Supporting Information

to

Ring-Opening Metathesis Polymerization-Derived, Polymer-Bound Cu-Catalysts for Click-Chemistry and Hydrosilylation Reactions Under Micellar Conditions

by

G. Pawar, B., Bantu, J. Weckesser, S. Blechert*, K. Wurst, M. R. Buchmeiser*

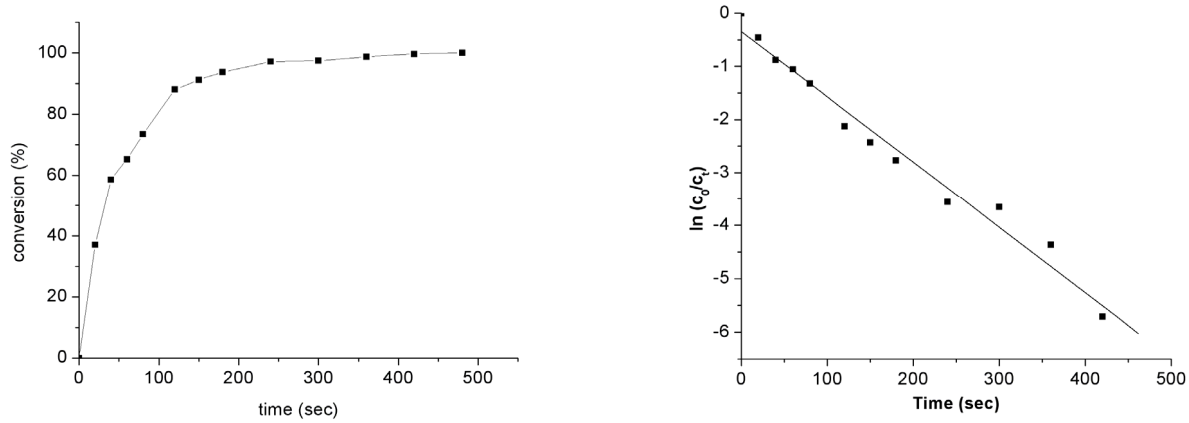

Figure S1: Kinetics of ROMP of **M1** by the action of $RuCl_2(Py)_2(IMesH_2)(CHPh)$ and first-order kinetics plot.

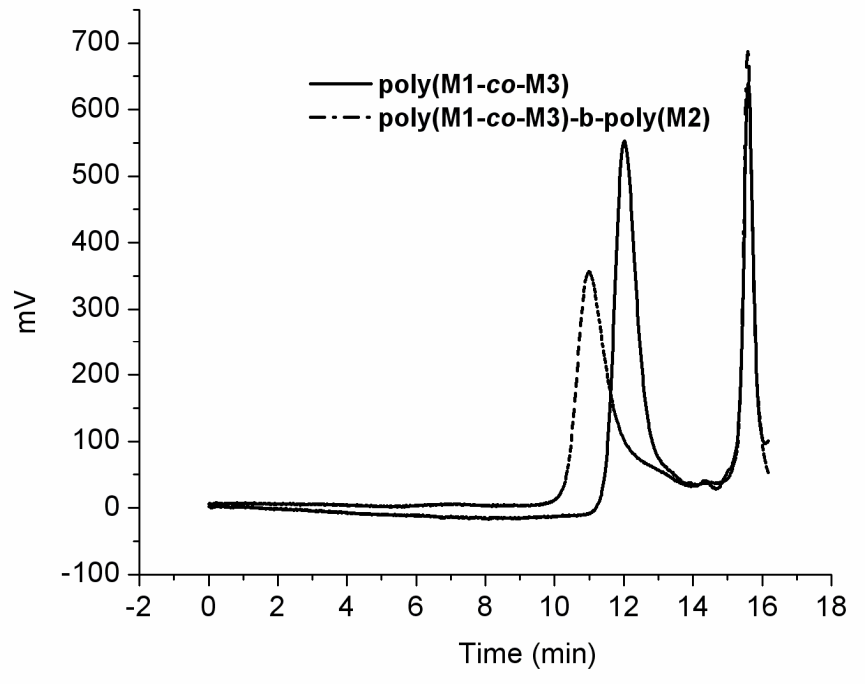

Figure S2. Overlay of GPC traces for **poly(M1-*co*-M3)** and **poly(M1-*co*-M3)-*b*-poly(M2)**.

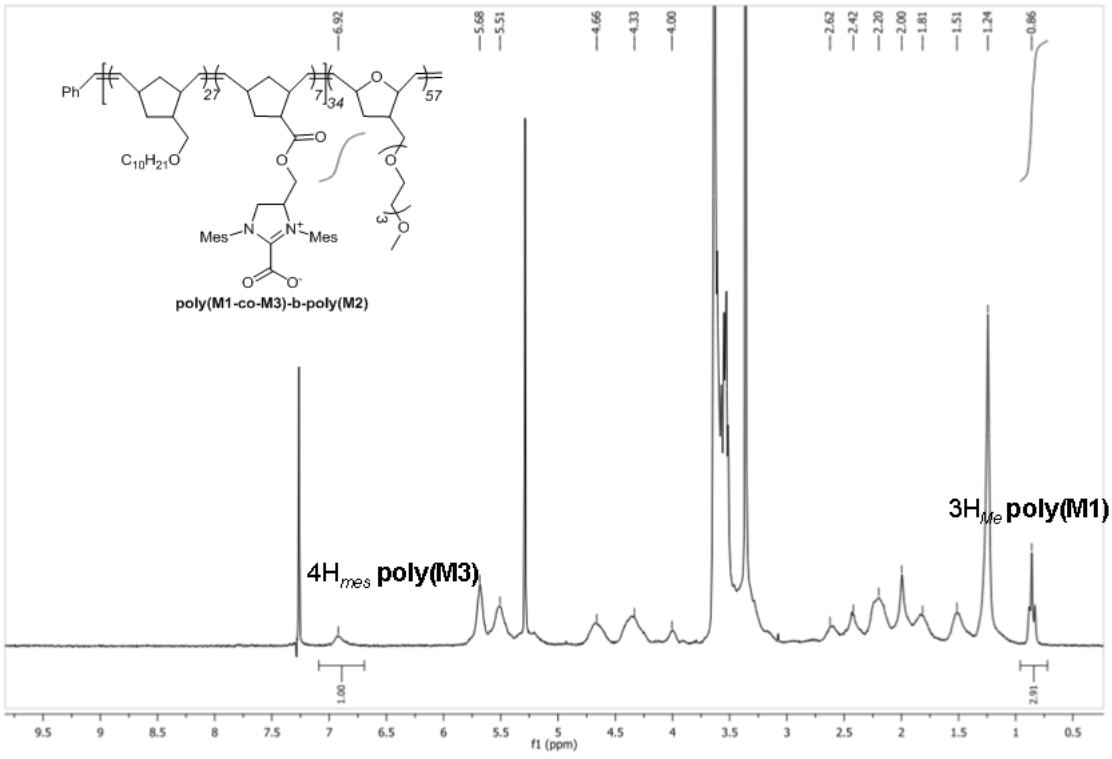

Figure S3. ^{1}H-NMR of **poly(M1-*co*-M3)-*b*-poly(M2)**.

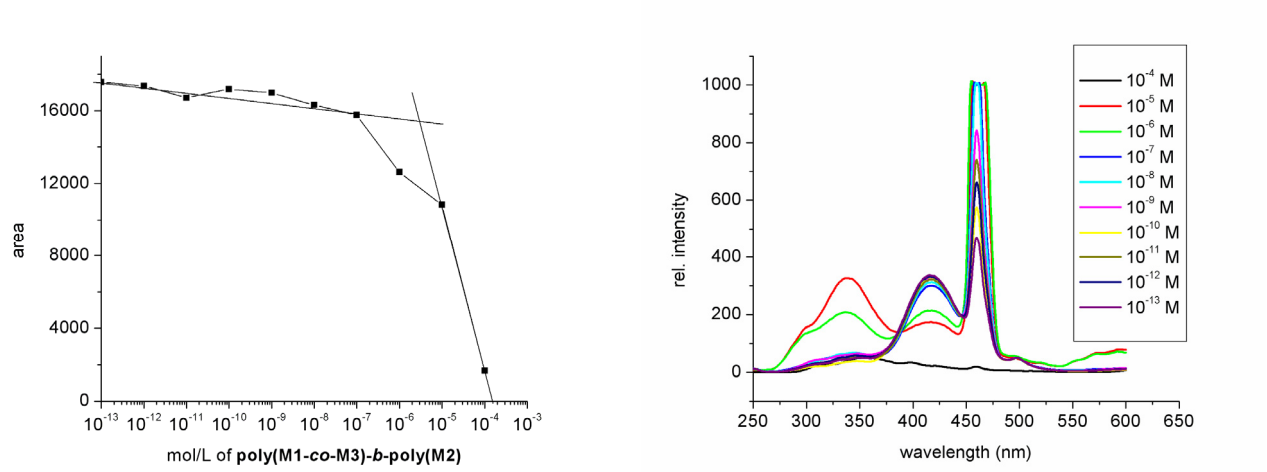

Figure S4. *cmc* measurements for **poly(M1-*co*-M3)-*b*-poly(M2)** in water.

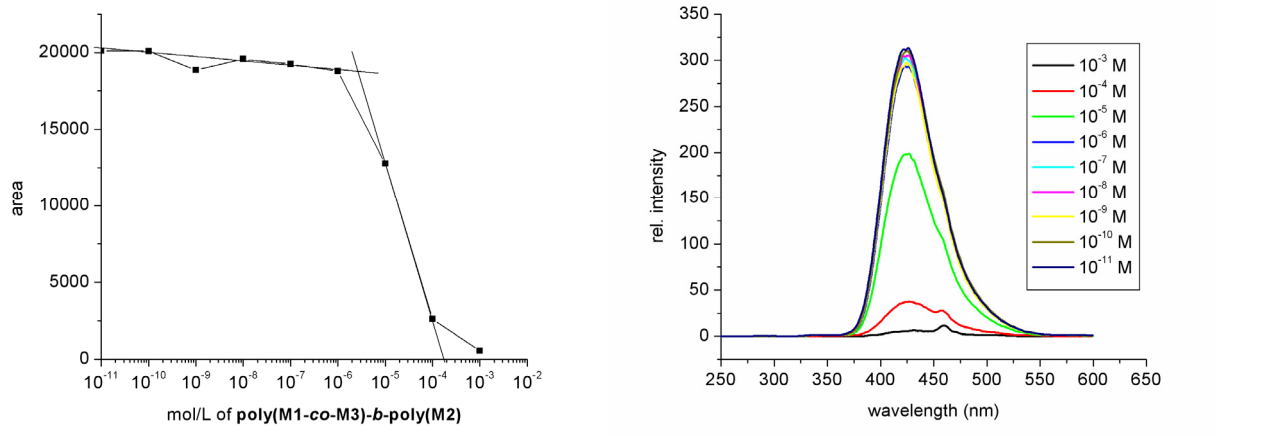

Figure S5. *cmc* measurements for **poly(M1-*co*-M3)-*b*-poly(M2)** in DMF.

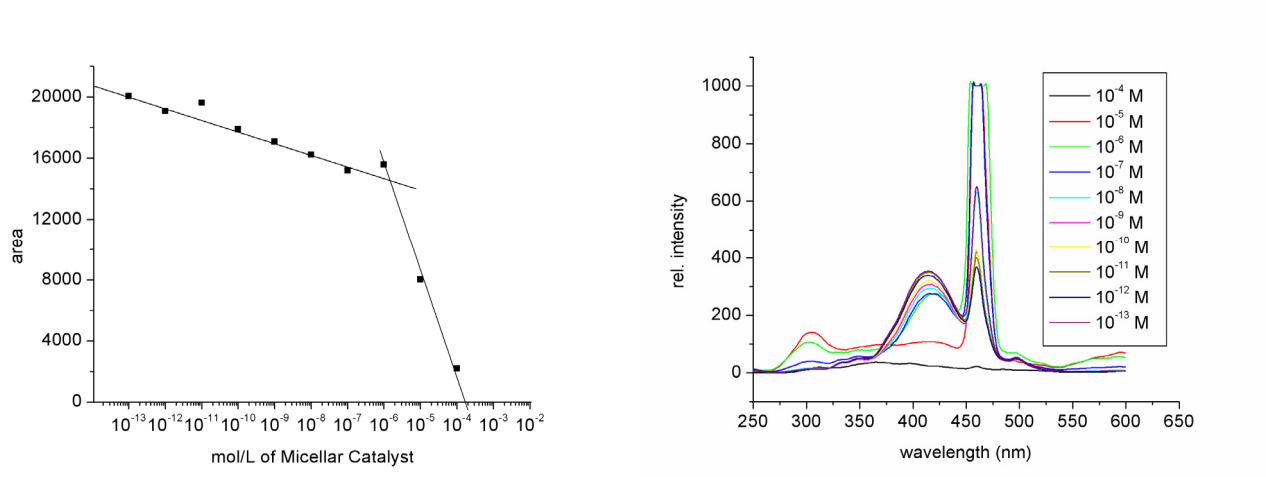

Figure S6. *cmc* measurements for **poly(M1-*co*-M3)-*b*-poly(M2)-Cu** in water.

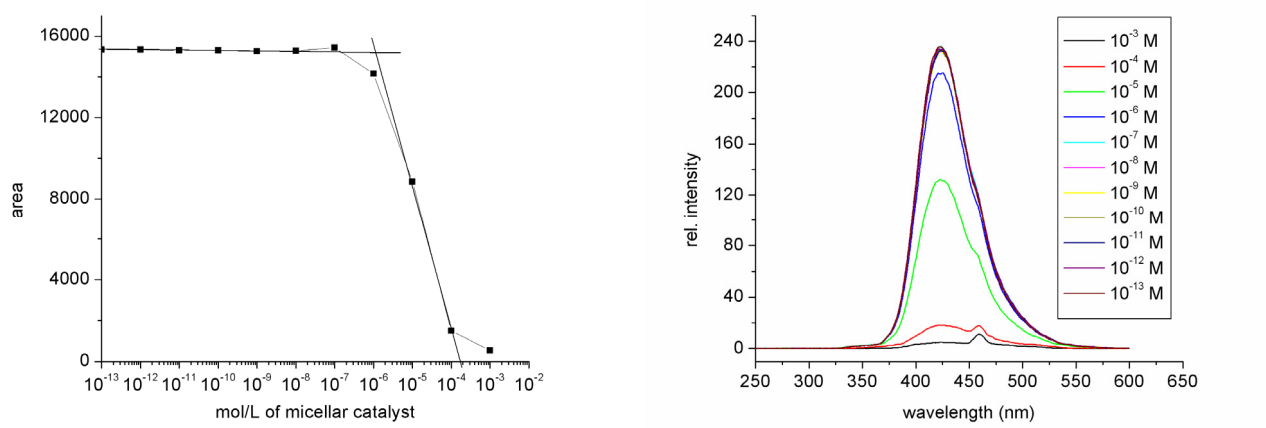

Figure S7. *cmc* measurements for **poly(M1-*co*-M3)-*b*-poly(M2)-Cu** in DMF.

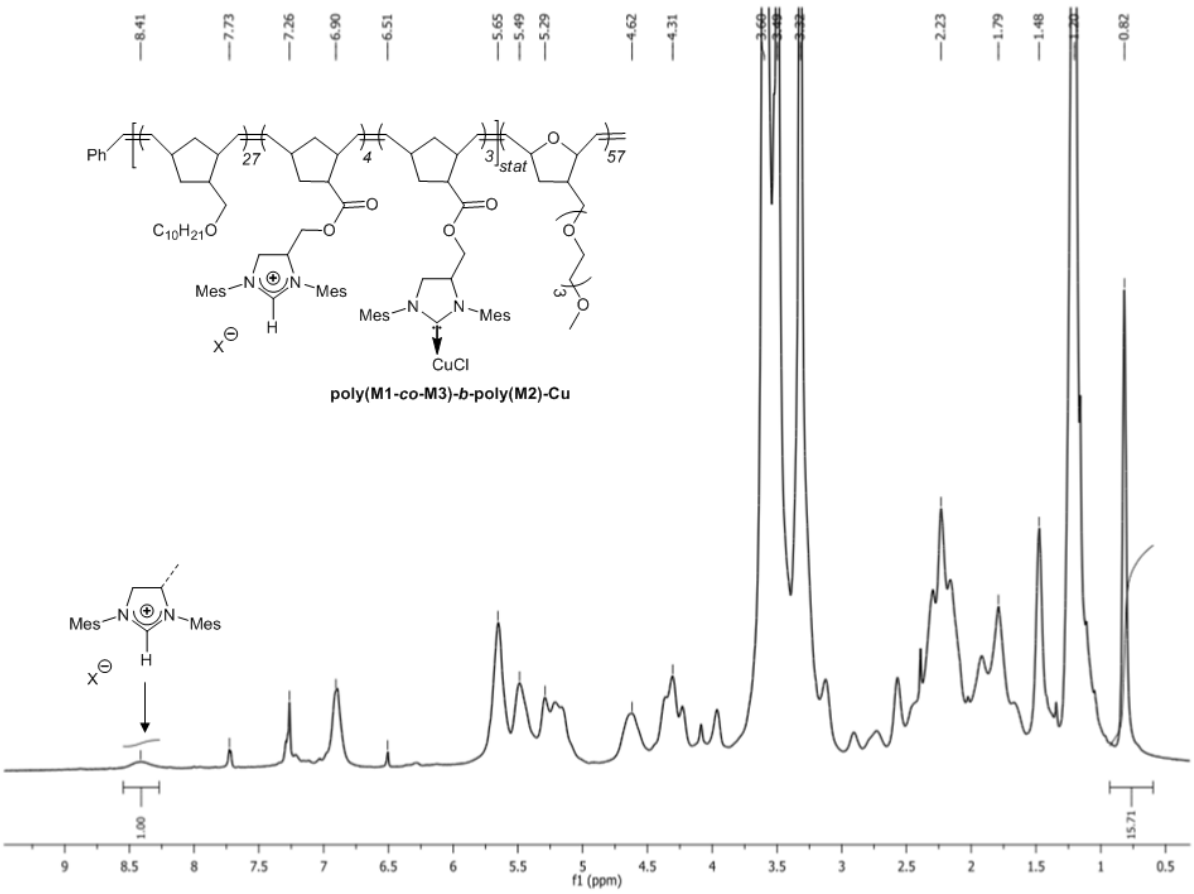

Figure S8. ^{1}H-NMR of **poly(M1-*co*-M3)-*b*-poly(M2)-Cu** ($CDCl_3$).

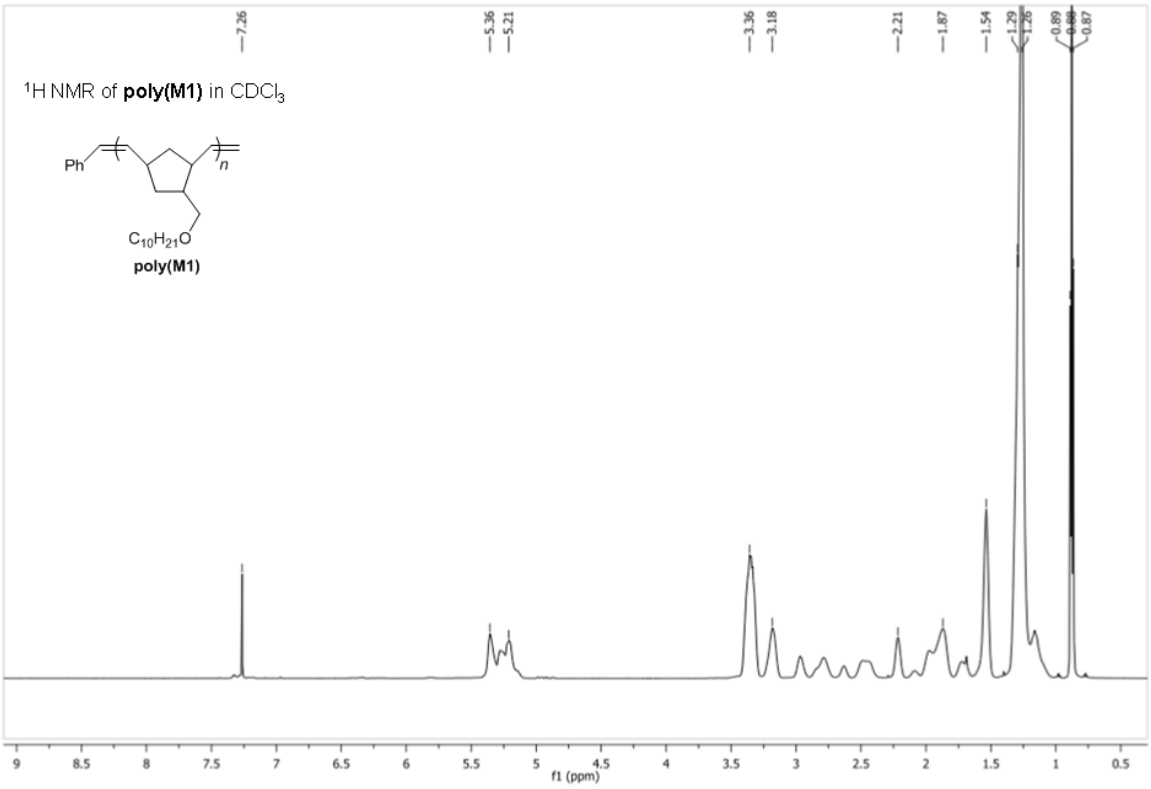

Figure S9. ^{1}H-NMR of **poly(M1)**.

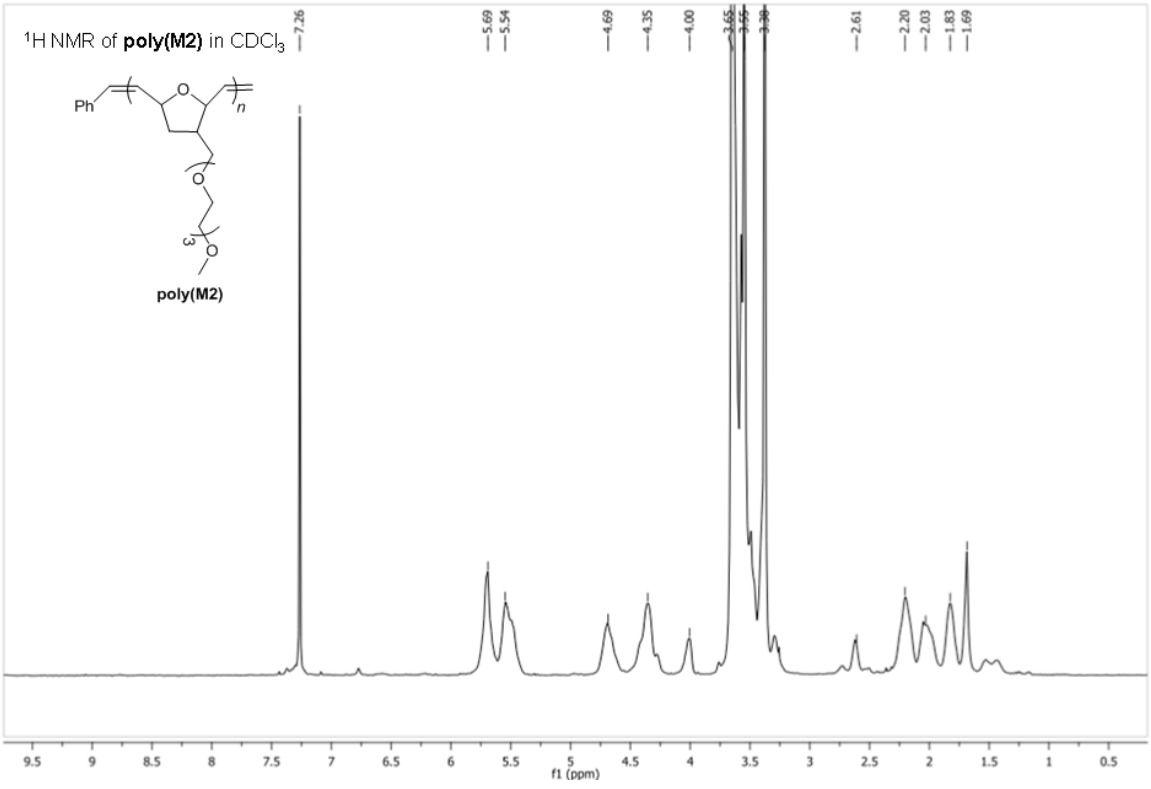

Figure S10. ^{1}H-NMR of **poly(M2)**.

Table S1. Crystal data and structure refinement for **1**.

Empirical formula	C22 H28 Cl Cu N2	
Formula weight	419.45	
Temperature	233(2) K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	Pbcn (no.60)	
Unit cell dimensions	a = 30.4627(5) Å	α= 90°.
	b = 8.9030(2) Å	β= 90°.
	c = 15.8730(3) Å	γ = 90°.
Volume	4304.91(14) $Å^3$	
Z	8	
Density (calculated)	1.294 Mg/m^3	
Absorption coefficient	1.146 mm^{-1}	
F(000)	1760	
Crystal size	0.3 x 0.3 x 0.07 mm^3	
Theta range for data collection	1.34 to 25.00°.	
Index ranges	-36<=h<=35, -10<=k<=10, -18<=l<=18	
Reflections collected	18276	
Independent reflections	3761 [R(int) = 0.0313]	
Reflections [I>2sigma(I)]	3253	
Completeness to theta = 25.00°	98.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3761 / 0 / 241	
Goodness-of-fit on F^2	1.072	
Final R indices [I>2sigma(I)]	R1 = 0.0444, wR2 = 0.1108	
R indices (all data)	R1 = 0.0521, wR2 = 0.1146	
Largest diff. peak and hole	0.562 and -0.494 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	1257(1)	2007(1)	2540(1)	40(1)
Cl(1)	1234(1)	3394(1)	1470(1)	69(1)
N(1)	1035(1)	1304(3)	4202(1)	38(1)
N(2)	1544(1)	-318(3)	3658(1)	35(1)
C(1)	1280(1)	874(3)	3548(2)	33(1)
C(2)	1058(1)	647(4)	5056(2)	53(1)
C(3)	1502(1)	-81(4)	5184(2)	56(1)
C(4)	1589(1)	-1136(3)	4459(2)	44(1)
C(5)	739(1)	2565(4)	4087(2)	41(1)
C(6)	309(1)	2272(4)	3842(2)	54(1)
C(7)	30(1)	3505(6)	3747(3)	68(1)
C(8)	167(1)	4953(5)	3900(2)	63(1)
C(9)	592(1)	5180(4)	4158(2)	56(1)
C(10)	890(1)	4010(4)	4248(2)	45(1)
C(11)	1798(1)	-869(3)	2954(2)	34(1)
C(12)	1604(1)	-1888(3)	2401(2)	39(1)
C(13)	1860(1)	-2438(4)	1745(2)	44(1)
C(14)	2291(1)	-2005(4)	1636(2)	45(1)
C(15)	2474(1)	-1005(4)	2202(2)	46(1)
C(16)	2233(1)	-430(3)	2873(2)	38(1)
C(61)	148(1)	688(5)	3683(3)	83(1)
C(81)	-148(2)	6254(6)	3793(3)	95(2)
C(101)	1359(1)	4304(4)	4494(3)	61(1)
C(121)	1134(1)	-2375(5)	2487(2)	59(1)
C(141)	2561(1)	-2618(5)	909(2)	65(1)
C(161)	2444(1)	631(4)	3494(2)	54(1)

Table S3. Bond lengths [Å] and angles [°] for **1**.

Cu(1)-C(1)	1.892(3)
Cu(1)-Cl(1)	2.1011(9)
N(1)-C(1)	1.336(3)
N(1)-C(5)	1.451(4)
N(1)-C(2)	1.479(4)
N(2)-C(1)	1.343(4)
N(2)-C(11)	1.443(3)
N(2)-C(4)	1.472(3)
C(2)-C(3)	1.512(5)
C(3)-C(4)	1.509(4)
C(5)-C(10)	1.390(5)
C(5)-C(6)	1.391(5)
C(6)-C(7)	1.395(5)
C(6)-C(61)	1.514(6)
C(7)-C(8)	1.376(6)
C(8)-C(9)	1.373(5)
C(8)-C(81)	1.514(5)
C(9)-C(10)	1.388(4)
C(10)-C(101)	1.505(5)
C(11)-C(16)	1.388(4)
C(11)-C(12)	1.393(4)
C(12)-C(13)	1.390(4)
C(12)-C(121)	1.504(5)
C(13)-C(14)	1.380(5)
C(14)-C(15)	1.381(5)
C(14)-C(141)	1.518(4)
C(15)-C(16)	1.390(4)
C(16)-C(161)	1.509(4)
C(1)-Cu(1)-Cl(1)	176.20(9)
C(1)-N(1)-C(5)	118.2(2)
C(1)-N(1)-C(2)	124.8(2)
C(5)-N(1)-C(2)	116.9(2)
C(1)-N(2)-C(11)	119.2(2)
C(1)-N(2)-C(4)	123.9(2)
C(11)-N(2)-C(4)	116.9(2)
N(1)-C(1)-N(2)	117.5(2)
N(1)-C(1)-Cu(1)	118.8(2)

N(2)-C(1)-Cu(1)	123.61(19)
N(1)-C(2)-C(3)	109.6(2)
C(4)-C(3)-C(2)	108.8(3)
N(2)-C(4)-C(3)	109.6(2)
C(10)-C(5)-C(6)	122.4(3)
C(10)-C(5)-N(1)	119.2(3)
C(6)-C(5)-N(1)	118.3(3)
C(5)-C(6)-C(7)	117.1(4)
C(5)-C(6)-C(61)	121.7(3)
C(7)-C(6)-C(61)	121.2(3)
C(8)-C(7)-C(6)	122.3(3)
C(9)-C(8)-C(7)	118.4(3)
C(9)-C(8)-C(81)	121.2(4)
C(7)-C(8)-C(81)	120.3(4)
C(8)-C(9)-C(10)	122.4(4)
C(9)-C(10)-C(5)	117.4(3)
C(9)-C(10)-C(101)	121.1(3)
C(5)-C(10)-C(101)	121.5(3)
C(16)-C(11)-C(12)	121.9(3)
C(16)-C(11)-N(2)	119.1(2)
C(12)-C(11)-N(2)	118.9(2)
C(13)-C(12)-C(11)	117.7(3)
C(13)-C(12)-C(121)	120.1(3)
C(11)-C(12)-C(121)	122.2(3)
C(14)-C(13)-C(12)	121.9(3)
C(13)-C(14)-C(15)	118.8(3)
C(13)-C(14)-C(141)	120.6(3)
C(15)-C(14)-C(141)	120.6(3)
C(14)-C(15)-C(16)	121.5(3)
C(11)-C(16)-C(15)	118.1(3)
C(11)-C(16)-C(161)	121.5(3)
C(15)-C(16)-C(161)	120.4(3)

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. 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)	43(1)	47(1)	31(1)	5(1)	1(1)	12(1)
Cl(1)	81(1)	77(1)	48(1)	25(1)	7(1)	26(1)
N(1)	43(1)	40(1)	31(1)	1(1)	5(1)	9(1)
N(2)	41(1)	35(1)	28(1)	1(1)	1(1)	6(1)
C(1)	33(1)	37(2)	30(1)	-3(1)	-1(1)	2(1)
C(2)	68(2)	55(2)	35(2)	6(2)	13(2)	15(2)
C(3)	79(2)	53(2)	35(2)	9(2)	-1(2)	15(2)
C(4)	57(2)	38(2)	35(2)	9(1)	2(1)	9(1)
C(5)	41(2)	50(2)	31(1)	0(1)	7(1)	13(1)
C(6)	46(2)	69(2)	47(2)	-7(2)	2(2)	9(2)
C(7)	41(2)	106(3)	58(2)	0(2)	0(2)	22(2)
C(8)	60(2)	74(3)	55(2)	12(2)	13(2)	34(2)
C(9)	63(2)	49(2)	56(2)	11(2)	17(2)	19(2)
C(10)	47(2)	50(2)	40(2)	3(1)	8(1)	12(2)
C(11)	39(1)	32(2)	30(1)	3(1)	1(1)	7(1)
C(12)	39(2)	43(2)	35(2)	-1(1)	-1(1)	2(1)
C(13)	55(2)	43(2)	34(2)	-5(1)	-3(1)	7(2)
C(14)	52(2)	47(2)	37(2)	6(1)	8(1)	17(2)
C(15)	40(2)	49(2)	49(2)	7(2)	8(1)	6(1)
C(16)	42(2)	32(2)	40(2)	5(1)	-1(1)	2(1)
C(61)	57(2)	95(3)	98(3)	-23(3)	-10(2)	-9(2)
C(81)	82(3)	113(4)	90(3)	33(3)	18(3)	60(3)
C(101)	58(2)	52(2)	72(2)	-6(2)	-4(2)	6(2)
C(121)	45(2)	78(3)	52(2)	-15(2)	-1(1)	-14(2)
C(141)	73(2)	72(2)	51(2)	-4(2)	20(2)	22(2)
C(161)	52(2)	51(2)	58(2)	-3(2)	0(2)	-13(2)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **1**.

	x	y	z	U(eq)
H(2A)	826	-104	5126	63
H(2B)	1014	1435	5479	63
H(3A)	1731	691	5208	67
H(3B)	1505	-637	5716	67
H(4A)	1886	-1551	4507	52
H(4B)	1379	-1971	4475	52
H(7)	-261	3340	3572	82
H(9)	685	6164	4277	67
H(13)	1736	-3127	1364	53
H(15)	2767	-706	2133	55
H(61A)	-156	716	3506	125
H(61B)	174	104	4197	125
H(61C)	325	229	3245	125
H(81A)	-358	6256	4254	143
H(81B)	-304	6149	3263	143
H(81C)	14	7190	3794	143
H(10A)	1373	5197	4843	91
H(10B)	1534	4453	3990	91
H(10C)	1472	3452	4807	91
H(12A)	942	-1574	2296	88
H(12B)	1071	-2598	3073	88
H(12C)	1084	-3265	2148	88
H(14A)	2865	-2714	1082	98
H(14B)	2542	-1936	434	98
H(14C)	2448	-3595	747	98
H(16A)	2487	119	4027	80
H(16B)	2255	1495	3578	80
H(16C)	2725	960	3277	80