Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

First Structural Example of a Metal Un-coordinated Mesoionic Imidazo[1,5-a]pyridine and Its Precursor Intermediate Copper Complex: An Insight to The Catalytic Cycle

Suprakash Roy[a)], Saleem Javed[b)], Marilyn M. Olmstead[c)], Apurba K. Patra*[a]

[a)]*Department of Chemistry, National Institute of Technology Durgapur, Mahatma Gandhi Avenue, Durgapur 713 209, India*

[b)]*Department of Chemistry, Indian Institute of Technology, Kanpur 208 016, India*

[c)] *Department of Chemistry, University of California Davis, CA 95616 (USA)*

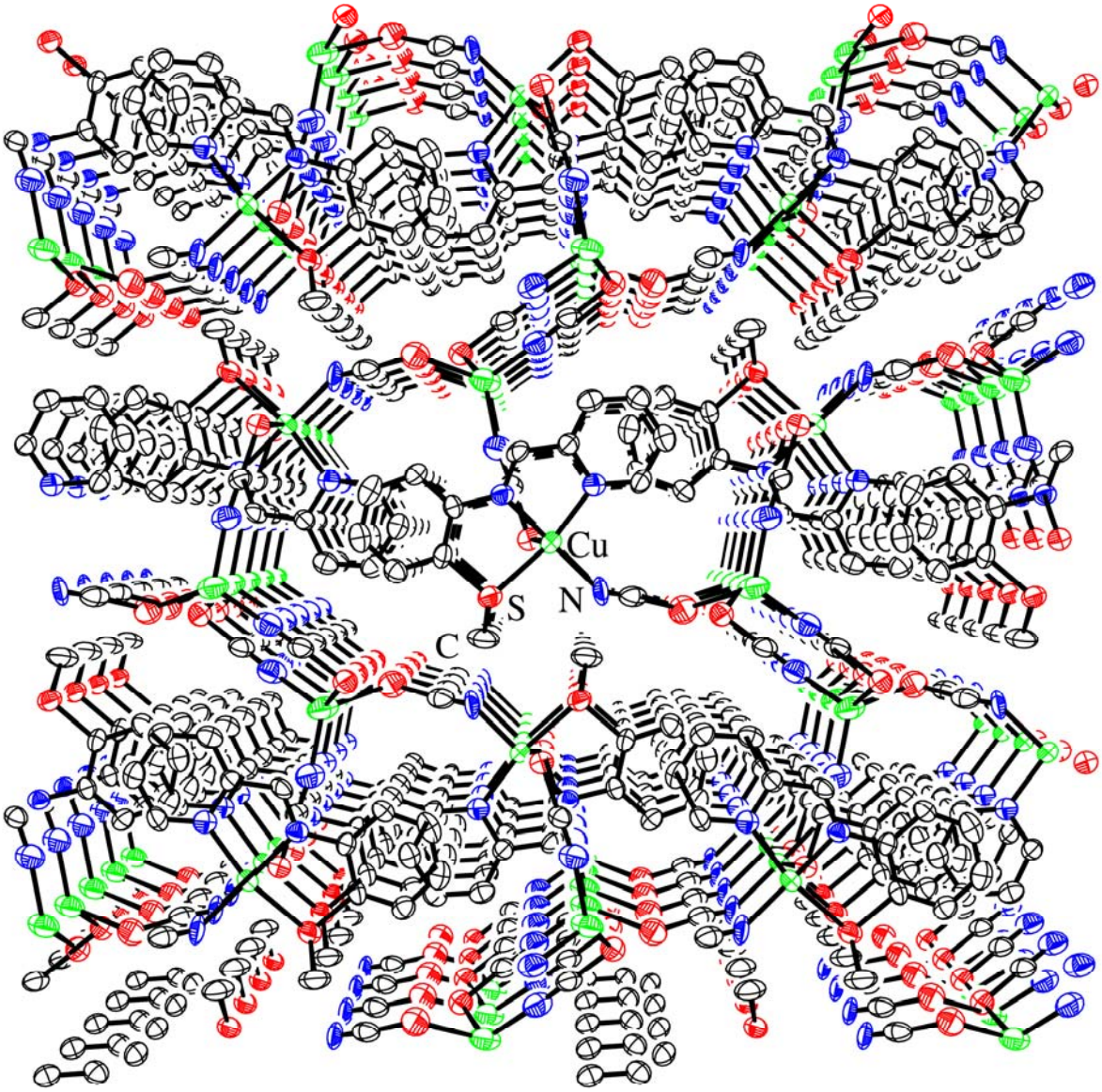


Fig. S1 ORTEP diagram of 3-dimensional network of $[(L^1)Cu_2(SCN)_3]_n$ (**1**) shown normal to 'a' axis (green: Cu, red: S, black: C, blue:N)

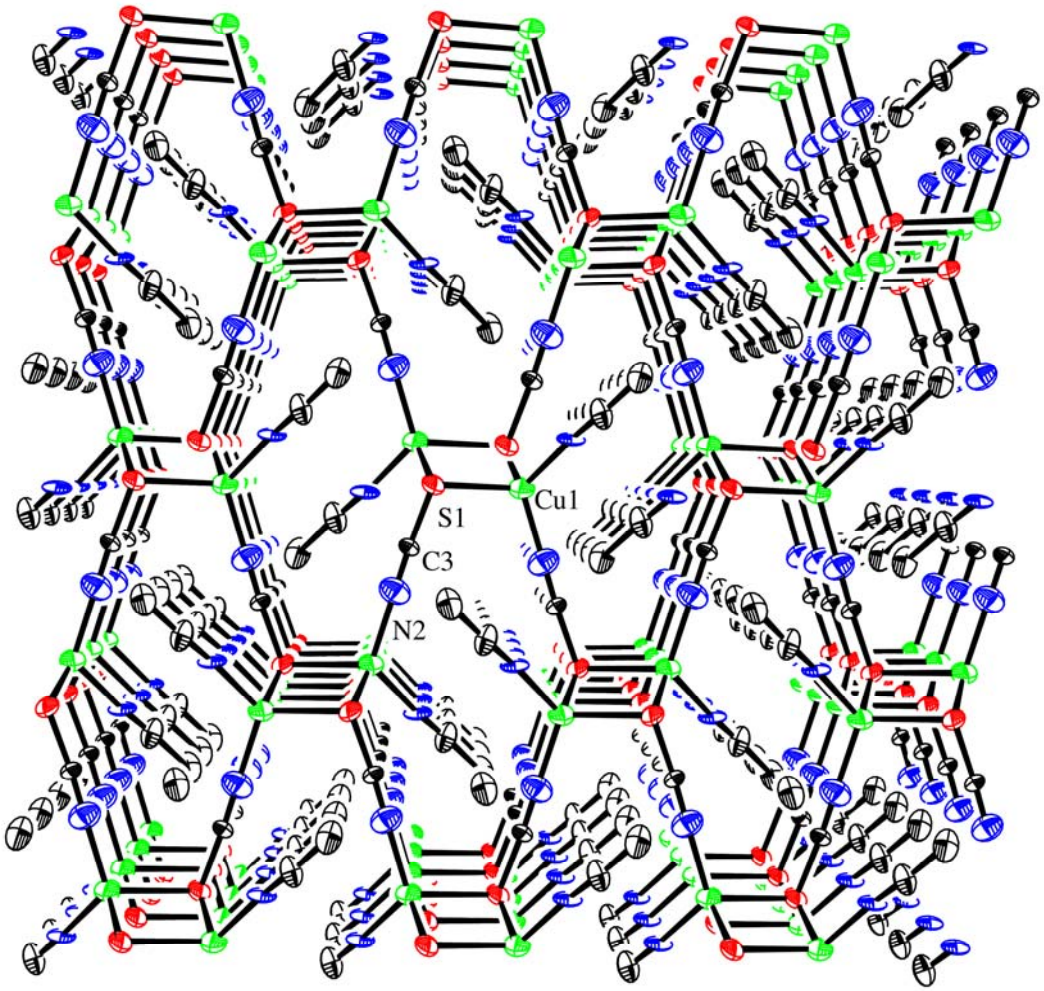


Fig. S2. ORTEP diagram of the polymeric 3-D network of **3**, Cu: green, N: blue, C: black, S: red; view normal to 'a' axis, 30% ellipsoid

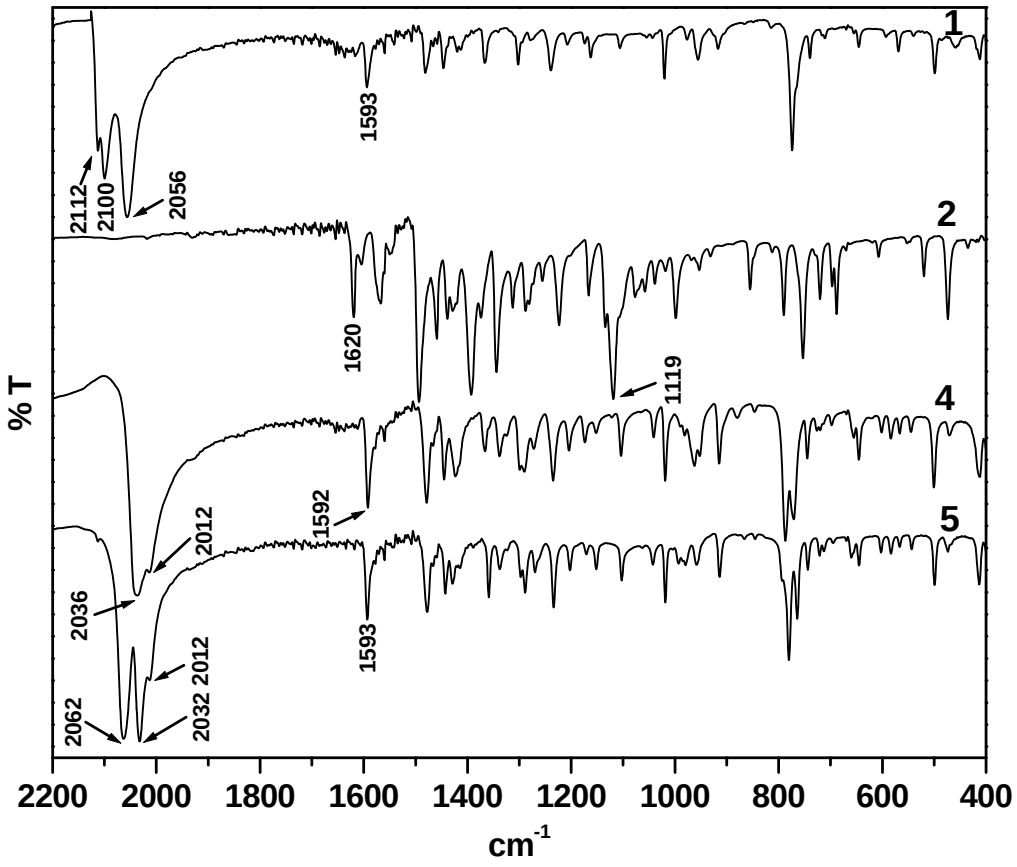


Fig. S3. FT-IR spectra of **1**, **2**, **4** and **5** (KBr disk)

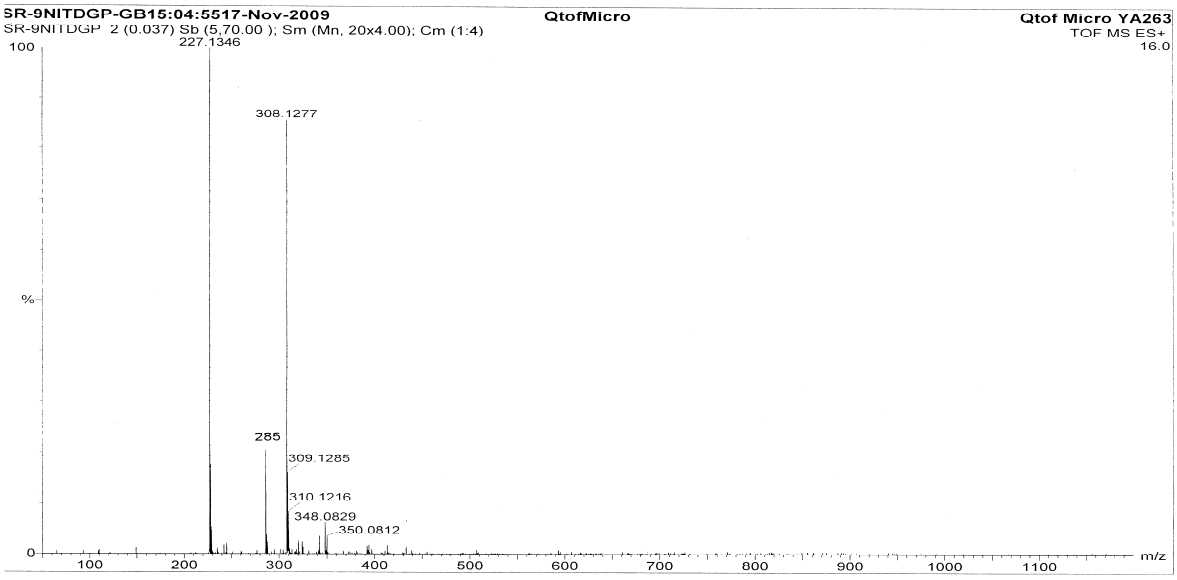


Fig. S4: Mass spectrum of **2**

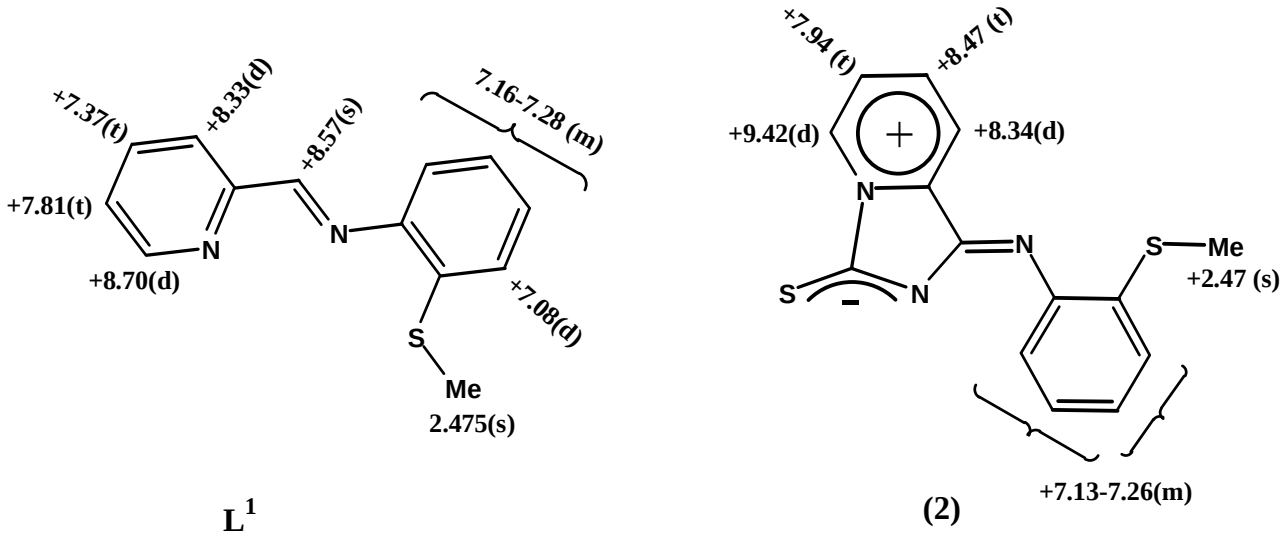


Fig. S5: ^{1}H NMR shifts of **2** compared to L^{1}, δ values are shown on their corresponding positions.

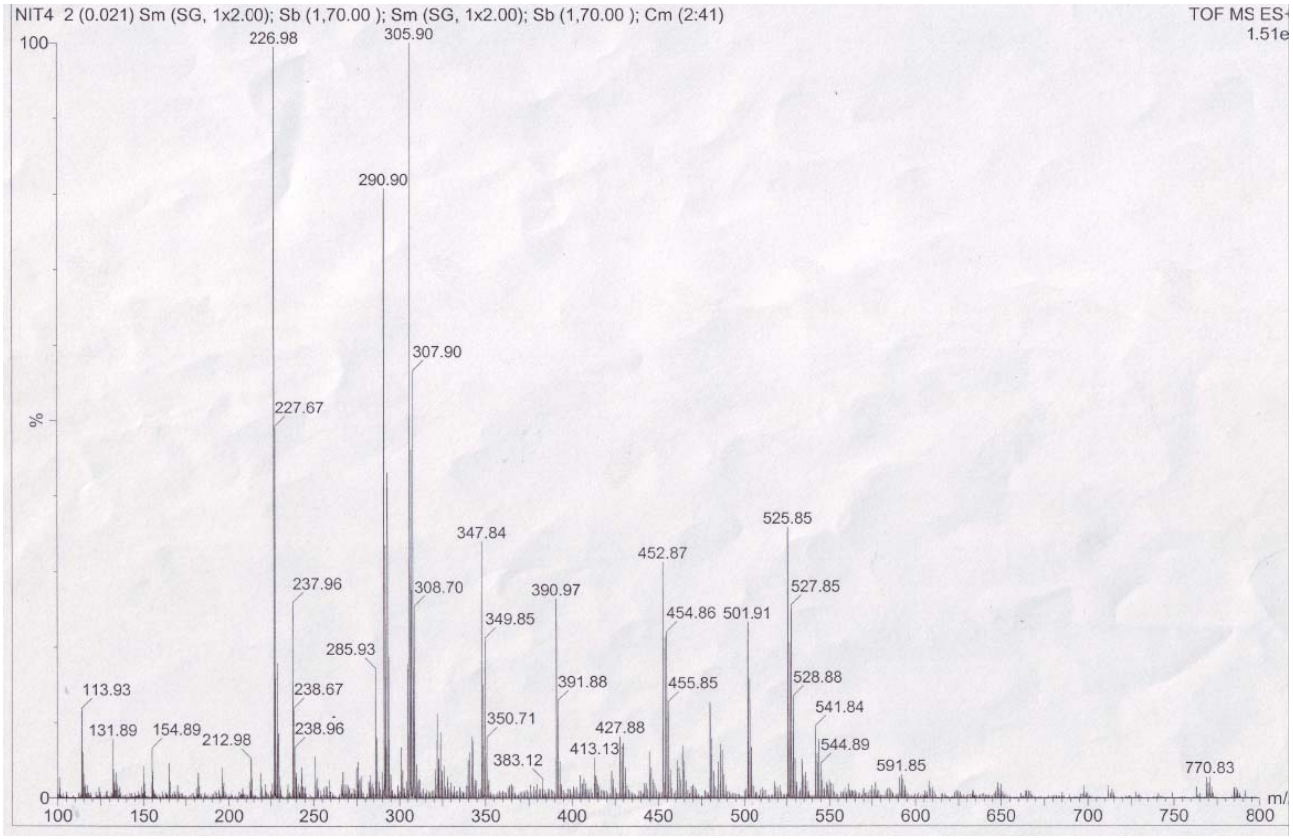
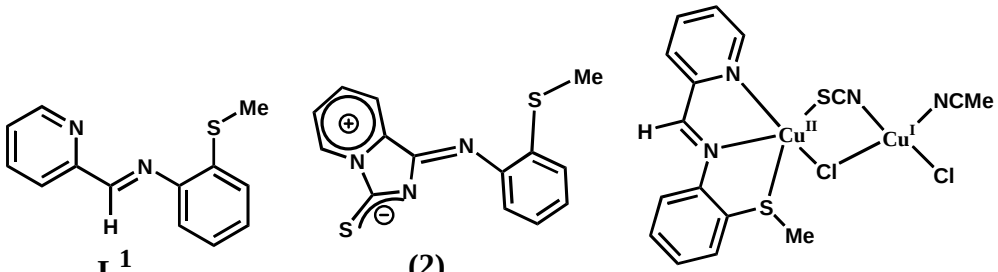


Fig. S6: Mass spectrum of the aliquot taken during the course of the reaction

$L^1 = C_{13}H_{12}N_2S = 228$, **2** + $1H^+ = 286$, L^1 + Cu = 291, **2** + $Na^+ = 308$, L1 + Cu + Cl^- = 326, **2** + Cu = 348, (L^1 + Cu + SCN + MeCN) + $1H^+ = 391$, L^1 + 2Cu + SCN + MeCN = 453, L^1 + Cu^{II} + μ_2-SCN +μ_2-Cl + Cu^I + Cl + MeCN + $1H^+ = 526$



L^1 **(2)** **Mass = 525**

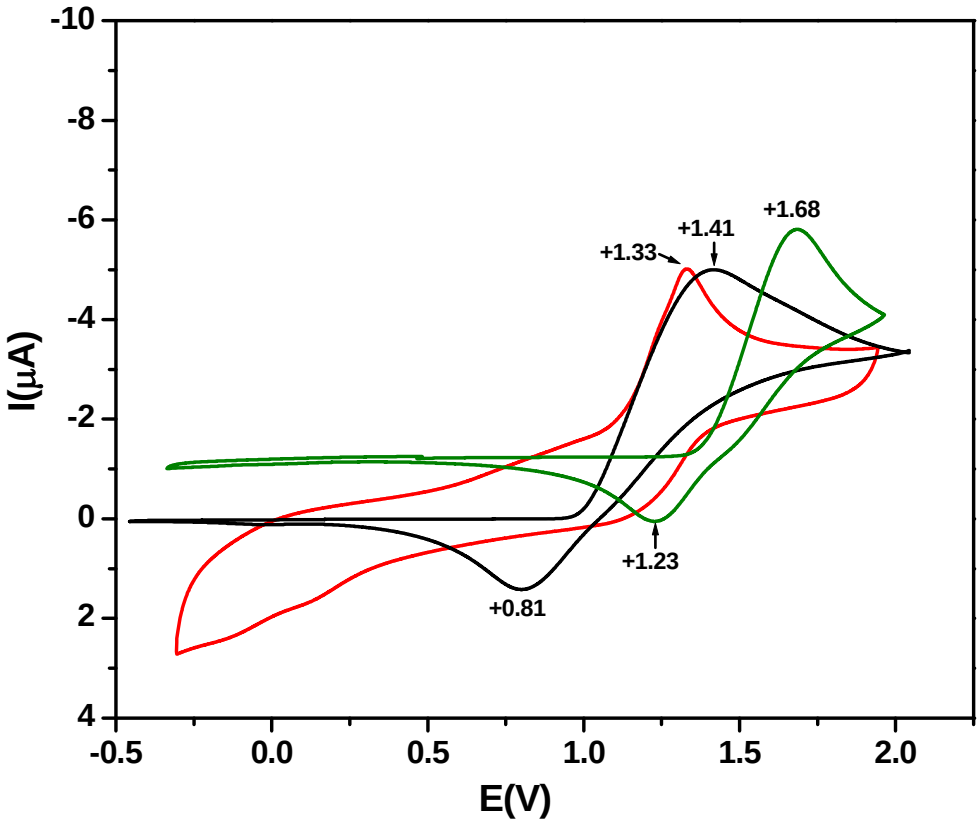


Fig. S7. Cyclic voltammogram (scan rate 50 mV/s) of LiCl (green trace), KSCN (black trace) and NaN3 (red trace) measured in MeCN solution of 0.1 M TBAP, using platinum as working electrode. Potentials are *vs* NHE.

Table S1. Crystal data and structure refinement for $[(L^1)Cu_2(SCN)_3]_n$ (**1**)

Identification code	sr8	
Empirical formula	C16 H12 Cu2 N5 S4	
Formula weight	529.63	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 6.7778(3) Å	α= 90°.
	b = 15.2422(8) Å	β= 90°.
	c = 18.9036(9) Å	γ = 90°.
Volume	1952.90(16) Å^3	
Z	4	
Density (calculated)	1.801 Mg/m^3	
Absorption coefficient	2.617 mm^{-1}	
F(000)	1060	
Crystal size	0.25 x 0.20 x 0.18 mm^3	
Theta range for data collection	1.72 to 23.29°.	
Index ranges	-7<=h<=7, -16<=k<=16, -21<=l<=21	
Reflections collected	19783	
Independent reflections	2816 [R(int) = 0.0692]	
Completeness to theta = 23.29°	99.8 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2816 / 0 / 245	
Goodness-of-fit on F^2	1.085	
Final R indices [I>2sigma(I)]	R1 = 0.0506, wR2 = 0.1184	
R indices (all data)	R1 = 0.0604, wR2 = 0.1249	
Absolute structure parameter	0.53(3)	
Largest diff. peak and hole	1.574 and -0.791 e.Å^{-3}	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for $[(L^1)Cu_2(SCN)_3]_n$ (**1**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	2159(2)	7791(1)	6602(1)	44(1)
Cu(2)	2031(2)	11541(1)	5937(1)	69(1)
S(1)	3094(4)	6674(1)	5800(1)	47(1)
S(2)	-1745(4)	7376(1)	6645(1)	48(1)
S(3)	-75(4)	10258(2)	5593(1)	66(1)
S(4)	5020(4)	11054(2)	5492(1)	51(1)
N(1)	2456(10)	8590(4)	7458(3)	41(2)
N(2)	2737(10)	6894(4)	7311(3)	39(2)
N(3)	-1945(13)	6787(5)	8035(4)	63(2)
N(4)	1842(14)	8711(5)	5881(4)	57(2)
N(5)	6059(13)	12464(6)	4617(4)	62(2)
C(1)	2287(13)	9457(5)	7509(4)	44(2)
C(2)	2371(12)	9890(5)	8159(4)	46(2)
C(3)	2654(13)	9409(5)	8756(4)	48(2)
C(4)	2823(13)	8515(6)	8714(4)	46(2)
C(5)	2740(13)	8115(5)	8061(4)	39(2)
C(6)	2880(13)	7185(5)	7951(4)	40(2)
C(7)	2779(12)	5991(5)	7132(4)	35(2)
C(8)	2694(13)	5305(5)	7615(4)	43(2)
C(9)	2563(12)	4457(6)	7374(5)	52(2)
C(10)	2515(13)	4268(5)	6673(5)	53(2)
C(11)	2612(12)	4928(5)	6187(4)	45(2)
C(12)	2770(13)	5794(4)	6408(4)	38(2)
C(13)	1115(17)	6532(7)	5168(5)	68(3)
C(14)	-1880(13)	7043(5)	7458(4)	42(2)
C(15)	1147(15)	9313(7)	5795(5)	55(3)
C(16)	5649(15)	11871(6)	4982(4)	50(2)

Table S3. Bond lengths [Å] and angles [°] for $[(L^1)Cu_2(SCN)_3]_n$ (**1**)

Cu(1)-N(2)	1.956(6)
Cu(1)-N(4)	1.966(8)
Cu(1)-N(1)	2.035(6)
Cu(1)-S(1)	2.367(2)
Cu(1)-S(2)	2.722(3)
Cu(2)-N(5)#1	1.958(9)
Cu(2)-N(3)#2	1.981(8)
Cu(2)-S(4)	2.315(3)
Cu(2)-S(3)	2.506(3)
S(1)-C(12)	1.780(7)
S(1)-C(13)	1.809(10)
S(2)-C(14)	1.622(9)
S(3)-C(15)	1.705(12)
S(4)-C(16)	1.632(10)
N(1)-C(1)	1.331(10)
N(1)-C(5)	1.365(9)
N(2)-C(6)	1.291(9)
N(2)-C(7)	1.417(9)
N(3)-C(14)	1.158(10)
N(3)-Cu(2)#3	1.981(8)
N(4)-C(15)	1.044(11)
N(5)-C(16)	1.170(11)
N(5)-Cu(2)#4	1.958(9)
C(1)-C(2)	1.396(11)
C(1)-H(1)	0.9300
C(2)-C(3)	1.359(11)
C(2)-H(2)	0.9300
C(3)-C(4)	1.370(11)
C(3)-H(3)	0.9300
C(4)-C(5)	1.377(11)
C(4)-H(4)	0.9300
C(5)-C(6)	1.437(10)
C(6)-H(6)	0.9300
C(7)-C(8)	1.389(10)
C(7)-C(12)	1.401(11)
C(8)-C(9)	1.373(12)
C(8)-H(8)	0.9300
C(9)-C(10)	1.356(13)
C(9)-H(9)	0.9300
C(10)-C(11)	1.365(12)
C(10)-H(10)	0.9300
C(11)-C(12)	1.389(11)
C(11)-H(11)	0.9300
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
N(2)-Cu(1)-N(4)	174.7(3)
N(2)-Cu(1)-N(1)	81.6(2)
N(4)-Cu(1)-N(1)	97.8(3)
N(2)-Cu(1)-S(1)	83.22(18)

N(4)-Cu(1)-S(1)	95.7(2)
N(1)-Cu(1)-S(1)	156.0(2)
N(2)-Cu(1)-S(2)	90.7(2)
N(4)-Cu(1)-S(2)	94.6(3)
N(1)-Cu(1)-S(2)	102.18(19)
S(1)-Cu(1)-S(2)	96.46(8)
N(5)#1-Cu(2)-N(3)#2	111.6(3)
N(5)#1-Cu(2)-S(4)	110.4(3)
N(3)#2-Cu(2)-S(4)	116.3(3)
N(5)#1-Cu(2)-S(3)	105.9(3)
N(3)#2-Cu(2)-S(3)	112.7(3)
S(4)-Cu(2)-S(3)	98.86(10)
C(12)-S(1)-C(13)	104.2(5)
C(12)-S(1)-Cu(1)	95.5(3)
C(13)-S(1)-Cu(1)	108.1(3)
C(14)-S(2)-Cu(1)	99.0(3)
C(15)-S(3)-Cu(2)	108.9(3)
C(16)-S(4)-Cu(2)	101.5(4)
C(1)-N(1)-C(5)	118.6(7)
C(1)-N(1)-Cu(1)	130.1(5)
C(5)-N(1)-Cu(1)	111.2(5)
C(6)-N(2)-C(7)	123.8(6)
C(6)-N(2)-Cu(1)	114.6(5)
C(7)-N(2)-Cu(1)	121.3(5)
C(14)-N(3)-Cu(2)#3	171.3(7)
C(15)-N(4)-Cu(1)	141.7(8)
C(16)-N(5)-Cu(2)#4	173.5(8)
N(1)-C(1)-C(2)	122.0(7)
N(1)-C(1)-H(1)	119.0
C(2)-C(1)-H(1)	119.0
C(3)-C(2)-C(1)	118.9(7)
C(3)-C(2)-H(2)	120.6
C(1)-C(2)-H(2)	120.6
C(2)-C(3)-C(4)	120.0(8)
C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0
C(3)-C(4)-C(5)	119.3(8)
C(3)-C(4)-H(4)	120.4
C(5)-C(4)-H(4)	120.4
N(1)-C(5)-C(4)	121.4(7)
N(1)-C(5)-C(6)	114.3(7)
C(4)-C(5)-C(6)	124.3(7)
N(2)-C(6)-C(5)	118.0(7)
N(2)-C(6)-H(6)	121.0
C(5)-C(6)-H(6)	121.0
C(8)-C(7)-C(12)	118.7(7)
C(8)-C(7)-N(2)	124.9(7)
C(12)-C(7)-N(2)	116.2(6)
C(9)-C(8)-C(7)	119.6(8)
C(9)-C(8)-H(8)	120.2
C(7)-C(8)-H(8)	120.2
C(10)-C(9)-C(8)	121.7(8)
C(10)-C(9)-H(9)	119.1
C(8)-C(9)-H(9)	119.1

C(9)-C(10)-C(11)	120.0(8)
C(9)-C(10)-H(10)	120.0
C(11)-C(10)-H(10)	120.0
C(10)-C(11)-C(12)	120.1(8)
C(10)-C(11)-H(11)	120.0
C(12)-C(11)-H(11)	120.0
C(11)-C(12)-C(7)	119.9(7)
C(11)-C(12)-S(1)	122.1(6)
C(7)-C(12)-S(1)	117.9(5)
S(1)-C(13)-H(13A)	109.5
S(1)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
S(1)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(3)-C(14)-S(2)	178.3(9)
N(4)-C(15)-S(3)	175.3(10)
N(5)-C(16)-S(4)	178.6(10)

Symmetry transformations used to generate equivalent atoms:
#1 x-1/2,-y+5/2,-z+1 #2 -x,y+1/2,-z+3/2 #3 -x,y-1/2,-z+3/2
#4 x+1/2,-y+5/2,-z+1

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for $[(L^1)Cu_2(SCN)_3]_n$ (**1**) The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	60(1)	37(1)	37(1)	6(1)	-1(1)	1(1)
Cu(2)	77(1)	86(1)	44(1)	11(1)	9(1)	26(1)
S(1)	55(1)	48(1)	39(1)	5(1)	5(1)	5(1)
S(2)	58(1)	46(1)	41(1)	2(1)	-3(1)	1(1)
S(3)	64(2)	70(2)	65(2)	2(1)	-13(1)	7(1)
S(4)	56(2)	50(1)	49(1)	0(1)	2(1)	5(1)
N(1)	37(4)	45(4)	41(4)	1(3)	0(3)	-7(3)
N(2)	40(4)	43(4)	33(3)	2(3)	3(3)	-3(3)
N(3)	65(6)	73(5)	50(5)	-4(4)	1(5)	-13(5)
N(4)	79(6)	20(3)	70(5)	-8(3)	27(5)	3(4)
N(5)	65(6)	74(6)	47(5)	-9(4)	5(4)	-22(4)
C(1)	49(6)	36(4)	47(5)	10(4)	-2(4)	-5(4)
C(2)	37(5)	41(4)	60(5)	-6(4)	-5(4)	4(4)
C(3)	48(6)	51(5)	44(5)	-5(4)	-6(4)	-2(4)
C(4)	40(5)	57(5)	41(4)	7(4)	-3(4)	-3(5)
C(5)	40(5)	38(4)	38(4)	3(3)	-2(4)	-2(4)
C(6)	42(5)	42(4)	37(4)	11(4)	-3(4)	14(5)
C(7)	32(4)	32(4)	42(4)	-4(3)	1(4)	2(4)
C(8)	49(5)	42(5)	39(4)	8(4)	-5(4)	5(4)
C(9)	34(6)	48(5)	75(6)	21(5)	-3(5)	-3(4)
C(10)	44(6)	41(4)	72(6)	-6(4)	1(5)	2(4)
C(11)	43(5)	46(5)	47(5)	-6(4)	0(4)	7(4)
C(12)	38(5)	29(4)	48(5)	6(3)	7(4)	5(4)
C(13)	84(8)	87(7)	32(5)	-7(5)	-10(5)	20(7)
C(14)	43(5)	45(5)	37(5)	-5(4)	4(4)	-4(4)
C(15)	64(7)	68(7)	35(5)	-1(5)	5(5)	-32(6)
C(16)	56(7)	59(6)	34(5)	-6(5)	-5(4)	-10(5)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for $[(L^1)Cu_2(SCN)_3]_n$ (**1**)

	x	y	z	U(eq)
H(1)	2108	9785	7099	53
H(2)	2236	10496	8183	55
H(3)	2732	9687	9193	57
H(4)	2993	8181	9121	55
H(6)	3068	6803	8329	49
H(8)	2725	5420	8098	52
H(9)	2506	4001	7700	63
H(10)	2415	3688	6524	63
H(11)	2573	4797	5706	54
H(13A)	1186	6986	4817	101
H(13B)	-130	6565	5409	101
H(13C)	1240	5970	4944	101

Table S6. Crystal data and structure refinement for **2**

Identification code	purple_final
Empirical formula	C14 H11 N3 S2
Formula weight	285.38
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 7.416(7) A a = 74.754(12) deg. b = 8.040(7) A b = 79.687(12) deg. c = 12.085(10) A g = 63.974(11) deg.
Volume	623.1(9) A^3
Z, Calculated density	2, 1.521 Mg/m^3
Absorption coefficient	0.414 mm^-1
F(000)	296
Crystal size	0.30 x 0.26 x 0.21 mm
Theta range for data collection	1.75 to 24.05 deg.
Limiting indices	-8<=h<=8, -9<=k<=9, -13<=l<=13
Reflections collected / unique	4047 / 1952 [R(int) = 0.0566]
Completeness to theta = 24.05	98.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1952 / 0 / 172
Goodness-of-fit on F^2	0.964
Final R indices [I>2sigma(I)]	R1 = 0.0638, wR2 = 0.1516
R indices (all data)	R1 = 0.0938, wR2 = 0.1704
Largest diff. peak and hole	0.669 and -0.393 e.A^-3

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(13)	1236(7)	2407(7)	4084(4)	34(1)
S(2)	3618(2)	7695(2)	-3854(1)	30(1)
S(1)	1720(2)	2881(2)	2549(1)	30(1)
N(1)	3556(5)	4402(5)	-2515(3)	23(1)
N(3)	2953(5)	6675(5)	-1525(3)	24(1)
C(6)	2800(6)	5120(6)	-759(4)	26(1)
N(2)	2399(5)	4746(5)	336(3)	25(1)
C(11)	1174(7)	6270(6)	3075(4)	31(1)
C(7)	1976(6)	5972(6)	1077(4)	24(1)
C(9)	1365(7)	8871(7)	1606(4)	32(1)
C(14)	3349(7)	6388(6)	-2583(4)	24(1)
C(1)	3981(7)	3485(6)	-3377(4)	28(1)
C(8)	1842(7)	7833(6)	772(4)	29(1)
C(4)	3238(7)	1858(6)	-1099(4)	27(1)
C(2)	4057(7)	1681(6)	-3097(4)	28(1)
C(12)	1610(6)	5192(6)	2237(4)	24(1)
C(5)	3195(7)	3661(6)	-1413(4)	26(1)
C(3)	3666(7)	865(6)	-1960(4)	29(1)
C(10)	1044(7)	8098(7)	2739(4)	33(1)

Table S8. Bond lengths [A] and angles [deg] for **2**

C(13)-S(1)	1.795(4)
S(2)-C(14)	1.651(5)
S(1)-C(12)	1.764(5)
N(1)-C(5)	1.340(6)
N(1)-C(1)	1.347(5)
N(1)-C(14)	1.516(5)
N(3)-C(14)	1.318(5)
N(3)-C(6)	1.383(6)
C(6)-N(2)	1.287(6)
C(6)-C(5)	1.480(6)
N(2)-C(7)	1.402(5)
C(11)-C(10)	1.382(6)
C(11)-C(12)	1.407(6)
C(7)-C(8)	1.406(6)
C(7)-C(12)	1.408(6)
C(9)-C(10)	1.373(7)
C(9)-C(8)	1.376(6)
C(1)-C(2)	1.378(6)
C(4)-C(3)	1.385(6)
C(4)-C(5)	1.386(6)
C(2)-C(3)	1.397(6)
C(12)-S(1)-C(13)	103.1(2)
C(5)-N(1)-C(1)	123.6(4)
C(5)-N(1)-C(14)	108.0(3)
C(1)-N(1)-C(14)	128.4(4)
C(14)-N(3)-C(6)	110.5(4)
N(2)-C(6)-N(3)	133.6(4)
N(2)-C(6)-C(5)	118.2(4)
N(3)-C(6)-C(5)	108.2(4)
C(6)-N(2)-C(7)	125.4(4)
C(10)-C(11)-C(12)	119.4(4)
N(2)-C(7)-C(8)	127.1(4)
N(2)-C(7)-C(12)	113.4(4)
C(8)-C(7)-C(12)	119.5(4)
C(10)-C(9)-C(8)	120.6(4)
N(3)-C(14)-N(1)	107.1(4)
N(3)-C(14)-S(2)	133.9(4)
N(1)-C(14)-S(2)	119.0(3)
N(1)-C(1)-C(2)	117.4(4)
C(9)-C(8)-C(7)	119.9(4)
C(3)-C(4)-C(5)	117.7(4)
C(1)-C(2)-C(3)	120.7(4)
C(11)-C(12)-C(7)	119.4(4)
C(11)-C(12)-S(1)	123.7(4)
C(7)-C(12)-S(1)	117.0(3)
N(1)-C(5)-C(4)	120.6(4)
N(1)-C(5)-C(6)	106.1(4)
C(4)-C(5)-C(6)	133.3(4)
C(4)-C(3)-C(2)	119.9(4)
C(9)-C(10)-C(11)	121.3(4)

Table S9. Anisotropic displacement parameters (A^2 x 10^3) for **2**
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(13)	50(3)	39(3)	18(3)	-2(2)	-4(2)	-24(3)
S(2)	45(1)	26(1)	24(1)	-4(1)	-1(1)	-19(1)
S(1)	41(1)	27(1)	24(1)	-5(1)	-1(1)	-17(1)
N(1)	28(2)	23(2)	21(2)	-5(2)	0(2)	-15(2)
N(3)	28(2)	21(2)	23(2)	-3(2)	-3(2)	-11(2)
C(6)	28(3)	21(3)	31(3)	-6(2)	-3(2)	-12(2)
N(2)	36(2)	23(2)	18(2)	-3(2)	-1(2)	-15(2)
C(11)	34(3)	30(3)	29(3)	-6(2)	-1(2)	-13(2)
C(7)	25(3)	26(3)	25(3)	-8(2)	-3(2)	-10(2)
C(9)	44(3)	26(3)	34(3)	-8(2)	-2(2)	-21(2)
C(14)	27(3)	23(2)	24(3)	-5(2)	-3(2)	-11(2)
C(1)	41(3)	29(3)	18(2)	-5(2)	-1(2)	-18(2)
C(8)	35(3)	26(3)	26(3)	-5(2)	1(2)	-15(2)
C(4)	36(3)	23(3)	25(3)	0(2)	-5(2)	-16(2)
C(2)	39(3)	26(3)	25(3)	-9(2)	-3(2)	-16(2)
C(12)	27(3)	20(2)	24(3)	-2(2)	-2(2)	-11(2)
C(5)	30(3)	28(3)	24(3)	-6(2)	0(2)	-16(2)
C(3)	38(3)	22(2)	33(3)	-6(2)	-3(2)	-18(2)
C(10)	35(3)	38(3)	32(3)	-17(2)	3(2)	-18(2)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **2**

	x	y	z	U(eq)
H(13A)	1266	1160	4342	51
H(13B)	-64	3321	4292	51
H(13C)	2248	2486	4438	51
H(11)	975	5757	3848	37
H(9)	1258	10108	1400	39
H(1)	4215	4048	-4134	33
H(8)	2075	8362	8	34
H(4)	2988	1333	-336	33
H(2)	4371	999	-3670	34
H(3)	3693	-343	-1782	35
H(10)	734	8818	3292	39

Table S11. Crystal data and structure refinement for **3**

Identification code	sr9
Empirical formula	C3 H3 Cu N2 S
Formula weight	162.67
Temperature	150(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions	a = 6.648(10) A alpha = 90 deg.
	b = 7.368(10) A beta = 105.08(3) deg.
	c = 11.379(16) A gamma = 90 deg.
Volume	538.2(13) A^3
Z, Calculated density	5, 2.510 Mg/m^3
Absorption coefficient	5.377 mm^-1
F(000)	400
Crystal size	0.15 x 0.11 x 0.13 mm
Theta range for data collection	4.21 to 22.73 deg.
Limiting indices	-7<=h<=7, -8<=k<=8, -11<=l<=12
Reflections collected / unique	2179 / 558 [R(int) = 0.1603]
Completeness to theta = 22.73	77.1 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	558 / 0 / 64
Goodness-of-fit on F^2	0.867
Final R indices [I>2sigma(I)]	R1 = 0.0604, wR2 = 0.0901
R indices (all data)	R1 = 0.1050, wR2 = 0.1006
Largest diff. peak and hole	0.461 and -0.325 e.A^-3

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **3**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(2)	4567(12)	2579(12)	7839(9)	53(2)
C(3)	3947(13)	3037(12)	6848(9)	33(2)
C(1)	8779(15)	4376(14)	11175(11)	42(3)
C(2)	10254(14)	5607(13)	11975(10)	52(3)
Cu(1)	5632(2)	1802(2)	9497(1)	51(1)
S(1)	2825(4)	3818(3)	5444(2)	42(1)
N(1)	7623(12)	3405(13)	10607(7)	45(2)

Table S13. Bond lengths [A] and angles [deg] for **3**.

N(2)-C(3)	1.145(11)
N(2)-Cu(1)	1.923(10)
C(3)-S(1)	1.680(10)
C(1)-N(1)	1.123(11)
C(1)-C(2)	1.466(14)
Cu(1)-N(1)	1.967(9)
Cu(1)-S(1)#1	2.420(4)
Cu(1)-S(1)#2	2.428(4)
S(1)-Cu(1)#3	2.420(4)
S(1)-Cu(1)#4	2.428(4)
C(3)-N(2)-Cu(1)	179.4(8)
N(2)-C(3)-S(1)	173.7(8)
N(1)-C(1)-C(2)	176.8(13)
N(2)-Cu(1)-N(1)	117.8(4)
N(2)-Cu(1)-S(1)#1	110.1(3)
N(1)-Cu(1)-S(1)#1	108.5(3)
N(2)-Cu(1)-S(1)#2	111.2(2)
N(1)-Cu(1)-S(1)#2	107.1(3)
S(1)#1-Cu(1)-S(1)#2	100.70(11)
C(3)-S(1)-Cu(1)#3	101.8(3)
C(3)-S(1)-Cu(1)#4	98.9(3)
Cu(1)#3-S(1)-Cu(1)#4	79.30(11)
C(1)-N(1)-Cu(1)	175.5(9)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y-1/2,-z+3/2 #2 x,-y+1/2,z+1/2
#3 -x+1,y+1/2,-z+3/2 #4 x,-y+1/2,z-1/2

Table S14. Anisotropic displacement parameters (A^2 x 10^3) for **3**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(2)	57(6)	62(7)	47(7)	11(5)	24(5)	0(5)
C(3)	54(6)	26(6)	19(6)	5(5)	12(5)	-6(4)
C(1)	39(7)	31(6)	58(8)	-10(6)	14(5)	2(5)
C(2)	35(6)	40(6)	59(8)	8(6)	-27(5)	-9(4)
Cu(1)	73(1)	43(1)	28(1)	1(1)	-6(1)	-7(1)
S(1)	57(2)	33(2)	25(2)	6(1)	-8(1)	-1(1)
N(1)	60(6)	52(6)	10(4)	-3(4)	-14(4)	-2(4)

Table S15. Crystal data and structure refinement for **4**.

Identification code	sr21
Empirical formula	C12 H12 Cl Cu N5 S
Formula weight	357.32
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P $\bar{1}$
Unit cell dimensions	a = 6.950(2) A alpha = 89.315(10) deg. b = 7.115(2) A beta = 83.557(9) deg. c = 14.846(5) A gamma = 79.712(9) deg.
Volume	717.7(4) A^3
Z, Calculated density	2, 1.654 Mg/m^3
Absorption coefficient	1.849 mm^-1
F(000)	362
Crystal size	0.33 x 0.30 x 0.22 mm
Theta range for data collection	1.38 to 24.68 deg.
Limiting indices	-8<=h<=8, -8<=k<=8, -17<=l<=17
Reflections collected / unique	8141 / 2439 [R(int) = 0.0554]
Completeness to theta = 24.68	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2439 / 0 / 238
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0405, wR2 = 0.0979
R indices (all data)	R1 = 0.0576, wR2 = 0.1054
Largest diff. peak and hole	0.663 and -0.448 e.A^-3

Table S16. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **4**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cu(1)	2056(1)	7013(1)	7600(1)	22(1)
S(1)	3051(2)	4773(2)	6400(1)	23(1)
Cl(1)	3290(2)	4844(2)	8780(1)	34(1)
N(3)	4174(5)	8498(5)	7273(3)	27(1)
N(4)	5281(6)	8161(5)	6635(3)	31(1)
N(5)	6453(7)	7884(6)	5995(3)	49(1)
C(7)	-635(6)	4368(5)	7198(3)	21(1)
C(12)	1005(6)	3564(6)	6609(3)	20(1)
C(10)	-601(7)	997(6)	6273(3)	28(1)
C(9)	-2243(7)	1827(6)	6844(3)	28(1)
C(11)	1021(7)	1869(6)	6154(3)	23(1)
C(8)	-2242(6)	3487(6)	7305(3)	23(1)
N(2)	-501(5)	6078(5)	7652(2)	21(1)
C(6)	-1897(7)	7014(6)	8183(3)	25(1)
C(5)	-1538(6)	8778(6)	8588(3)	24(1)
C(1)	786(7)	10713(6)	8693(3)	26(1)
C(3)	-2457(7)	11651(6)	9454(3)	30(1)
C(4)	-2952(7)	10005(7)	9115(3)	29(1)
C(2)	-564(7)	11984(6)	9241(3)	29(1)
N(1)	320(5)	9123(5)	8366(2)	22(1)
C(13)	2372(9)	6092(7)	5398(3)	30(1)

Table S17. Bond lengths [A] and angles [deg] for **4**.

Cu(1)-N(3)	1.975(4)
Cu(1)-N(2)	1.999(3)
Cu(1)-N(1)	2.022(3)
Cu(1)-S(1)	2.3634(13)
Cu(1)-Cl(1)	2.4468(14)
S(1)-C(12)	1.786(4)
S(1)-C(13)	1.812(5)
N(3)-N(4)	1.150(5)
N(4)-N(5)	1.174(6)
C(7)-C(8)	1.369(6)
C(7)-C(12)	1.395(6)
C(7)-N(2)	1.420(5)
C(12)-C(11)	1.387(6)
C(10)-C(11)	1.375(6)
C(10)-C(9)	1.387(6)
C(9)-C(8)	1.371(6)
N(2)-C(6)	1.271(5)
C(6)-C(5)	1.471(6)
C(5)-N(1)	1.361(5)
C(5)-C(4)	1.371(6)
C(1)-N(1)	1.342(5)
C(1)-C(2)	1.380(6)
C(3)-C(2)	1.379(7)
C(3)-C(4)	1.393(6)

N(3)-Cu(1)-N(2)	161.85(15)
N(3)-Cu(1)-N(1)	94.54(15)
N(2)-Cu(1)-N(1)	80.65(13)
N(3)-Cu(1)-S(1)	95.36(11)
N(2)-Cu(1)-S(1)	84.04(10)
N(1)-Cu(1)-S(1)	158.50(10)
N(3)-Cu(1)-Cl(1)	104.23(12)
N(2)-Cu(1)-Cl(1)	93.87(10)
N(1)-Cu(1)-Cl(1)	100.64(10)
S(1)-Cu(1)-Cl(1)	95.35(5)
C(12)-S(1)-C(13)	99.3(2)
C(12)-S(1)-Cu(1)	96.19(14)
C(13)-S(1)-Cu(1)	104.41(18)
N(4)-N(3)-Cu(1)	122.2(3)
N(3)-N(4)-N(5)	176.9(4)
C(8)-C(7)-C(12)	119.2(4)
C(8)-C(7)-N(2)	124.4(4)
C(12)-C(7)-N(2)	116.4(4)
C(11)-C(12)-C(7)	120.3(4)
C(11)-C(12)-S(1)	119.7(3)
C(7)-C(12)-S(1)	119.9(3)
C(11)-C(10)-C(9)	119.6(4)
C(8)-C(9)-C(10)	120.5(4)
C(10)-C(11)-C(12)	119.8(4)
C(7)-C(8)-C(9)	120.7(4)
C(6)-N(2)-C(7)	123.7(4)
C(6)-N(2)-Cu(1)	115.0(3)

C(7)-N(2)-Cu(1)	120.9(3)
N(2)-C(6)-C(5)	117.1(4)
N(1)-C(5)-C(4)	122.7(4)
N(1)-C(5)-C(6)	113.8(4)
C(4)-C(5)-C(6)	123.5(4)
N(1)-C(1)-C(2)	121.7(4)
C(2)-C(3)-C(4)	118.6(4)
C(5)-C(4)-C(3)	118.7(5)
C(3)-C(2)-C(1)	120.0(4)
C(1)-N(1)-C(5)	118.3(4)
C(1)-N(1)-Cu(1)	128.9(3)
C(5)-N(1)-Cu(1)	112.8(3)

Symmetry transformations used to generate equivalent atoms:

Table S18. Anisotropic displacement parameters (A^2 x 10^3) for **4**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	16(1)	27(1)	24(1)	-6(1)	-1(1)	-6(1)
S(1)	18(1)	28(1)	24(1)	-4(1)	-1(1)	-6(1)
Cl(1)	26(1)	39(1)	37(1)	-6(1)	-6(1)	-2(1)
N(3)	24(2)	32(2)	28(2)	-9(2)	0(2)	-13(2)
N(4)	33(2)	26(2)	39(3)	-1(2)	-10(2)	-18(2)
N(5)	50(3)	58(3)	46(3)	-16(2)	9(2)	-32(2)
C(7)	21(2)	19(2)	23(2)	-1(2)	-7(2)	-2(2)
C(12)	20(2)	23(2)	20(2)	5(2)	-4(2)	-7(2)
C(10)	33(3)	23(2)	30(3)	-1(2)	-9(2)	-6(2)
C(9)	26(3)	30(2)	33(3)	3(2)	-7(2)	-13(2)
C(11)	20(2)	23(2)	25(3)	-3(2)	-1(2)	0(2)
C(8)	16(2)	24(2)	26(3)	0(2)	-2(2)	1(2)
N(2)	15(2)	24(2)	21(2)	-4(2)	-2(2)	-2(1)
C(6)	18(2)	31(2)	25(3)	2(2)	1(2)	-3(2)
C(5)	22(2)	28(2)	23(3)	-2(2)	-5(2)	-3(2)
C(1)	29(3)	23(2)	28(3)	-2(2)	-6(2)	-5(2)
C(3)	36(3)	30(2)	21(3)	-6(2)	-2(2)	4(2)
C(4)	23(3)	36(3)	26(3)	-4(2)	-1(2)	-1(2)
C(2)	39(3)	22(2)	26(3)	0(2)	-10(2)	-4(2)
N(1)	20(2)	26(2)	20(2)	-3(2)	-3(2)	-3(2)
C(13)	34(3)	32(3)	24(3)	-5(2)	-4(2)	-11(3)

Table S19. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **4**.

	x	y	z	U(eq)
H(7)	-3070(60)	6740(50)	8370(30)	11(10)
H(5)	-3270(60)	3960(50)	7660(20)	7(10)
H(4)	-3360(60)	1380(50)	6900(20)	9(10)
H(8)	-340(60)	13190(60)	9420(30)	28(12)
H(2)	1940(60)	1360(50)	5830(30)	8(11)
H(6)	-4080(70)	9670(60)	9270(30)	22(12)
H(3)	-600(70)	-90(70)	5930(30)	39(13)
H(9)	2080(70)	10970(60)	8470(30)	28(12)
H(10)	-3350(70)	12570(60)	9820(30)	33(12)
H(13)	2390(60)	5320(60)	4910(30)	25(12)
H(14)	1200(80)	6600(70)	5480(30)	45(17)
H(15)	3200(70)	6840(60)	5310(30)	34(14)

Table S20. Torsion angles [deg] for **4**.

N(3)-Cu(1)-S(1)-C(12)	-174.19(17)
N(2)-Cu(1)-S(1)-C(12)	-12.42(16)
N(1)-Cu(1)-S(1)-C(12)	-57.1(3)
Cl(1)-Cu(1)-S(1)-C(12)	80.93(13)
N(3)-Cu(1)-S(1)-C(13)	-72.9(2)
N(2)-Cu(1)-S(1)-C(13)	88.9(2)
N(1)-Cu(1)-S(1)-C(13)	44.2(3)
Cl(1)-Cu(1)-S(1)-C(13)	-177.8(2)
N(2)-Cu(1)-N(3)-N(4)	-83.2(6)
N(1)-Cu(1)-N(3)-N(4)	-156.9(4)
S(1)-Cu(1)-N(3)-N(4)	4.0(4)
Cl(1)-Cu(1)-N(3)-N(4)	100.9(4)
Cu(1)-N(3)-N(4)-N(5)	-178(100)
C(8)-C(7)-C(12)-C(11)	-1.5(6)
N(2)-C(7)-C(12)-C(11)	178.4(4)
C(8)-C(7)-C(12)-S(1)	175.7(3)
N(2)-C(7)-C(12)-S(1)	-4.3(5)
C(13)-S(1)-C(12)-C(11)	84.1(4)
Cu(1)-S(1)-C(12)-C(11)	-170.1(3)
C(13)-S(1)-C(12)-C(7)	-93.2(4)
Cu(1)-S(1)-C(12)-C(7)	12.6(3)
C(11)-C(10)-C(9)-C(8)	-1.3(7)
C(9)-C(10)-C(11)-C(12)	0.3(7)
C(7)-C(12)-C(11)-C(10)	1.2(6)
S(1)-C(12)-C(11)-C(10)	-176.1(3)
C(12)-C(7)-C(8)-C(9)	0.5(6)
N(2)-C(7)-C(8)-C(9)	-179.5(4)
C(10)-C(9)-C(8)-C(7)	1.0(7)
C(8)-C(7)-N(2)-C(6)	-2.7(6)
C(12)-C(7)-N(2)-C(6)	177.3(4)
C(8)-C(7)-N(2)-Cu(1)	170.2(3)
C(12)-C(7)-N(2)-Cu(1)	-9.8(5)
N(3)-Cu(1)-N(2)-C(6)	-83.2(6)
N(1)-Cu(1)-N(2)-C(6)	-7.4(3)
S(1)-Cu(1)-N(2)-C(6)	-172.2(3)
Cl(1)-Cu(1)-N(2)-C(6)	92.8(3)
N(3)-Cu(1)-N(2)-C(7)	103.3(5)
N(1)-Cu(1)-N(2)-C(7)	179.1(3)
S(1)-Cu(1)-N(2)-C(7)	14.3(3)
Cl(1)-Cu(1)-N(2)-C(7)	-80.7(3)
C(7)-N(2)-C(6)-C(5)	-178.9(3)
Cu(1)-N(2)-C(6)-C(5)	7.8(5)
N(2)-C(6)-C(5)-N(1)	-3.0(6)
N(2)-C(6)-C(5)-C(4)	174.8(4)
N(1)-C(5)-C(4)-C(3)	-1.4(7)
C(6)-C(5)-C(4)-C(3)	-179.1(4)
C(2)-C(3)-C(4)-C(5)	0.3(7)
C(4)-C(3)-C(2)-C(1)	0.9(7)
N(1)-C(1)-C(2)-C(3)	-1.1(7)
C(2)-C(1)-N(1)-C(5)	0.0(6)
C(2)-C(1)-N(1)-Cu(1)	-177.2(3)
C(4)-C(5)-N(1)-C(1)	1.3(6)

C(6)-C(5)-N(1)-C(1)	179.2(4)
C(4)-C(5)-N(1)-Cu(1)	178.9(3)
C(6)-C(5)-N(1)-Cu(1)	-3.2(4)
N(3)-Cu(1)-N(1)-C(1)	-14.8(4)
N(2)-Cu(1)-N(1)-C(1)	-177.2(4)
S(1)-Cu(1)-N(1)-C(1)	-132.0(3)
Cl(1)-Cu(1)-N(1)-C(1)	90.6(4)
N(3)-Cu(1)-N(1)-C(5)	167.8(3)
N(2)-Cu(1)-N(1)-C(5)	5.5(3)
S(1)-Cu(1)-N(1)-C(5)	50.6(5)
Cl(1)-Cu(1)-N(1)-C(5)	-86.7(3)

Symmetry transformations used to generate equivalent atoms:

Table S21. Crystal data and structure refinement for **5**.

Identification code	sr24
Empirical formula	C3.50 H3 Cu N1.50 S
Formula weight	161.67
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, $P\ 2_1/c$
Unit cell dimensions	a = 9.9433(8) A alpha = 90 deg. b = 10.6557(8) A beta = 90.237(2) deg. c = 14.4837(11) A gamma = 90 deg.
Volume	1534.6(2) A^3
Z, Calculated density	4, 0.700 Mg/m^3
Absorption coefficient	1.508 mm^-1
F(000)	318
Crystal size	0.14 x 0.12 x 0.10 mm
Theta range for data collection	2.05 to 20.09 deg.
Limiting indices	-9<=h<=9, -8<=k<=10, -13<=l<=14
Reflections collected / unique	10735 / 1450 [R(int) = 0.0893]
Completeness to theta = 20.09	99.9 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1450 / 0 / 209
Goodness-of-fit on F^2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0395, wR2 = 0.0859
R indices (all data)	R1 = 0.0584, wR2 = 0.0939
Largest diff. peak and hole	0.319 and -0.421 e.A^-3

Table S22. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **5**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
N(6)	7812(6)	2749(6)	5171(4)	19(2)
C(14)	7079(9)	3109(7)	4740(6)	21(2)
S(3)	5885(2)	3698(2)	4013(2)	42(1)
Cu(1)	8996(1)	2474(1)	6387(1)	19(1)
S(1)	7558(2)	3548(2)	7443(1)	21(1)
C(12)	7971(7)	5082(6)	7044(4)	14(2)
C(7)	9194(6)	5262(6)	6596(4)	13(2)
C(8)	9614(7)	6463(7)	6369(5)	21(2)
C(11)	7147(7)	6092(7)	7226(5)	21(2)
C(10)	7558(7)	7285(7)	6975(5)	21(2)
C(9)	8789(7)	7454(7)	6565(4)	20(2)
N(2)	9912(6)	4152(5)	6368(4)	17(1)
C(6)	11144(7)	4129(7)	6107(5)	20(2)
C(4)	12995(7)	2774(7)	5520(5)	21(2)
C(2)	12582(7)	576(7)	5430(5)	24(2)
C(3)	13445(7)	1570(7)	5306(5)	22(2)
C(1)	11292(7)	805(7)	5752(4)	17(2)
C(5)	11703(7)	2913(6)	5845(5)	18(2)
N(1)	10848(6)	1946(5)	5961(4)	17(2)
N(5)	6074(7)	260(6)	6563(4)	29(2)
N(3)	8401(6)	764(5)	6707(4)	22(2)
N(4)	7214(8)	534(5)	6632(4)	25(2)
C(13)	5850(7)	3402(7)	7019(5)	32(2)

Table S23. Bond lengths [A] and angles [deg] for **5**.

N(6)-C(14)	1.031(8)
N(6)-Cu(1)	2.135(7)
C(14)-S(3)	1.703(10)
Cu(1)-N(3)	1.971(6)
Cu(1)-N(2)	2.007(5)
Cu(1)-N(1)	2.025(6)
Cu(1)-S(1)	2.3895(19)
S(1)-C(12)	1.782(7)
S(1)-C(13)	1.810(7)
C(12)-C(11)	1.379(9)
C(12)-C(7)	1.394(9)
C(7)-C(8)	1.387(9)
C(7)-N(2)	1.421(8)
C(8)-C(9)	1.368(9)
C(11)-C(10)	1.384(9)
C(10)-C(9)	1.375(9)
N(2)-C(6)	1.283(8)
C(6)-C(5)	1.461(9)
C(4)-C(5)	1.378(9)
C(4)-C(3)	1.394(10)
C(2)-C(3)	1.375(9)
C(2)-C(1)	1.389(9)
C(1)-N(1)	1.329(8)
C(5)-N(1)	1.347(8)
N(5)-N(4)	1.175(9)
N(3)-N(4)	1.209(8)

C(14)-N(6)-Cu(1)	159.4(7)
N(6)-C(14)-S(3)	179.1(9)
N(3)-Cu(1)-N(2)	164.4(2)
N(3)-Cu(1)-N(1)	95.1(2)
N(2)-Cu(1)-N(1)	80.2(2)
N(3)-Cu(1)-N(6)	99.0(2)
N(2)-Cu(1)-N(6)	96.6(2)
N(1)-Cu(1)-N(6)	106.6(2)
N(3)-Cu(1)-S(1)	96.41(18)
N(2)-Cu(1)-S(1)	81.67(17)
N(1)-Cu(1)-S(1)	151.11(17)
N(6)-Cu(1)-S(1)	97.64(17)
C(12)-S(1)-C(13)	100.8(3)
C(12)-S(1)-Cu(1)	95.3(2)
C(13)-S(1)-Cu(1)	107.7(2)
C(11)-C(12)-C(7)	120.2(6)
C(11)-C(12)-S(1)	121.0(5)
C(7)-C(12)-S(1)	118.7(5)
C(8)-C(7)-C(12)	120.1(6)
C(8)-C(7)-N(2)	124.1(6)
C(12)-C(7)-N(2)	115.7(6)
C(9)-C(8)-C(7)	118.8(7)
C(12)-C(11)-C(10)	119.3(6)
C(9)-C(10)-C(11)	119.9(7)
C(8)-C(9)-C(10)	121.6(7)

C(6)-N(2)-C(7)	124.4(6)
C(6)-N(2)-Cu(1)	114.9(5)
C(7)-N(2)-Cu(1)	120.6(4)
N(2)-C(6)-C(5)	117.2(6)
C(5)-C(4)-C(3)	118.3(6)
C(3)-C(2)-C(1)	119.1(7)
C(2)-C(3)-C(4)	118.6(6)
N(1)-C(1)-C(2)	123.1(7)
N(1)-C(5)-C(4)	123.4(6)
N(1)-C(5)-C(6)	113.9(6)
C(4)-C(5)-C(6)	122.7(7)
C(1)-N(1)-C(5)	117.5(6)
C(1)-N(1)-Cu(1)	128.9(5)
C(5)-N(1)-Cu(1)	113.6(4)
N(4)-N(3)-Cu(1)	117.4(5)
N(5)-N(4)-N(3)	177.3(7)

Symmetry transformations used to generate equivalent atoms:

Table S24. Anisotropic displacement parameters (A^2 x 10^3) for **5**.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
N(6)	24(4)	10(4)	22(4)	-4(3)	6(3)	-8(3)
C(14)	31(6)	8(5)	25(6)	-7(4)	18(5)	-15(4)
S(3)	39(1)	39(2)	48(2)	5(1)	-6(1)	3(1)
Cu(1)	19(1)	10(1)	27(1)	0(1)	1(1)	-1(1)
S(1)	24(1)	11(1)	27(1)	2(1)	5(1)	-2(1)
C(12)	17(4)	9(4)	15(4)	-3(3)	-7(4)	1(4)
C(7)	12(4)	11(5)	16(4)	-2(3)	-2(4)	5(4)
C(8)	23(4)	15(5)	24(5)	-5(4)	-1(4)	-2(4)
C(11)	24(5)	20(5)	20(4)	0(4)	-3(4)	-5(4)
C(10)	20(4)	21(5)	21(4)	-1(4)	-3(4)	6(4)
C(9)	30(5)	6(4)	22(4)	4(4)	-7(4)	0(4)
N(2)	17(4)	15(4)	18(4)	0(3)	-1(3)	-1(3)
C(6)	22(5)	14(5)	24(5)	-1(4)	-1(4)	-9(4)
C(4)	15(5)	23(5)	25(5)	5(4)	-3(4)	-3(4)
C(2)	34(5)	11(5)	26(5)	5(4)	0(4)	2(4)
C(3)	23(5)	22(5)	21(4)	1(4)	-1(4)	9(4)
C(1)	22(5)	18(5)	10(4)	3(3)	-5(4)	-4(4)
C(5)	22(5)	10(5)	21(5)	2(3)	-3(4)	-1(4)
N(1)	22(4)	5(4)	24(4)	-2(3)	-4(3)	1(3)
N(5)	27(4)	18(4)	41(4)	-2(3)	12(4)	-4(3)
N(3)	15(4)	7(4)	44(4)	-3(3)	-3(3)	0(3)
N(4)	46(5)	8(4)	22(4)	1(3)	9(4)	2(4)
C(13)	21(5)	16(5)	58(6)	-6(4)	13(4)	-3(4)

Table S25. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **5**.

	x	y	z	U(eq)
H(5)	10442	6593	6088	25
H(2)	6323	5973	7515	25
H(3)	7003	7971	7084	25
H(4)	9068	8263	6417	24
H(7)	11659	4857	6086	24
H(9)	13554	3467	5446	25
H(11)	12860	-238	5300	28
H(10)	14310	1442	5083	27
H(12)	10711	128	5824	20
H(14A)	5262	3901	7393	48
H(14B)	5576	2539	7048	48
H(14C)	5805	3687	6391	48