"Click-Triazole: coordination of 2-(1,2,3-triazol-4-yl)-pyridine to cations of traditional tetrahedral geometry"

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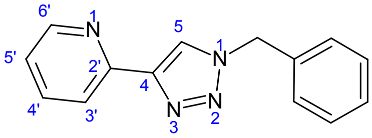
ELECTRONIC SUPPORTING INFORMATION

A) Synthesis and characterizations:

General comments: All commercially available chemicals (copper(II) sulfate, sodium ascorbate, sodium azide, 2-ethynylpyridine, benzylazide, methyl iodide) were used as received. TLC was performed on silica coated plates, with a pore diameter of 60 Å. Anhydrous dichloromethane and tetrahydrofuran were dried by passing through an activated alumina column according to the manufacturer's instructions (Innovative Technology). Chemical shifts (δ) are reported in ppm and are indirectly referenced to TMS *via* the residual solvent signal ($CDCl_3$: δ ^1H = 7.26 ^{13}C = 77.16, CD_3CN: δ ^1H = 1.94, CD_3OD: δ ^1H = 3.31). In the ^1H NMR spectra multiplicities are denoted as br (broad), s (singlet), d (doublet), t (triplet) and m (multiplet). Chemical shifts of heterocyclic ligands appeared to be fairly sensitive to solvent. In particular, it was sometimes noticed that ^1H chemical shift differed between different batches of $CDCl_3$, possibly due to various amounts of trace HCl / DCl in such solvent. As a result, most chemical shifts are reported here in $CDCl_3$ which has been freshly filtered through a plug of basic alumina (this method lead to reproducible chemical shifts). Filtered $CDCl_3$ is denoted here with an asterisk ($CDCl_3$*). ^1H and ^{13}C NMR were recorded at 300 MHz and 125 MHz, respectively. 2D heteronuclear [^1H-^{13}C] NMR data (HSQC, HMBC) were recorded on Bruker Avance 500 spectrometer (^1H, 500 MHz; ^{13}C, 125 MHz). Melting points were recorded on a Mel-TempII apparatus and were uncorrected. Microwave reactions were performed on a Biotage Iniator 2.5 using 0.5-2 mL microwave vials.

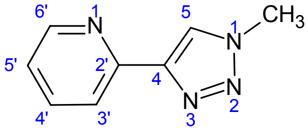
Caution: organic azides are potentially explosive. Handle with care.

1-Benzyl-4-(2-pyridyl)-1,2,3-triazole (L1): Benzylazide (68 mg, 0.48 mmol, 1.0 eq.) and 2-ethynylpyridine (50 mg, 0.48 mmol, 1.0 eq.) were dissolved in *t*-BuOH (1 mL) into a microwave vial. A 10 mL solution of $CuSO_4$ (7.6 mg, 10 mol%) was prepared and 1 mL of this solution was used to dissolve sodium ascorbate (9.5 mg, 10 mol%). The latter solution was transferred to the starting microwave vial. The reaction mixture was stirred at 125 °C using 100 W irradiation power for 30 min. Upon cooling to room temperature, water (10 mL) was added to the homogeneous orange solution and the precipitate was filtered and rinsed with water (3 × 10 mL). The crude material obtained was stirred in water at room temperature and the aqueous solution filtered to give the expected compound as a white solid (90 mg, 80%). ^1H NMR ($CDCl_3$*, 300 MHz, 25 °C): 8.55 (d, ^3J = 4.2 Hz, 1 H, H6'), 8.19 (d, ^3J = 8.1 Hz, 1 H, H3'), 8.06 (s, 1 H, H5), 7.78 (dt, ^3J = 8.0 Hz, ^4J =1.5 Hz, 1 H, H4'), 7.37 (m, 5 H, Ph), 7.22 (m, 1 H, H5'),



5.60 (s, 2 H, CH_2). Mp: 110-112 °C; lit.: 110-112°C from Z. Gonda, Z. Novák, *Dalton Trans*. 2010, **39**, 726-729.
CAS n°: 862675-34-1

1-Methyl-4-(2-pyridyl)-1,2,3-triazole (L2): Sodium azide (138 mg, 2.13 mmol, 2.2 eq), copper(II) sulfate (15 mg, 10 mol%) and sodium ascorbate (95 mg, 0.48 mmol, 0.5 eq) were dissolved in water (0.5 mL) in a microwave vial. To this mixture were added iodomethane (152 mg, 1.07 mmol, 1.1 eq) dissolved in DMF (1 mL) and 2-ethynylpyridine (100 mg, 0.97 mmol, 1.0 eq) in DMF (1 mL). The reaction mixture was stirred at room temperature for 3 days during which a white precipitate appeared. The reaction mixture was then heated at 150 °C using microwave irradiation of 130 W for 10 min., resulting in the disappearance of the observed precipitate. The reaction mixture was diluted in water (10 mL), poured into a solution of EDTA (10 mL) and the remaining solution was extracted with Et_2O (5 ×10 mL). The combined organic layers were washed with brine (50 mL), dried over Na_2SO_4 and concentrated to give **L2** as a light beige solid (102 mg, 65%). ^{1}H NMR ($CDCl_3$*, 300 MHz, 25 °C): 8.58 (br, 1 H, H6'), 8.17 (d, ^3J = 8.1 Hz, 1 H, H5'), 8.12 (s, 1 H, H5), 7.78 (dt, ^3J = 7.8 Hz, ^4J = 1.5 Hz, 1 H, H4'), 7.23 (m, 1 H, H3'), 4.17 (s, 3 H, -CH_3). ^{13}C NMR ($CDCl_3$*, 125 MHz, 25°C): 150.3 (C2'), 149.4 (C6'), 148.7 (C4), 137.0 (C4'), 123.1 (C5), 122.9 (C3'), 120.3 (C5'), 36.9 (CH_3).



Mp: 103-104 °C. Rf (1.0:0.2 CH_2Cl_2/Et_2O) = 0.23. HR-ESI-MS: calc. for $C_8H_8N_4.H^+$ 161.0827, found 161.0825; calc. for $C_8H_8N_4.Na^+$: 183.0647, found: 183.0572.

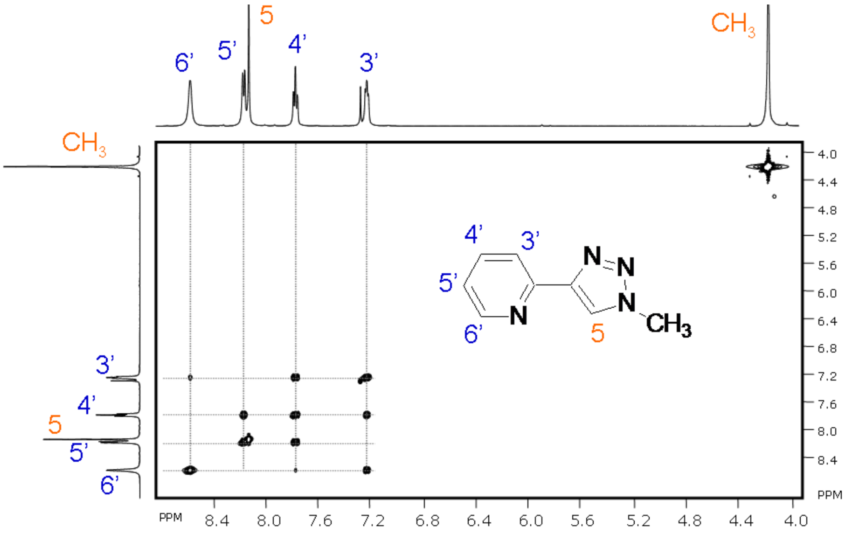


Figure S1: COSY NMR spectrum of **L2** (300 MHz, $CDCl_3$*, 25 °C).

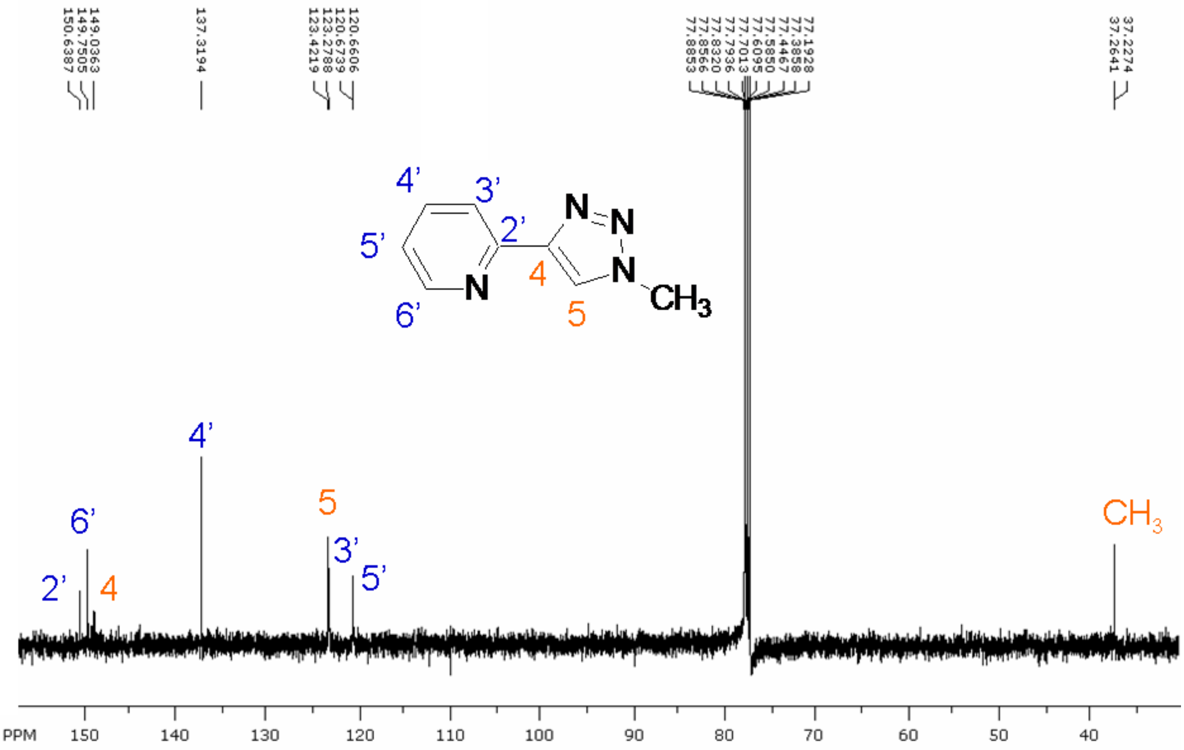


Figure S2: ^{13}C NMR spectrum of **L2** (125 MHz, $CDCl_3$*, 25 °C).

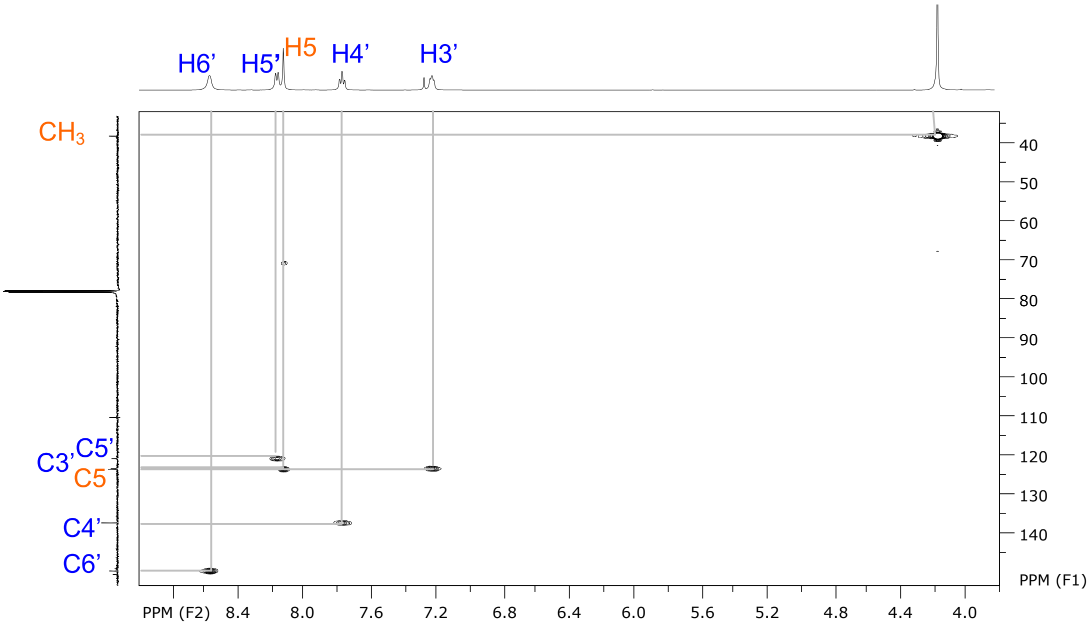


Figure S3: HSQC NMR spectrum of **L2** (^{1}H, 500 MHz; ^{13}C, 125 MHz, $CDCl_3$*, 25 °C).

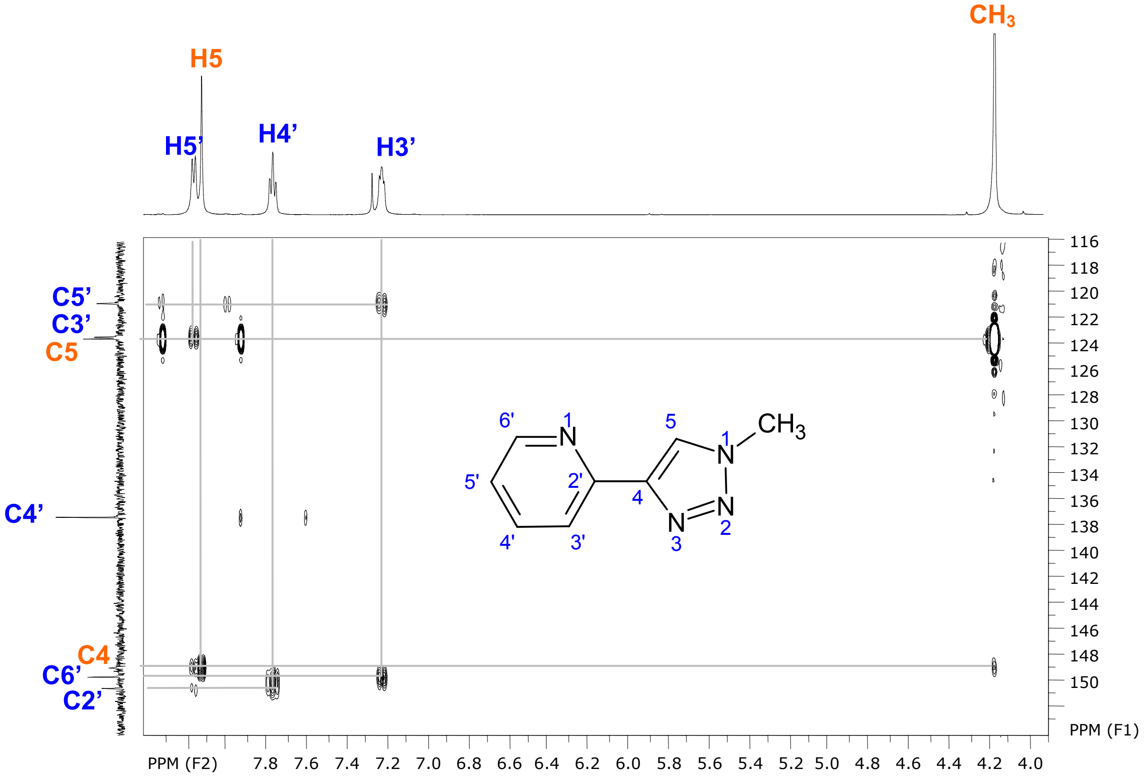


Figure S4: HMBC NMR spectrum of **L2** (^{1}H, 500 MHz; ^{13}C, 125 MHz, CDCl$_3$*, 25 °C).

B) ^{1}H NMR and mass spectrometry analysis of complexation

a) Coordination of Cu(I) to **L1**

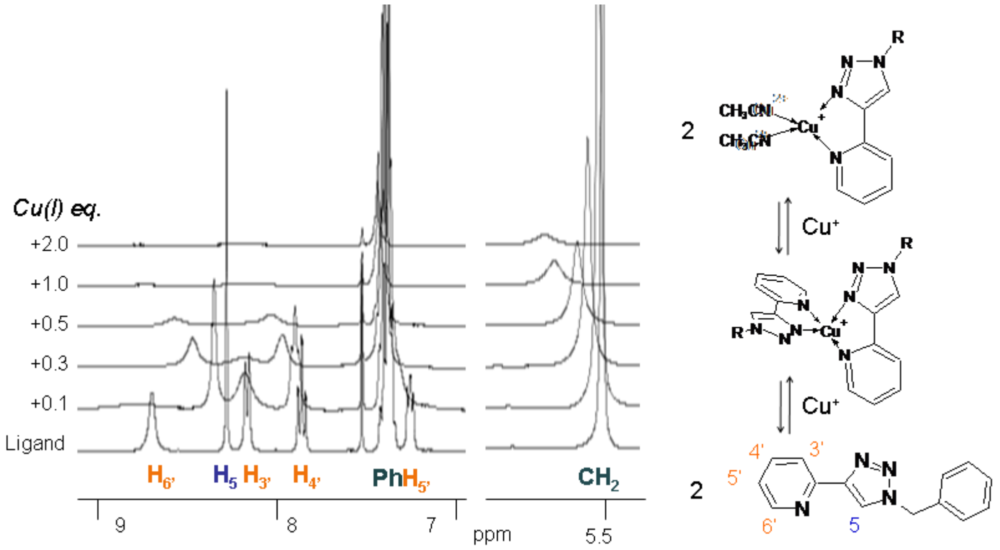


Figure S5: Excerpt from the ^{1}H NMR titration of **L1**with Cu(CH$_3$CN)$_4$BF$_4$ in degassed 1:1 CDCl$_3$/CD$_3$CN ([**L1**]$_0$ = 35 mM).

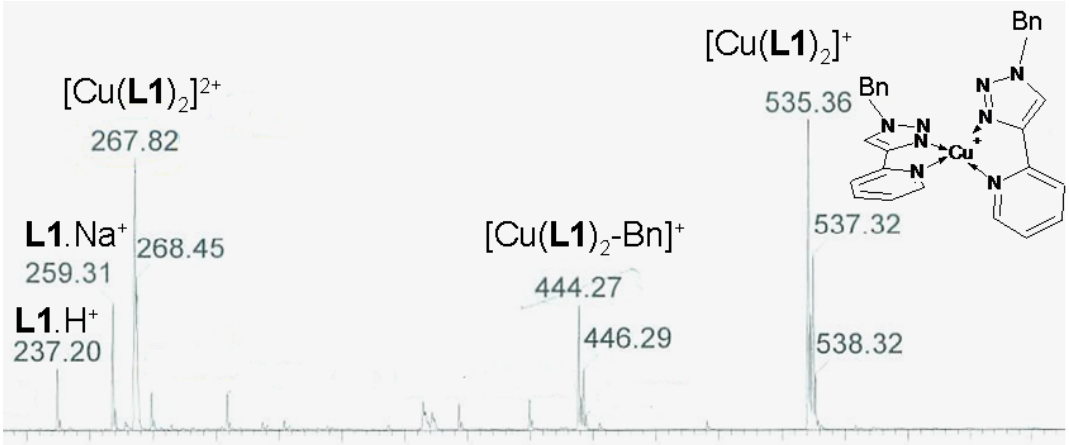


Figure S6: ESI-MS analysis of a 1+1 mixture between **L1** and $Cu(CH_3CN)_4.BF_4$. The mixture was prepared in 1:1 $CHCl_3/CH_3CN$; the sample was diluted with CH_3CN in order to favour vaporization.

b) Coordination of Ag(I) to **L1**

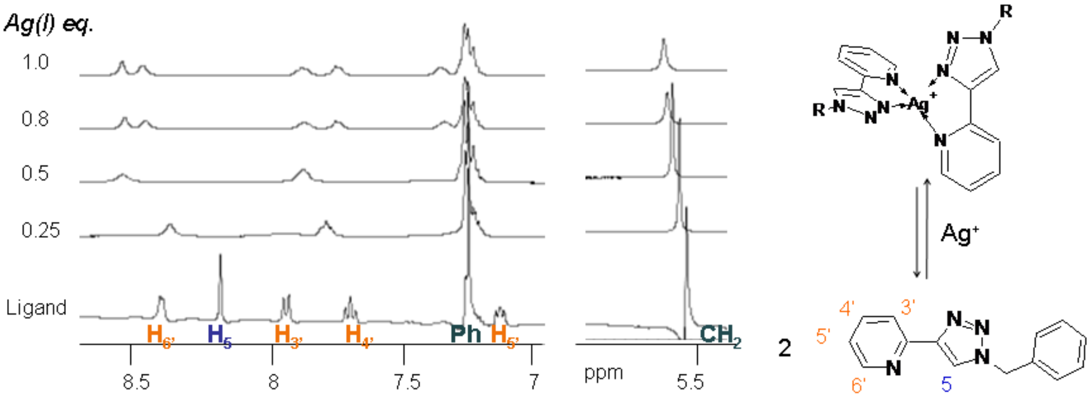


Figure S7: Excerpt from the ^{1}H NMR titration of **L1** with Ag(OTf) in 1:1 $CDCl_3/CD_3NO_2$ ([**L1**]$_0$ = 36 mM).

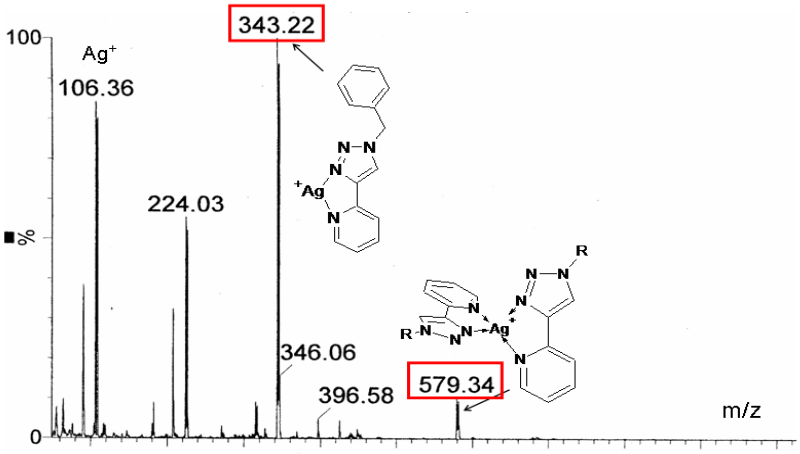


Figure S8: ESI-MS analysis of a 1+1 mixture between **L1** and Ag(OTf). The mixture was prepared in 1:1 $CHCl_3/CH_3NO_2$, CH_3CN was added to favour vaporization (competition with ligand **L1**). M(**L1**) = 236 g/mol.

C) UV-vis analysis

a) **General methods**: UV titrations were performed on a Cary Bio 300 spectrophotometer with a thermostat controlling the temperature at 25 °C, unless otherwise specified. For Cu(I) titrations, spectrograde chloroform was filtered onto basic alumina and degassed with argon. Acetonitrile was degassed with argon. Mixtures were then prepared and quickly degassed before use. The spectral data obtained in the titrations were processed with Microsoft Excel and fitted with Hyperquad 2006 (http://www.hyperquad.co.uk/).

b) Cu(I) titration of 6,6'-dimethyl-2,2'-bipyridine in $CHCl_3/CH_3CN$

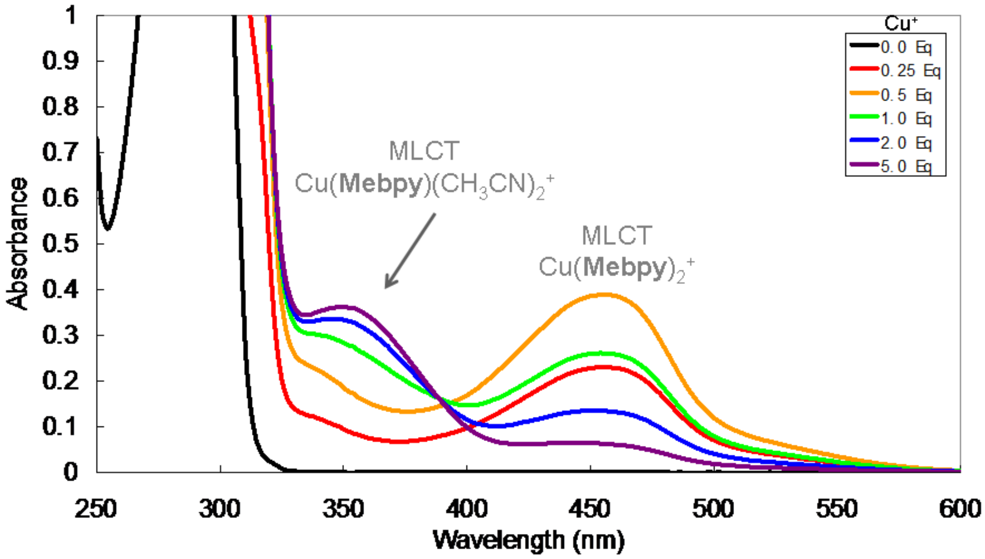
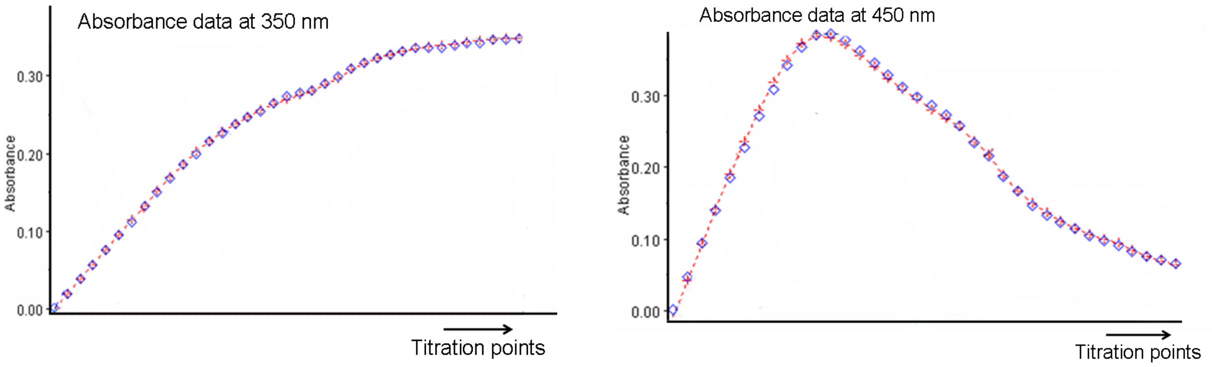


Figure S9: UV-vis titration of 6,6'-dimethyl-2,2'-bipyridine (~1.5 10^{-4} M) with $Cu(CH_3CN)_4.BF_4$.


Absorbance data at 350 nm

Absorbance data at 450 nm

Figure S10: UV-vis analysis of the above titration at 350 nm (left) and 450 nm (right); blue diamonds: experimental points; dashed red signals: calculated (fitted) points.

c) Cu(I) titration of 2,2'-bipyridine in $CHCl_3/CH_3CN$

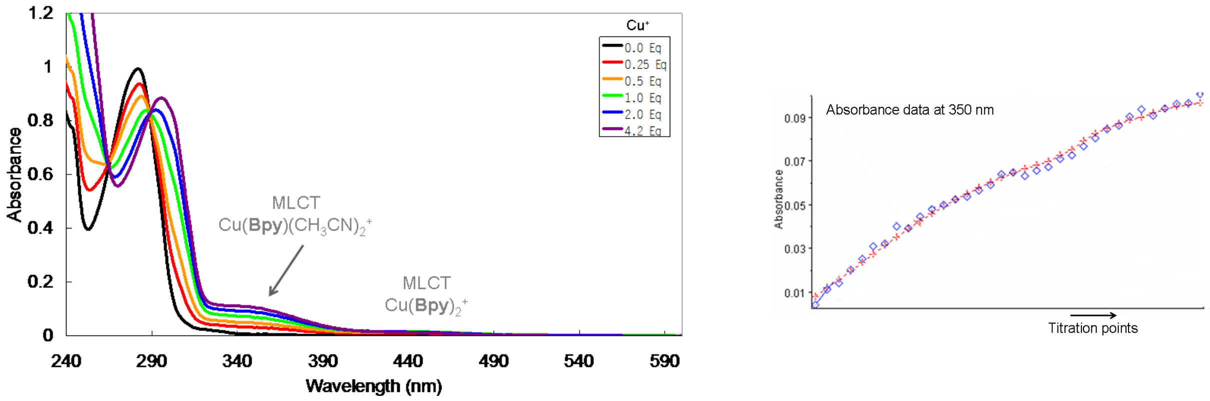


Figure S11: left) UV-vis titration of 2,2'-bipyridine (~6.7 10^{-4} M) with $Cu(CH_3CN)_4.BF_4$ (the MLCT for Cu(**Bpy**)$_2^+$ is less intense than that for Cu(**Mebpy**)$_2^+$, as reported in S. Kitagawa, M. Munakata, and A. Higashie, *Inorg. Chim. Acta* 1984, **84**, 79-84), and right) fitting analysis of the above titration at 350 nm (see Fig. S10 for colour coding).

d) Cu(I) titration of L1 in $CHCl_3/CH_3CN$

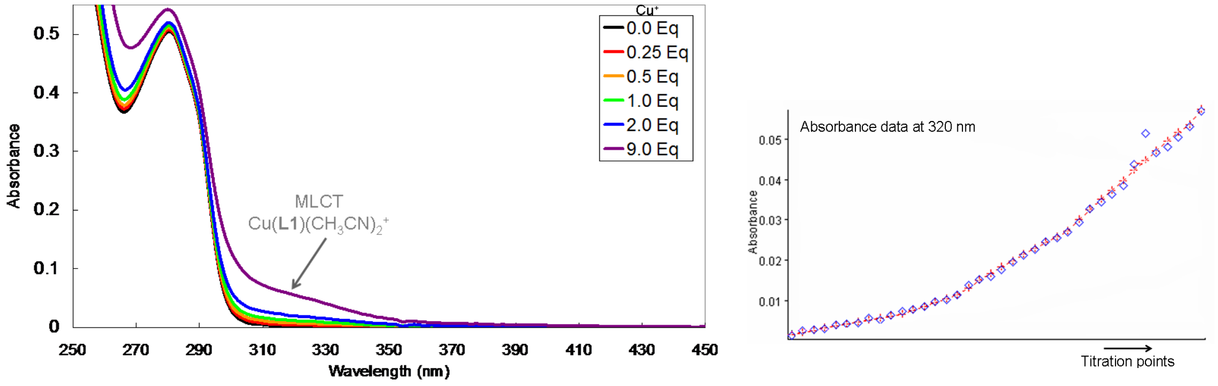


Figure S12: UV-vis titration of **L1** (~1.5 10^{-4} M) with $Cu(CH_3CN)_4.BF_4$ (left) and fitting analysis at 320 nm; blue diamonds: experimental points; dashed red signals: calculated (fitted) points.

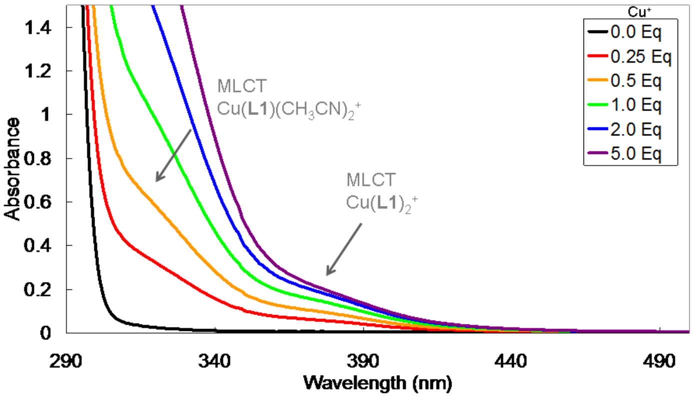


Figure S13: UV-vis titration of **L1** (~1.0 10^{-3} M) with $Cu(CH_3CN)_4.BF_4$.

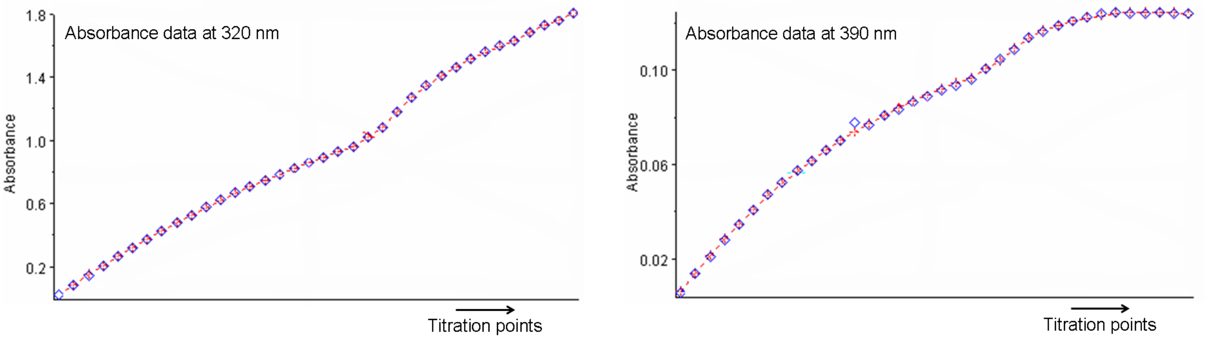
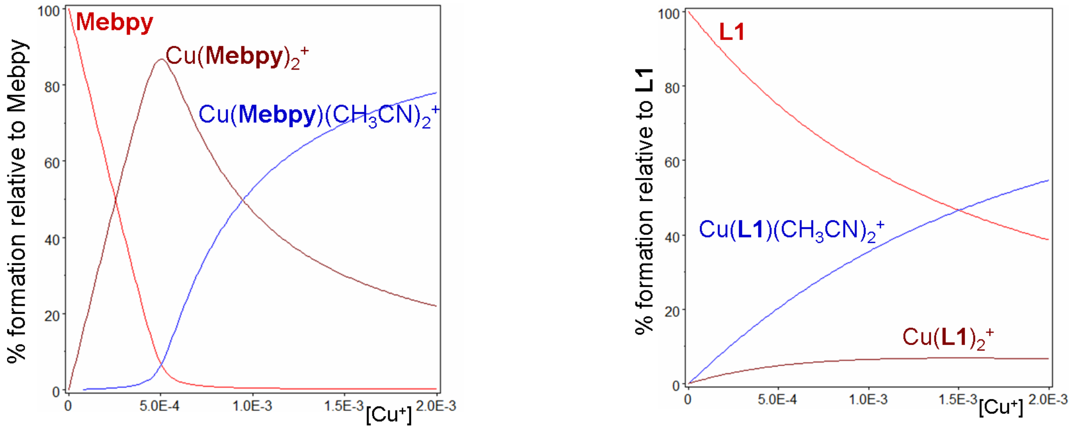


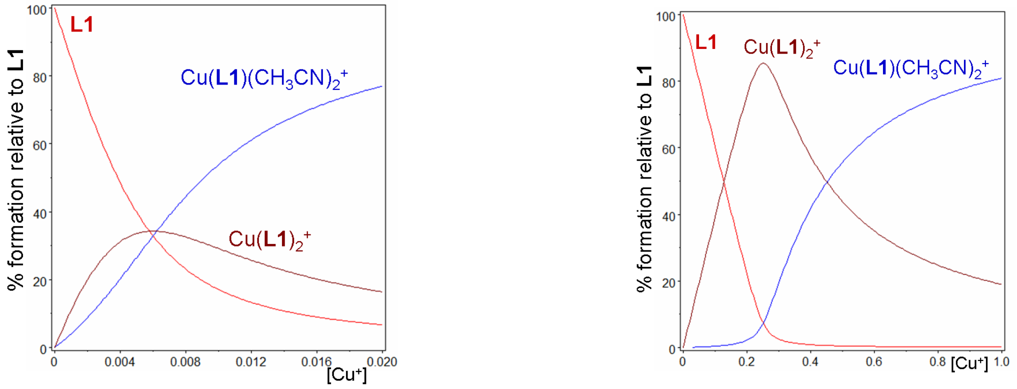
Figure S14: Fitting analysis of the above titration at 320 nm (left) and 390 nm (right); blue diamonds: experimental points; dashed red signals: calculated (fitted) points.

d) Species distribution simulation in 1:1 $CHCl_3/CH_3CN$


[Mebpy] = 1 mM

[L1] = 1 mM

Figure S15: Simulation of the species distribution in 1:1 $CHCl_3/CH_3CN$, with [**L1**]= **1 mM**, [Cu^+] from 0 to 2 mM for : *left*: the **Mebpy** ligand, *right*: ligand **L1**, based on the binding constants determined experimentally. HySS2009 4.0.10 (Protonic Software) was used to perform the simulations.


[L1] = 10 mM

[L1] = 0.5 M

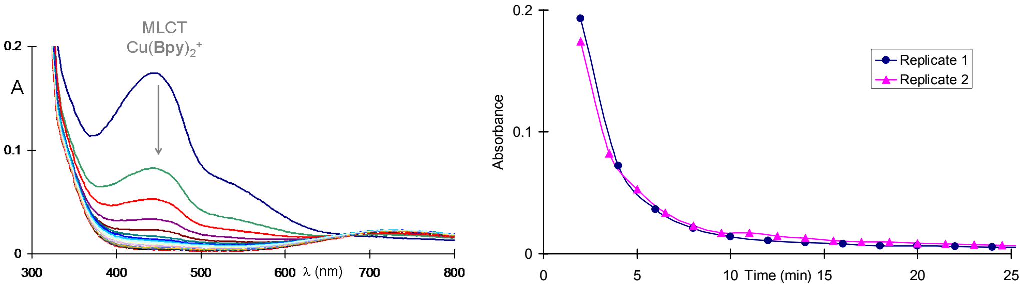
Figure S16: Simulation of the species distribution for species involving **L1** ([Cu^+] from 0 to 2 × [**L1**]).

e) **Comparative oxidation studies**

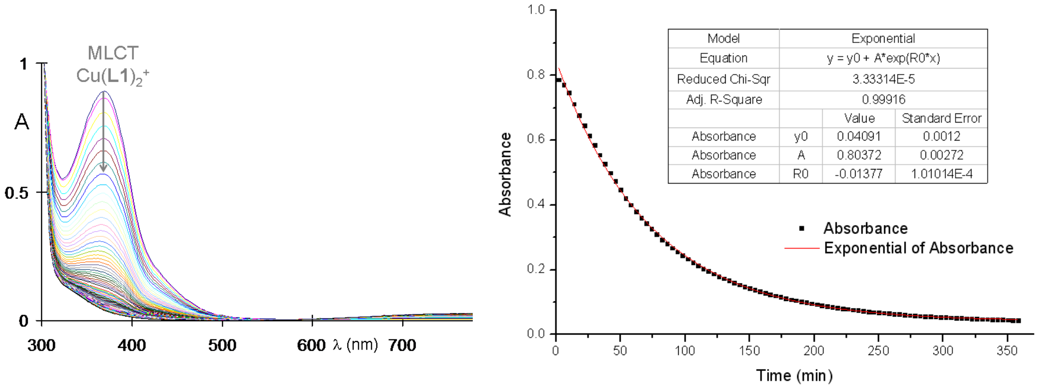
Method: To solutions of ligand in (non-degassed) spectrograde $CHCl_3$* ($[L]_0$ = 0.50 mM) was added $Cu(CH_3CN)_4.BF_4$ (0.5 equivalent) as a solid. The mixture was quickly sonicated and some of the resulting solution transferred to a (stoppered) quartz UV-vis cuvette. The absorbance of the MLCT was monitored as a function of time, and the resulting curve fitted (exponential) to yield the half-life of the complex. Experiments were performed in duplicate.

Results:

$Cu(\mathbf{Bpy})_2^+$

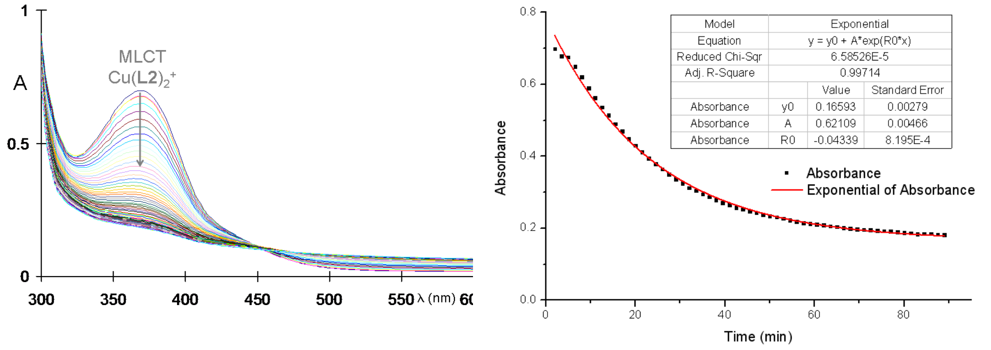


$Cu(\mathbf{L1})_2^+$



Model	Exponential		
Equation	y = y0 + A*exp(R0*x)		
Reduced Chi-Sqr	3.33314E-5		
Adj. R-Square	0.99916		
		Value	Standard Error
Absorbance	y0	0.04091	0.0012
Absorbance	A	0.80372	0.00272
Absorbance	R0	-0.01377	1.01014E-4

$Cu(\mathbf{L2})_2^+$



Model	Exponential		
Equation	y = y0 + A*exp(R0*x)		
Reduced Chi-Sqr	6.58526E-5		
Adj. R-Square	0.99714		
		Value	Standard Error
Absorbance	y0	0.16593	0.00279
Absorbance	A	0.62109	0.00466
Absorbance	R0	-0.04339	8.195E-4

Figure S17: UV-vis analysis of the susceptibility to O_2 ($[complex]_0$ = 0.2 mM, $CHCl_3$*, 25 °C).

D) DFT calculations

Methods: Electronic structure calculations of species Cu(**Bpy**)$_2^+$, Cu(**L1**)(CH_3CN)$_2^+$ and Cu(**L1**)$_2^+$ were performed at the B3LYP/6-31G(d,p) level of theory[1] using the Gaussian 03 software package.[2] The structures of these systems were optimized fully and frequency calculations were performed to ensure that the optimized structures corresponded to minima on the potential energy surface. The highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO, respectively) were then calculated using the optimized structures.

[1]. Becke, A.D., *J. Chem. Phys.* **1993**, *98*, 5648; [2]. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03, Revision C.02;* Gaussian, Inc., Wallingford CT., 2004.

Results: frontier orbitals

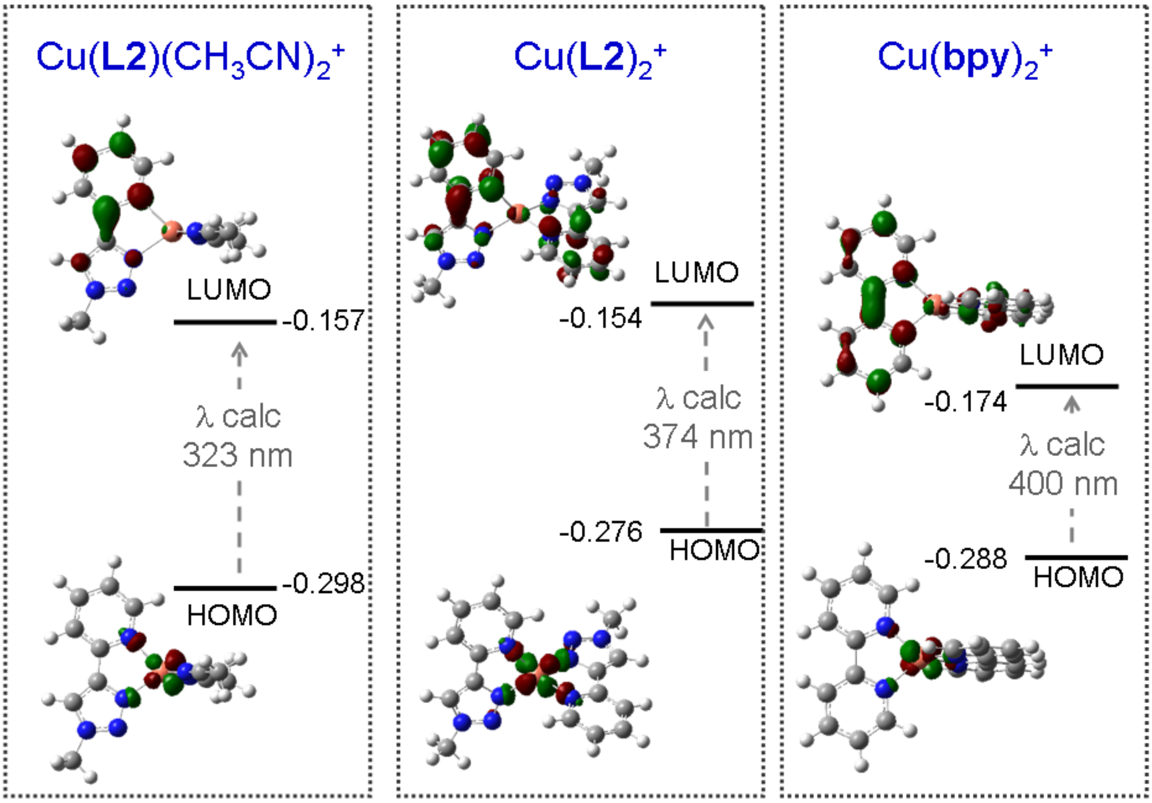


Figure S18: Graphical representation of DFT calculations. Energies are indicated in Hartree (isosurface value 0.05).

E) Electrochemical characterization of the CuL$_2$ complexes

General methods: Anhydrous dichloromethane and tetrahydrofuran were stored over molecular sieve 4Å and degassed under argon prior to use. Cyclic voltammetry experiments were performed on a CHInstrument Model 600B series, Electrochemical Analyzer Workstation. Data were recorded with the CHinstrument software version 5.1. Glassy carbon electrode was used as working electrode, platinum wire as counter electrode, non aqueous Ag/Ag$^+$ electrode as reference electrode and were all purchased from CHInstrument. Tetrabutylammonium hexafluorophosphate (TBAHF) was used as supporting electrolyte at a concentration of 0.1 M in each solvent and ferrocene as reference at a concentration of 2 mM.

The anodic (E_{pa}) and the cathodic (E_{pc}) peak potentials, as well as the corresponding anodic (i_{pa}) and cathodic (i_{pc}) peak currents, were obtained at the same scan rate of 0.1 V.s^{-1}.

$E_{1/2}$ (Fc+/Fc, CH_2Cl_2) in 0.10 M supporting electrolyte was taken as **0.60 V vs SCE** as reported by D. Bao, B. Millare, W. Xia, B. G. Steyer, A. A. Gerasimenko, A. Ferreira, A. Contreras and V. I. Vullev in *J. Phys. Chem*. 2009, **113**, 1259-1267. **$E_{1/2}$ (Fc+/Fc, THF)** was taken as 100 mV lower than in CH_2Cl_2 (i.e. **0.50 V vs SCE**) as reported by I. Noviandri, K. N. Brown, D. S. Fleming, P. T. Gulyas, P. A. Lay, A. F. Masters and L. Philips in *J. Phys. Chem*. 1999, **103**, 6713-6722.

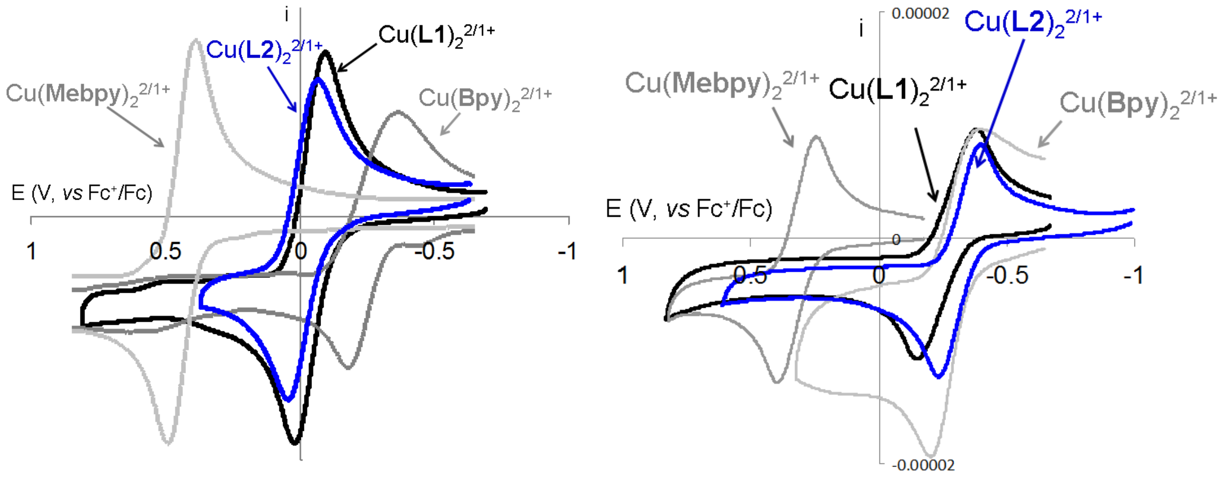


Figure S19: Comparative electrochemistry in CH_2Cl_2. (left) and in THF (right) 0.1 M $NBu_4.PF_6$, [complex]= 0.6-0.9 mM, scan rate: 100 mV/s.

Table S1. Electrochemical data for Cu(**Mebpy**)$_2$, Cu(**bpy**)$_2$, Cu(**L1**)$_2$ and Cu(**L2**)$_2$ **in CH_2Cl_2**

CH_2Cl_2	E_{pa} (V)	E_{pc} (V)	ΔE (V)	$E_{1/2}$ (V)	$E_{1/2}$ *vs* Fc/Fc$^+$(V)	$E_{1/2}$ *vs* SCE (V)
Cu(**Mebpy**)$_2$	0.667	0.563	0.104	0.615	0.437	1.04
Cu(**Bpy**)$_2$	-0.004	-0.174	0.170	-0.089	-0.267	0.33
Cu(**L1**)$_2$	0.208	0.097	0.111	0.152	-0.039	0.56
Cu(**L2**)$_2$	0.175	0.065	0.110	0.120	-0.015	0.59

Table S2. Electrochemical data for Cu(**Mebpy**)$_2$, Cu(**bpy**)$_2$, Cu(**L1**)$_2$ and Cu(**L2**)$_2$ **in THF**

THF	E_{pa} (V)	E_{pc} (V)	ΔE (V)	$E_{1/2}$ (V)	$E_{1/2}$ *vs* Fc/Fc$^+$(V)	$E_{1/2}$ *vs* SCE (V)
Cu(**Mebpy**)$_2$	0.573	0.420	0.153	0.496	0.317	0.82[a]
Cu(**Bpy**)$_2$	-0.028	-0.221	0.193	-0.124	-0.303	0.23[b]
Cu(**L1**)$_2$	0.019	-0.214	0.233	-0.097	-0.266	0.20
Cu(**L2**)$_2$	-0.046	-0.201	0.155	-0.124	-0.316	0.18

a $E_{1/2}$ (Cu(**Mebpy**)$_2^{2/1+}$, THF) = 0.82 V *vs* SCE is to be compared to $E_{1/2}$ (Cu(**Mebpy**)$_2^{2/1+}$, CH_3CN) = 0.73 V *vs* SCE in CH_3CN reported by P. Federlin, J.-M. Kern, A. Rastegar, C. Dietrich-Buchecker, P. A. Marnot and J.-P. Sauvage in *New J. Chem*. 1990, **14**, 9-12.

b Similarly, $E_{1/2}$ (Cu(**Bpy**)$_2^{2/1+}$, THF) = 0.23 V *vs* SCE is to be compared to $E_{1/2}$ (Cu(**Bpy**)$_2^{2/1+}$, CH_3CN) = 0.18 V *vs* SCE in CH_3CN (*ibid*.).

F) X-ray details

Methods: A crystal of the compound (yellow, block-shaped, size 0.25 × 0.25 × 0.20 mm) was mounted on a glass fiber with grease and cooled to -93 °C in a stream of nitrogen gas controlled with Cryostream Controller 700. Data collection was performed on a Bruker SMART APEX II X-ray diffractometer with graphite-monochromated Mo K_α radiation (λ = 0.71073 Å), operating at 50 kV and 30 mA over 2θ ranges of 3.28 ~ 52.00º. No significant decay was observed during the data collection.

Data were processed on a PC using the Bruker AXS Crystal Structure Analysis Package:[1] Data collection: APEX2 (Bruker, 2006); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT (Bruker, 2005); structure solution: XPREP (Bruker, 2005) and SHELXTL (Bruker, 2000); structure refinement: SHELXTL; molecular graphics: SHELXTL; publication materials: SHELXTL. Neutral atom scattering factors were taken from Cromer and Waber.[2] The crystal is monoclinic space group $P2_1/n$, based on the systematic absences, E statistics and successful refinement of the structure. The structure was solved by direct methods. Full-matrix least-square refinements minimizing the function $\sum w\ (F_o^2 - F_c^2)^{\ 2}$ were applied to the compound. All non-hydrogen atoms were refined anisotropically. All H atoms were placed in geometrically calculated positions, with C-H = 0.95 (aromatic) and 0.99(CH_2) Å, and refined as riding atoms, with Uiso(H) = 1.2 Ueq(C). The anion, BF_4^-, is disordered. SHELX commands, SADI, SUMP, EADP and PART were used to resolve the disorder.

Convergence to final R_1 = 0.0587 and wR_2 = 0.1353 for 3342 (I>2σ(I)) independent reflections, and R_1 = 0.1022 and wR_2 = 0.1574 for all 5846 (R(int) = 0.0594) independent reflections, with 400 parameters and 73 restraints, were achieved.[3] The largest residual peak and hole to be 0.514 and – 0.538 e/Å^3, respectively.

Crystallographic data, atomic coordinates and equivalent isotropic displacement parameters, bond lengths and angles, anisotropic displacement parameters, hydrogen coordinates and isotropic displacement parameters, and torsion angles are given in Table S3 to S9. The molecular structure and the cell packing are shown in Figure S20.

[1] Bruker AXS Crystal Structure Analysis Package:

Bruker (2000). SHELXTL. Version 6.14. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2005). XPREP. Version 2005/2. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2005). SAINT. Version 7.23A. Bruker AXS Inc., Madison,Wisconsin, USA.

Bruker (2006). APEX2. Version 2.0-2. Bruker AXS Inc., Madison, Wisconsin, USA.

[2] Cromer, D. T.; Waber, J. T. *International Tables for X-ray Crystallography*; Kynoch Press: Birmingham, UK, 1974; Vol. 4, Table 2.2 A.

[3] $R_1 = \sum | |Fo| - |Fc| | / \sum |Fo|$

$wR_2 = \{\sum [w (Fo^2 - Fc^2)^2] / \sum [w(Fo^2)^2]\}^{1/2}$

$(w = 1 / [\sigma^2(Fo^2) + (0.0674P)^2]$, where $P = [\mathrm{Max}\ (Fo^2, 0) + 2Fc^2] / 3)$

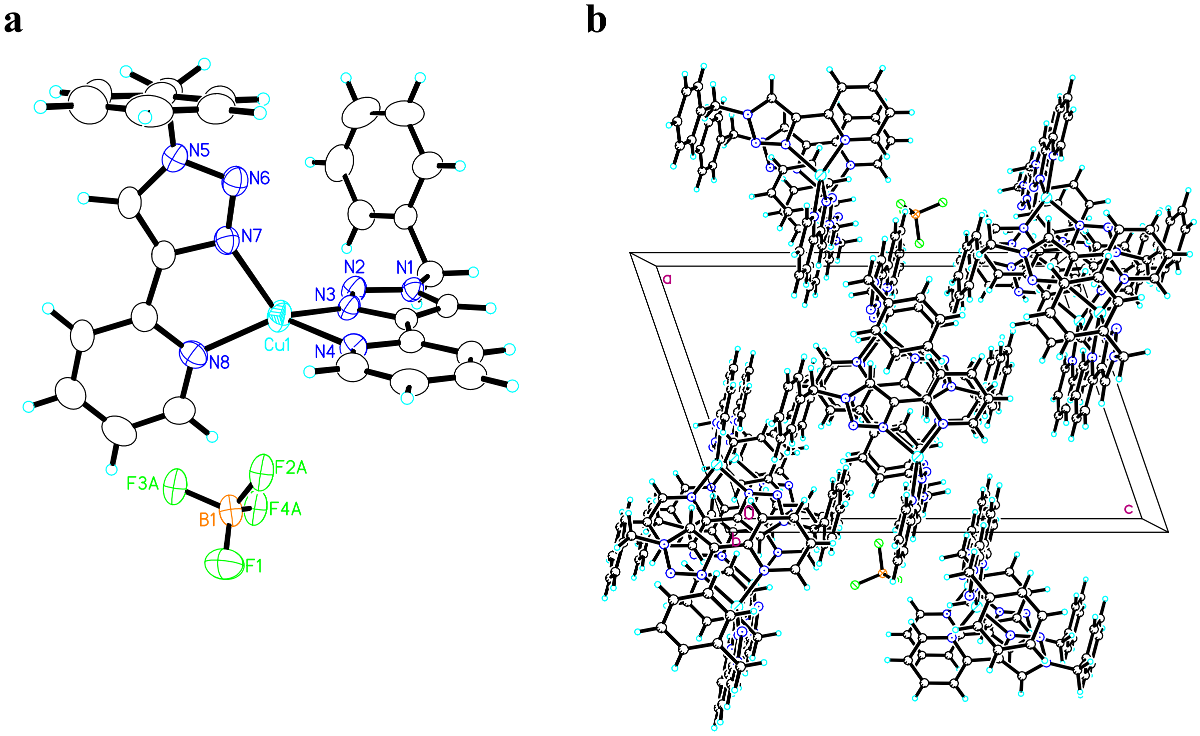


Figure S20. a) Molecular Structure (Displacement ellipsoids for non-H atoms are shown at the 50% probability level and H atoms are represented by circles of arbitrary size); b) Unit cell packing.

Table S3. Crystal data and structure refinement for ap12

Identification code	ap12	
Empirical formula	C28 H24 B Cu F4 N8	
Formula weight	622.90	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 13.2589(6) Å	α= 90°.
	b = 11.2087(5) Å	β= 108.960(2)°.

	c = 19.7397(8) Å	γ = 90°.
Volume	2774.5(2) Å^3	
Z	4	
Density (calculated)	1.491 Mg/m^3	
Absorption coefficient	0.849 mm^{-1}	
F(000)	1272	
Crystal size	0.25 x 0.25 x 0.20 mm^3	
Theta range for data collection	1.64 to 26.00°.	
Index ranges	-14<=h<=16, -11<=k<=13, -24<=l<=24	
Reflections collected	11984	
Independent reflections	5426 [R(int) = 0.0594]	
Completeness to theta = 26.00°	99.5 %	
Absorption correction	Multi-scan	
Max. and min. transmission	0.8486 and 0.8158	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5426 / 73 / 400	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0587, wR2 = 0.1353	
R indices (all data)	R1 = 0.1022, wR2 = 0.1574	
Largest diff. peak and hole	0.514 and -0.538 e.Å^{-3}	

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for ap12. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	7710(1)	4398(1)	9916(1)	40(1)
N(1)	6174(3)	7635(3)	9722(2)	29(1)
N(2)	7104(3)	7056(3)	9996(2)	34(1)
N(3)	6887(3)	5923(3)	9836(2)	29(1)
N(4)	6201(3)	3734(3)	9450(2)	31(1)
N(5)	9790(3)	3689(3)	8757(2)	32(1)
N(6)	8833(3)	4132(3)	8717(2)	35(1)
N(7)	8769(3)	4047(3)	9370(2)	32(1)
N(8)	8891(3)	3681(3)	10734(2)	35(1)
C(1)	5366(3)	6893(4)	9389(2)	29(1)

C(2)	5823(3)	5789(4)	9475(2)	27(1)
C(3)	5427(3)	4579(4)	9256(2)	28(1)
C(4)	4374(3)	4309(4)	8869(2)	34(1)
C(5)	4107(4)	3131(4)	8680(2)	39(1)
C(6)	4894(4)	2269(4)	8878(2)	41(1)
C(7)	5919(4)	2611(4)	9257(2)	38(1)
C(8)	6153(3)	8937(4)	9830(2)	33(1)
C(9)	6965(3)	9552(4)	9568(2)	30(1)
C(10)	7897(4)	9998(4)	10045(3)	44(1)
C(11)	8645(4)	10540(5)	9785(3)	59(2)
C(12)	8449(5)	10634(5)	9053(4)	64(2)
C(13)	7531(5)	10194(5)	8589(3)	61(2)
C(14)	6789(4)	9659(4)	8841(2)	43(1)
C(15)	10324(3)	3301(4)	9422(2)	33(1)
C(16)	9665(3)	3533(4)	9814(2)	30(1)
C(17)	9763(3)	3336(4)	10564(2)	32(1)
C(18)	10642(3)	2827(4)	11055(2)	43(1)
C(19)	10648(4)	2674(5)	11741(3)	57(2)
C(20)	9783(4)	3021(5)	11930(3)	56(1)
C(21)	8917(4)	3507(4)	11412(2)	43(1)
C(22)	10078(4)	3568(4)	8104(2)	40(1)
C(23)	9768(4)	2335(4)	7775(2)	35(1)
C(24)	8733(4)	2108(4)	7359(2)	41(1)
C(25)	8429(4)	972(5)	7095(2)	44(1)
C(26)	9162(5)	66(5)	7248(2)	51(1)
C(27)	10204(5)	288(5)	7663(3)	52(1)
C(28)	10507(4)	1418(5)	7919(2)	46(1)
B(1)	8231(4)	5707(6)	13131(3)	54(2)
F(1)	7913(3)	4737(4)	13416(2)	88(1)
F(2A)	7790(8)	5688(11)	12379(5)	52(2)
F(4A)	8049(8)	6840(7)	13367(6)	52(2)
F(3A)	9349(7)	5610(13)	13284(7)	52(2)
F(2B)	7600(11)	6385(19)	12641(8)	130(6)
F(3B)	9245(11)	5580(30)	13102(9)	130(6)
F(4B)	8417(12)	6298(16)	13834(6)	130(6)
F(3C)	9244(7)	5965(11)	13387(6)	68(2)

F(2C)	7983(8)	5305(11)	12386(4)	68(2)
F(4C)	7509(7)	6603(8)	13090(5)	68(2)

Table S5. Bond lengths [Å] for ap12

Cu(1)-N(3)	2.006(3)	C(6)-C(7)	1.376(6)	C(20)-H(20A)	0.9500
Cu(1)-N(8)	2.017(3)	C(6)-H(6A)	0.9500	C(21)-H(21A)	0.9500
Cu(1)-N(4)	2.051(3)	C(7)-H(7A)	0.9500	C(22)-C(23)	1.524(6)
Cu(1)-N(7)	2.067(3)	C(8)-C(9)	1.506(6)	C(22)-H(22A)	0.9900
N(1)-N(2)	1.342(4)	C(8)-H(8A)	0.9900	C(22)-H(22B)	0.9900
N(1)-C(1)	1.347(5)	C(8)-H(8B)	0.9900	C(23)-C(24)	1.375(6)
N(1)-C(8)	1.476(5)	C(9)-C(10)	1.381(6)	C(23)-C(28)	1.385(6)
N(2)-N(3)	1.318(5)	C(9)-C(14)	1.382(6)	C(24)-C(25)	1.386(6)
N(3)-C(2)	1.366(5)	C(10)-C(11)	1.395(7)	C(24)-H(24A)	0.9500
N(4)-C(7)	1.333(5)	C(10)-H(10A)	0.9500	C(25)-C(26)	1.370(7)
N(4)-C(3)	1.357(5)	C(11)-C(12)	1.388(8)	C(25)-H(25A)	0.9500
N(5)-N(6)	1.342(5)	C(11)-H(11A)	0.9500	C(26)-C(27)	1.380(7)
N(5)-C(15)	1.345(5)	C(12)-C(13)	1.356(7)	C(26)-H(26A)	0.9500
N(5)-C(22)	1.464(5)	C(12)-H(12A)	0.9500	C(27)-C(28)	1.374(7)
N(6)-N(7)	1.322(5)	C(13)-C(14)	1.374(7)	C(27)-H(27A)	0.9500
N(7)-C(16)	1.355(5)	C(13)-H(13A)	0.9500	C(28)-H(28A)	0.9500
N(8)-C(21)	1.340(5)	C(14)-H(14A)	0.9500	B(1)-F(2B)	1.300(11)
N(8)-C(17)	1.361(5)	C(15)-C(16)	1.366(5)	B(1)-F(3C)	1.304(10)
C(1)-C(2)	1.364(6)	C(15)-H(15A)	0.9500	B(1)-F(1)	1.354(7)
C(1)-H(1A)	0.9500	C(16)-C(17)	1.461(6)	B(1)-F(3B)	1.371(12)
C(2)-C(3)	1.468(6)	C(17)-C(18)	1.374(6)	B(1)-F(4C)	1.372(8)
C(3)-C(4)	1.389(5)	C(18)-C(19)	1.363(6)	B(1)-F(4A)	1.400(9)
C(4)-C(5)	1.387(6)	C(18)-H(18A)	0.9500	B(1)-F(2A)	1.408(10)
C(4)-H(4A)	0.9500	C(19)-C(20)	1.372(7)	B(1)-F(3A)	1.417(10)
C(5)-C(6)	1.381(6)	C(19)-H(19A)	0.9500	B(1)-F(2C)	1.470(9)
C(5)-H(5A)	0.9500	C(20)-C(21)	1.378(6)	B(1)-F(4B)	1.484(11)

Table S6. Angles [Å] for ap12

N(3)-Cu(1)-N(8)	131.61(14)	C(10)-C(9)-C(8)	120.8(4)	C(25)-C(26)-H(26A)	120.0
N(3)-Cu(1)-N(4)	81.25(14)	C(14)-C(9)-C(8)	119.9(4)	C(27)-C(26)-H(26A)	120.0
N(8)-Cu(1)-N(4)	127.27(15)	C(9)-C(10)-C(11)	119.5(5)	C(28)-C(27)-C(26)	120.1(5)
N(3)-Cu(1)-N(7)	124.39(14)	C(9)-C(10)-H(10A)	120.3	C(28)-C(27)-H(27A)	120.0

N(8)-Cu(1)-N(7)	81.92(14)	C(11)-C(10)-H(10A)	120.3	C(26)-C(27)-H(27A)	120.0
N(4)-Cu(1)-N(7)	115.18(13)	C(12)-C(11)-C(10)	120.1(5)	C(27)-C(28)-C(23)	120.4(5)
N(2)-N(1)-C(1)	112.3(3)	C(12)-C(11)-H(11A)	120.0	C(27)-C(28)-H(28A)	119.8
N(2)-N(1)-C(8)	118.5(3)	C(10)-C(11)-H(11A)	120.0	C(23)-C(28)-H(28A)	119.
C(1)-N(1)-C(8)	129.1(4)	C(13)-C(12)-C(11)	119.9(5)	F(2B)-B(1)-F(3C)	119.5(12)
N(3)-N(2)-N(1)	105.5(3)	C(13)-C(12)-H(12A)	120.1	F(2B)-B(1)-F(1)	124.5(9)
N(2)-N(3)-C(2)	109.9(3)	C(11)-C(12)-H(12A)	120.1	F(3C)-B(1)-F(1)	115.9(8)
N(2)-N(3)-Cu(1)	137.0(3)	C(12)-C(13)-C(14)	120.4(5)	F(2B)-B(1)-F(3B)	115.7(11)
C(2)-N(3)-Cu(1)	113.0(3)	C(12)-C(13)-H(13A)	119.8	F(3C)-B(1)-F(3B)	30.7(10)
C(7)-N(4)-C(3)	117.6(4)	C(14)-C(13)-H(13A)	119.8	F(1)-B(1)-F(3B)	112.0(12)
C(7)-N(4)-Cu(1)	127.8(3)	C(13)-C(14)-C(9)	120.9(5)	F(2B)-B(1)-F(4C)	42.3(8)
C(3)-N(4)-Cu(1)	114.3(3)	C(13)-C(14)-H(14A)	119.6	F(3C)-B(1)-F(4C)	118.2(8)
N(6)-N(5)-C(15)	111.4(3)	C(9)-C(14)-H(14A)	119.6	F(1)-B(1)-F(4C)	107.8(6)
N(6)-N(5)-C(22)	119.6(3)	N(5)-C(15)-C(16)	105.2(4)	F(3B)-B(1)-F(4C)	138.7(14)
C(15)-N(5)-C(22)	128.7(4)	N(5)-C(15)-H(15A)	127.4	F(2B)-B(1)-F(4A)	65.1(10)
N(7)-N(6)-N(5)	105.9(3)	C(16)-C(15)-H(15A)	127.4	F(3C)-B(1)-F(4A)	86.4(7)
N(6)-N(7)-C(16)	109.9(3)	N(7)-C(16)-C(15)	107.6(3)	F(1)-B(1)-F(4A)	118.6(6)
N(6)-N(7)-Cu(1)	139.8(3)	N(7)-C(16)-C(17)	119.4(4)	F(3B)-B(1)-F(4A)	112.9(14)
C(16)-N(7)-Cu(1)	110.2(3)	C(15)-C(16)-C(17)	133.0(4)	F(4C)-B(1)-F(4A)	33.2(4)
C(21)-N(8)-C(17)	117.1(4)	N(8)-C(17)-C(18)	122.6(4)	F(2B)-B(1)-F(2A)	43.7(9)
C(21)-N(8)-Cu(1)	128.2(3)	N(8)-C(17)-C(16)	113.8(4)	F(3C)-B(1)-F(2A)	115.8(9)
C(17)-N(8)-Cu(1)	114.7(3)	C(18)-C(17)-C(16)	123.6(4)	F(1)-B(1)-F(2A)	110.3(7)
N(1)-C(1)-C(2)	104.4(4)	C(19)-C(18)-C(17)	118.8(4)	F(3B)-B(1)-F(2A)	91.8(9)
N(1)-C(1)-H(1A)	127.8	C(19)-C(18)-H(18A)	120.6	F(4C)-B(1)-F(2A)	84.7(6)
C(2)-C(1)-H(1A)	127.8	C(17)-C(18)-H(18A)	120.6	F(4A)-B(1)-F(2A)	107.9(7)
C(1)-C(2)-N(3)	107.9(4)	C(18)-C(19)-C(20)	120.0(5)	F(2B)-B(1)-F(3A)	125.4(12)
C(1)-C(2)-C(3)	134.4(4)	C(18)-C(19)-H(19A)	120.0	F(3C)-B(1)-F(3A)	20.1(6)
N(3)-C(2)-C(3)	117.7(4)	C(20)-C(19)-H(19A)	120.0	F(1)-B(1)-F(3A)	107.2(8)
N(4)-C(3)-C(4)	122.4(4)	C(19)-C(20)-C(21)	118.6(5)	F(3B)-B(1)-F(3A)	14.0(10)
N(4)-C(3)-C(2)	113.4(3)	C(19)-C(20)-H(20A)	120.7	F(4C)-B(1)-F(3A)	136.9(9)
C(4)-C(3)-C(2)	124.2(4)	C(21)-C(20)-H(20A)	120.7	F(4A)-B(1)-F(3A)	106.3(7)
C(5)-C(4)-C(3)	118.6(4)	N(8)-C(21)-C(20)	122.9(5)	F(2A)-B(1)-F(3A)	105.7(7)
C(5)-C(4)-H(4A)	120.7	N(8)-C(21)-H(21A)	118.5	F(2B)-B(1)-F(2C)	63.5(10)
C(3)-C(4)-H(4A)	120.7	C(20)-C(21)-H(21A)	118.5	F(3C)-B(1)-F(2C)	108.9(7)
C(6)-C(5)-C(4)	119.1(4)	N(5)-C(22)-C(23)	110.3(3)	F(1)-B(1)-F(2C)	99.9(7)
C(6)-C(5)-H(5A)	120.4	N(5)-C(22)-H(22A)	109.6	F(3B)-B(1)-F(2C)	80.2(9)

C(4)-C(5)-H(5A)	120.4	C(23)-C(22)-H(22A)	109.6	F(4C)-B(1)-F(2C)	103.9(6)
C(7)-C(6)-C(5)	118.7(4)	N(5)-C(22)-H(22B)	109.6	F(4A)-B(1)-F(2C)	127.2(8)
C(7)-C(6)-H(6A)	120.6	C(23)-C(22)-H(22B)	109.6	F(2A)-B(1)-F(2C)	19.7(5)
C(5)-C(6)-H(6A)	120.6	H(22A)-C(22)-H(22B)	108.1	F(3A)-B(1)-F(2C)	93.9(7)
N(4)-C(7)-C(6)	123.6(4)	C(24)-C(23)-C(28)	119.2(4)	F(2B)-B(1)-F(4B)	107.8(10)
N(4)-C(7)-H(7A)	118.2	C(24)-C(23)-C(22)	120.1(4)	F(3C)-B(1)-F(4B)	72.6(7)
C(6)-C(7)-H(7A)	118.2	C(28)-C(23)-C(22)	120.7(4)	F(1)-B(1)-F(4B)	87.1(8)
N(1)-C(8)-C(9)	110.7(3)	C(23)-C(24)-C(25)	120.4(5)	F(3B)-B(1)-F(4B)	102.7(9)
N(1)-C(8)-H(8A)	109.5	C(23)-C(24)-H(24A)	119.8	F(4C)-B(1)-F(4B)	68.2(7)
C(9)-C(8)-H(8A)	109.5	C(25)-C(24)-H(24A)	119.8	F(4A)-B(1)-F(4B)	43.8(6)
N(1)-C(8)-H(8B)	109.5	C(26)-C(25)-C(24)	120.0(5)	F(2A)-B(1)-F(4B)	151.4(9)
C(9)-C(8)-H(8B)	109.5	C(26)-C(25)-H(25A)	120.0	F(3A)-B(1)-F(4B)	89.5(8)
H(8A)-C(8)-H(8B)	108.1	C(24)-C(25)-H(25A)	120.0	F(2C)-B(1)-F(4B)	170.9(9)
C(10)-C(9)-C(14)	119.2(4)	C(25)-C(26)-C(27)	119.9(5)		

Table S7. Anisotropic displacement parameters ($Å^2 \times 10^3$) for ap12. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	31(1)	36(1)	52(1)	2(1)	13(1)	7(1)
N(1)	26(2)	27(2)	35(2)	1(2)	13(2)	4(2)
N(2)	31(2)	26(2)	45(2)	-4(2)	14(2)	1(2)
N(3)	22(2)	30(2)	36(2)	0(2)	10(2)	-1(2)
N(4)	34(2)	24(2)	36(2)	-2(2)	13(2)	0(2)
N(5)	27(2)	31(2)	37(2)	-2(2)	12(2)	0(2)
N(6)	31(2)	31(2)	42(2)	0(2)	11(2)	1(2)
N(7)	31(2)	30(2)	34(2)	0(2)	10(2)	4(2)
N(8)	42(2)	28(2)	35(2)	1(2)	12(2)	1(2)
C(1)	23(2)	32(3)	31(2)	4(2)	8(2)	0(2)
C(2)	26(2)	35(3)	21(2)	2(2)	8(2)	2(2)
C(3)	29(2)	31(3)	27(2)	0(2)	12(2)	-2(2)
C(4)	29(2)	41(3)	31(2)	-1(2)	10(2)	-3(2)
C(5)	40(3)	47(3)	29(2)	-3(2)	9(2)	-12(2)
C(6)	55(3)	36(3)	35(2)	-5(2)	18(2)	-16(2)
C(7)	46(3)	30(3)	41(3)	1(2)	18(2)	1(2)

C(8)	40(3)	22(2)	39(2)	-3(2)	16(2)	3(2)
C(9)	31(2)	23(2)	39(2)	0(2)	14(2)	4(2)
C(10)	46(3)	35(3)	48(3)	-1(2)	10(2)	1(2)
C(11)	42(3)	42(3)	87(4)	-5(3)	13(3)	-9(3)
C(12)	69(4)	42(3)	96(5)	-2(3)	48(4)	-16(3)
C(13)	83(4)	56(4)	56(3)	5(3)	39(3)	-8(3)
C(14)	47(3)	40(3)	47(3)	-5(2)	22(2)	-4(2)
C(15)	24(2)	28(2)	41(3)	-2(2)	3(2)	0(2)
C(16)	26(2)	24(2)	38(2)	0(2)	8(2)	0(2)
C(17)	31(2)	25(2)	38(2)	-3(2)	6(2)	-5(2)
C(18)	29(3)	47(3)	48(3)	8(2)	7(2)	6(2)
C(19)	45(3)	71(4)	48(3)	18(3)	7(3)	2(3)
C(20)	63(4)	62(4)	39(3)	12(3)	11(3)	0(3)
C(21)	48(3)	39(3)	47(3)	3(2)	20(2)	-4(2)
C(22)	39(3)	45(3)	40(3)	1(2)	18(2)	-4(2)
C(23)	39(3)	37(3)	32(2)	-1(2)	18(2)	-2(2)
C(24)	39(3)	46(3)	40(3)	6(2)	16(2)	0(2)
C(25)	42(3)	57(3)	34(3)	-3(2)	12(2)	-15(3)
C(26)	79(4)	43(3)	38(3)	-9(2)	30(3)	-9(3)
C(27)	70(4)	43(3)	44(3)	-6(2)	22(3)	10(3)
C(28)	38(3)	58(3)	41(3)	-6(3)	14(2)	4(3)
B(1)	38(4)	63(5)	57(4)	15(4)	9(3)	13(3)
F(1)	80(2)	100(3)	87(2)	35(2)	29(2)	-9(2)
F(2A)	32(3)	53(4)	63(4)	-7(3)	6(3)	6(3)
F(4A)	32(3)	53(4)	63(4)	-7(3)	6(3)	6(3)
F(3A)	32(3)	53(4)	63(4)	-7(3)	6(3)	6(3)
F(2B)	121(9)	181(14)	94(8)	45(8)	45(7)	-9(8)
F(3B)	121(9)	181(14)	94(8)	45(8)	45(7)	-9(8)
F(4B)	121(9)	181(14)	94(8)	45(8)	45(7)	-9(8)
F(3C)	50(4)	82(5)	56(4)	-18(3)	-3(3)	14(3)
F(2C)	50(4)	82(5)	56(4)	-18(3)	-3(3)	14(3)
F(4C)	50(4)	82(5)	56(4)	-18(3)	-3(3)	14(3)

Table S8. Hydrogen coordinates (× 10^4) and isotropic displacement parameters (Å^2 × 10^3) for ap12.

	x	y	z	U(eq)
H(1A)	4641	7093	9149	35
H(4A)	3849	4919	8737	40
H(5A)	3393	2919	8419	47
H(6A)	4730	1456	8754	49
H(7A)	6456	2013	9388	46
H(8A)	6306	9109	10346	40
H(8B)	5433	9248	9568	40
H(10A)	8028	9937	10546	53
H(11A)	9289	10846	10110	70
H(12A)	8958	11005	8876	77
H(13A)	7399	10255	8088	73
H(14A)	6147	9359	8510	52
H(15A)	11010	2943	9584	39
H(18A)	11236	2586	10919	51
H(19A)	11250	2328	12089	68
H(20A)	9781	2927	12408	67
H(21A)	8312	3729	11540	52
H(22A)	10856	3685	8219	48
H(22B)	9707	4188	7755	48
H(24A)	8222	2735	7251	49
H(25A)	7712	820	6809	53
H(26A)	8955	-714	7068	61
H(27A)	10712	-341	7772	62
H(28A)	11228	1570	8197	55

Table S9. Torsion angles [°] for ap12.

C(1)-N(1)-N(2)-N(3)	0.0(4)	C(4)-C(5)-C(6)-C(7)	0.1(6)
C(8)-N(1)-N(2)-N(3)	178.6(3)	C(3)-N(4)-C(7)-C(6)	-0.2(6)
N(1)-N(2)-N(3)-C(2)	-1.1(4)	Cu(1)-N(4)-C(7)-C(6)	-172.9(3)
N(1)-N(2)-N(3)-Cu(1)	173.2(3)	C(5)-C(6)-C(7)-N(4)	0.3(6)

N(8)-Cu(1)-N(3)-N(2)	47.2(5)	N(2)-N(1)-C(8)-C(9)	54.6(5)
N(4)-Cu(1)-N(3)-N(2)	-179.7(4)	C(1)-N(1)-C(8)-C(9)	-126.9(4)
N(7)-Cu(1)-N(3)-N(2)	-65.1(4)	N(1)-C(8)-C(9)-C(10)	-105.9(4)
N(8)-Cu(1)-N(3)-C(2)	-138.6(3)	N(1)-C(8)-C(9)-C(14)	73.1(5)
N(4)-Cu(1)-N(3)-C(2)	-5.6(3)	C(14)-C(9)-C(10)-C(11)	-0.4(7)
N(7)-Cu(1)-N(3)-C(2)	109.1(3)	C(8)-C(9)-C(10)-C(11)	178.6(4)
N(3)-Cu(1)-N(4)-C(7)	178.6(4)	C(9)-C(10)-C(11)-C(12)	0.3(8)
N(8)-Cu(1)-N(4)-C(7)	-44.8(4)	C(10)-C(11)-C(12)-C(13)	-0.2(8)
N(7)-Cu(1)-N(4)-C(7)	54.6(4)	C(11)-C(12)-C(13)-C(14)	0.2(9)
N(3)-Cu(1)-N(4)-C(3)	5.7(3)	C(12)-C(13)-C(14)-C(9)	-0.4(8)
N(8)-Cu(1)-N(4)-C(3)	142.4(3)	C(10)-C(9)-C(14)-C(13)	0.5(7)
N(7)-Cu(1)-N(4)-C(3)	-118.3(3)	C(8)-C(9)-C(14)-C(13)	-178.5(5)
C(15)-N(5)-N(6)-N(7)	1.3(4)	N(6)-N(5)-C(15)-C(16)	-0.8(5)
C(22)-N(5)-N(6)-N(7)	175.2(4)	C(22)-N(5)-C(15)-C(16)	-174.0(4)
N(5)-N(6)-N(7)-C(16)	-1.3(4)	N(6)-N(7)-C(16)-C(15)	0.8(5)
N(5)-N(6)-N(7)-Cu(1)	-178.4(3)	Cu(1)-N(7)-C(16)-C(15)	178.8(3)
N(3)-Cu(1)-N(7)-N(6)	-46.7(5)	N(6)-N(7)-C(16)-C(17)	-179.2(4)
N(8)-Cu(1)-N(7)-N(6)	177.6(4)	Cu(1)-N(7)-C(16)-C(17)	-1.2(5)
N(4)-Cu(1)-N(7)-N(6)	50.1(5)	N(5)-C(15)-C(16)-N(7)	0.0(5)
N(3)-Cu(1)-N(7)-C(16)	136.2(3)	N(5)-C(15)-C(16)-C(17)	-179.9(4)
N(8)-Cu(1)-N(7)-C(16)	0.5(3)	C(21)-N(8)-C(17)-C(18)	0.1(6)
N(4)-Cu(1)-N(7)-C(16)	-127.0(3)	Cu(1)-N(8)-C(17)-C(18)	-179.8(3)
N(3)-Cu(1)-N(8)-C(21)	50.9(4)	C(21)-N(8)-C(17)-C(16)	178.9(4)
N(4)-Cu(1)-N(8)-C(21)	-64.0(4)	Cu(1)-N(8)-C(17)-C(16)	-1.0(5)
N(7)-Cu(1)-N(8)-C(21)	-179.6(4)	N(7)-C(16)-C(17)-N(8)	1.6(6)
N(3)-Cu(1)-N(8)-C(17)	-129.2(3)	C(15)-C(16)-C(17)-N(8)	-178.5(4)
N(4)-Cu(1)-N(8)-C(17)	115.9(3)	N(7)-C(16)-C(17)-C(18)	-179.7(4)
N(7)-Cu(1)-N(8)-C(17)	0.3(3)	C(15)-C(16)-C(17)-C(18)	0.3(8)
N(2)-N(1)-C(1)-C(2)	1.2(4)	N(8)-C(17)-C(18)-C(19)	-0.8(7)
C(8)-N(1)-C(1)-C(2)	-177.4(4)	C(16)-C(17)-C(18)-C(19)	-179.4(5)
N(1)-C(1)-C(2)-N(3)	-1.8(4)	C(17)-C(18)-C(19)-C(20)	0.3(8)
N(1)-C(1)-C(2)-C(3)	179.8(4)	C(18)-C(19)-C(20)-C(21)	0.7(8)
N(2)-N(3)-C(2)-C(1)	1.9(4)	C(17)-N(8)-C(21)-C(20)	1.1(7)
Cu(1)-N(3)-C(2)-C(1)	-173.9(3)	Cu(1)-N(8)-C(21)-C(20)	-179.0(4)
N(2)-N(3)-C(2)-C(3)	-179.4(3)	C(19)-C(20)-C(21)-N(8)	-1.5(8)
Cu(1)-N(3)-C(2)-C(3)	4.8(4)	N(6)-N(5)-C(22)-C(23)	-91.4(5)

C(7)-N(4)-C(3)-C(4)	-0.2(6)	C(15)-N(5)-C(22)-C(23)	81.3(5)
Cu(1)-N(4)-C(3)-C(4)	173.4(3)	N(5)-C(22)-C(23)-C(24)	81.1(5)
C(7)-N(4)-C(3)-C(2)	-178.3(3)	N(5)-C(22)-C(23)-C(28)	-95.7(5)
Cu(1)-N(4)-C(3)-C(2)	-4.7(4)	C(28)-C(23)-C(24)-C(25)	1.0(6)
C(1)-C(2)-C(3)-N(4)	178.2(4)	C(22)-C(23)-C(24)-C(25)	-175.9(4)
N(3)-C(2)-C(3)-N(4)	0.0(5)	C(23)-C(24)-C(25)-C(26)	-0.2(6)
C(1)-C(2)-C(3)-C(4)	0.2(7)	C(24)-C(25)-C(26)-C(27)	-0.1(7)
N(3)-C(2)-C(3)-C(4)	-178.1(3)	C(25)-C(26)-C(27)-C(28)	-0.5(7)
N(4)-C(3)-C(4)-C(5)	0.5(6)	C(26)-C(27)-C(28)-C(23)	1.3(7)
C(2)-C(3)-C(4)-C(5)	178.4(4)	C(24)-C(23)-C(28)-C(27)	-1.6(7)
C(3)-C(4)-C(5)-C(6)	-0.5(6)	C(22)-C(23)-C(28)-C(27)	175.3(4)