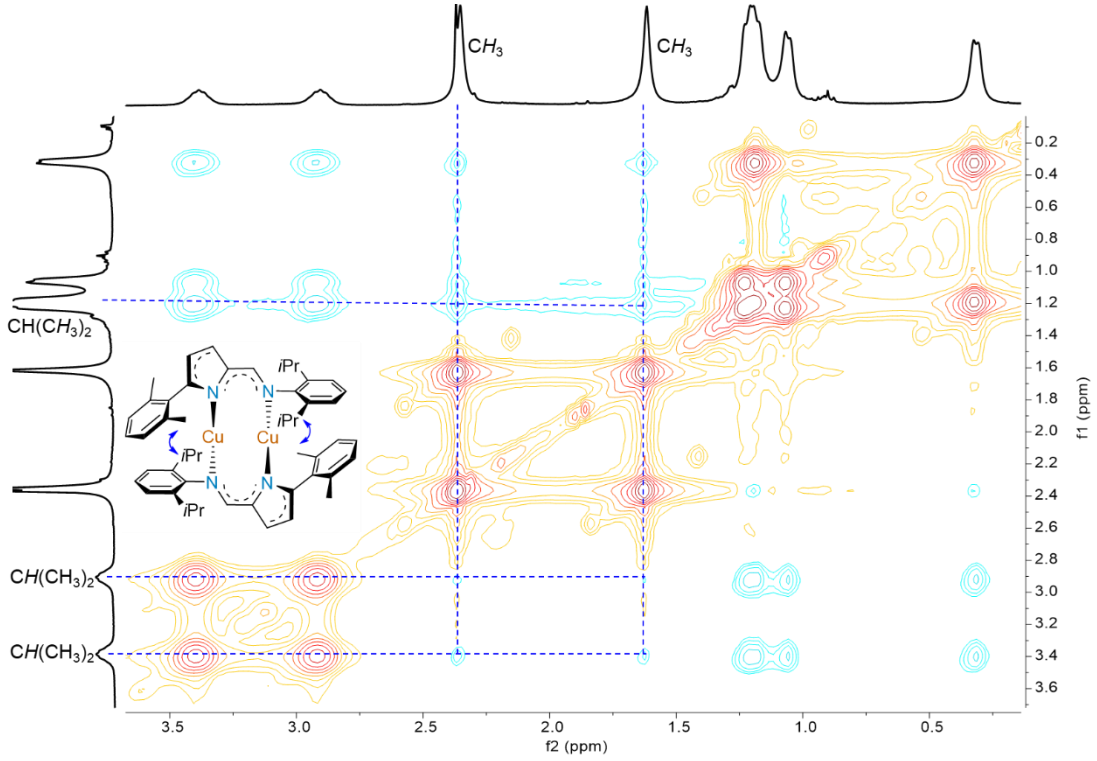

Figure S14 Magnification of the ^{1}H-^{1}H NOESY NMR spectrum (300 MHz, $CDCl_3$, 298 K) of complex **1b**, showing the NOE off-diagonal cross peaks between the methyl protons of the 5-aryl ring and the methinic and methyl protons of the isopropyl groups of the *N*-aryl ring. The off-diagonal cross peaks presented in blue and orange-red correspond to NOE (through-space dipolar interactions) and chemical exchange resonances, respectively.

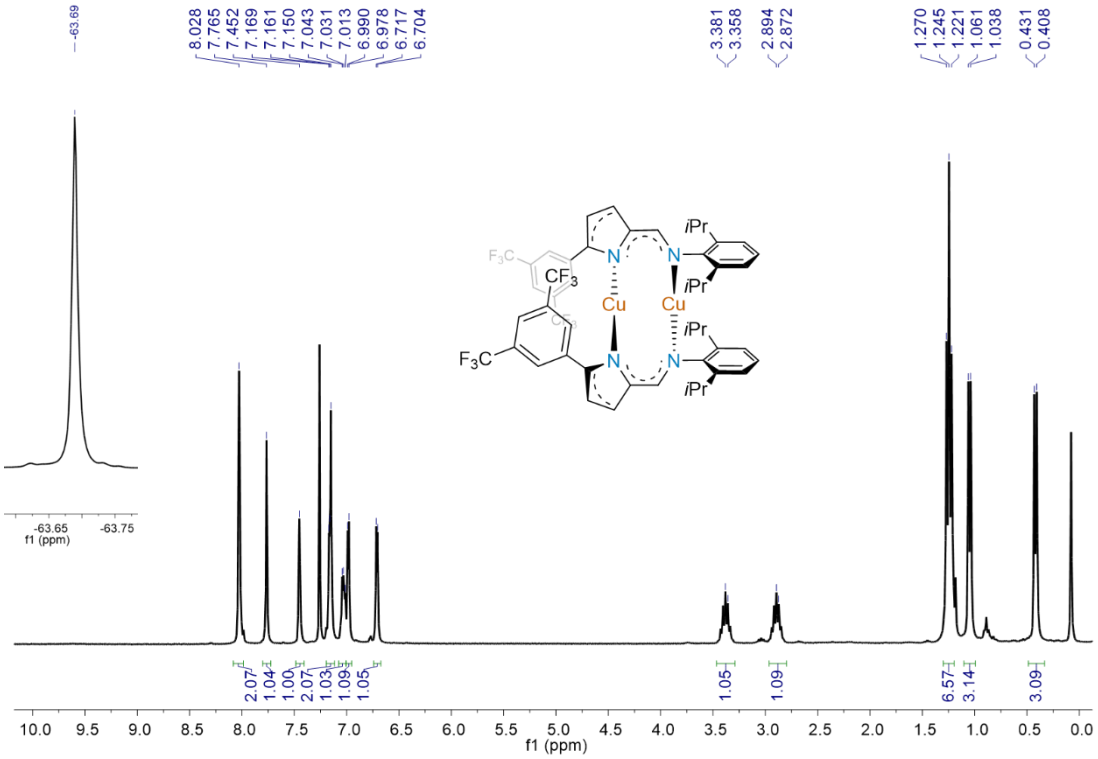

Figure S15 ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) of complex **1c**, the inset showing the respective $^{19}F\{^{1}H\}$ NMR spectrum (300 MHz, $CDCl_3$, 298 K).

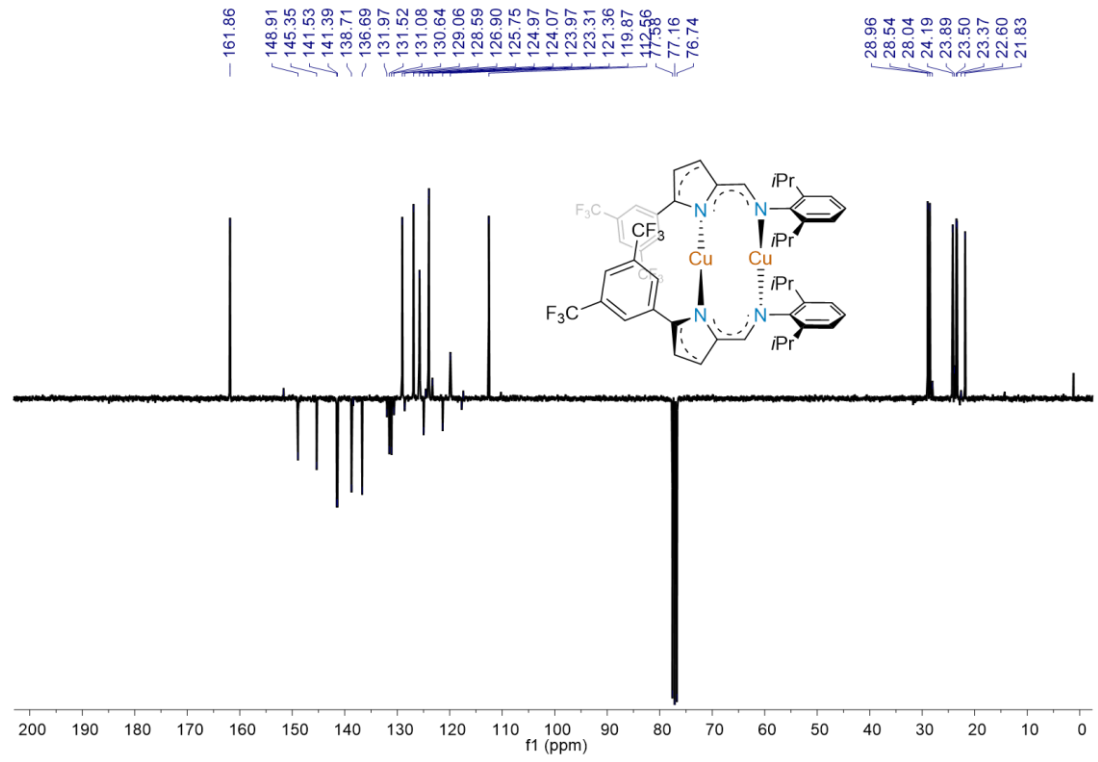

Figure S16 ^{13}C APT NMR spectrum (75 MHz, $CDCl_3$, 298 K) of complex **1c**.

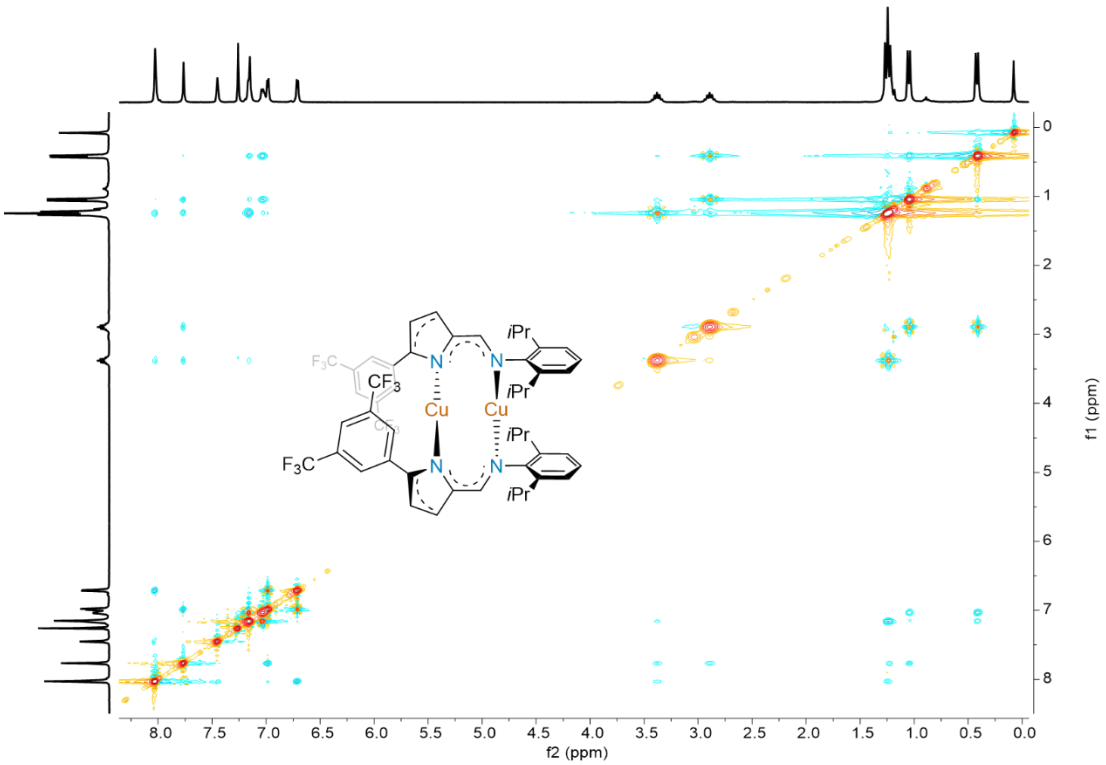

Figure S17 ^{1}H-^{1}H NOESY NMR (300 MHz, $CDCl_3$, 298 K) of complex **1c**. The off-diagonal cross peaks presented in blue correspond to NOE (through-space dipolar interactions) resonances.

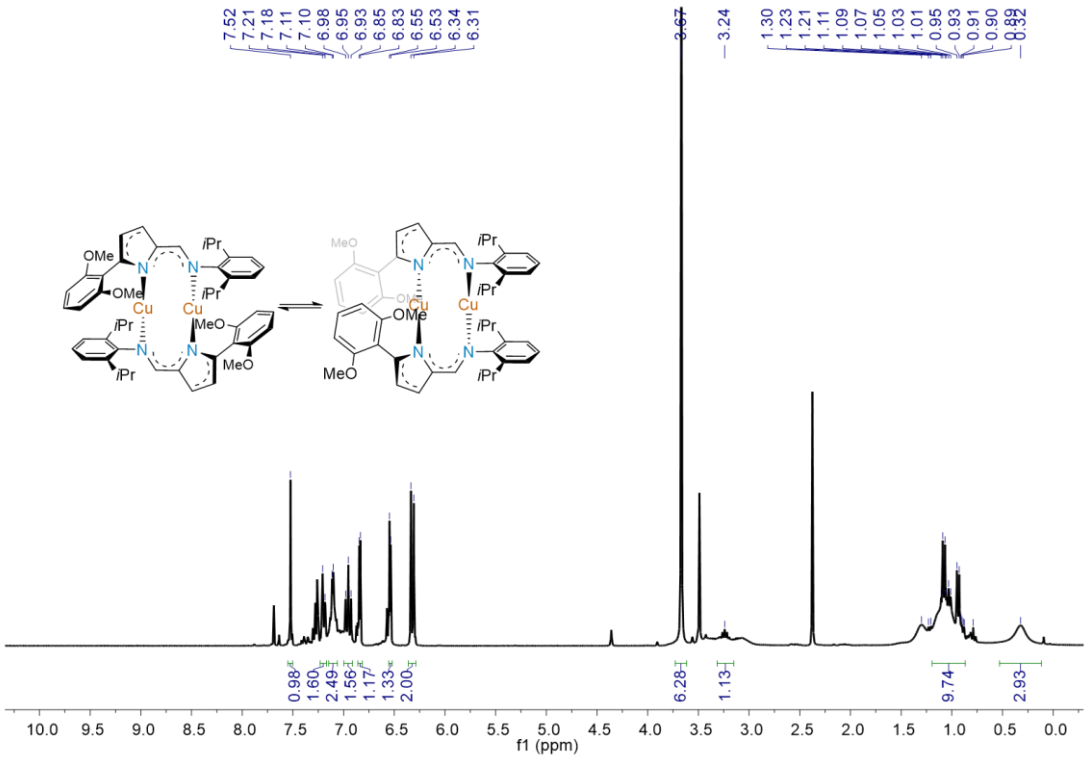

Figure S18 ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) of complex **1d**.

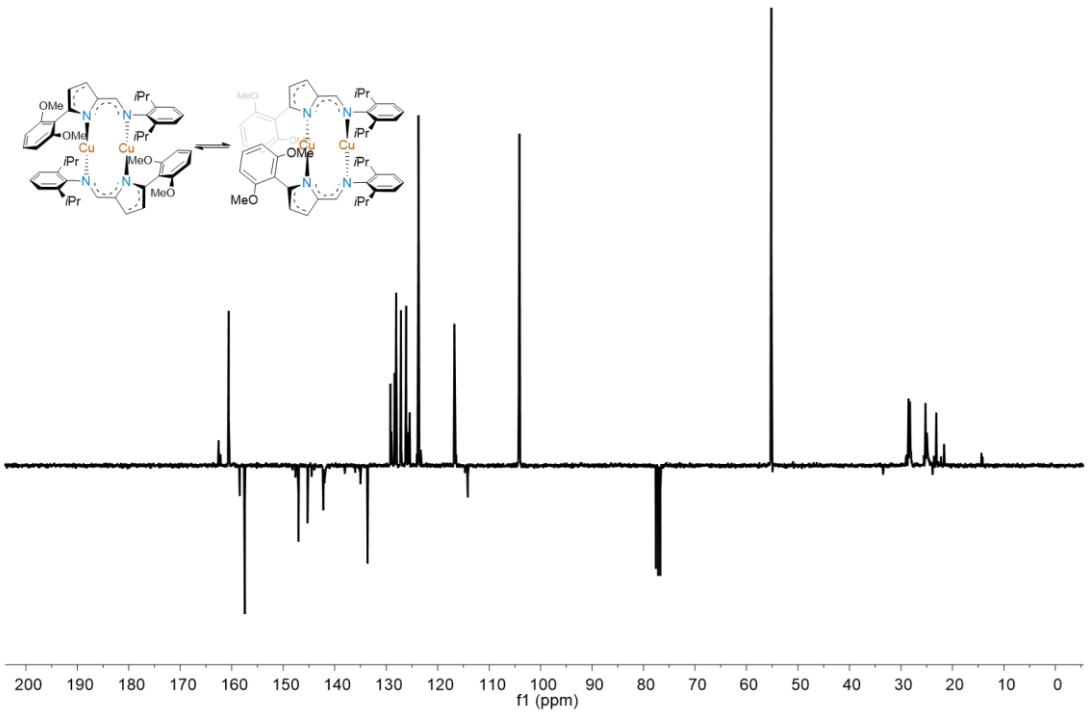

Figure S19 ^{13}C APT NMR spectrum (75 MHz, $CDCl_3$, 298 K) of complex **1d**.

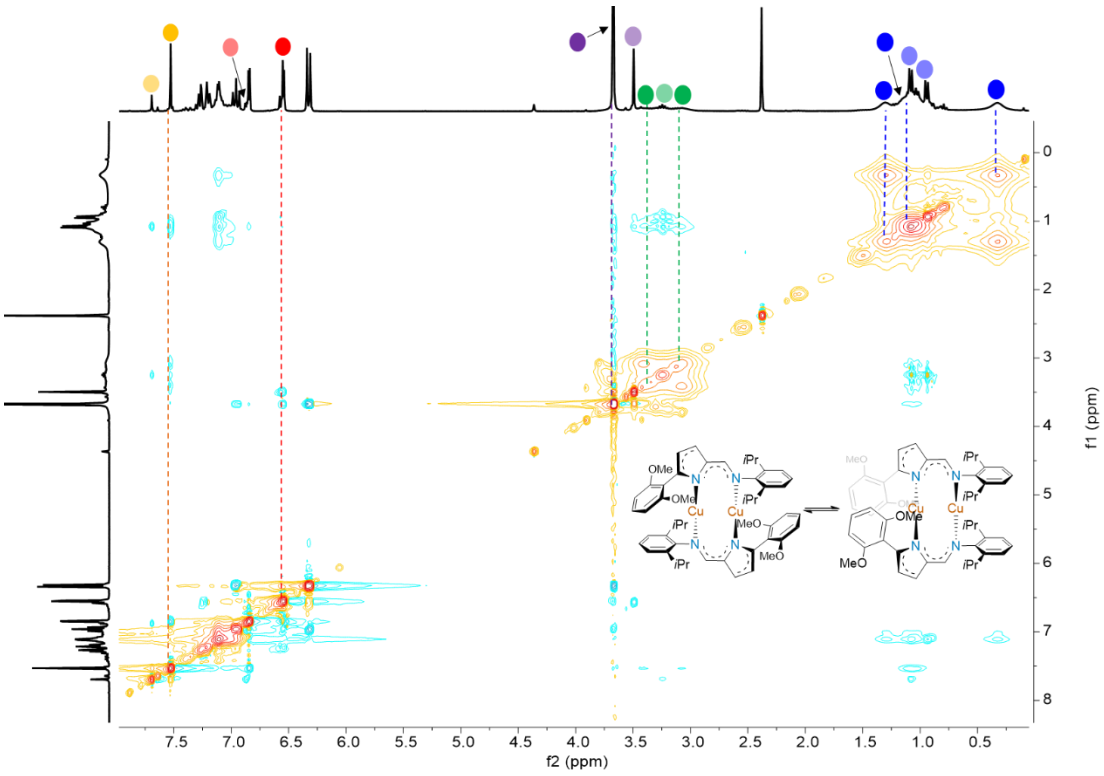

Figure S20 ^{1}H-^{1}H NOESY NMR (300 MHz, $CDCl_3$, 298 K) of complex **1d**. Some examples of the assignment of the N=C*H* (orange circles), H3 + H4 (red circles), OMe (violet circles), C*H*$(CH_3)_2$ (green circles) and CH$(CH_3)_2$ (blue circles) resonances of the major and minor isomers are distinguished by the corresponding darker and lighter colored circles, respectively. The off-diagonal cross peaks presented in blue and orange-red correspond to NOE (through-space dipolar interactions) and chemical exchange resonances, respectively, and have been highlighted by dashed lines for the major isomer for clarity.

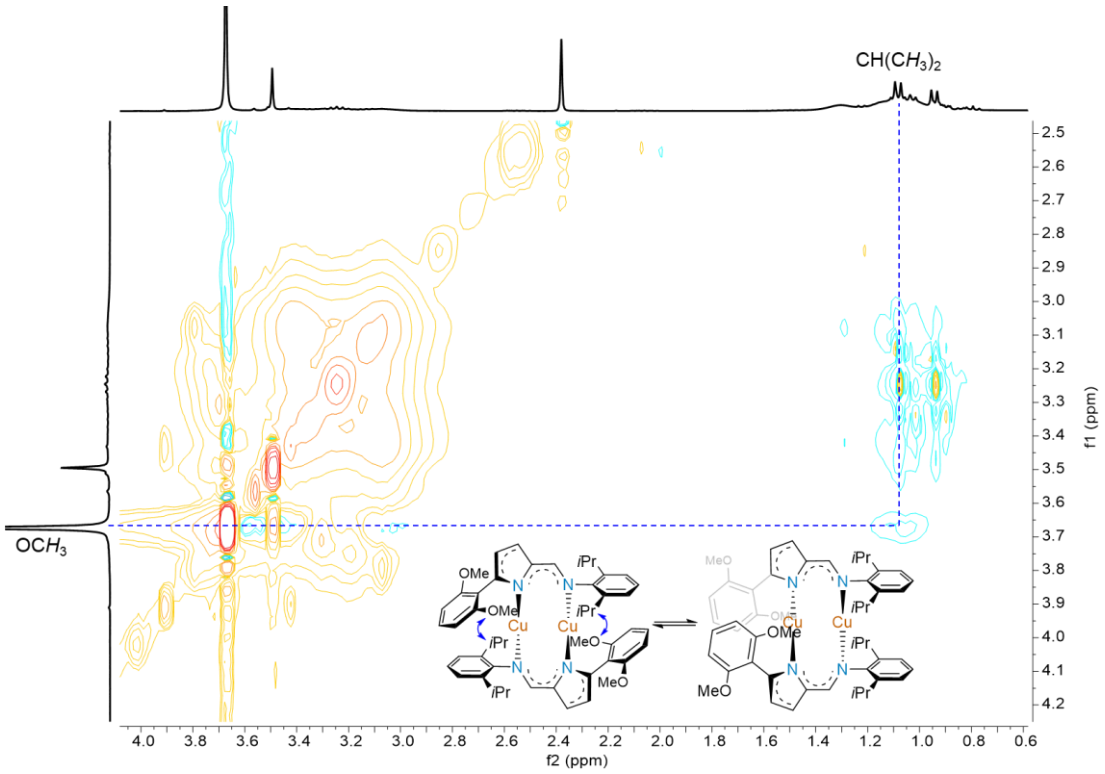

Figure S21 Magnification of the ^{1}H-^{1}H NOESY NMR spectrum (300 MHz, $CDCl_3$, 298 K) of complex **1d**, showing the NOE off-diagonal cross peaks between the methoxy protons of the 5-aryl ring and the methyl protons of the isopropyl groups of the N-aryl ring. The off-diagonal cross peaks presented in blue and orange-red correspond to NOE (through-space dipolar interactions) and chemical exchange resonances, respectively.

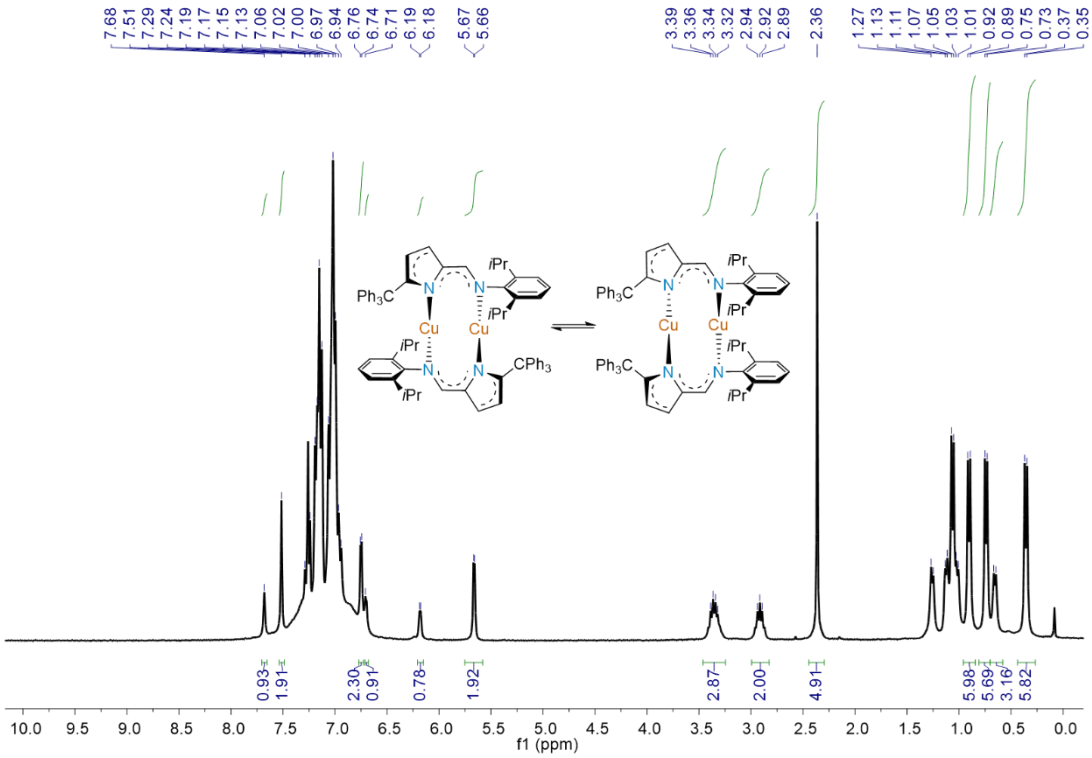

Figure S22 ^{1}H NMR spectrum (300 MHz, $CDCl_3$, 298 K) of complex **1e**.

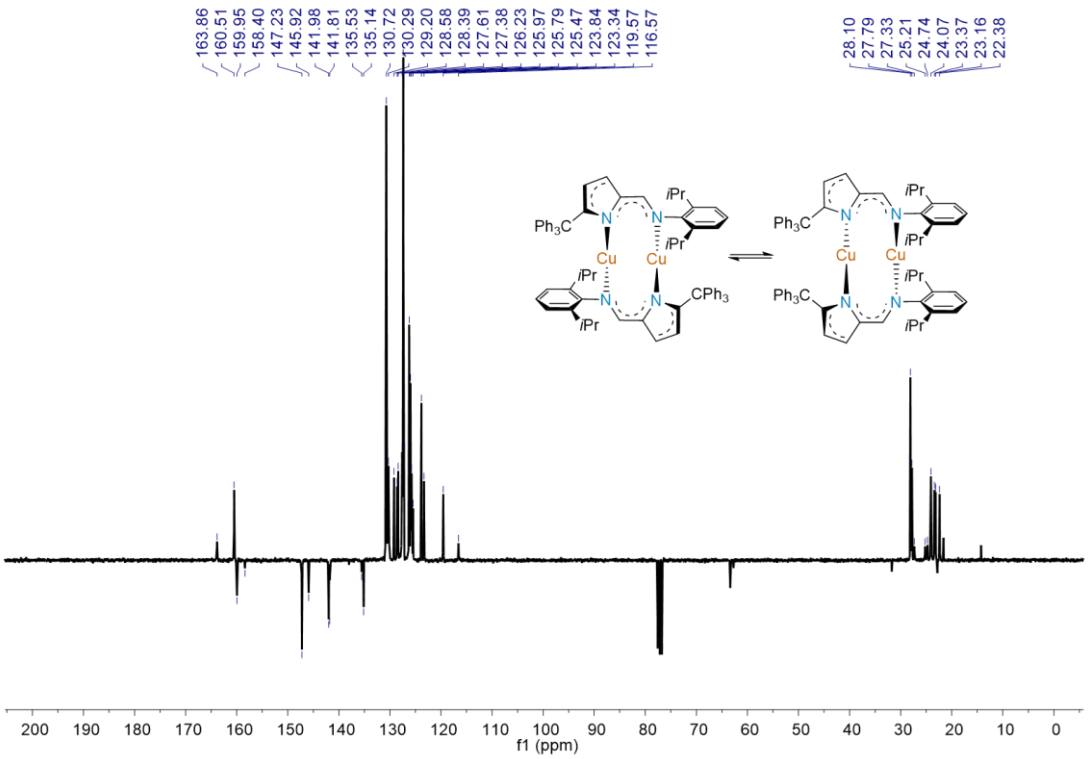

Figure S23 ^{13}C APT NMR spectrum (75 MHz, $CDCl_3$, 298 K) of complex **1e**.

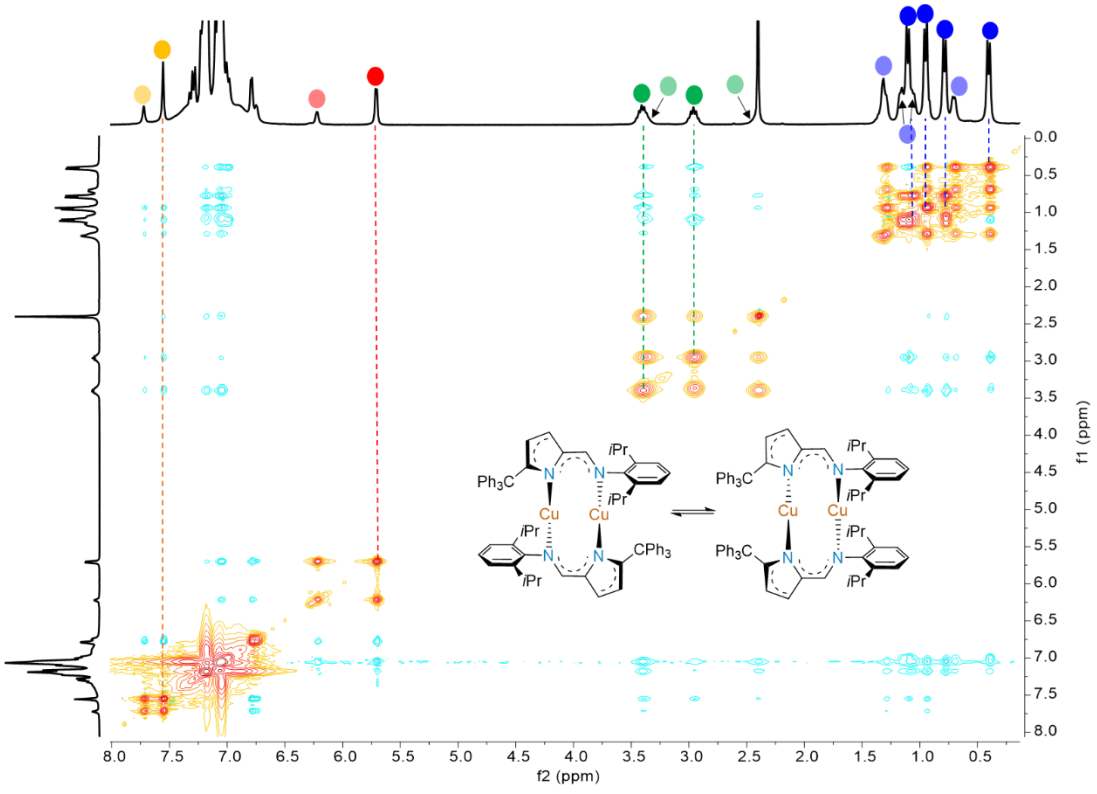

Figure S24 ^{1}H-^{1}H NOESY NMR (300 MHz, $CDCl_3$, 298 K) of complex **1e**. Some examples of the assignment of the N=C*H* (orange circles), H3 + H4 (red circles), C*H*$(CH_3)_2$ (green circles) and CH$(CH_3)_2$ (blue circles) resonances of the major and minor isomers are distinguished by the corresponding darker and lighter colored circles, respectively. The off-diagonal cross peaks presented in blue and orange-red correspond to NOE (through-space dipolar interactions) and chemical exchange resonances, respectively, and have been highlighted in dashed lines for the major isomer for clarity.

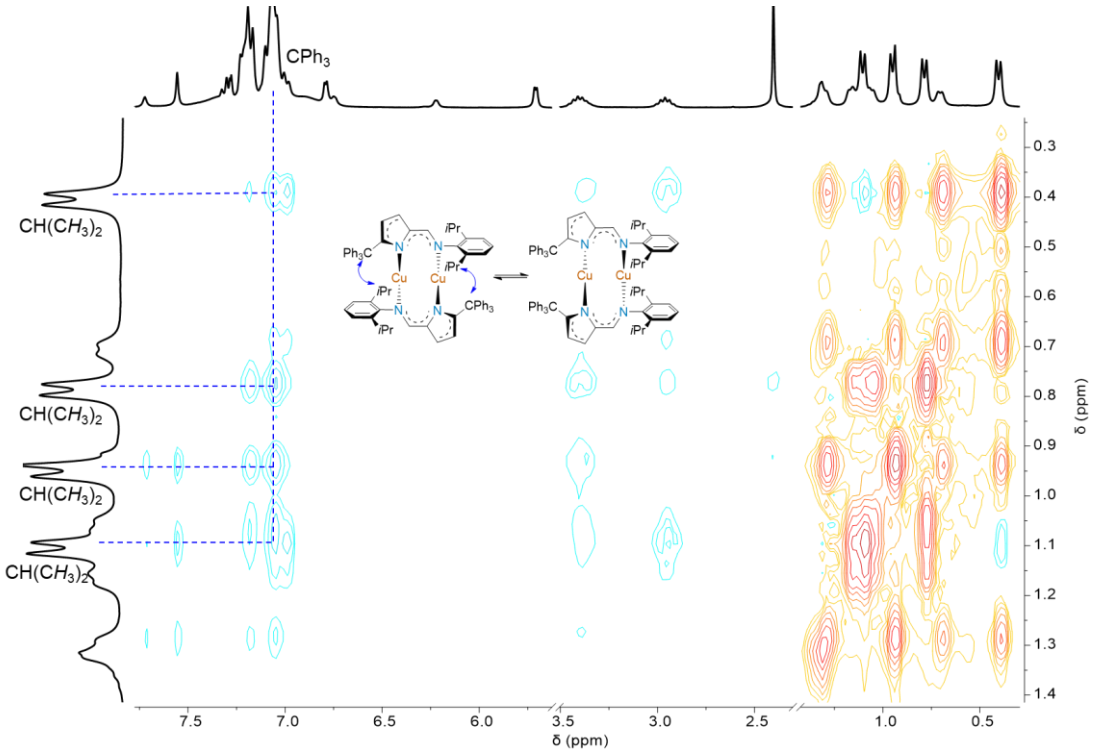

Figure S25 Magnification of the ^{1}H-^{1}H NOESY NMR spectrum (300 MHz, $CDCl_3$, 298 K) of complex **1e**, showing the NOE off-diagonal cross peaks between the 5-trityl protons and the methyl protons of the isopropyl groups of the N-aryl ring. The off-diagonal cross peaks presented in blue and orange-red correspond to NOE (through-space dipolar interactions) and chemical exchange resonances, respectively.

Selection of bond lengths and angles of complexes 1a and 1c-e

Table S1 Selected bond distances (Å) and bond angles (º) for complexes **1a** and **1c-e**.

	1a	**1c**	**1d**	**1e**
Distances (Å)				
Cu(1)-N(1)	1.841(4)	1.8616(16)	1.865(5)	1.917(5)
Cu(1)-N(4)	1.873(4)	1.8616(15)	1.882(5)	1.916(5)
Cu(1)-Cu(2)	2.5677(11)	2.4969(5)	2.4806(10)	2.5355(12)
Cu(2)-N(3)	1.844(4)	1.8660(16)	1.877(5)	1.853(5)
Cu(2)-N(2)	1.876(5)	1.8659(16)	1.891(5)	1.861(5)
O(1)-C(12)	-	-	1.428(7)	-
O(2)-C(13)	-	-	1.423(7)	-
N(1)-C(5)	1.365(7)	1.367(2)	1.367(7)	1.357(8)
N(1)-C(2)	1.392(7)	1.379(2)	1.383(7)	1.386(8)
N(2)-C(6)	1.290(7)	1.299(2)	1.305(7)	1.319(8)
C(2)-C(3)	1.407(8)	1.402(3)	1.412(8)	1.391(9)
C(2)-C(6)	1.412(8)	1.416(3)	1.419(8)	1.393(9)
C(3)-C(4)	1.366(9)	1.381(3)	1.383(8)	1.363(9)
C(4)-C(5)	1.417(8)	1.396(3)	1.399(8)	1.382(9)
Angles (º)				
N(1)-Cu(1)-N(4)	171.6(2)	169.45(9)	176.7(2)	175.2(2)
N(1)-Cu(1)-Cu(2)	92.66(15)	95.27(5)	89.07(14)	89.28(16)
N(4)-Cu(1)-Cu(2)	95.36(14)	95.27(5)	94.04(15)	85.98(16)
N(3)-Cu(2)-N(2)	172.6(2)	166.13(10)	176.9(2)	170.9(2)
N(3)-Cu(2)-Cu(1)	92.90(14)	96.94(5)	87.19(14)	94.03(17)
N(2)-Cu(2)-Cu(1)	94.27(16)	96.94(5)	95.20(14)	95.06(17)
C(11)-O(1)-C(12)	-	-	117.8(5)	-
C(5)-N(1)-C(2)	106.1(4)	105.93(15)	106.6(5)	106.0(5)
C(5)-N(1)-Cu(1)	124.0(4)	122.39(13)	124.8(4)	128.8(4)
C(2)-N(1)-Cu(1)	127.4(4)	129.30(13)	127.8(4)	118.6(4)
C(6)-N(2)-Cu(2)	131.0(4)	132.30(14)	122.0(4)	125.1(4)
N(1)-C(2)-C(3)	109.4(5)	109.76(17)	108.8(5)	109.3(5)
N(1)-C(2)-C(6)	127.7(5)	126.51(17)	127.5(6)	129.2(6)
C(3)-C(2)-C(6)	122.9(5)	123.64(18)	123.7(5)	121.2(6)
C(4)-C(3)-C(2)	107.5(5)	107.02(18)	107.6(5)	106.8(6)
C(3)-C(4)-C(5)	107.0(5)	106.68(17)	106.4(5)	107.9(6)
N(1)-C(5)-C(4)	110.1(5)	110.61(17)	110.7(5)	110.0(5)
N(2)-C(6)-C(2)	127.4(5)	128.10(18)	127.4(5)	129.4(6)

Crystallographic data of complexes 1a and 1c-e

Table S2 Crystallographic data for complexes **1a** and **1c-e**.

	1a	**1c**	**1d**	**1e**
Formula	$C_{64}H_{86}Cu_2N_4$	$C_{25}H_{23}CuF_6N_2$	$C_{50}H_{56}Cu_2N_4O_4$	$C_{72}H_{70}Cu_2N_4$
M	1038.44	528.99	904.06	1118.40
λ (Å)	0.71073	0.71073	0.71073	0.71073
T (K)	150	150	150	150
Crystal system	Monoclinic	Monoclinic	Triclinic	Triclinic
Space group	$P2_1/c$	C2/c	P-1	P-1
a (Å)	17.148(2)	18.8775(7)	10.5418(9)	12.766(2)
b (Å)	17.406(2)	16.6289(6)	11.9349(11)	13.503(3)
c (Å)	25.948(3)	16.1945(6)	21.971(2)	20.234(3)
α (Å)	90	90	83.347(6)	83.795(8)
β (Å)	105.459(6)	108.6830(10)	80.624(6)	87.004(8)
γ (Å)	90	90	80.833(5)	73.957(5)
V ($Å^3$)	7464.7(17)	4815.8(3)	2681.0(4)	3331.6(10)
Z	4	8	2	2
ρ_{calc} ($g.cm^{-3}$)	0.924	1.459	1.120	1.115
μ (mm^{-1})	0.602	0.968	0.834	0.679
Crystal size (mm)	0.20×0.05×0.05	0.10×0.05×0.05	0.08×0.08×0.02	0.10×0.10×0.06
θ_{max} (º)	25.798	30.355	25.826	25.912
Total data	47595	33648	9920	26884
Unique data	14170	7210	5305	12774
R_{int}	0.1528	0.0632	0.1038	0.0738
R [$I > 2\sigma(I)$]	0.0772	0.0419	0.0755	0.1083
R_w	0.2145	0.1126	0.1879	0.2981
Goodness of fit	0.837	1.034	0.864	1.057
ρ_{min}	-0.525	-0.618	-0.503	-0.757
ρ_{max}	0.531	1.102	0.997	4.394

Supplementary cyclic voltammetry data

Table S3 Electrochemical data for complexes **1a-e** in a $[N(n\text{-}Bu)_4][BF_4]/CH_2Cl_2$ solution at 200 mV/s scan rate. Potentials in Volts measured versus FcH/FcH^+.

Complex	1st Oxidation			2nd Oxidation	1st Oxidation	i_p^{1st}/ i_p^{2nd} Oxidation
	E_p [ox (I)]	E_p (red)	$E_{1/2}$	E_p [ox (II)]	i_p [ox (I)]/i_p (red)	i_p [ox(I)]/i_p [ox(II)]
1a	0.79	0.71	0.75	1.09	1.23	0.5
1b	0.94			1.13		2.0
1c	1.00			1.31		1.7
1d	0.37	0.06	0.22	1.02	3.13	0.4
1e	0.63	0.50	0.57		1.12	
1-H	0.93					

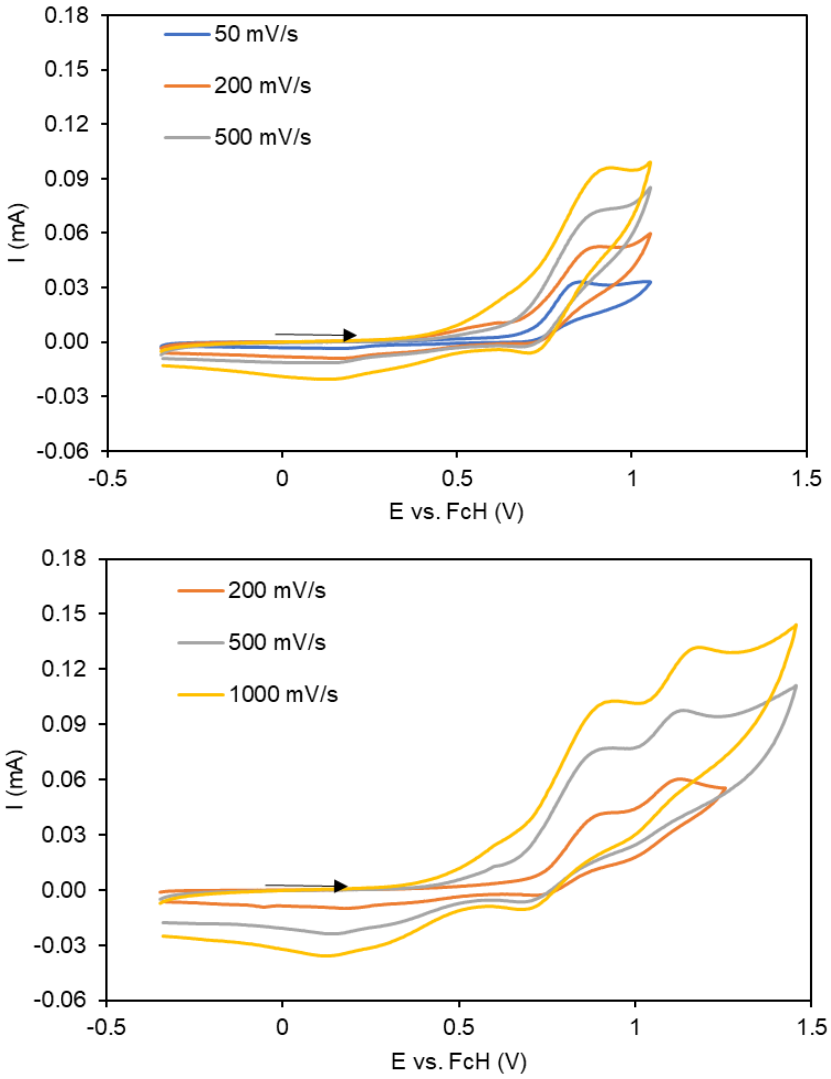

Figure S26 Cyclic voltammogram for the oxidation of complex **1b**, in a $[N(n\text{-}Bu)_4][BF_4]/CH_2Cl_2$ solution at various scan rates and two different potential ranges. Potentials in Volts measured versus FcH/FcH^+. The black arrow indicates the initial potential scanning direction.

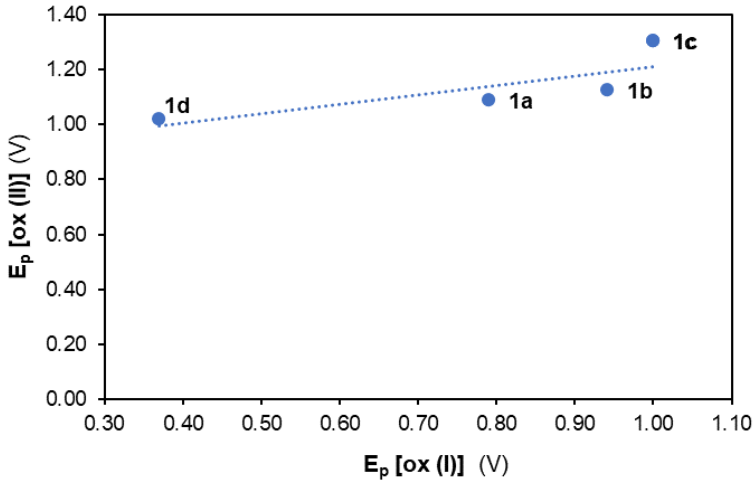

Figure S27 Correlation between the first and second oxidation potentials (E_p [ox(I)] and E_p [ox(II)], respectively) for complexes **1a-e** in a [N(*n*-Bu)$_4$][BF$_4$]/CH_2Cl_2 solution at 200 mV/s scan rate. Potentials in Volts measured versus FcH/FcH^+. The dashed line is a linear correlation visual guide.

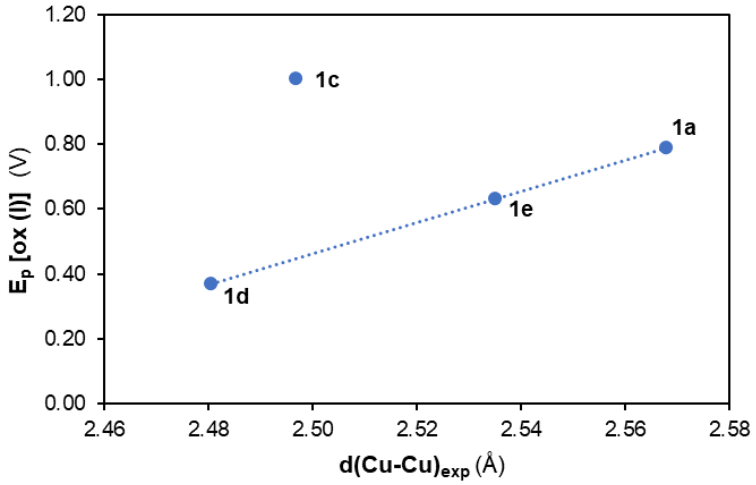

Figure S28 Correlation between the first oxidation potential (E_p [ox(I)]) for complexes **1a-e** and the Cu···Cu distance measured by X-ray diffraction.

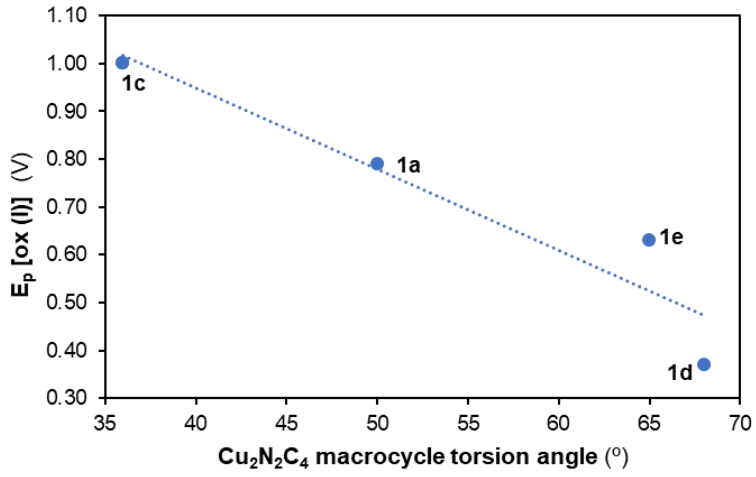

Figure S29 Correlation between the first oxidation potential (E_p [ox(I)]) for complexes **1a-e** and the $Cu_2N_2C_4$ macrocycle torsion angle measured by X-Ray diffraction. The dashed line is a linear correlation visual guide.

Variable temperature NMR spectra of complexes 1a-e

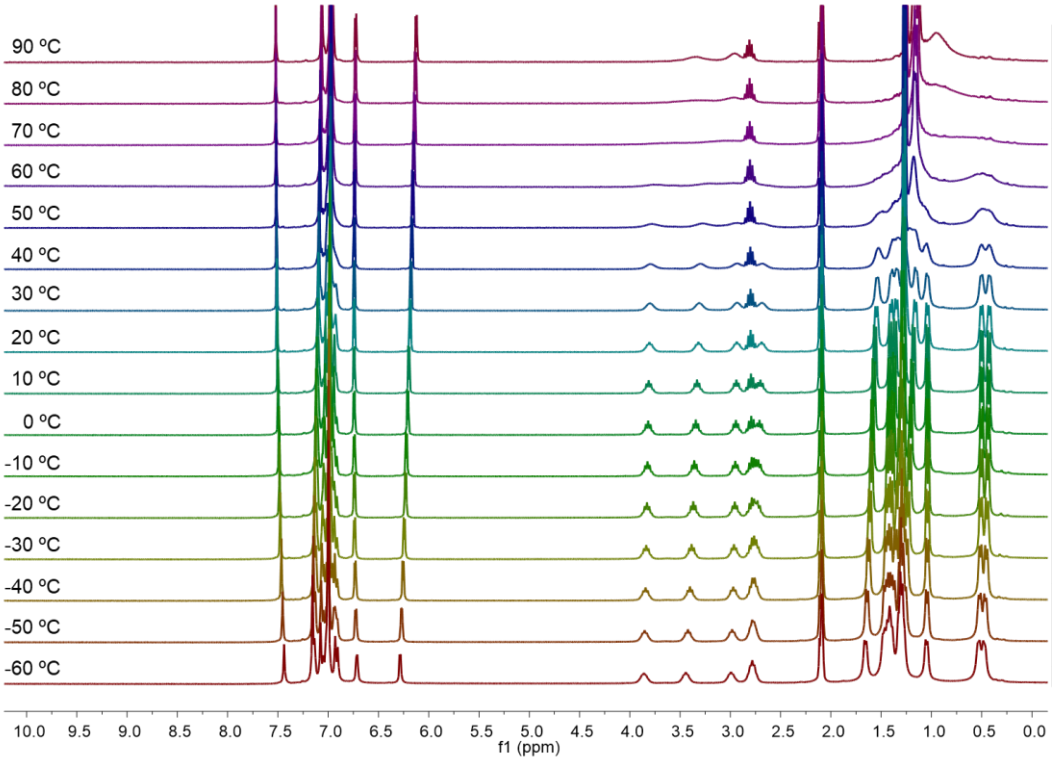

Figure S30 Variable temperature ^{1}H NMR spectra (300 MHz, toluene-d_8) of complex **1a**.

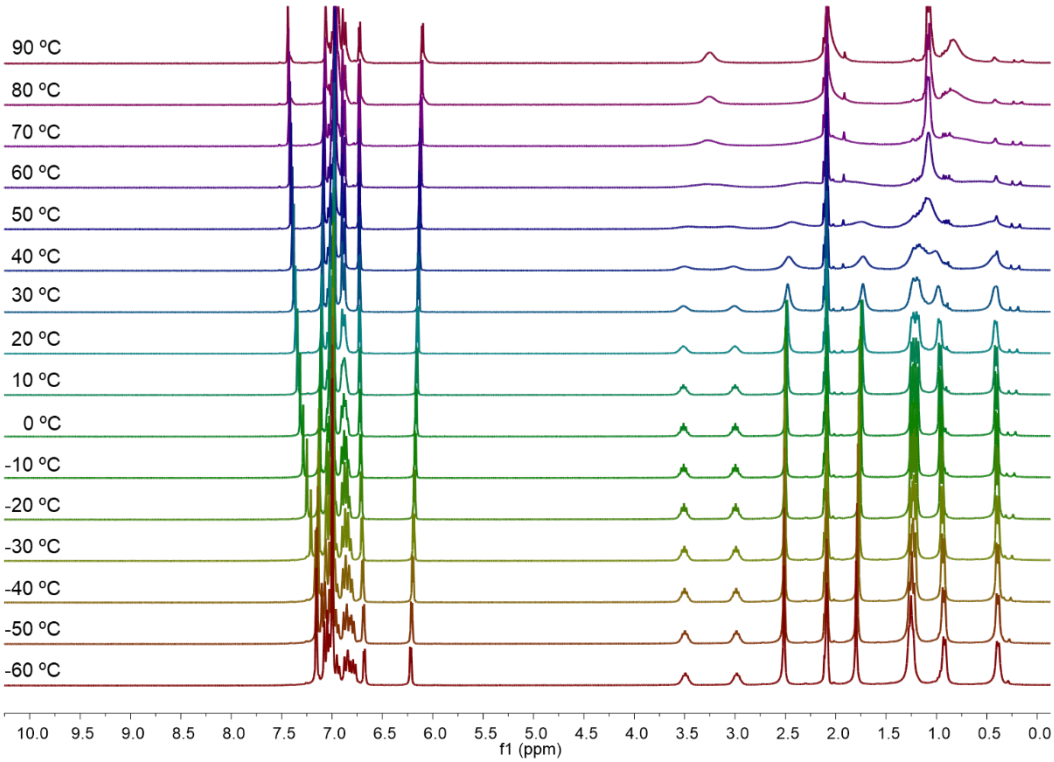

Figure S31 Variable temperature ^{1}H NMR spectra (300 MHz, toluene-d_8) of complex **1b**.

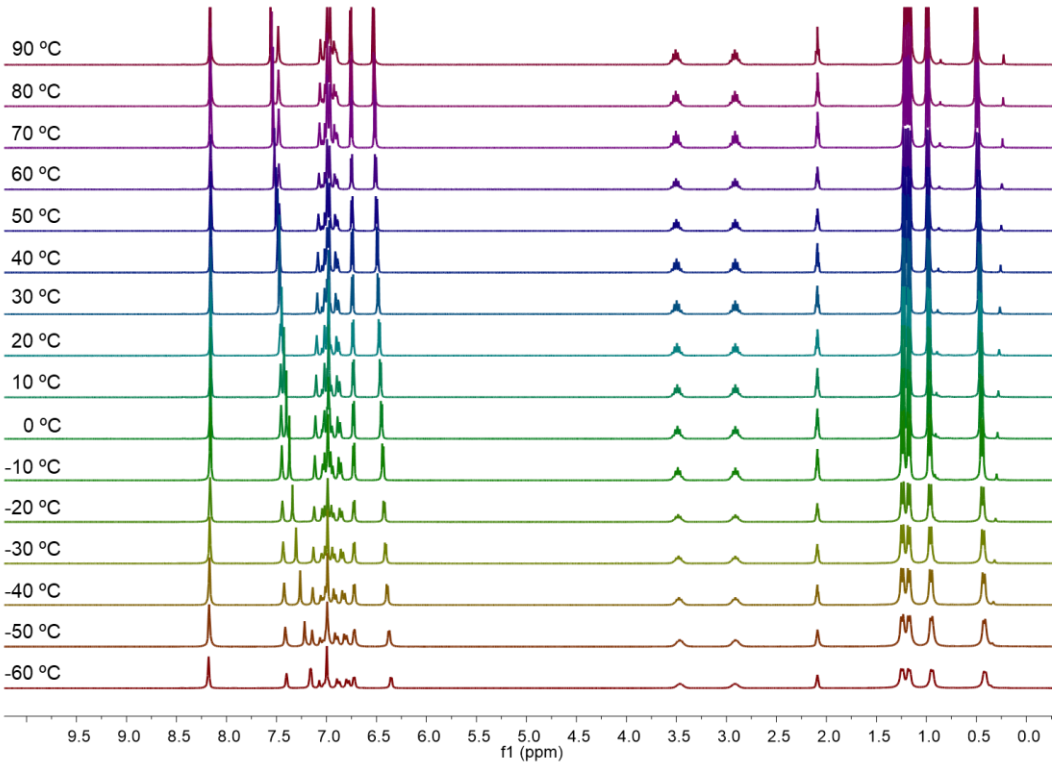

Figure S32 Variable temperature ^{1}H NMR spectra (300 MHz, toluene-d_8) of complex **1c**.

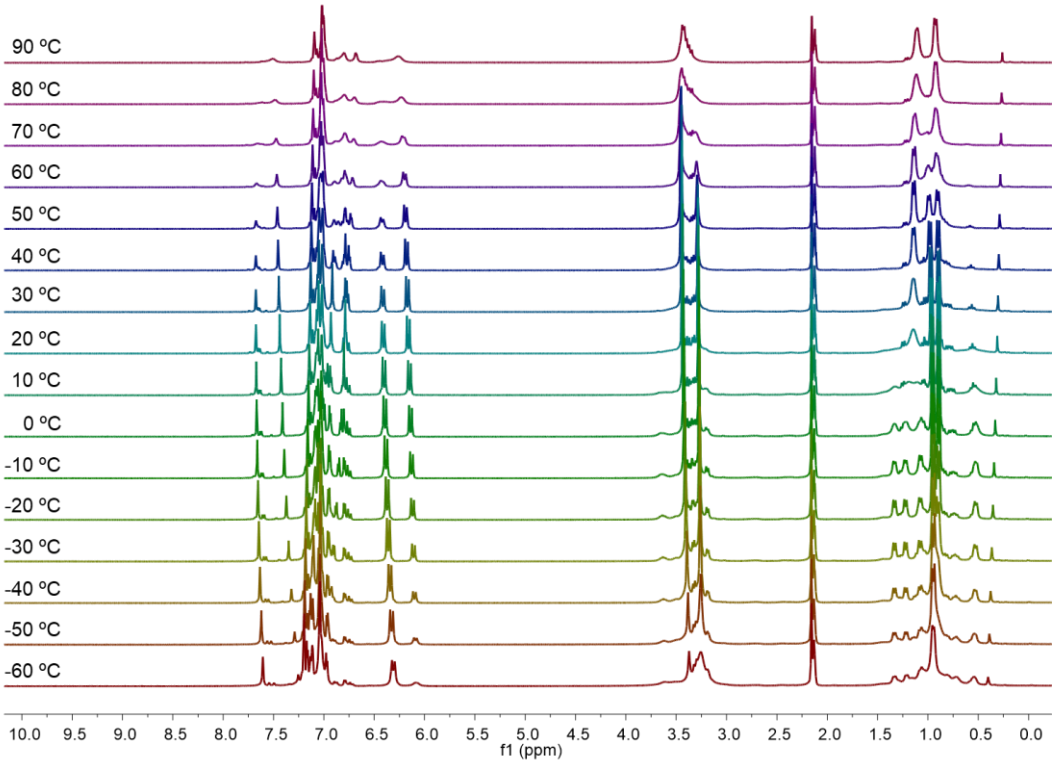

Figure S33 Variable temperature ^{1}H NMR spectra (300 MHz, toluene-d_8) of complex **1d**.

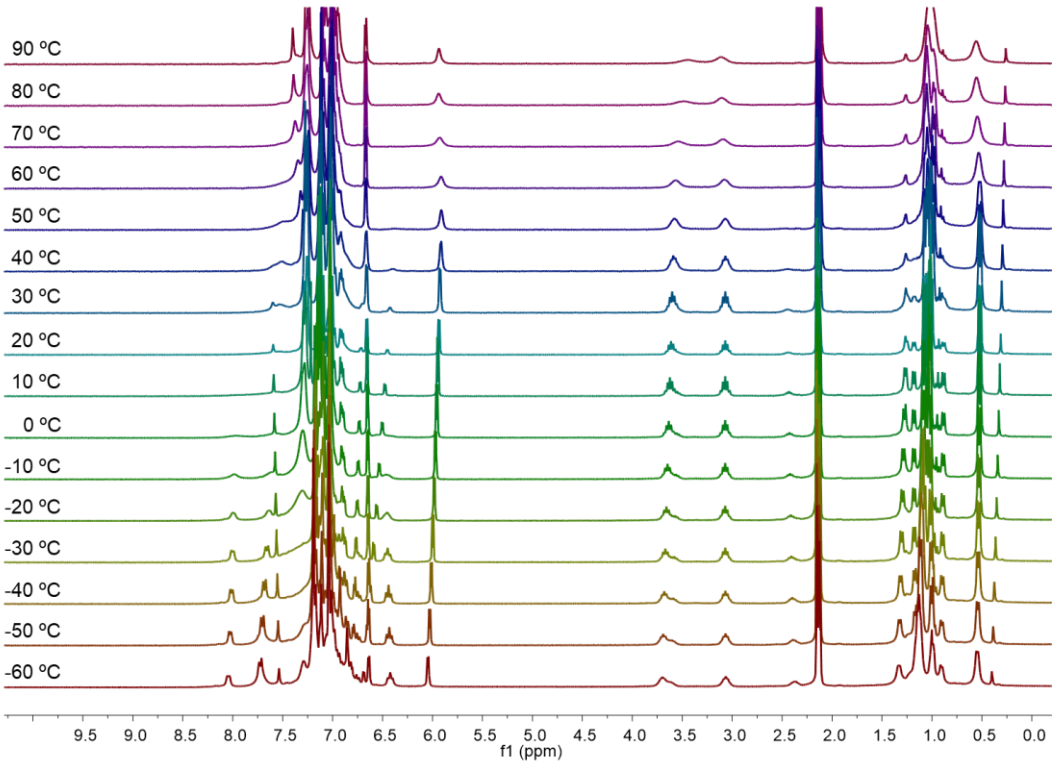

Figure S34 Variable temperature ^{1}H NMR spectra (300 MHz, toluene-d_8) of complex **1e**.

Kinetic and thermodynamic data derived from VT-NMR studies in complexes 1a-e

Rotation kinetic barriers determined by the coalescence temperature method

From the VT-NMR experiments it was possible to estimate the values of the isopropyl rotation barriers in complexes **1a-e** and of the rotation of the 5-(2,6-$Me_2C_6H_3$) ring in complex **1b**, according to the coalescence temperature method. In this method, the process rate constant, k_C, at the coalescence temperature, T_C, is calculated by the equation:

$$k_C = (\pi/\sqrt{2})\sqrt{\Delta\nu^2+J_{AB}^2}$$

where $\Delta\nu$ is the frequency difference of the resonances corresponding to the static spectrum and J_{AB} is the coupling between exchanging nuclei A and B.[2] The activation energies, $\Delta G^{\ddagger}$ were calculated by the Eyring equation ($\Delta G^{\ddagger}=RT_C\ln(k_Ch/k_BT_C)$, R, h and k_B being the gas, Planck and Boltzmann constants, respectively) using the determined k_C and T_C values.

Table S4 Values of $\Delta G^{\ddagger}$ for the rotation of the isopropyl groups of the *N*-(2,6-*i*$Pr_2C_6H_3$) substituent in complexes **1a-e**, determined by the coalescence temperature method.

Process	Complex	$\Delta\nu$[a]	J_{AB}	k_C (s^{-1})	T_C (ºC)	T_C (K)	$\Delta G^{\ddagger}$
*i*Pr group rotation[b]	**1a**	132	6.9	293.2	70	343.15	16.32
	1b	123	6.6	273.2	60	333.15	15.88
	1c	[c]	[c]	[c]	[c]	[c]	[c]
	1d	[d]	[d]	[d]	[d]	[d]	[d]
	1e	190.2	6.9	422.5	100	373.15	17.54
5-(2,6-$Me_2C_6H_3$) ring rotation[e]	**1b**	213	0	473.2	60	333.15	15.51

[a] Determined at -60 ºC. [b] Parameters determined utilizing the respective C*H*$(CH_3)_2$ resonances. [c] Parameters not determined since no coalescence of the C*H*$(CH_3)_2$ resonances was observed. [d] No parameters were determined for complex **1d**, owing to the overlapping and broadening of the respective C*H*$(CH_3)_2$ and O(C*H*$_3$) ^{1}H NMR resonances. [e] Parameters determined utilizing the respective 5-Ph-C*H*$_3$ resonances.

Isomer equilibria observed in complexes 1d,e determined by van't Hoff analysis

The isomer equilibria observed in complexes **1d,e** was subject of van't Hoff ($\Delta G^{o}=-RT\ln(K_{eq})$, K_{eq} being the equilibrium constant) analyses. The equilibrium constants were calculated considering the reaction [$\mathbf{A}^{\#}$] $\rightleftharpoons$ [$\mathbf{A}^{*}$], in which **A** represents the complexes **1d,e** and # and * represent the two possible conformers, in which K_{eq} = [$\mathbf{A}^{*}$]/[$\mathbf{A}^{\#}$]. The relative concentrations of the two species in equilibrium were calculated by relative integration of the respective resonances, $I_{\mathbf{A}\#}$ or $I_{\mathbf{A}*}$ in the NMR spectra, at the different temperatures, making K_{eq} = $I_{\mathbf{A}*}$/ $I_{\mathbf{A}\#}$. To validate the method, several resonances were used, whenever possible. The van't

Hoff plots for the different complexes are presented in Figures S27 and S28 and the respective results summarized in Table S4.

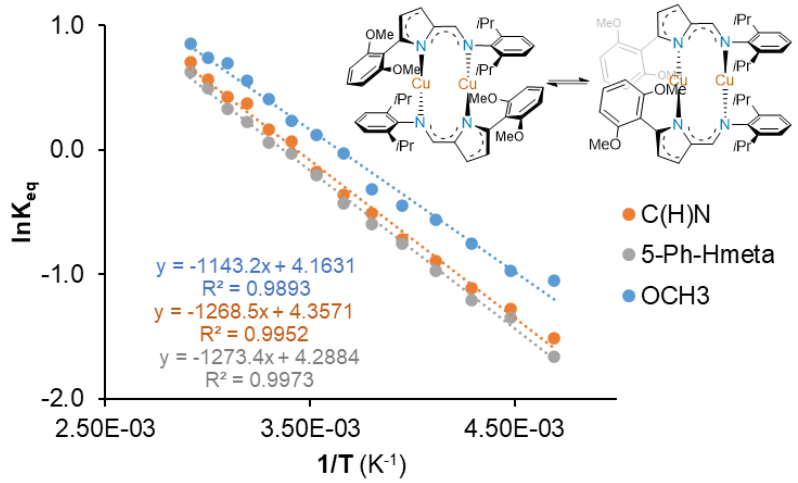

Figure S35 van't Hoff plot of the chemical exchange occurring in complex **1d**.

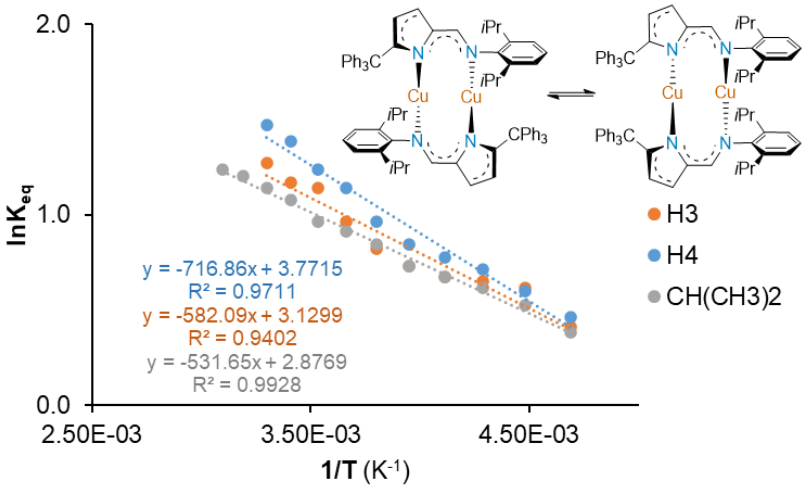

Figure S36 van't Hoff plot of the chemical exchange occurring in complex **1e**.

Table S5 Calculated values of ΔH°, ΔS°, and ΔG° (at 298 K) from the van't Hoff plots using different resonances and their average values for the *transoid-cisoid* isomerization occurring in complexes **1d,e**.

Complex	Resonance	ΔH° (kcal mol^{-1})	ΔH° (av.) (kcal mol^{-1})	ΔS° (cal mol^{-1} K^{-1})	ΔS° (av.) (cal mol^{-1} K^{-1})	ΔG° (kcal mol^{-1})	ΔG° (av.) (kcal mol^{-1})
	N=C*H*	2.27		8.28		-0.19	
1d	5-Ph-H$_{meta}$	2.53	2.4±0.2	8.53	8.5±0.2	-0.01	-0.1±0.1
	OC*H*$_3$	2.52		8.67		-0.06	
	H3	1.16		6.23		-0.70	
1e	H4	1.43	1.2±0.2	7.50	6.4±0.9	-0.81	-0.7±0.1
	C*H*(CH$_3$)$_2$	1.06		5.72		-0.65	

NMR data of the products obtained in the catalytic azide-alkyne cycloaddition reactions

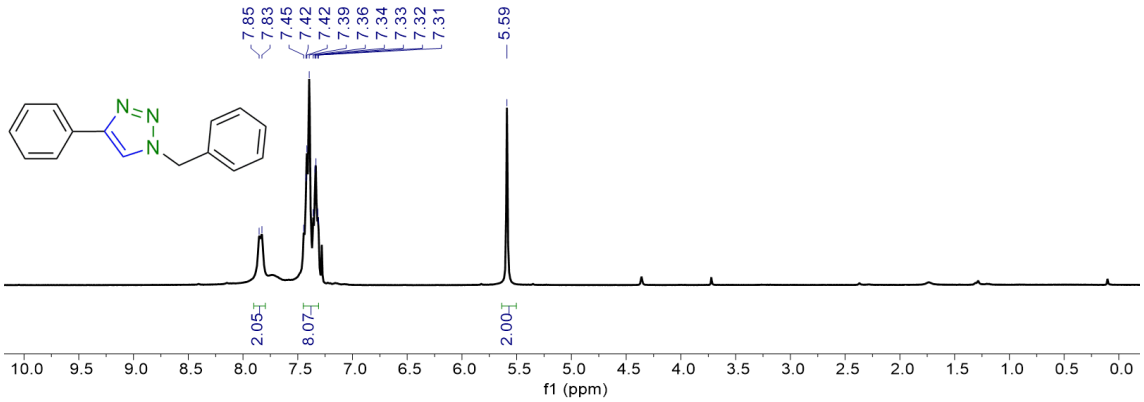

Figure S37 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of the cycloaddition product of phenylacetylene and (azidomethyl)benzene, 1-benzyl-4-phenyl-1*H*-1,2,3-triazole.

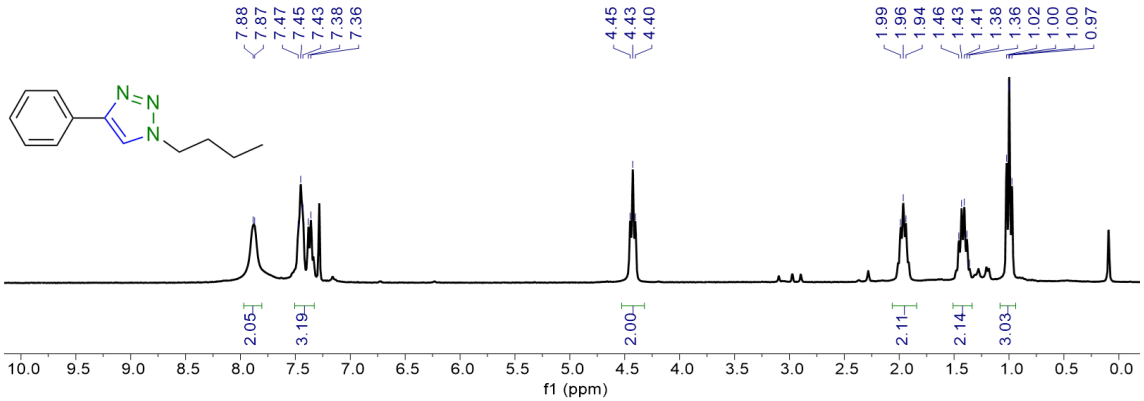

Figure S38 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of the cycloaddition product of phenylacetylene and 1-azidobutane, 1-(*n*-butyl)-4-phenyl-1*H*-1,2,3-triazole.

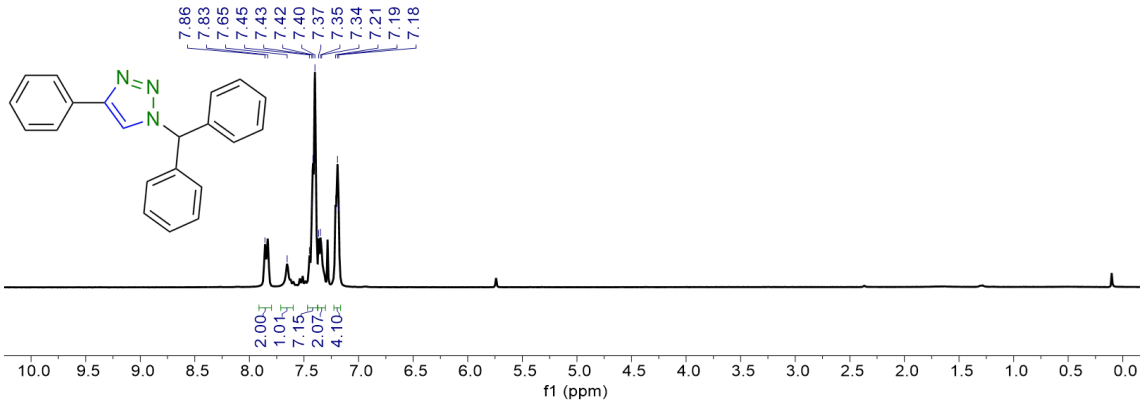

Figure S39 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of the cycloaddition product of phenylacetylene and (azidomethylene)dibenzene, 1-benzhydryl-4-phenyl-1*H*-1,2,3-triazole.

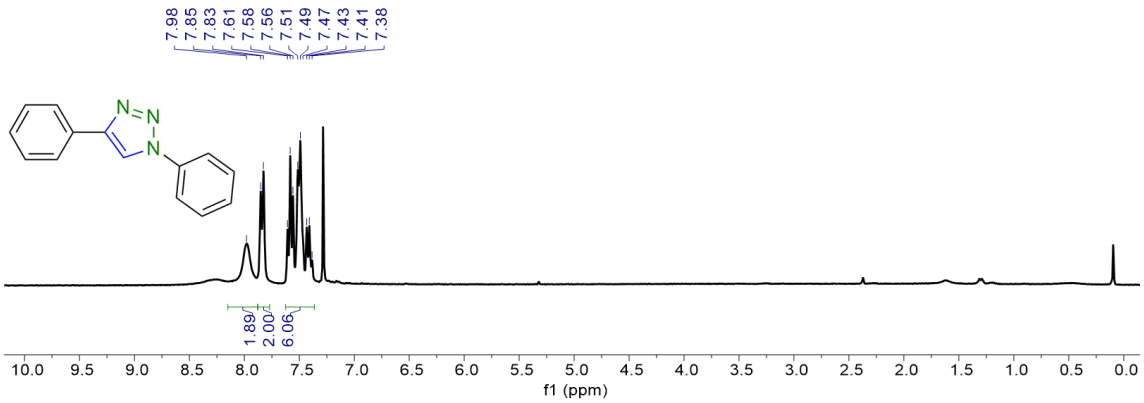

Figure S40 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of the cycloaddition product of phenylacetylene and azidodibenzene, 1,4-diphenyl-1*H*-1,2,3-triazole.

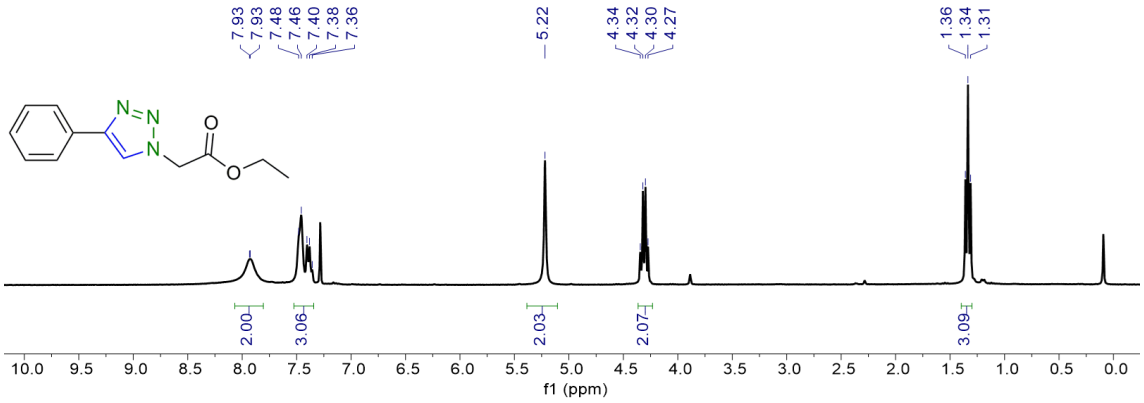

Figure S41 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of the cycloaddition product of phenylacetylene and ethyl 2-azidoacetate, ethyl 2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)acetate.

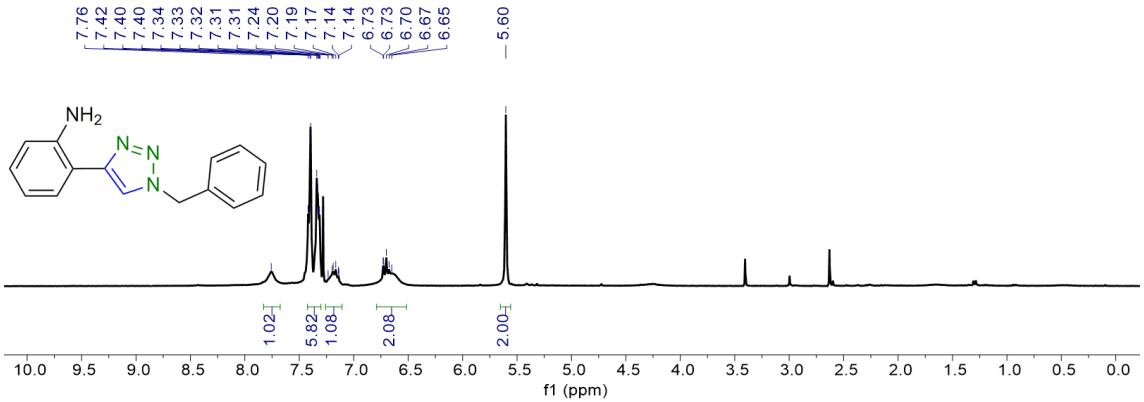

Figure S42 ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of the cycloaddition product of 2-ethynylaniline and 2-(1-benzyl-1*H*-1,2,3-triazol-4-yl)aniline.

Relationship between catalytic Turnover Frequency and the first oxidation potential of complexes 1a-e

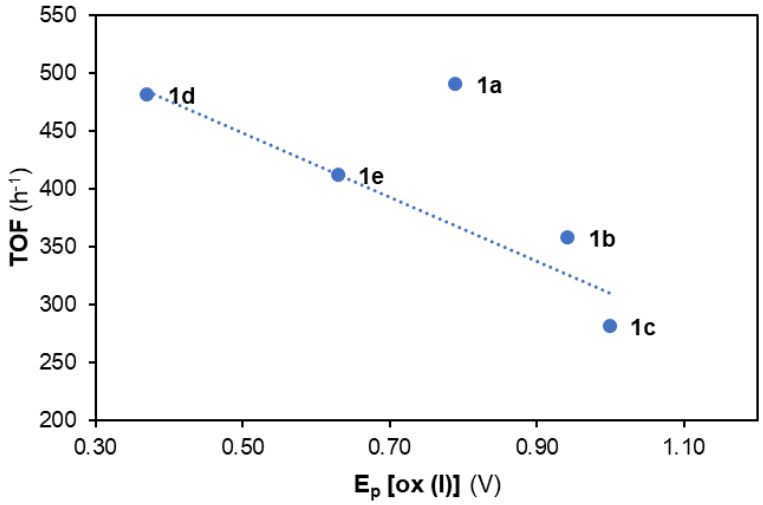

Figure S43 Trend observed between the catalytic activity (expressed in TOF) obtained in the catalytic cycloaddition of phenylacetylene to (azidomethyl)benzene and the first oxidation potential (E_p [ox(I)]) for catalyst precursors **1a-e**. The dashed line is a linear correlation visual guide.

Atomic coordinates of the optimized geometries

1a-*cisoid*

Cu	4.733034	7.126568	13.569220
Cu	5.439082	4.939773	14.853044
N	3.640669	7.656034	15.024996
N	5.489969	5.662790	16.581830
C	3.878655	7.512804	16.384614
N	5.500123	3.815226	13.355444
C	6.249267	4.902313	17.531804
C	6.536730	0.415866	14.443521
N	5.792410	6.663430	12.067658
C	2.564929	8.477157	14.917289
C	2.942889	8.271770	17.115918
C	4.768504	6.645804	17.050838
C	0.426749	9.949471	11.488949
C	0.442553	8.589649	11.786066
C	6.604413	1.779802	14.154281
C	4.218998	0.348326	13.818411
C	1.937088	8.944554	13.657337
C	6.429090	3.005394	19.004621
C	5.441472	2.416661	13.669745
C	5.357997	-0.300661	14.272661
C	2.100676	8.861361	16.191380
C	1.181659	8.068126	12.851092
C	1.203540	10.793852	12.281585
C	5.682279	3.728155	18.072723
C	7.208228	9.634180	12.240831
C	1.954412	10.326505	13.358658
C	7.428649	11.011052	12.156289
C	5.968825	5.397526	11.526265
C	7.544896	5.319686	17.888332
C	5.769989	4.132880	12.117106
C	8.248981	4.562605	18.828182
C	5.771520	9.803089	10.275534
C	6.030603	11.172689	10.234716
C	6.382867	9.012465	11.279098
C	6.316165	7.534101	11.165671
C	6.871904	11.798670	11.153249
C	6.594603	5.498486	10.267508
C	7.699629	3.418340	19.388318
C	4.233073	1.712346	13.515756
C	6.834174	6.841976	10.051307
H	9.245760	4.878995	19.124394
H	8.261096	2.844601	20.120289
H	6.006939	2.105077	19.441086
H	4.813249	6.810790	18.131901
H	2.890198	8.327702	18.196287
H	1.246883	9.498742	16.376358
H	1.219895	11.857458	12.048734
H	-0.153027	7.908419	11.185035
H	5.566409	11.766167	9.450127
H	8.087620	11.484127	12.881678
H	7.325805	7.304355	9.206716
H	6.867238	4.662476	9.635240
H	5.915347	3.299550	11.422592
H	3.296437	-0.212550	13.692316
H	5.328541	-1.363013	14.497957
H	7.424005	-0.094931	14.805883
C	2.965884	2.385587	13.025334
H	3.170162	3.457799	12.947227
C	7.910089	2.536093	14.321257
C	8.671592	2.144963	15.588352
C	8.796765	2.373930	13.081330
H	7.660500	3.601625	14.408352
C	4.283982	3.276258	17.690747
H	4.059196	3.710942	16.707494
C	8.180196	6.561154	17.293532
H	7.520123	6.918484	16.496996
C	1.811147	2.209879	14.015299
H	0.921887	2.746097	13.666285
H	1.533254	1.156884	14.132478
H	2.074506	2.599476	15.003676
C	2.577883	1.881448	11.631748
H	3.382754	2.048457	10.909093
H	2.362272	0.807236	11.646205
H	1.683201	2.397316	11.266971
C	9.540966	6.258918	16.660522
H	10.272151	5.927510	17.405710

H	9.459775	5.476859	15.898999
H	9.947195	7.156991	16.182502
C	8.296844	7.675189	18.338651
H	7.318667	7.937311	18.753777
H	8.939494	7.368040	19.171324
H	8.729894	8.579097	17.896727
C	4.159410	1.758450	17.554696
H	3.175331	1.500455	17.150559
H	4.916973	1.350295	16.879484
H	4.250725	1.251992	18.521922
C	3.245192	3.818160	18.679406
H	2.237301	3.498774	18.392966
H	3.444802	3.445449	19.690407
H	3.252199	4.911468	18.717852
C	2.770366	11.322390	14.165852
H	3.305733	10.765510	14.941163
C	1.068409	6.583966	13.153992
H	1.810879	6.337812	13.919640
C	7.952387	8.851855	13.309144
H	7.575259	7.824787	13.302474
C	4.832889	9.218643	9.231407
H	4.725213	8.149236	9.437268
C	7.222150	13.269083	11.039279
H	7.770163	13.539929	11.952016
C	8.157772	13.506797	9.848782
H	9.061532	12.894977	9.926564
H	7.661132	13.248127	8.907011
H	8.458559	14.558782	9.792416
C	5.992211	14.173874	10.951624
H	5.411861	13.972848	10.044524
H	5.330683	14.032357	11.810597
H	6.293339	15.226456	10.920034
C	3.439531	9.845021	9.323742
H	2.764326	9.370928	8.602357
H	3.012457	9.723763	10.322360
H	3.463707	10.917020	9.096904
C	5.396069	9.363097	7.814521
H	6.377627	8.889398	7.718245
H	4.722950	8.898760	7.085599
H	5.508744	10.417122	7.536956
C	7.707736	9.422364	14.707648
H	6.642201	9.413488	14.960159
H	8.240542	8.829649	15.457707
H	8.064613	10.454031	14.797000
C	9.449513	8.793211	12.987275
H	9.895462	9.794260	12.987097
H	9.981696	8.187837	13.729741
H	9.621161	8.349660	12.001699
C	-0.431189	10.539647	10.386066
H	0.112891	11.410912	9.995109
C	-1.758274	11.046265	10.964742
H	-2.363849	11.530125	10.190410
H	-2.338195	10.213618	11.378385
H	-1.591209	11.767332	11.770499
C	-0.683459	9.590956	9.216439
H	-1.198501	10.117623	8.406661
H	0.251301	9.184216	8.819016
H	-1.321487	8.749792	9.509349
C	3.817940	12.018489	13.295447
H	4.431155	12.692214	13.904930
H	4.483101	11.296850	12.814079
H	3.349887	12.617709	12.506285
C	1.875937	12.346240	14.870419
H	1.319263	12.953231	14.147639
H	1.147097	11.859025	15.525430
H	2.479018	13.027080	15.480906
C	-0.313089	6.257250	13.731322
H	-1.107027	6.480708	13.009807
H	-0.383153	5.194722	13.990627
H	-0.507968	6.841262	14.635972
C	1.372634	5.723469	11.926192
H	2.381417	5.915942	11.545934
H	1.300669	4.661522	12.180994
H	0.665829	5.908855	11.110418
H	9.538065	2.801277	15.719126
H	9.052321	1.118931	15.537710
H	8.043483	2.234726	16.479518
H	9.730110	2.935113	13.198724
H	8.298761	2.735964	12.176808
H	9.051751	1.319727	12.924517

1a-*transoid*

Cu	-1.054874	2.154191	7.673545
Cu	1.470056	1.731884	7.069404
N	-0.743732	3.915535	8.243038
N	1.411169	-0.073611	7.572893
N	-1.626668	0.454600	7.074224
N	1.751781	3.482194	6.417406
C	-3.920096	-0.266862	7.635054
C	5.464071	0.642014	9.732871
H	5.693902	1.092784	10.696626
C	0.130362	4.835285	7.691189
C	0.372422	-0.962780	7.359811
C	-1.553379	4.608468	9.080223
C	-2.679301	4.024869	9.850140
C	4.137743	0.321375	9.433267
C	-4.839886	3.203209	11.472652
C	-0.977244	-0.680491	7.062656
H	-1.558942	-1.569874	6.803706
C	3.847027	-0.281198	8.192824
C	3.063019	0.601803	10.468652
H	2.102702	0.287800	10.047393
C	6.510350	0.387680	8.849696
C	-2.441073	3.252949	11.005074
C	-4.005486	4.359211	9.491815
C	-2.538512	1.686107	4.606420
H	-1.518862	1.542213	4.980390
C	-4.852308	0.991119	5.308370
H	-5.218160	1.470782	4.404129
C	2.492399	-0.817915	7.909255
C	4.887118	-0.510588	7.263900
C	-3.528195	2.859241	11.789432
H	-3.346256	2.275086	12.689941
C	2.864267	3.598128	5.519760
C	-1.040753	2.867605	11.448901
H	-0.334930	3.255069	10.707205
C	0.829016	-2.280077	7.564287
H	0.223233	-3.174016	7.480594
C	1.423377	2.534612	3.688265
H	0.685323	2.616676	4.493291
C	6.194676	-0.174898	7.613097
H	6.992235	-0.368013	6.899152
C	-2.791393	3.193140	4.511128
H	-3.805574	3.405216	4.154713
H	-2.087257	3.658501	3.812763
H	-2.671303	3.677601	5.485593
C	-3.485421	1.020055	5.587938
C	1.201794	4.603890	6.803968
H	1.637467	5.522585	6.400504
C	-0.152052	6.119141	8.198746
H	0.386345	7.025004	7.948490
C	-5.054584	3.944429	10.311082
H	-6.071094	4.216217	10.035305
C	-5.747507	0.349950	6.154432
H	-6.807751	0.333312	5.918691
C	-5.276628	-0.275636	7.299752
H	-5.978449	-0.781539	7.957558
C	4.077326	4.168628	5.963831
C	-3.629291	-2.486627	8.792388
H	-4.678607	-2.765755	8.645624
H	-3.276221	-2.979721	9.704311
H	-3.062713	-2.891077	7.947655
C	-0.872215	1.346101	11.492104
H	-1.565184	0.883859	12.203827
H	0.144426	1.077013	11.797601
H	-1.057417	0.900975	10.508729
C	-1.200767	5.972257	9.092010
H	-1.677381	6.735775	9.691501
C	-3.479163	-0.965636	8.911148
H	-2.420000	-0.745668	9.075175
C	2.161763	-2.187137	7.931498
H	2.839715	-2.989233	8.189812
C	0.890067	3.333872	2.495324
H	0.758281	4.389814	2.751267
H	-0.077911	2.939027	2.168664
H	1.571022	3.281504	1.638794
C	4.623079	-1.119999	5.897279
H	3.537840	-1.215508	5.781930
C	-4.235709	-0.451144	10.137973
H	-4.132441	0.631499	10.246923
H	-3.844456	-0.923721	11.045642
H	-5.303901	-0.688752	10.081007
C	-4.325007	5.168332	8.245356

H	-3.391297	5.303820	7.688835
C	2.726610	3.118532	4.201058
C	8.720638	-0.613531	9.488370
H	8.790266	-1.207701	8.570401
H	8.229682	-1.230393	10.246997
H	9.740262	-0.399292	9.826941
C	3.820715	3.214160	3.340218
H	3.725931	2.850458	2.320367
C	-5.984650	2.814536	12.386753
H	-5.576888	2.120367	13.134101
C	7.944308	0.684220	9.241839
H	7.909626	1.235923	10.191099
C	5.137742	4.247665	5.057291
H	6.077656	4.685601	5.382931
C	-5.309562	4.439407	7.326546
H	-4.947569	3.442707	7.058354
H	-5.456133	5.009405	6.402268
H	-6.291871	4.322172	7.797530
C	-2.618030	1.021483	3.228658
H	-2.408188	-0.050814	3.292226
H	-1.892773	1.471025	2.542094
H	-3.610856	1.140173	2.781195
C	8.666233	1.565701	8.220752
H	8.757570	1.062199	7.252308
H	9.679004	1.801062	8.564965
H	8.132102	2.506316	8.058641
C	4.280765	4.692941	7.375757
H	3.396957	4.436299	7.967411
C	-4.849887	6.561126	8.606872
H	-5.784962	6.494676	9.174391
H	-5.048216	7.146026	7.702069
H	-4.128829	7.113556	9.216685
C	2.965688	2.099910	10.771459
H	3.902964	2.488131	11.185412
H	2.174723	2.297403	11.502889
H	2.736803	2.672064	9.866093
C	5.020576	3.774465	3.758294
H	5.860432	3.844092	3.072919
C	1.569873	1.050408	3.340668
H	2.294816	0.899741	2.532970
H	0.611263	0.635848	3.010077
H	1.908373	0.471580	4.206188
C	-7.111485	2.090156	11.647348
H	-7.883362	1.761567	12.351412
H	-6.737210	1.211732	11.113737
H	-7.594355	2.745647	10.914628
C	5.221405	-2.525450	5.786255
H	6.311004	-2.501460	5.900826
H	4.997844	-2.963183	4.807267
H	4.819231	-3.191292	6.555589
C	4.426619	6.218577	7.390689
H	4.540235	6.583034	8.417166
H	3.558655	6.718083	6.948567
H	5.309723	6.534313	6.824153
C	-0.689068	3.501829	12.797904
H	-0.780566	4.591399	12.756377
H	0.340852	3.258043	13.081858
H	-1.346983	3.139938	13.595708
C	3.293362	-0.207131	11.748568
H	4.234805	0.070576	12.235177
H	3.329954	-1.279670	11.535064
H	2.484603	-0.030791	12.466517
C	5.129969	-0.220491	4.766828
H	4.702483	0.784324	4.830323
H	4.858114	-0.645641	3.794207
H	6.220969	-0.121249	4.787268
C	5.481084	4.033290	8.058289
H	6.420586	4.296441	7.559510
H	5.390826	2.943974	8.060536
H	5.556198	4.370901	9.097711
C	-6.521645	4.039348	13.134536
H	-6.941522	4.769453	12.433649
H	-5.728026	4.538426	13.698599
H	-7.313461	3.752622	13.835292
C	-3.024907	0.392635	6.763613

1b-*cisoid*

Cu	4.820829	7.084975	13.572340
Cu	5.447674	4.936747	14.823916
N	3.612022	7.578558	14.924314
N	5.400066	5.677839	16.552787
C	3.737235	7.460819	16.296426

N	5.593694	3.842431	13.300565
C	6.199902	4.969955	17.508627
C	6.308220	0.321230	14.259728
N	6.000963	6.674144	12.168552
C	2.574885	8.418335	14.702447
C	2.758129	8.254765	16.928385
C	4.617710	6.621341	17.008304
C	1.198287	9.546526	10.818556
C	1.004012	8.248465	11.274858
C	6.513879	1.679499	14.006719
C	3.978188	0.520183	13.706630
C	2.128275	8.798425	13.342488
C	6.461209	3.191818	19.108304
C	5.414239	2.447110	13.574061
C	5.056047	-0.259756	14.106673
C	2.014451	8.849150	15.920969
C	1.457704	7.857489	12.536260
C	1.854295	10.471319	11.622362
C	5.656047	3.857094	18.180509
C	7.230691	9.603418	12.686468
C	2.326701	10.116798	12.887192
C	7.190451	10.979028	12.922452
C	6.248962	5.452172	11.570770
C	7.529534	5.381133	17.725880
C	5.990889	4.170890	12.098773
C	8.292068	4.682916	18.663725
C	5.651669	9.907504	10.843268
C	5.641977	11.278333	11.106789
C	6.448817	9.066025	11.644376
C	6.514346	7.617258	11.345203
C	6.402923	11.813976	12.139047
C	6.921614	5.653734	10.347888
C	7.765287	3.600132	19.356473
C	4.130681	1.882046	13.440941
C	7.100987	7.021225	10.211465
H	9.315302	4.994859	18.855116
H	8.372620	3.071665	20.085883
H	6.055421	2.338863	19.645837
H	4.617076	6.779796	18.091240
H	2.612555	8.338612	17.998371
H	1.163564	9.509183	16.023345
H	2.008433	11.487382	11.267505
H	0.833909	9.838743	9.837360
H	0.480110	7.526271	10.653422
H	5.025220	11.929126	10.491833
H	6.386342	12.883608	12.330125
H	7.798468	11.397052	13.721063
H	7.598669	7.549949	9.409710
H	7.256730	4.870503	9.679048
H	6.177371	3.348738	11.400733
H	2.998749	0.062917	13.595737
H	4.918920	-1.319219	14.303969
H	7.146690	-0.290898	14.580966
C	2.946264	2.717943	12.993958
H	3.235472	3.769542	13.098587
C	7.894417	2.283604	14.188383
C	8.479534	1.980924	15.570419
C	8.845810	1.828752	13.076913
H	7.791558	3.371670	14.109628
C	4.236735	3.379578	17.930606
H	3.853227	3.922846	17.059942
C	8.119091	6.565588	16.984283
H	7.436859	6.802760	16.160571
C	1.707739	2.496851	13.863912
H	0.915384	3.195381	13.575379
H	1.304028	1.484416	13.754844
H	1.932287	2.656849	14.923147
C	2.629885	2.473427	11.514982
H	3.491156	2.700502	10.878862
H	2.354800	1.426760	11.342318
H	1.793803	3.101647	11.188954
C	9.484435	6.250196	16.370398
H	10.245438	6.064336	17.136002
H	9.435010	5.367508	15.724981
H	9.830604	7.094377	15.764928
C	8.193900	7.798570	17.890272
H	7.207679	8.067300	18.281675
H	8.853432	7.615651	18.746201
H	8.585807	8.660409	17.339367
C	4.182293	1.886872	17.595312
H	3.157307	1.593337	17.344709
H	4.820983	1.644039	16.740799

H	4.500201	1.268756	18.442050
C	3.327139	3.709861	19.118505
H	2.299450	3.387474	18.919733
H	3.669438	3.202237	20.027345
H	3.310817	4.784592	19.325583
C	3.046347	11.130606	13.733058
H	2.507985	11.337846	14.663174
H	4.043851	10.775929	14.012080
H	3.166512	12.071246	13.190223
C	1.200996	6.458677	13.025919
H	0.503657	5.937985	12.363753
H	2.126293	5.874173	13.072226
H	0.783117	6.462908	14.037891
C	8.128043	8.726873	13.516184
H	7.551431	8.079596	14.185684
H	8.730034	8.065619	12.884426
H	8.802842	9.332091	14.128033
C	4.811398	9.351684	9.726757
H	5.428361	8.932710	8.925374
H	4.159410	8.547991	10.083175
H	4.177973	10.131037	9.296145
H	9.435154	2.500609	15.697852
H	8.670880	0.910677	15.705417
H	7.808771	2.307819	16.370713
H	9.831745	2.289680	13.199807
H	8.465955	2.100113	12.086899
H	8.977958	0.741074	13.094809

1b-*transoid*

Cu	-1.047746	2.175561	7.607291
Cu	1.433846	1.741159	7.037898
N	-0.700587	3.943875	8.131306
N	1.305077	-0.073161	7.499593
N	-1.675987	0.514225	6.964014
N	1.763673	3.465658	6.340490
C	-3.985219	-0.110934	7.554580
C	5.004490	0.607486	10.094633
H	5.088922	0.938215	11.126859
C	0.081211	4.864481	7.457062
C	0.290768	-0.946331	7.151603
C	-1.529554	4.653759	8.931045
C	-2.499300	4.025532	9.859627
C	3.766769	0.172081	9.619065
C	-4.315009	3.024993	11.727492
C	-1.054088	-0.631224	6.865864
H	-1.652156	-1.488623	6.543251
C	3.665327	-0.269811	8.284268
C	6.125500	0.602993	9.272100
C	-2.032728	3.534047	11.095978
C	-3.872922	4.003008	9.553174
C	-2.574260	1.853505	4.546614
H	-1.556503	1.666104	4.905611
C	-4.906882	1.266494	5.291162
H	-5.269399	1.792024	4.411246
C	2.379244	-0.834090	7.811975
C	4.792736	-0.261579	7.440633
C	-2.954775	3.034484	12.016334
H	-2.599824	2.664126	12.974888
C	2.915678	3.508315	5.489168
C	0.759349	-2.272108	7.242811
H	0.171107	-3.160784	7.049423
C	1.528815	2.379007	3.656094
H	0.762837	2.513162	4.427401
C	6.015560	0.176903	7.954003
H	6.889459	0.180059	7.307290
C	-2.765896	3.370465	4.466316
H	-3.773292	3.627918	4.120664
H	-2.050482	3.810395	3.762825
H	-2.612965	3.843771	5.441679
C	-3.533592	1.212284	5.533116
C	1.175218	4.601801	6.606165
H	1.593913	5.493923	6.131346
C	-0.286847	6.167955	7.845111
H	0.174734	7.082187	7.492555
C	-4.766614	3.501256	10.502850
H	-5.829206	3.487742	10.273052
C	-5.813260	0.648693	6.143262
H	-6.878597	0.696194	5.936074
C	-5.348439	-0.036613	7.256850
H	-6.059638	-0.522975	7.919290
C	4.120698	4.074242	5.958403
C	-3.758265	-2.374995	8.633411

H	-4.820916	-2.606648	8.500204
H	-3.407466	-2.911643	9.521324
H	-3.224995	-2.773235	7.764316
C	-1.296825	6.034856	8.787547
H	-1.811169	6.817591	9.328870
C	-3.542223	-0.866261	8.796926
H	-2.470668	-0.695011	8.936237
C	2.076524	-2.202255	7.673303
H	2.753547	-3.019512	7.883162
C	1.074356	3.160180	2.419101
H	0.970105	4.227325	2.638731
H	0.107508	2.788999	2.062351
H	1.790180	3.058655	1.595991
C	-4.241820	-0.357844	10.059566
H	-4.090510	0.715753	10.196366
H	-3.845750	-0.873528	10.941058
H	-5.320784	-0.545771	10.028839
C	2.829848	2.938400	4.202150
C	3.972224	2.931483	3.400877
H	3.919118	2.498785	2.404963
C	5.230206	4.052363	5.109160
H	6.165103	4.487526	5.452277
C	-2.697037	1.205674	3.163803
H	-2.525904	0.125824	3.214333
H	-1.965512	1.635511	2.471109
H	-3.691685	1.364831	2.733241
C	4.256707	4.703769	7.334960
H	3.346298	4.483657	7.900910
C	5.167211	3.482106	3.845597
H	6.045098	3.473020	3.205760
C	1.628055	0.880338	3.359099
H	2.389250	0.671560	2.599129
H	0.671335	0.500320	2.984237
H	1.885494	0.312609	4.259140
C	4.390931	6.227570	7.234853
H	4.458199	6.674021	8.232697
H	3.539377	6.681370	6.717960
H	5.295480	6.504798	6.682011
C	5.427429	4.114619	8.125149
H	6.390297	4.346132	7.656360
H	5.346387	3.028299	8.211042
H	5.447234	4.536380	9.135876
C	-3.079410	0.523845	6.677158
C	-4.385174	4.475824	8.220470
H	-3.861263	5.372117	7.878049
H	-4.242004	3.703243	7.454929
H	-5.455533	4.693807	8.268711
C	-0.567976	3.572583	11.435089
H	-0.395302	3.238976	12.461616
H	0.014793	2.933171	10.763599
H	-0.165464	4.585443	11.327539
C	4.694454	-0.685587	6.000712
H	5.687901	-0.845243	5.573199
H	4.113202	-1.604295	5.885087
H	4.197759	0.086745	5.401080
C	2.571832	0.148632	10.532377
H	1.805560	0.861012	10.208290
H	2.097500	-0.838414	10.536396
H	2.859163	0.398945	11.556925
H	-5.023792	2.644644	12.458107
H	7.085669	0.933437	9.658974

1c-*cisoid*

Cu	-1.296667	2.212440	3.835028
Cu	-1.297165	-0.310191	3.835403
N	-3.086320	2.303033	4.414871
N	-3.060468	-0.498070	3.207794
C	-4.104769	0.252942	3.427859
H	-5.072231	-0.135180	3.095525
F	1.496938	4.402241	6.115755
C	-1.519578	4.238252	6.050734
H	-1.251163	3.207802	6.266292
C	-5.361494	2.188446	4.361253
H	-6.358531	1.799370	4.197239
C	-1.597481	-0.692784	-0.745600
H	-0.733152	-1.264871	-0.393881
H	-1.236248	0.263277	-1.137630
H	-2.043522	-1.235600	-1.585854
F	0.523407	3.974704	7.994655
C	-3.263666	-1.718825	2.483286
C	-3.025820	-1.719259	1.093421
C	-3.644753	-2.885427	3.171214

F	1.266892	5.969386	7.588961
C	-0.664546	5.268331	6.427361
C	-4.159401	1.522682	4.045572
C	-5.010446	3.399184	4.938368
H	-5.669803	4.160681	5.332394
C	-2.737161	4.516973	5.418225
C	-3.220018	-2.912101	0.396769
H	-3.053258	-2.936640	-0.675972
C	-3.828567	-4.053032	2.425063
H	-4.134137	-4.963764	2.933565
C	-3.855772	-2.904225	4.674159
H	-3.539981	-1.931650	5.066823
C	-2.603045	-0.447905	0.379221
H	-2.109180	0.188974	1.124758
C	-3.603944	3.434560	4.951011
C	0.659271	4.910602	7.036927
C	-3.089113	5.854689	5.213116
H	-4.023576	6.089856	4.712509
C	-3.625206	-4.069745	1.052041
H	-3.776207	-4.987318	0.490491
C	-5.336155	-3.084166	5.024604
H	-5.952742	-2.295187	4.582360
H	-5.480473	-3.059908	6.109921
H	-5.714901	-4.044606	4.657667
C	-1.009436	6.597303	6.203554
H	-0.340057	7.398845	6.490727
C	-3.822851	0.321980	-0.141128
H	-4.353812	-0.262981	-0.900563
H	-3.519902	1.273606	-0.589669
H	-4.532189	0.546581	0.661144
C	-2.994751	-3.970450	5.357120
H	-3.280064	-4.980950	5.044940
H	-3.116641	-3.916167	6.444100
H	-1.932823	-3.835200	5.130092
F	-3.829183	8.579637	5.884439
C	-2.642601	8.296105	5.320577
F	-2.786759	8.506233	3.998769
C	-2.232463	6.879120	5.603007
F	-1.753574	9.184870	5.777741
N	0.492989	2.302098	3.255002
N	0.466044	-0.498475	4.463158
C	1.510655	0.251995	4.242754
H	2.477962	-0.136370	4.575254
F	-4.090161	4.404918	1.555715
C	-1.073297	4.237664	1.619007
H	-1.342536	3.207289	1.404115
C	2.768121	2.186582	3.308429
H	3.765012	1.797155	3.472500
C	-0.996522	-0.690456	8.416933
H	-1.861168	-1.262377	8.065725
H	-1.357275	0.265974	8.808504
H	-0.550524	-1.232983	9.257398
F	-3.117754	3.973722	-0.322942
C	0.668677	-1.718958	5.188278
C	0.430990	-1.718559	6.578174
C	1.049020	-2.886111	4.500886
F	-3.858814	5.969798	0.080321
C	-1.927797	5.268119	1.242208
C	1.565781	1.521447	3.624489
C	2.417518	3.397218	2.730835
H	3.077168	4.158258	2.336416
C	0.144744	4.515889	2.250861
C	0.624610	-2.911160	7.275397
H	0.457923	-2.935074	8.348164
C	1.232299	-4.053441	5.247598
H	1.537305	-4.964592	4.739516
C	1.259842	-2.905708	2.997926
H	0.944039	-1.933308	2.604822
C	0.008925	-0.446631	7.291774
H	-0.484804	0.190067	6.545990
C	1.011022	3.433202	2.718352
C	-3.252216	4.911051	0.633561
C	0.497698	5.853486	2.455044
H	1.432565	6.088310	2.955052
C	1.029106	-4.069348	6.620657
H	1.179670	-4.986722	7.182648
C	2.740186	-3.085873	2.647416
H	3.356843	-2.296676	3.089172
H	2.884398	-3.062205	1.562072
H	3.118928	-4.046127	3.014847
C	-1.581928	6.596982	1.465172
H	-2.250899	7.398829	1.177901

C	1.229159	0.322994	7.811504
H	1.759960	-0.261793	8.571186
H	0.926711	1.275007	8.259565
H	1.938485	0.546831	7.009009
C	0.398717	-3.972230	2.315568
H	0.684090	-4.982606	2.628095
H	0.520427	-3.918389	1.228546
H	-0.663174	-3.836891	2.542715
F	1.239578	8.577411	1.782459
C	0.052790	8.295137	2.346520
F	0.197121	8.505988	3.668189
C	-0.358431	6.878287	2.064990
F	-0.835575	9.184289	1.888814

1c-*transoid*

Cu	-1.085815	2.145066	7.493647
Cu	1.375309	1.788345	6.927925
N	-0.611740	3.863859	8.112231
N	1.169639	-0.005963	7.482965
N	-1.755182	0.532450	6.777556
N	1.716821	3.488541	6.173343
C	-4.111435	0.052615	7.291550
C	4.348813	1.494469	10.011743
C	0.035947	4.820556	7.360102
C	0.230802	-0.887421	6.990368
C	-1.382046	4.537068	9.005004
C	-2.135345	3.842987	10.048591
C	3.250542	0.949869	9.352851
C	-3.509552	2.538635	12.130803
C	-1.106761	-0.589544	6.630814
H	-1.661902	-1.433580	6.212226
C	3.397264	-0.169796	8.527177
C	5.610588	0.930375	9.872596
C	-1.666980	2.630863	10.570240
C	-3.305063	4.392692	10.588027
C	-2.478106	1.624782	4.168479
H	-1.484442	1.450644	4.594907
C	-4.856133	1.101591	4.800405
H	-5.151773	1.511895	3.838326
C	2.234964	-0.757816	7.862458
C	4.671657	-0.737727	8.391709
C	-2.353008	1.985623	11.593217
C	2.839772	3.569488	5.280691
C	0.736466	-2.200683	7.044269
H	0.198762	-3.095028	6.755224
C	1.437114	2.418663	3.470678
H	0.664842	2.578015	4.231122
C	5.760230	-0.190786	9.057124
C	-2.645768	3.136404	3.985169
H	-3.628471	3.378688	3.566008
H	-1.885104	3.531372	3.303419
H	-2.552128	3.663095	4.940715
C	-3.502975	1.078326	5.143685
C	1.088175	4.600869	6.437102
H	1.435072	5.501374	5.923274
C	-0.363808	6.104691	7.778266
H	0.013693	7.041006	7.386722
C	-3.978520	3.745458	11.616805
C	-5.825315	0.606465	5.660840
H	-6.872932	0.626984	5.374476
C	-5.449321	0.087254	6.892271
H	-6.212182	-0.293720	7.564668
C	4.048475	4.142751	5.731263
C	-3.680674	-2.042691	8.625903
H	-4.654947	-2.464497	8.354335
H	-3.404602	-2.431245	9.611763
H	-2.946910	-2.411791	7.903351
C	-1.258878	5.926155	8.824272
H	-1.725215	6.691968	9.429211
C	-3.743466	-0.510907	8.652849
H	-2.744668	-0.141069	8.908628
C	2.005355	-2.120181	7.601153
H	2.669750	-2.937318	7.847631
C	0.960216	3.098630	2.183951
H	0.827821	4.175458	2.327977
H	0.003452	2.678269	1.857755
H	1.672829	2.958014	1.364435
C	-4.698676	-0.047045	9.755163
H	-4.812638	1.040976	9.760023
H	-4.316694	-0.354583	10.732906
H	-5.694234	-0.490022	9.645484
C	2.723582	3.039550	3.980842

C	3.834297	3.099733	3.138088
H	3.759414	2.694083	2.132681
C	5.122310	4.194291	4.838835
H	6.057877	4.640187	5.164070
C	-2.538522	0.888198	2.827268
H	-2.394145	-0.188864	2.958237
H	-1.761623	1.255134	2.148587
H	-3.503097	1.035399	2.329786
C	4.228650	4.687990	7.138016
H	3.397838	4.326495	7.752107
C	5.025363	3.677218	3.555121
H	5.876541	3.722879	2.881868
C	1.593762	0.907286	3.274052
H	2.360173	0.684149	2.523615
H	0.652546	0.461324	2.934584
H	1.885610	0.412293	4.206385
C	4.198540	6.220683	7.157434
H	4.328040	6.592835	8.179105
H	3.255741	6.619935	6.771447
H	5.007086	6.632345	6.543038
C	5.520528	4.182851	7.786816
H	6.409540	4.609014	7.310067
H	5.598121	3.093496	7.727692
H	5.548518	4.470217	8.841682
C	-3.140502	0.542940	6.393519
H	2.263796	1.380367	9.495396
H	6.465620	1.363457	10.379451
H	4.812963	-1.596703	7.744665
H	-0.743983	2.207230	10.185592
H	-3.693812	5.326036	10.194291
H	-4.040305	2.037741	12.932384
C	4.133193	2.670224	10.920520
F	3.313165	3.579011	10.359904
F	3.568251	2.301066	12.079450
F	5.283599	3.295601	11.216441
C	7.122992	-0.810625	8.931887
F	8.063858	0.120293	8.704981
F	7.471778	-1.449543	10.060832
F	7.182487	-1.702127	7.932533
C	-1.791854	0.708898	12.149932
F	-0.800439	0.939309	13.022778
F	-2.727914	-0.011090	12.790630
F	-1.283745	-0.067848	11.175596
C	-5.273751	4.304258	12.132519
F	-5.356742	5.629655	11.944926
F	-6.325861	3.748433	11.507562
F	-5.426157	4.066415	13.444318

1d-*cisoid*

Cu	4.812255	7.067999	13.591956
Cu	5.449849	4.917578	14.846623
N	3.841029	7.760689	15.046874
N	5.494345	5.643755	16.584279
C	4.031817	7.613523	16.405188
N	5.515594	3.769684	13.353880
C	6.251640	4.867554	17.519862
C	6.404478	0.336613	14.470876
N	5.720836	6.553867	12.025854
C	2.929928	8.747896	14.891454
C	3.221336	8.540409	17.100877
C	4.834742	6.667890	17.067920
C	1.463500	10.184011	11.137040
C	1.481757	8.816250	11.373826
C	6.537554	1.691679	14.162018
C	4.073340	0.382781	13.890818
C	2.459238	9.222774	13.578605
C	6.413592	3.010706	19.044487
C	5.401518	2.382359	13.690962
C	5.187178	-0.319312	14.330861
C	2.520131	9.250113	16.146734
C	1.969314	8.341062	12.594476
C	1.934956	11.085636	12.081605
C	5.658756	3.738620	18.122511
C	6.592939	9.546470	12.376908
C	2.434688	10.603216	13.293530
C	6.560011	10.936678	12.517265
C	5.913315	5.304042	11.474380
C	7.583171	5.230572	17.801094
C	5.763443	4.052724	12.098646
C	8.295011	4.471987	18.732903
C	5.378300	9.723311	10.299379
C	5.353470	11.114218	10.426966

C	5.999938	8.909694	11.268290
C	6.069777	7.450879	11.075703
C	5.946106	11.702993	11.535821
C	6.386025	5.438486	10.148316
C	7.717968	3.374261	19.357052
C	4.153351	1.740443	13.573030
C	6.492319	6.792256	9.899466
H	9.318800	4.747364	18.972647
H	8.285294	2.798046	20.082623
H	5.970230	2.145686	19.529527
H	4.893912	6.816639	18.150851
H	3.159596	8.635408	18.178089
H	1.804474	10.045038	16.298375
H	1.919637	12.147264	11.869388
H	1.067913	10.555998	10.195566
H	1.110655	8.133378	10.620250
H	4.871519	11.732755	9.680334
H	5.933292	12.785104	11.635939
H	7.013915	11.419735	13.373163
H	6.819172	7.280643	8.992975
H	6.637618	4.619637	9.485397
H	5.893874	3.200465	11.424195
H	3.121028	-0.131783	13.791273
H	5.106960	-1.376044	14.570083
H	7.270513	-0.215746	14.824033
C	2.919768	2.485670	13.098927
H	3.170316	3.551770	13.097351
C	7.881212	2.384160	14.295406
C	8.629256	1.994254	15.570899
C	8.747880	2.134819	13.055972
H	7.685810	3.462833	14.346662
C	4.227663	3.339153	17.813118
H	3.960113	3.808910	16.858309
C	8.237680	6.423118	17.129787
H	7.577326	6.734071	16.313106
C	1.729298	2.296512	14.041873
H	0.883164	2.911929	13.716816
H	1.385117	1.256921	14.063317
H	1.985009	2.587517	15.065182
C	2.554002	2.087989	11.665373
H	3.376421	2.291252	10.972524
H	2.322244	1.018859	11.602521
H	1.673831	2.641530	11.318903
C	9.593668	6.069783	16.514362
H	10.329898	5.793362	17.276779
H	9.504728	5.234171	15.813538
H	10.000958	6.927382	15.967432
C	8.365554	7.600303	18.101861
H	7.389179	7.904445	18.491676
H	8.997749	7.335728	18.957044
H	8.818028	8.467698	17.607893
C	4.054849	1.828907	17.644764
H	3.036649	1.604261	17.310395
H	4.749893	1.424278	16.903181
H	4.207905	1.292001	18.587485
C	3.267175	3.882483	18.876830
H	2.233610	3.606609	18.641007
H	3.511043	3.472882	19.863688
H	3.316631	4.973344	18.945815
O	2.929473	11.413983	14.260839
H	3.448509	13.245589	14.884406
H	2.001972	13.231020	13.843463
C	2.997432	12.794434	13.999201
O	1.978340	7.024798	12.919536
C	1.550961	6.099430	11.946707
H	1.636560	5.117312	12.412304
H	2.188161	6.132871	11.054416
O	7.211936	8.732250	13.266616
C	7.800395	9.318822	14.404226
O	4.809684	9.069167	9.256803
H	8.252335	8.498182	14.961880
H	3.745009	9.112850	7.560419
C	4.134244	9.829665	8.285230
H	9.535405	2.600465	15.672410
H	8.946069	0.945479	15.555726
H	8.015220	2.154084	16.462087
H	9.708181	2.654350	13.145119
H	8.257902	2.488328	12.143670
H	8.950978	1.064682	12.934420
H	0.505286	6.268622	11.659121
H	3.625696	13.006989	13.124991
H	4.808223	10.527672	7.771236

H	3.298893	10.390487	8.723100
H	7.051185	9.813715	15.034528
H	8.582507	10.038407	14.129806

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Cu	2.653233	1.609565	3.941999
Cu	3.498443	-0.531871	4.853407
O	2.358689	-5.302009	4.333085
N	4.898474	0.378230	5.775812
N	4.372015	1.992038	3.257149
O	4.482603	5.238647	1.155876
O	2.767269	0.881847	1.146166
O	4.475917	-1.621455	2.358167
N	2.105082	-1.455576	3.974120
N	0.916474	1.257424	4.645096
C	3.569320	4.379049	0.641708
C	4.646104	2.668152	2.118360
C	5.106983	0.166222	7.168990
C	5.572125	1.818432	3.915612
C	5.310180	-1.149460	7.647414
C	0.891259	-3.140411	3.056480
H	0.666802	-4.102982	2.619974
C	2.675334	2.135696	0.647151
C	6.030842	2.932949	2.025606
H	6.512670	3.466480	1.218930
C	6.611953	2.413028	3.169092
H	7.659289	2.425618	3.444698
C	1.721076	3.812185	-0.788043
H	0.990621	4.101747	-1.538249
C	2.626862	4.756223	-0.319418
H	2.596626	5.768833	-0.702085
C	5.739762	1.176482	5.161915
C	3.492380	-4.806210	3.779742
C	5.453695	-1.344167	9.019494
H	5.611884	-2.348040	9.400621
C	4.664351	-5.556670	3.646083
H	4.707159	-6.586121	3.979458
C	0.258727	0.152840	4.382825
C	3.612576	3.063732	1.147382
C	5.460460	-2.307453	6.681218
H	4.777504	-2.127626	5.835403
C	2.174140	-2.702539	3.454789
C	0.256571	2.228038	5.452224
C	4.589121	-2.902868	2.776318
C	3.429984	-3.464001	3.352355
C	4.456622	6.577156	0.721776
H	4.647487	6.660799	-0.356045
H	5.254243	7.084367	1.266348
H	3.498941	7.060520	0.954609
C	1.731555	2.506296	-0.315912
H	1.020053	1.785038	-0.697952
C	0.008757	-2.121288	3.369894
H	-1.061784	-2.098049	3.207490
C	5.063002	1.264431	8.059720
C	0.779506	-1.076350	3.922996
C	0.692863	5.332641	3.245193
H	-0.203597	5.955294	3.346114
H	1.061200	5.456647	2.222182
H	1.454211	5.715821	3.931930
C	5.763856	-3.648775	2.638957
H	6.647091	-3.210759	2.191205
C	0.038310	0.508078	7.377763
H	0.616468	-0.108998	6.684411
C	5.084428	-3.666240	7.266710
H	5.800141	-3.996880	8.028236
H	5.085802	-4.418003	6.471463
H	4.087846	-3.648540	7.719045
C	5.223666	1.009264	9.425638
H	5.195699	1.842183	10.123255
C	5.785450	-4.967024	3.074816
H	6.696213	-5.549261	2.966435
C	0.395581	3.857516	3.501715
H	1.310692	3.300953	3.241680
C	5.581969	-1.009776	1.724090
H	6.441094	-0.937758	2.401091
H	5.247444	-0.007406	1.459665
H	5.873493	-1.559219	0.819871
C	1.898996	-0.116952	0.647567
H	0.849958	0.123557	0.855881
H	2.170777	-1.029413	1.176848
H	2.034508	-0.255123	-0.432738
C	5.410682	-0.276083	9.908504

H	5.528174	-0.448221	10.974728
C	0.054501	3.531677	4.942067
C	-0.711212	3.359898	2.565129
H	-0.883627	2.286558	2.687891
H	-0.438445	3.542870	1.520746
H	-1.653054	3.879444	2.775907
C	-0.538735	4.484478	5.767534
H	-0.703293	5.488316	5.389026
C	2.375028	-6.623832	4.816134
H	2.573052	-7.348735	4.015869
H	1.380087	-6.805713	5.224859
H	3.119705	-6.756469	5.611742
C	4.860051	2.707152	7.614692
H	4.627257	2.714697	6.546077
C	-0.142217	1.891595	6.767136
C	6.881918	-2.341296	6.108239
H	7.135745	-1.396589	5.618242
H	6.977566	-3.143529	5.369425
H	7.612079	-2.513900	6.907300
C	0.825268	0.538495	8.691148
H	0.323719	1.139281	9.457426
H	1.831066	0.941395	8.548068
H	0.930102	-0.477514	9.086489
C	-0.935169	4.170785	7.062882
H	-1.398899	4.927201	7.689851
C	-0.740889	2.886915	7.546772
H	-1.056319	2.644549	8.558400
C	-1.317132	-0.177347	7.586812
H	-1.936202	0.383446	8.295946
H	-1.179283	-1.187221	7.987434
H	-1.881008	-0.258280	6.652179
C	6.141365	3.525114	7.815939
H	6.003340	4.550460	7.456737
H	6.990996	3.090402	7.280319
H	6.412975	3.574534	8.876344
C	3.684093	3.387890	8.321378
H	3.829740	3.439137	9.405811
H	2.741779	2.868545	8.129850
H	3.575414	4.414869	7.956476
H	-0.822024	0.162668	4.557776
H	6.680906	1.399113	5.674941

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Cu	11.689235	5.846173	5.167638
Cu	11.676430	3.276293	5.394259
N	10.353313	5.906436	6.570004
N	13.012720	5.626682	3.769623
C	10.081467	6.938099	7.403696
N	13.538993	3.091487	5.487154
N	9.812203	3.102273	5.336184
C	14.331703	10.516189	2.018765
H	14.831200	11.116213	2.775043
C	13.274515	6.989405	7.127314
H	13.011099	6.051581	7.607394
C	8.139036	5.844119	7.160121
H	7.114523	5.501620	7.241584
C	13.052135	8.957460	0.109724
H	12.566621	8.357806	-0.652113
C	10.685412	6.803656	-0.011182
H	10.099070	7.655372	0.321052
C	13.287590	6.480039	2.753317
C	15.228064	5.449014	3.207297
H	16.251953	5.095449	3.194623
C	10.614615	8.989519	2.927593
H	11.270738	9.800647	2.634816
C	10.996095	7.665309	2.696409
C	14.016984	1.947314	6.201772
C	14.650064	6.402576	2.389718
H	15.122180	6.971962	1.601757
C	12.276834	7.286254	1.928702
C	9.327538	1.815496	4.938247
C	11.527360	7.333070	9.420864
C	9.077475	11.039198	7.204046
H	8.602663	11.462828	6.322816
C	10.291103	9.923637	9.438420
H	10.747688	9.498864	10.325353
C	8.720398	6.934287	7.779983
H	8.252317	7.645613	8.445583
C	9.378467	9.293764	3.497247
H	9.105560	10.335120	3.647850
C	12.640778	7.893418	10.064958
H	13.192497	8.691675	9.576423
C	13.670434	9.353183	2.392410

H	13.664619	9.049812	3.435487
C	12.159717	4.626036	-0.880648
H	12.746259	3.772224	-1.209139
C	9.162337	5.205675	6.432074
C	9.740107	9.822362	7.107191
H	9.767333	9.301067	6.154571
C	10.095062	6.652199	3.061925
H	10.337451	5.618384	2.833101
C	14.202007	4.962171	4.039109
C	10.848244	6.301441	10.071213
H	9.982133	5.847305	9.601519
C	9.618681	11.142675	9.539432
H	9.569348	11.644790	10.501772
C	11.020320	5.001597	-1.582903
H	10.707184	4.447574	-2.463309
C	12.384028	8.071067	7.218281
C	14.901098	8.349953	5.973757
H	15.871400	8.458303	5.498303
C	14.412254	3.832987	4.860174
H	15.459926	3.521522	4.926660
C	12.562222	5.336036	0.250540
H	13.457086	5.026542	0.779721
C	11.093438	7.895394	8.040970
C	12.366465	6.412863	11.951085
H	12.689555	6.056179	12.924998
C	10.283901	6.098853	-1.141004
H	9.391076	6.409939	-1.676560
C	14.027848	9.428596	6.053420
H	14.316531	10.396343	5.651159
C	8.947230	3.945104	5.835779
H	7.901399	3.621133	5.852920
C	11.265563	5.844505	11.321746
H	10.720884	5.035708	11.801265
C	13.722103	10.122172	-0.268522
H	13.742537	10.407708	-1.316717
C	14.544724	2.095402	7.498195
C	11.834095	6.437247	0.705876
C	10.368417	9.246956	8.220994
C	9.524274	2.565622	2.512945
H	10.214237	3.281742	2.976978
C	8.859716	6.956269	3.627504
H	8.181547	6.153435	3.895430
C	8.494839	8.280383	3.850878
H	7.530422	8.516386	4.290966
C	9.191458	1.526007	3.565539
C	9.039832	0.848629	5.923145
C	13.903800	0.676883	5.595797
C	13.053273	7.445162	11.314351
H	13.917030	7.902234	11.789526
C	9.012843	11.708745	8.425289
H	8.489688	12.657479	8.505423
C	14.518444	7.127911	6.519260
H	15.191944	6.278398	6.474584
C	14.361682	10.908294	0.681096
H	14.883130	11.814207	0.385094
C	13.011428	8.556371	1.445080
C	14.359608	-0.434209	6.305871
H	14.290289	-1.419293	5.854164
C	14.989489	0.950658	8.164997
H	15.405444	1.049177	9.164477
C	9.262524	1.100539	7.404607
H	9.703956	2.095527	7.515971
C	8.706762	0.269763	3.199944
H	8.579164	0.035025	2.147191
C	14.903940	-0.303522	7.578649
H	15.256710	-1.181465	8.112539
C	8.558889	-0.394814	5.503414
H	8.323035	-1.149928	6.249178
C	8.268072	3.337568	2.094440
H	7.541095	2.664937	1.625125
H	8.517968	4.125733	1.376038
H	7.778654	3.802837	2.956148
C	13.345004	0.524396	4.192720
H	12.692050	1.388262	4.007161
C	7.943045	1.091290	8.181987
H	7.246900	1.844143	7.798748
H	8.119501	1.300900	9.242364
H	7.447588	0.116607	8.112271
C	14.624249	3.444014	8.187044
H	14.155960	4.176148	7.523321
C	10.257506	0.097432	7.997403
H	9.873627	-0.927519	7.949224

H	10.448742	0.329368	9.050707
H	11.214716	0.122801	7.466786
C	10.231411	1.980363	1.290895
H	11.112873	1.399622	1.581590
H	10.557947	2.786416	0.626884
H	9.572714	1.325561	0.709608
C	12.491506	-0.730723	4.012552
H	12.023216	-0.724065	3.023208
H	11.692076	-0.783962	4.757598
H	13.088095	-1.647210	4.080667
C	16.075583	3.879195	8.409682
H	16.600440	3.184672	9.075111
H	16.112358	4.873144	8.868324
H	16.632644	3.915684	7.467510
C	14.469668	0.574712	3.152661
H	15.036488	1.508512	3.216979
H	14.061538	0.497002	2.138881
H	15.170901	-0.254342	3.300998
C	13.838605	3.455349	9.501100
H	12.796900	3.161196	9.339856
H	13.840266	4.456960	9.943416
H	14.271993	2.766096	10.234358
C	12.782649	9.291126	6.667559
H	12.134794	10.156724	6.741526
C	8.382168	-0.683805	4.157552
H	8.001116	-1.654583	3.853116

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Cu	3.083259	6.260714	0.139331
Cu	3.946168	4.053727	-1.128726
N	3.711178	7.340545	-1.280943
N	4.562585	3.341869	0.513855
N	2.269973	5.277042	1.545329
N	3.241781	4.596028	-2.808589
C	1.352398	6.205745	3.644888
C	3.422703	7.065118	-2.606066
C	3.783288	3.313302	1.657061
C	4.139835	8.627136	-1.242551
C	2.699009	4.140096	2.030758
H	2.169564	3.761285	2.908525
C	-0.221534	5.868035	0.132606
H	0.623391	5.256045	-0.203974
C	-1.072086	6.714610	2.336808
H	-2.011400	6.922888	1.832705
C	5.591525	2.483505	0.731393
C	2.969417	3.592941	-3.798411
C	4.326519	2.400680	2.580510
H	3.932108	2.193356	3.567536
C	1.142755	2.624335	-2.276290
H	1.321875	3.571754	-1.754990
C	-0.221391	7.163441	-0.686714
H	-1.057783	7.808513	-0.395656
H	-0.321092	6.940109	-1.754569
H	0.700289	7.735885	-0.543987
C	-0.020306	6.157908	1.608529
C	3.125667	5.830955	-3.227458
H	2.785416	5.957684	-4.258189
C	3.650311	8.212008	-3.390270
H	3.528009	8.274596	-4.464487
C	-0.948588	6.995704	3.690418
H	-1.785198	7.413128	4.243646
C	0.258280	6.746895	4.327018
H	0.362692	6.981836	5.382908
C	3.721522	3.557108	-4.998674
C	2.518212	4.922629	5.487556
H	1.763427	5.192881	6.234407
H	3.469725	4.781003	6.010842
H	2.221051	3.959768	5.060595
C	4.133078	9.187528	-2.535048
H	4.445251	10.189802	-2.790631
C	2.649521	6.018531	4.422503
H	3.437629	5.720954	3.724187
C	5.485125	1.901609	2.009775
H	6.180329	1.197245	2.443058
C	-0.362058	2.521195	-2.536157
H	-0.715962	3.328878	-3.184789
H	-0.910375	2.573297	-1.591175
H	-0.629113	1.570722	-3.010056
C	3.111485	7.321719	5.083726
H	3.224003	8.128841	4.355778
H	4.083952	7.171682	5.563873
H	2.410043	7.656069	5.855634

C	1.948221	2.646973	-3.562335
C	1.674722	1.698705	-4.548431
H	0.888134	0.970013	-4.376168
C	3.389984	2.595168	-5.957749
H	3.948348	2.569104	-6.889802
C	-1.499884	5.067048	-0.125445
H	-1.509119	4.130693	0.441586
H	-1.585484	4.826229	-1.189042
H	-2.395959	5.632881	0.150394
C	4.882167	4.494461	-5.308618
H	5.104971	5.084289	-4.414518
C	2.374720	1.674313	-5.746759
H	2.133827	0.938400	-6.508798
C	1.607724	1.486147	-1.361070
H	1.433143	0.513070	-1.833068
H	1.059520	1.508385	-0.412794
H	2.676823	1.553282	-1.136924
C	4.536787	5.463517	-6.446194
H	5.367625	6.153307	-6.628512
H	3.644632	6.059281	-6.230446
H	4.344904	4.918310	-7.376985
C	6.160625	3.727266	-5.663310
H	6.048698	3.158631	-6.592675
H	6.449523	3.030637	-4.872665
H	6.989212	4.429054	-5.803304
C	1.193763	5.883889	2.274583
C	6.582080	2.025573	-0.336921
C	4.367538	9.432058	0.034998
C	5.799236	0.996997	-1.181569
C	5.453931	1.216638	-2.515050
C	5.354971	-0.188348	-0.576947
C	4.727260	0.270027	-3.238261
C	4.636246	-1.135927	-1.294742
C	4.324814	-0.914571	-2.635647
H	5.753110	2.135750	-3.005348
H	5.581143	-0.368798	0.469437
H	4.470514	0.477870	-4.272376
H	4.316092	-2.050277	-0.802567
H	3.762953	-1.654554	-3.198657
C	7.193875	3.151060	-1.190628
C	8.067519	2.806302	-2.232433
C	7.027616	4.506423	-0.901777
C	8.725997	3.778510	-2.973562
C	7.692404	5.486438	-1.642545
C	8.538135	5.129518	-2.684366
H	8.246976	1.757625	-2.451110
H	6.382462	4.799198	-0.081479
H	9.397437	3.479206	-3.773640
H	7.552125	6.533357	-1.388583
H	9.057854	5.892207	-3.257173
C	7.815160	1.386368	0.345311
C	8.360411	0.168434	-0.064485
C	8.489113	2.107469	1.339690
C	9.528536	-0.325409	0.516183
C	9.648700	1.614576	1.924302
C	10.174978	0.390165	1.516125
H	7.872173	-0.408170	-0.843258
H	8.094722	3.068456	1.657537
H	9.929770	-1.277455	0.179551
H	10.146950	2.192242	2.698004
H	11.082759	0.003733	1.970590
C	5.143565	8.701070	1.145438
C	5.299055	9.335673	2.386338
C	5.812842	7.492735	0.943373
C	6.069388	8.770911	3.394268
C	6.591348	6.924386	1.954143
C	6.718360	7.554767	3.184717
H	4.820017	10.295511	2.556895
H	5.736048	6.995198	-0.016618
H	6.170724	9.287834	4.344561
H	7.107360	5.987120	1.766074
H	7.326851	7.113414	3.968803
C	2.949208	9.845779	0.481753
C	2.209624	10.742163	-0.303239
C	2.326082	9.292635	1.600808
C	0.915528	11.105930	0.048248
C	1.025102	9.650934	1.954801
C	0.317899	10.566736	1.186577
H	2.656540	11.159759	-1.200142
H	2.857298	8.570907	2.211102
H	0.370840	11.811686	-0.573020
H	0.570329	9.195862	2.829264

H	-0.693831	10.850562	1.462415
C	5.260928	10.654875	-0.277877
C	6.463521	10.456631	-0.968128
C	4.983321	11.937154	0.199779
C	7.341810	11.507578	-1.199960
C	5.866032	12.992861	-0.026713
C	7.045415	12.786222	-0.731568
H	6.709130	9.462654	-1.330793
H	4.067070	12.122036	0.751035
H	8.264167	11.325915	-1.744752
H	5.622901	13.981532	0.352889
H	7.730775	13.609644	-0.910881

1-H-*cisoid*

Cu	5.009198	7.020756	13.743321
Cu	5.553339	4.852434	14.942086
N	3.710814	7.490672	14.999708
N	5.379882	5.556577	16.679619
C	3.719276	7.330171	16.372127
N	5.806450	3.834909	13.378165
C	6.158194	4.846643	17.650725
C	6.277400	0.232480	14.182050
N	6.272241	6.697242	12.407706
C	2.706911	8.347852	14.727111
C	2.699514	8.119323	16.942621
C	4.557397	6.473411	17.116473
C	6.576914	1.586380	14.006279
C	3.989524	0.604386	13.544296
C	6.401593	3.065493	19.247239
C	5.545930	2.438812	13.567646
C	5.000617	-0.259799	13.948429
C	2.047130	8.756238	15.894037
C	5.606607	3.732038	18.310736
C	6.603129	5.511344	11.780128
C	7.485729	5.260362	17.882911
C	6.306351	4.207186	12.229480
C	8.237210	4.559901	18.826996
C	6.812519	7.681339	11.661682
C	7.354146	5.788976	10.619522
C	7.701506	3.474848	19.511189
C	4.235984	1.964243	13.353016
C	7.498483	7.169330	10.552140
H	9.258556	4.868370	19.030471
H	8.301270	2.944634	20.245590
H	5.991278	2.208969	19.775814
H	4.488842	6.596859	18.201792
H	2.468640	8.178687	17.998991
H	1.205997	9.433422	15.950905
H	8.024015	7.744564	9.802313
H	7.756407	5.047816	9.940082
H	6.542461	3.413122	11.514135
H	2.990104	0.214875	13.373941
H	4.790224	-1.316478	14.087619
H	7.061574	-0.445246	14.509370
C	3.133500	2.901564	12.895528
H	3.430552	3.917301	13.184539
C	7.978947	2.094888	14.290689
C	8.433605	1.747076	15.710844
C	8.978355	1.577951	13.251142
H	7.958002	3.187291	14.214428
C	4.196758	3.242753	18.031853
H	3.806060	3.817457	17.185423
C	8.067368	6.455078	17.149631
H	7.483883	6.586126	16.229804
C	1.787412	2.613994	13.561221
H	1.066647	3.395080	13.299160
H	1.361519	1.659262	13.233949
H	1.877914	2.587534	14.651674
C	3.001244	2.880070	11.368581
H	3.937748	3.166312	10.880099
H	2.733569	1.877325	11.016667
H	2.222369	3.575486	11.037726
C	9.526033	6.254152	16.737981
H	10.198510	6.224331	17.602257
H	9.658206	5.324763	16.175155
H	9.852872	7.084356	16.103780
C	7.906646	7.733690	17.979440
H	6.855867	7.933453	18.210961
H	8.448128	7.650676	18.928670
H	8.302415	8.599169	17.437131
C	4.176598	1.766302	17.625798
H	3.158258	1.459746	17.363897

H	4.818388	1.579905	16.759276
H	4.514478	1.117895	18.441652
C	3.274578	3.496723	19.228503
H	2.254192	3.166644	19.006248
H	3.618714	2.950428	20.113792
H	3.238001	4.559268	19.489314
H	2.505566	8.653708	13.707510
H	6.674594	8.720015	11.937035
H	9.415518	2.188338	15.912511
H	8.525456	0.664598	15.851949
H	7.733150	2.126387	16.461098
H	9.980873	1.970933	13.451290
H	8.693414	1.875833	12.237057
H	9.036745	0.483894	13.270874

1-H-*transoid*

Cu	-1.098744	2.156914	7.418025
Cu	1.391889	1.820461	6.919825
N	-0.887301	3.943744	7.920551
N	1.379716	0.016388	7.403962
N	-1.635027	0.410519	6.970175
N	1.728144	3.583012	6.355113
C	-3.949247	0.031193	7.709699
C	-0.012391	4.909220	7.463039
C	0.390261	-0.939124	7.280899
C	-1.815035	4.592767	8.652774
C	-0.979226	-0.718627	7.027003
H	-1.560990	-1.631561	6.866356
C	-2.504880	0.956137	4.255840
H	-1.500418	0.991123	4.690857
C	-4.843160	0.531057	5.100303
H	-5.197165	0.726520	4.091168
C	2.512714	-0.650655	7.702011
C	2.902591	3.671553	5.536866
C	0.943549	-2.216959	7.504235
H	0.394968	-3.150366	7.480665
C	1.427385	3.222803	3.502945
H	0.723400	2.977430	4.306193
C	-2.803537	2.341260	3.675597
H	-3.794696	2.378108	3.210585
H	-2.067829	2.601157	2.906451
H	-2.769976	3.111777	4.452533
C	-3.475163	0.602005	5.367581
C	1.153252	4.706092	6.695362
H	1.635597	5.627253	6.354004
C	-0.428309	6.174801	7.925357
H	0.077110	7.111779	7.726868
C	-5.756029	0.210634	6.096860
H	-6.816496	0.154104	5.868242
C	-5.307064	-0.032687	7.388041
H	-6.024942	-0.276495	8.166959
C	4.155482	3.907021	6.135717
C	-3.698798	-1.684132	9.537947
H	-4.756017	-1.967481	9.488445
H	-3.352272	-1.855706	10.562562
H	-3.144801	-2.357280	8.876139
C	-1.568695	5.971401	8.692329
H	-2.157687	6.712948	9.214284
C	-3.502459	-0.218182	9.139514
H	-2.431572	0.001253	9.199625
C	2.291662	-2.031740	7.783849
H	3.030785	-2.786529	8.014568
C	0.908554	4.484988	2.806652
H	0.824375	5.320814	3.508321
H	-0.080679	4.309671	2.369917
H	1.583727	4.793858	2.000591
C	-4.210810	0.715160	10.125515
H	-4.069197	1.764909	9.849152
H	-3.814059	0.572536	11.136128
H	-5.288560	0.524018	10.164175
C	2.777048	3.480635	4.146608
C	3.927669	3.568099	3.361929
H	3.848639	3.438363	2.285910
C	5.276375	3.984927	5.305544
H	6.250682	4.176588	5.747843
C	-2.493872	-0.115051	3.161534
H	-2.240018	-1.098031	3.570345
H	-1.757453	0.131302	2.388906
H	-3.472045	-0.199373	2.675037
C	4.316014	4.075751	7.636102
H	3.350193	3.857003	8.103224
C	5.169278	3.822657	3.930956

H	6.053185	3.891157	3.303177
C	1.456808	2.032520	2.542383
H	2.095083	2.221911	1.672753
H	0.449153	1.826049	2.165582
H	1.825554	1.130186	3.039844
C	4.690153	5.517167	7.995519
H	4.779266	5.634914	9.080703
H	3.937688	6.227265	7.638362
H	5.649437	5.797438	7.546369
C	5.333946	3.087900	8.212947
H	6.343176	3.274558	7.830491
H	5.070385	2.055109	7.963399
H	5.373171	3.175210	9.303758
C	-3.037217	0.333858	6.678859
H	-2.632900	4.050606	9.112008
H	3.447311	-0.118495	7.8326

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