Amido-bridged Cu_2N_2 diamond cores that minimize structural reorganization and facilitate reversible redox behavior between a Cu^1Cu^1 and a Class III delocalized $Cu^{1.5}Cu^{1.5}$ species.

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Supporting Information

S2 Graph 1: Plot of chemical shift (Hz) vs. X_2 from electron self-exchange experiments.
Graph 2: Plot of W_2, W_3, and W_{23} vs. X_2 from electron self-exchange experiments.

S3 Electronic structure calculation of **3**

S4 Figure 1: Cyclic voltammetry of **2** in THF and CH_2Cl_2.

S5 Figure 2: X-band EPR spectrum (9.38 GHz) of **3** at 5.2 K and simulation.

S6 Figure 3: $\chi_m T$ versus T for $[(SNS)Cu]_2[B(C_6H_3(CF_3)_2)_4]$, **3**

S7 Figure 4. Fully labeled drawing of $[(SNS)Cu]_2$, **2**

S8 Figure 5. Drawing of $[(SNS)Cu]_2[B(C_8H_3(CF_3)_2)_4]$, **3**

S9 Figure 6. Fully labeled drawing of $[(SNS)Cu]_2[B(C_8H_3(CF_3)_2)_4]$, anion omitted, **3**

S10 Figure 7. Fully labeled drawing of (SNS)CuCl, **4**

S11 Table 1. Crystal data and structure refinement for **2**

S12 Table 2. Atomic coordinates and equivalent isotropic displacement parameters for **2**

S13 Table 3. Bond lengths and angles for **2**

S16 Table 4. Anisotropic parameters for **2**

S17 Table 5. Hydrogen coordinates and isotropic displacement parameters for **2**

S18 Table 6. Crystal data and structure refinement for **3**

S19 Table 7. Atomic coordinates and equivalent isotropic displacement parameters for **3**

S22 Table 8. Bond lengths and angles for **3**

S28 Table 9. Anisotropic parameters for **3**

S31 Table 10. Hydrogen coordinates and isotropic displacement parameters for **3**

S33 Table 11. Crystal data and structure refinement for **4**

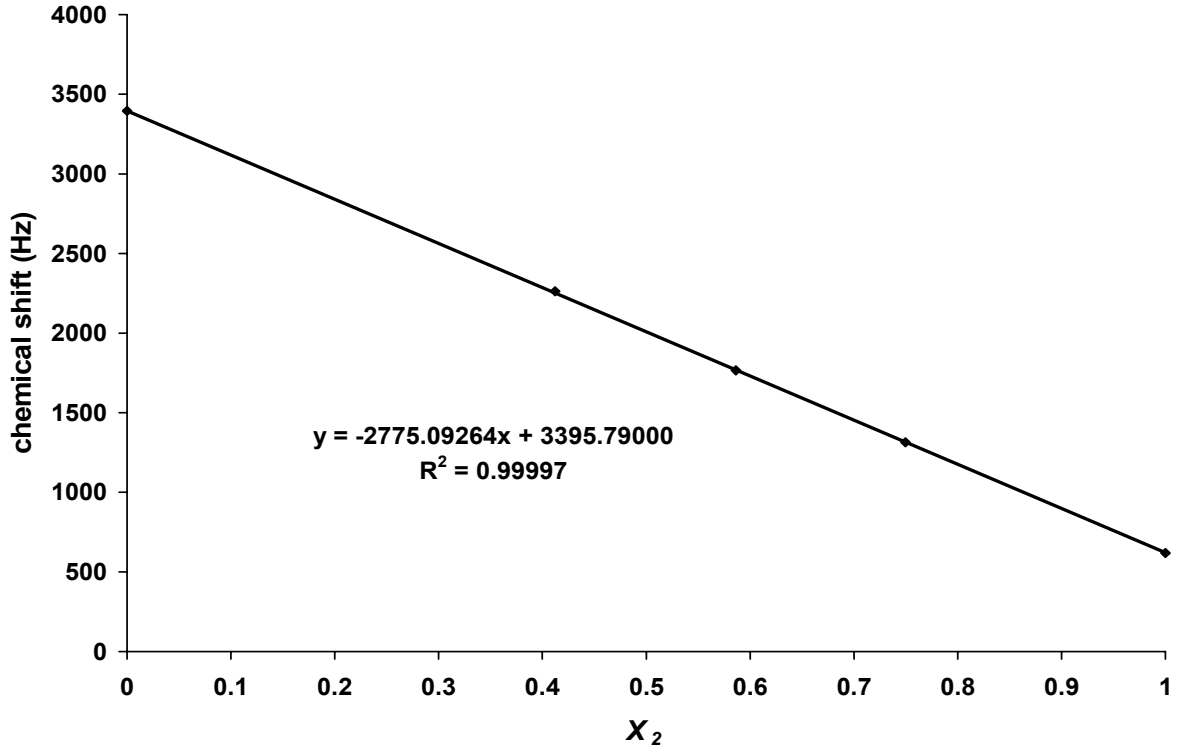
S34 Table 12. Atomic coordinates and equivalent isotropic displacement parameters for **4**

S35 Table 13. Bond lengths and angles for **4**

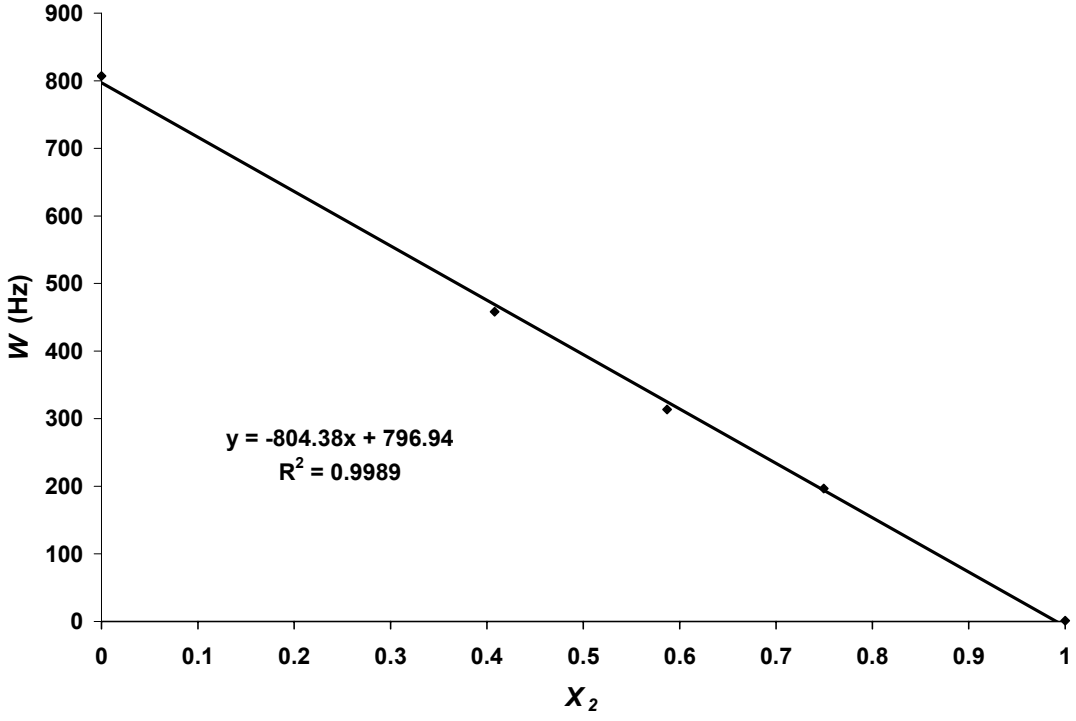
S37 Table 14. Anisotropic parameters for **4**

S38 Table 15. Hydrogen coordinates and isotropic displacement parameters for **4**

Graph 1: Plot of chemical shift (Hz) vs. χ_2 from electron self-exchange experiments.

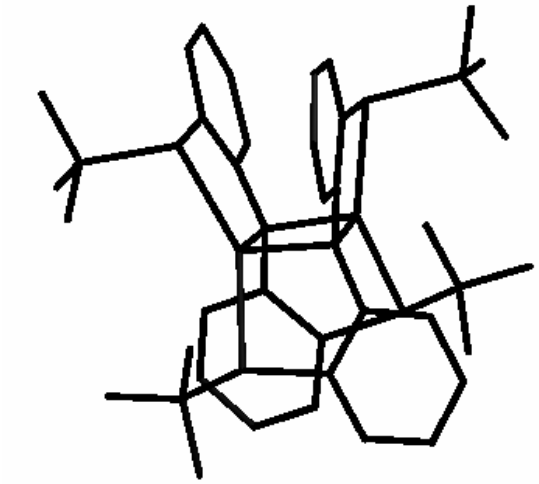


Graph 2: Plot of W_2, W_3, and W_{23} vs. χ_2 from electron self-exchange experiments.

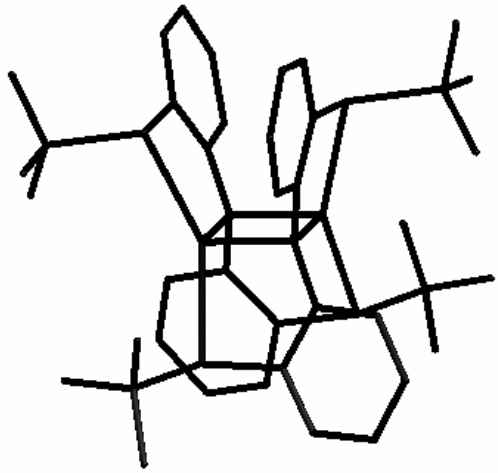


Electronic Structure Calculations. A hybrid density functional calculation was performed for complex **3** using Jaguar (version 4.0, release 20). The method used B3LYP with LACVP** as the basis set. A geometry optimization was carried out starting from coordinates based on the solid-state structure of cationic **3** that had been determined by an X-ray diffraction study. No symmetry constraints were imposed and the calculation was performed assuming a doublet electronic state. Optimization was considered converged when energy changes in successive iterations fell below 0.03 Kcal/mol.

Interatomic Distances (Å)	**From X-ray**	**From DFT**
Cu1-Cu2	2.4724 (4)	2.502
Cu1-N1	2.0887(16)	2.178
Cu1-N2	2.1011(17)	2.171
Cu1-S2	2.2805(6)	2.381
Cu1-S3	2.2805(6)	2.382
Cu2-N1	2.0641(16)	2.170
Cu2-N2	2.0568(16)	2.164
Cu2-S4	2.2797(6)	2.383
Cu2-S1	2.2834(6)	2.387
Interatomic Angles (deg.)		
Cu1-N1-Cu2	73.07(5)	70.38
Cu1-N2-Cu2	72.96(5)	70.36
N1-Cu1-N2	105.53(6)	109.35
N1-Cu2-N2	108.09(6)	109.91
S3-Cu1-S2	150.50(2)	150.45
S1-Cu2-S4	150.71(2)	150.16

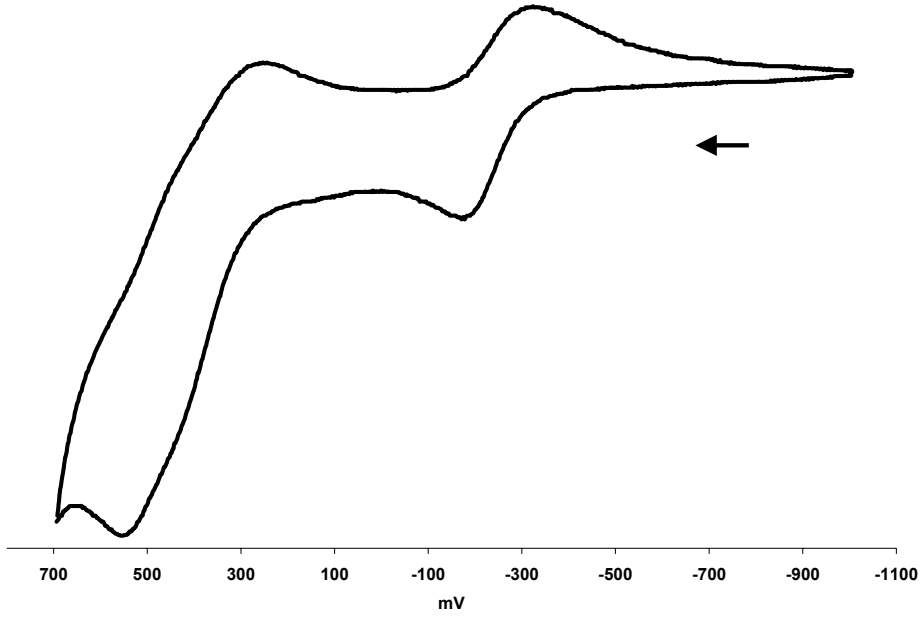


X-Ray



DFT

Figure 1: Cyclic voltamogram of **2** in THF (top) (0.35 M [^{n}Bu$_4$N][PF$_6$], 50 mV/s) and CH_2Cl_2 (0.30 M [^{n}Bu$_4$N][PF$_6$], 50 mV/s) (bottom), both referenced vs. Fc^+/Fc.



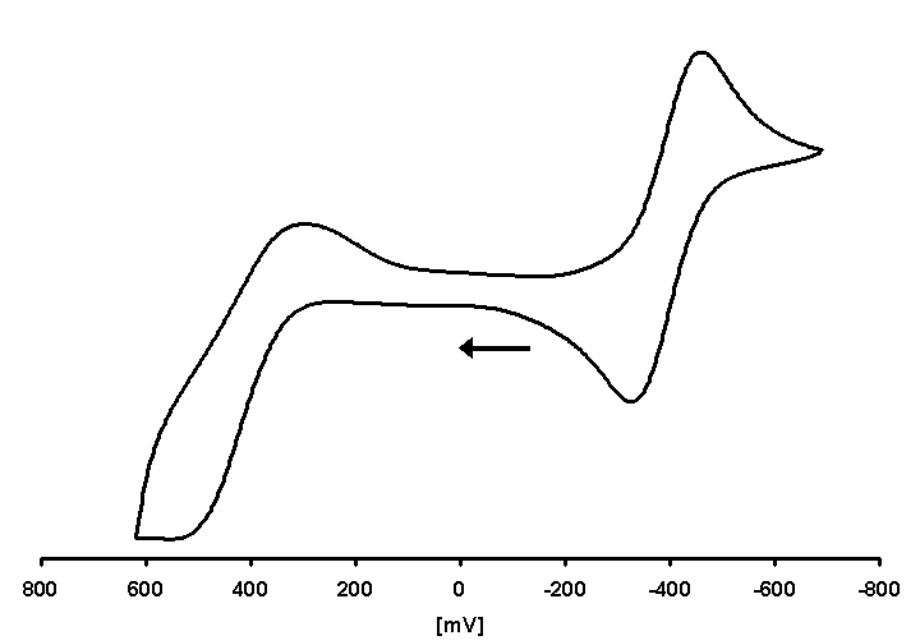


Figure 2: X-band EPR spectrum (9.38 GHz) of **3** at 5.2 K in 2-methyltetrahydrofuran (upper trace). Parameters used to obtain the simulated spectrum (lower trace): $g_1 = 2.013$, $g_2 = 2.065$, $g_3 = 2.069$, $A_1^{Cu} = 10$ G, $A_2^{Cu} = 18.5$ G, $A_3^{Cu} = 44$ G.

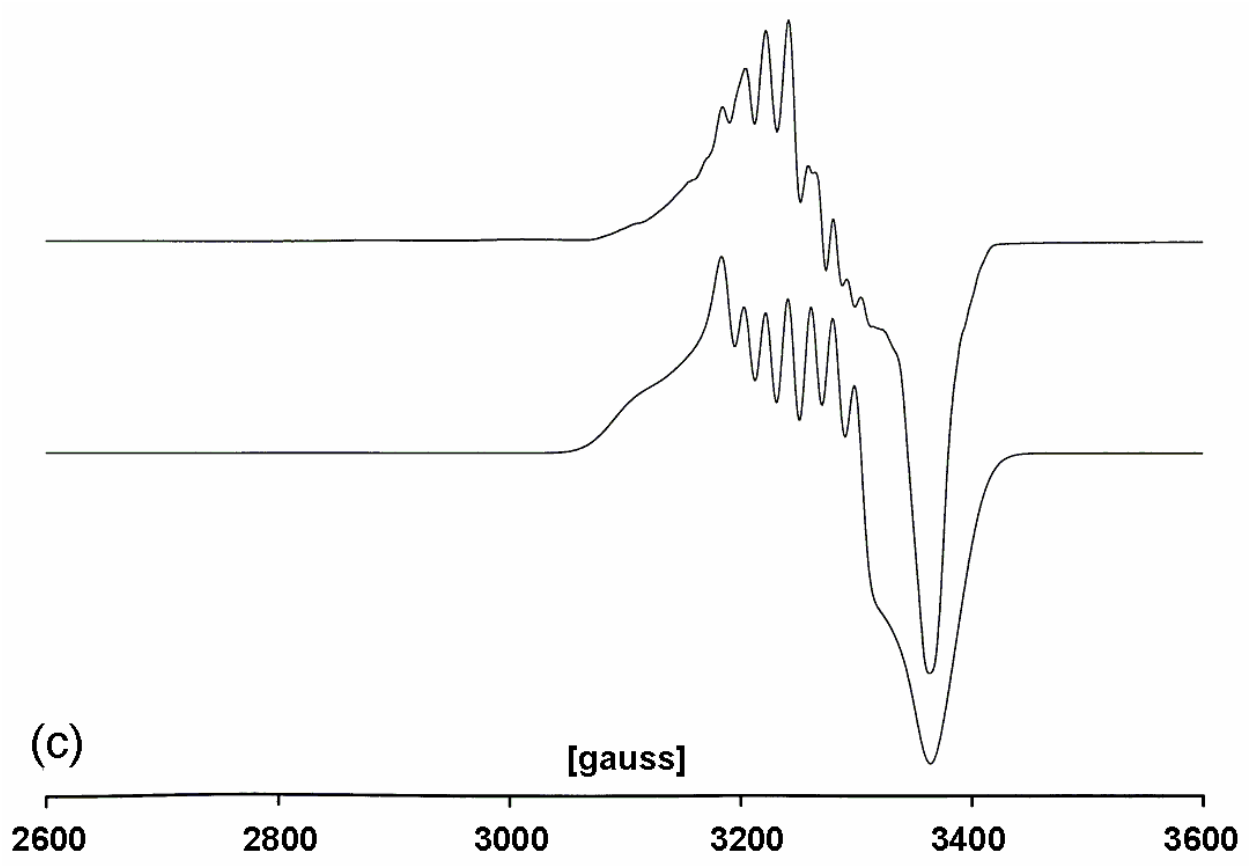


Figure 3: $\chi_m T$ versus T for $[(SNS)Cu]_2[B(C_6H_3(CF_3)_2)_4]$, **3.**

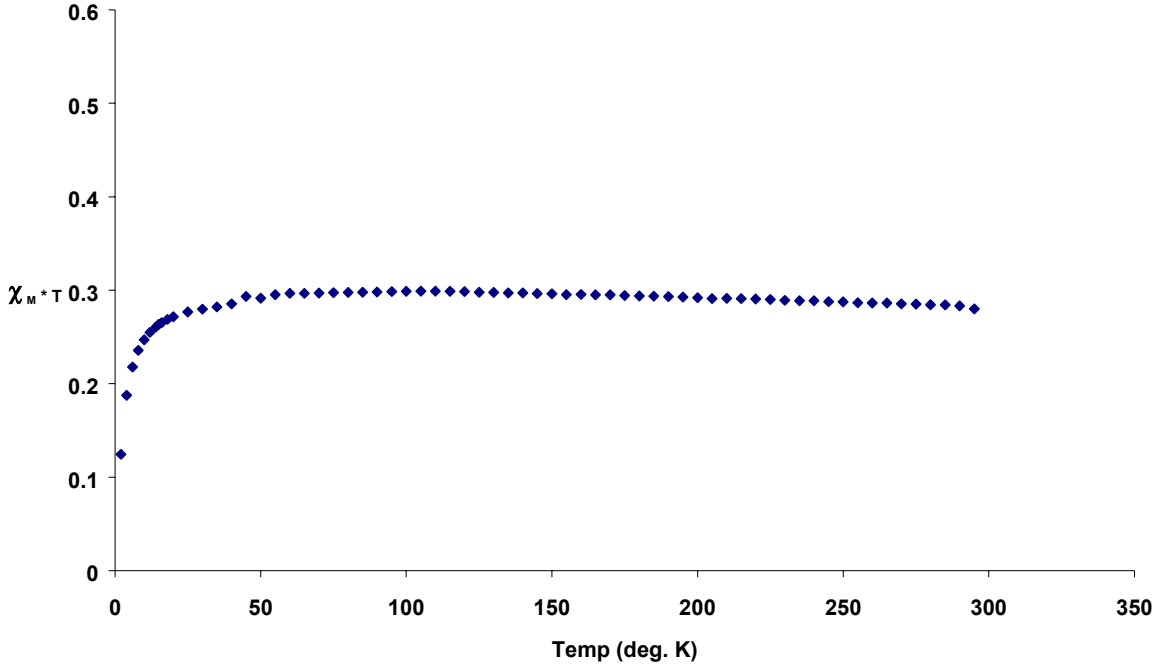


Figure 4. Fully labeled drawing of $[(SNS)Cu]_2$, **2**. Hydrogens have been omitted for clarity.

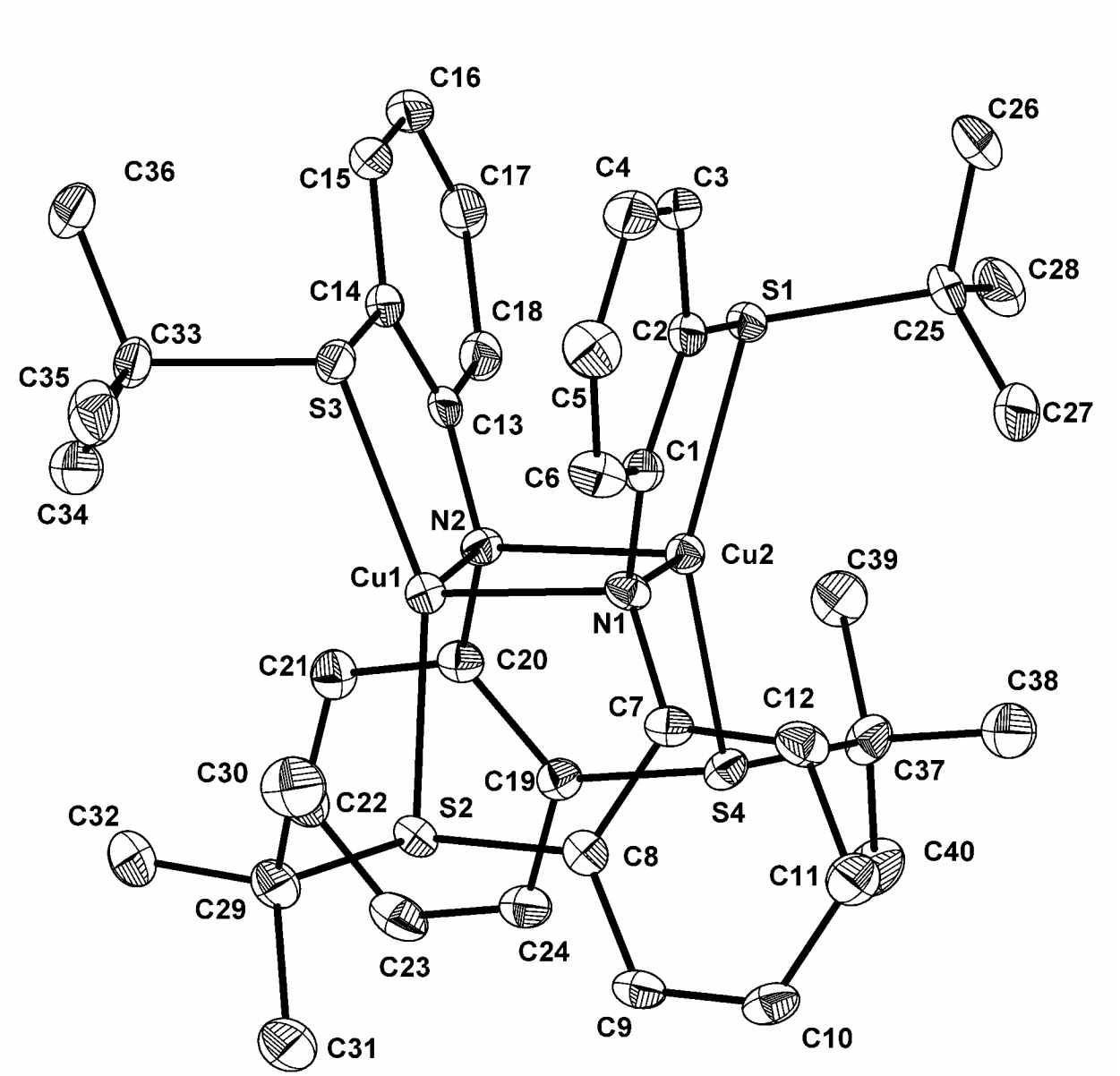


Figure 5. Drawing of $[(SNS)Cu]_2[B(C_6H_3(CF_3)_2)_4]$, **3**. Hydrogens and ½(ether) have been omitted for clarity.

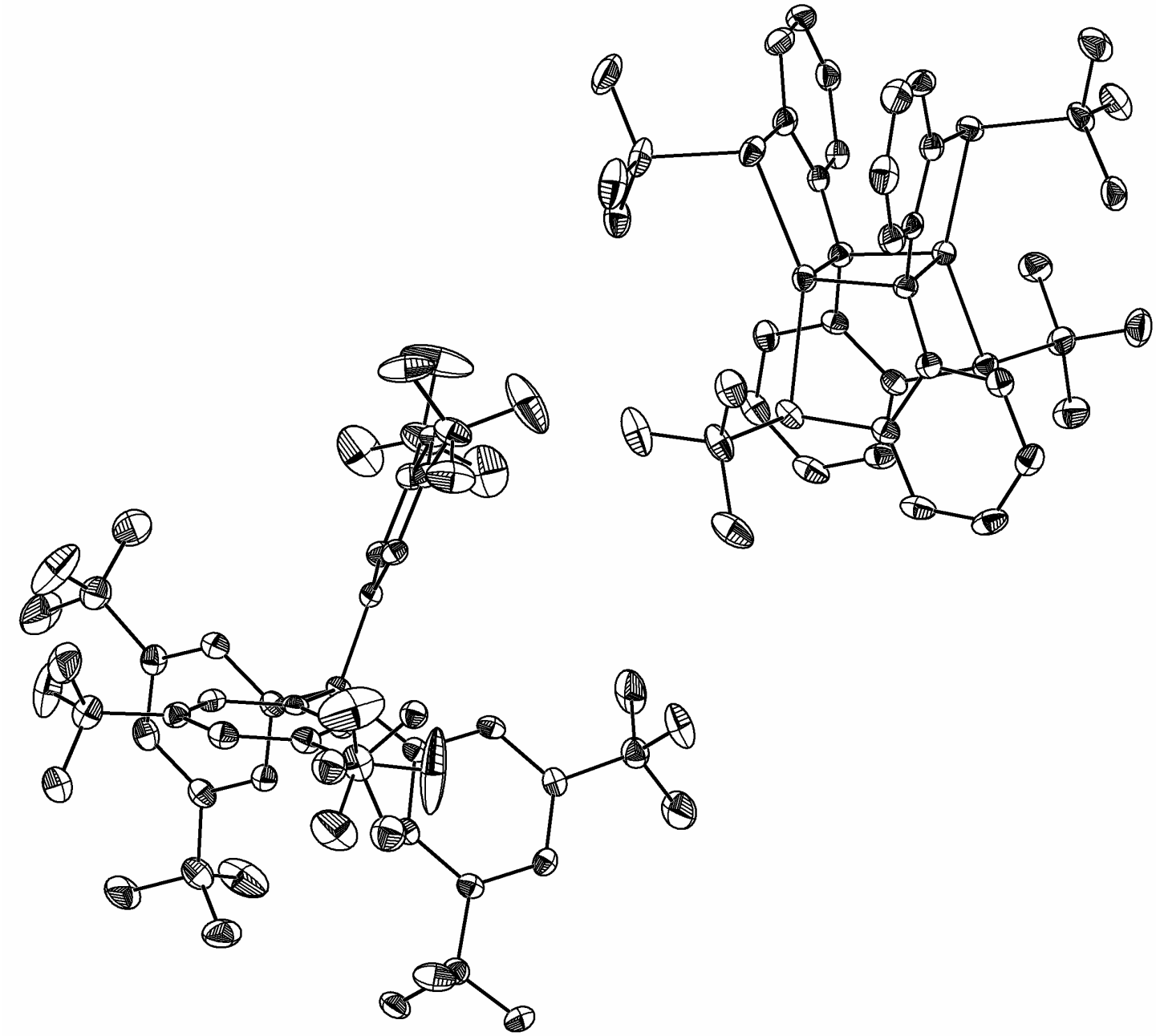


Figure 6. Fully labeled drawing of $[(SNS)Cu]_2[B(C_6H_3(CF_3)_2)_4]$, **3**. Anion, hydrogens and ½(ether) have been omitted for clarity.

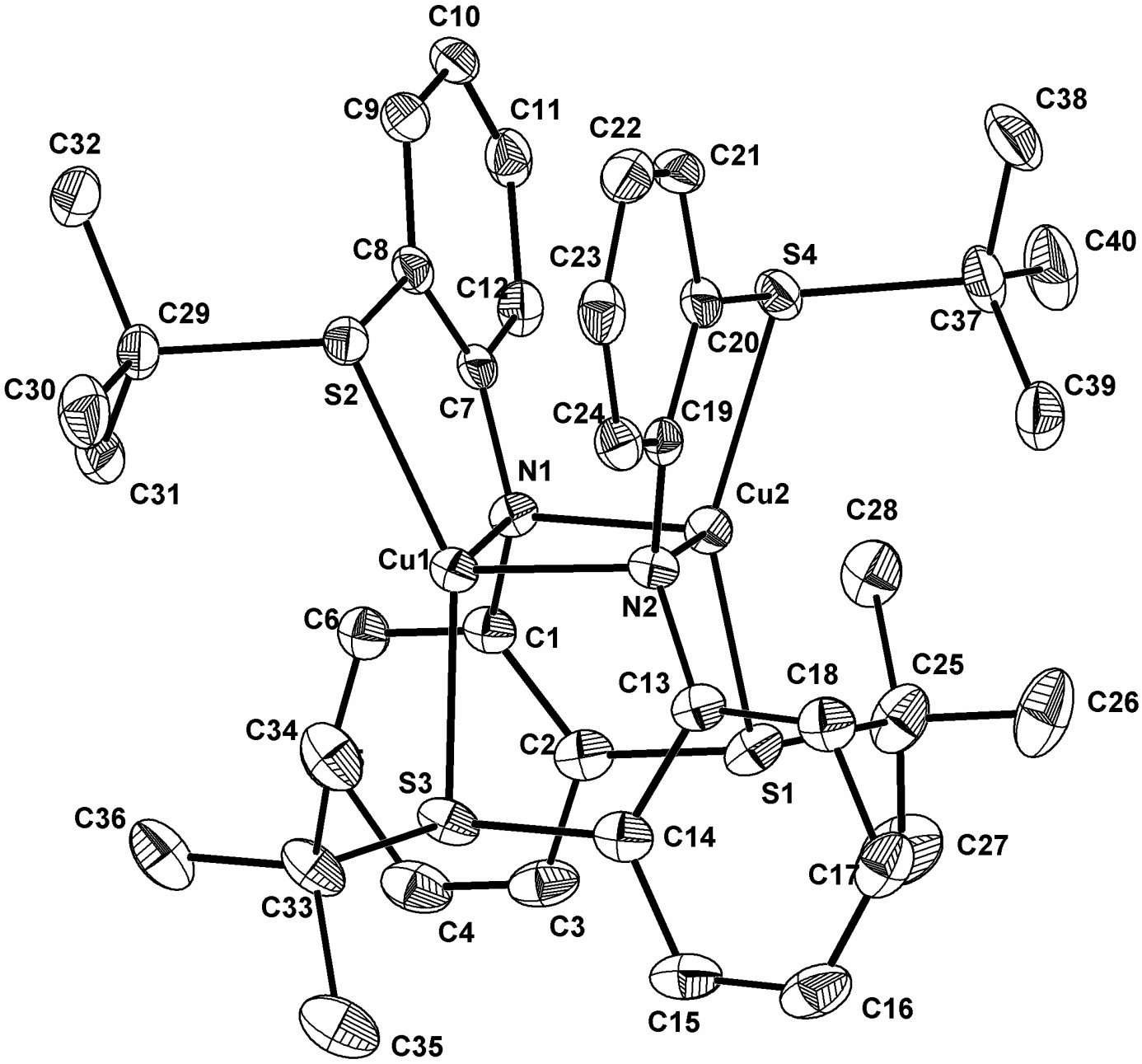


Figure 7. Drawing of (SNS)CuCl, **4**. Hydrogens have been omitted for clarity.

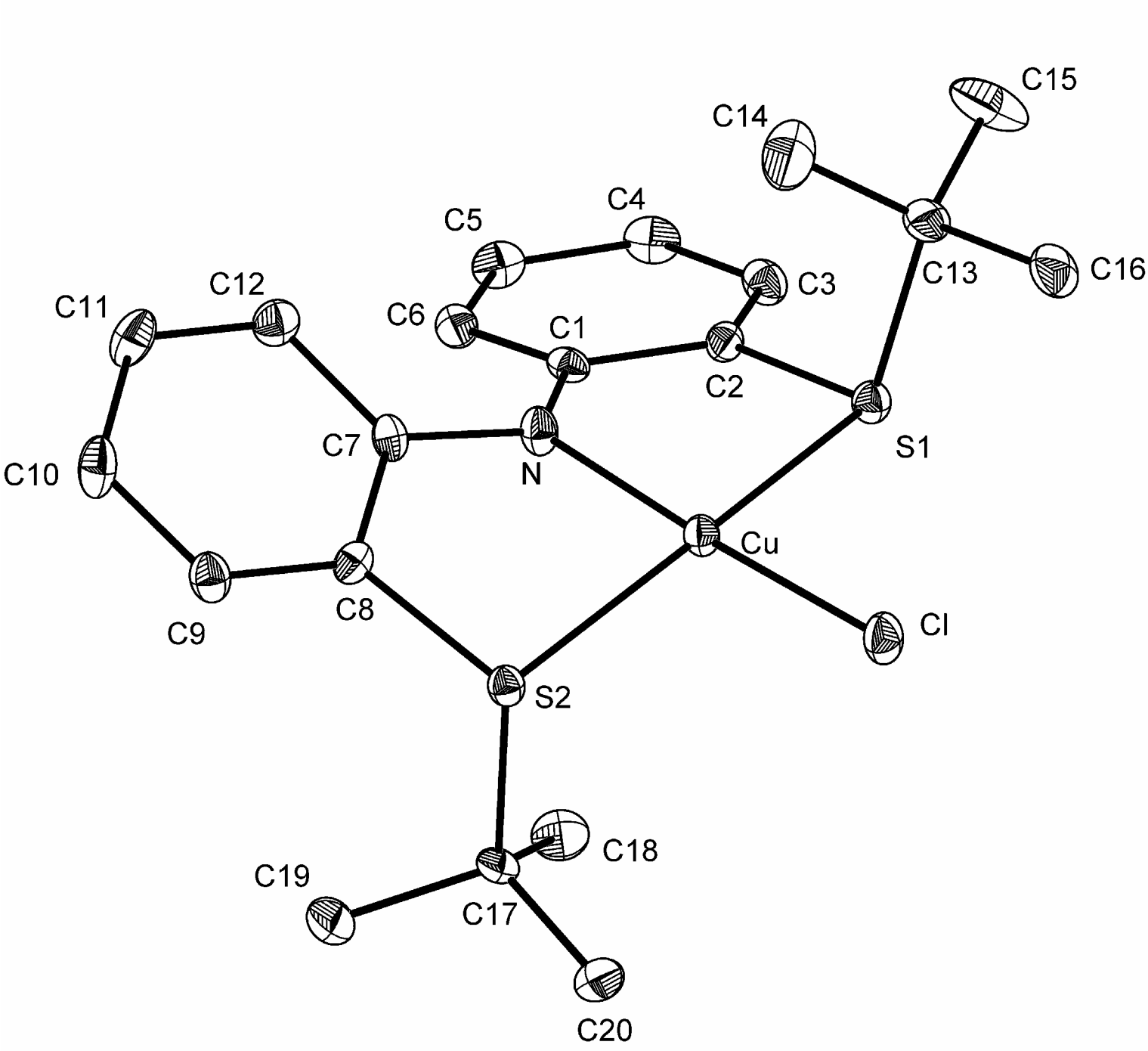


Table 1. Crystal data and structure refinement for **2**.

Name of Complex	$[(^t$Bu-SNS)Cu$]_2$	
Empirical formula	$C_{40}H_{52}Cu_2N_2S_4$	
Formula weight	816.206	
Temperature	98 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Crystal habit	rough block	
Crystal color	yellow	
Crystal size	0.33 x 0.28 x 0.21 mm^3	
Space group	P-1 (#2)	
Unit cell dimensions	a = 10.2263(9) Å	α= 94.017(2)°.
	b = 10.6226(9) Å	β= 90.634(2)°.
	c = 19.4884(17) Å	γ = 107.305(1)°.
Volume	2015.1(3) $Å^3$	
Z	2	
Density (calculated)	1.345 g/cm^3	
Absorption coefficient	1.292 mm^{-1}	
F(000)	856	
Theta range for data collection	2.01 to 28.40°.	
Index ranges	-13<=h<=13, -14<=k<=13, -25<=l<=25	
Reflections collected	42010	
Independent reflections	9371 [R(int) = 0.0507]	
Completeness to theta = 28.40°	92.4 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9371 / 0 / 445	
Goodness-of-fit on F^2	1.464	
Final R indices [I>2sigma(I)]	R1 = 0.0303, wR2 = 0.0660	
R indices (all data)	R1 = 0.0416, wR2 = 0.0685	
Largest diff. peak and hole	0.679 and -0.300 $e.Å^{-3}$	

Special Refinement Details

Refinement of F2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F2, conventional R-factors (R) are based on F, with F set to zero for negative F2. The threshold expression of F2 > 2□(F2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	y	z	U_{eq}
Cu(1)	3175(1)	6(1)	2339(1)	15(1)
Cu(2)	5267(1)	2114(1)	2544(1)	14(1)
N(1)	5277(1)	150(1)	2439(1)	15(1)
N(2)	3144(1)	2003(1)	2488(1)	14(1)
S(1)	5912(1)	2163(1)	3675(1)	16(1)
S(2)	3277(1)	-660(1)	1212(1)	16(1)
S(3)	2311(1)	-270(1)	3414(1)	18(1)
S(4)	5433(1)	2951(1)	1496(1)	16(1)
C(1)	5589(2)	-333(2)	3044(1)	17(1)
C(2)	5818(2)	461(2)	3674(1)	17(1)
C(3)	5904(2)	-99(2)	4294(1)	22(1)
C(4)	5811(2)	-1419(2)	4307(1)	26(1)
C(5)	5643(2)	-2201(2)	3690(1)	26(1)
C(6)	5532(2)	-1665(2)	3073(1)	22(1)
C(7)	5830(2)	-224(2)	1833(1)	16(1)
C(8)	5048(2)	-570(2)	1209(1)	16(1)
C(9)	5680(2)	-767(2)	595(1)	19(1)
C(10)	7047(2)	-674(2)	583(1)	22(1)
C(11)	7826(2)	-374(2)	1200(1)	24(1)
C(12)	7217(2)	-148(2)	1807(1)	21(1)
C(13)	2659(2)	2322(2)	3120(1)	16(1)
C(14)	2311(2)	1395(2)	3622(1)	18(1)
C(15)	2044(2)	1782(2)	4294(1)	24(1)
C(16)	2056(2)	3063(2)	4473(1)	28(1)
C(17)	2336(2)	3977(2)	3977(1)	26(1)
C(18)	2628(2)	3620(2)	3315(1)	21(1)
C(19)	3684(2)	2895(2)	1373(1)	16(1)
C(20)	2758(2)	2507(2)	1906(1)	15(1)
C(21)	1405(2)	2534(2)	1783(1)	20(1)
C(22)	982(2)	2853(2)	1161(1)	23(1)
C(23)	1893(2)	3161(2)	630(1)	24(1)
C(24)	3231(2)	3174(2)	737(1)	20(1)
C(25)	7756(2)	3045(2)	3880(1)	24(1)
C(26)	8155(2)	2805(2)	4604(1)	32(1)
C(27)	8642(2)	2583(2)	3352(1)	35(1)
C(28)	7857(2)	4489(2)	3844(1)	34(1)
C(29)	2352(2)	-2455(2)	1008(1)	24(1)
C(30)	2802(2)	-3275(2)	1519(1)	32(1)
C(31)	2615(2)	-2896(2)	273(1)	34(1)
C(32)	854(2)	-2524(2)	1065(1)	33(1)
C(33)	466(2)	-1246(2)	3363(1)	22(1)
C(34)	-285(2)	-757(2)	2811(1)	26(1)
C(35)	493(2)	-2647(2)	3174(1)	32(1)
C(36)	-202(2)	-1162(2)	4053(1)	33(1)
C(37)	6381(2)	4750(2)	1614(1)	20(1)
C(38)	7863(2)	4767(2)	1723(1)	27(1)
C(39)	5876(2)	5380(2)	2239(1)	26(1)
C(40)	6225(2)	5453(2)	975(1)	28(1)

Table 3. Bond lengths [Å] and angles [°] for **2**.

Cu(1)-Cu(2)	2.5989(3)	C(22)-C(23)	1.392(3)
Cu(1)-N(1)	2.1149(14)	C(22)-H(22)	0.9500
Cu(1)-N(2)	2.1303(14)	C(23)-C(24)	1.378(3)
Cu(1)-S(2)	2.2730(5)	C(23)-H(23)	0.9500
Cu(1)-S(3)	2.2854(5)	C(24)-H(24)	0.9500
Cu(2)-N(1)	2.0850(14)	C(25)-C(28)	1.514(3)
Cu(2)-N(2)	2.1395(14)	C(25)-C(26)	1.525(3)
Cu(2)-S(4)	2.2735(5)	C(25)-C(27)	1.527(3)
Cu(2)-S(1)	2.2853(5)	C(26)-H(26A)	0.9800
N(1)-C(1)	1.389(2)	C(26)-H(26B)	0.9800
N(1)-C(7)	1.398(2)	C(26)-H(26C)	0.9800
N(2)-C(13)	1.390(2)	C(27)-H(27A)	0.9800
N(2)-C(20)	1.389(2)	C(27)-H(27B)	0.9800
S(1)-C(2)	1.7825(18)	C(27)-H(27C)	0.9800
S(1)-C(25)	1.8637(18)	C(28)-H(28A)	0.9800
S(2)-C(8)	1.7856(18)	C(28)-H(28B)	0.9800
S(2)-C(29)	1.8707(18)	C(28)-H(28C)	0.9800
S(3)-C(14)	1.7870(19)	C(29)-C(32)	1.517(3)
S(3)-C(33)	1.8610(18)	C(29)-C(30)	1.521(3)
S(4)-C(19)	1.7848(18)	C(29)-C(31)	1.528(3)
S(4)-C(37)	1.8641(18)	C(30)-H(30A)	0.9800
C(1)-C(6)	1.403(3)	C(30)-H(30B)	0.9800
C(1)-C(2)	1.416(2)	C(30)-H(30C)	0.9800
C(2)-C(3)	1.396(2)	C(31)-H(31A)	0.9800
C(3)-C(4)	1.379(3)	C(31)-H(31B)	0.9800
C(3)-H(3)	0.9500	C(31)-H(31C)	0.9800
C(4)-C(5)	1.391(3)	C(32)-H(32A)	0.9800
C(4)-H(4)	0.9500	C(32)-H(32B)	0.9800
C(5)-C(6)	1.385(3)	C(32)-H(32C)	0.9800
C(5)-H(5)	0.9500	C(33)-C(35)	1.516(3)
C(6)-H(6)	0.9500	C(33)-C(36)	1.524(3)
C(7)-C(12)	1.398(2)	C(33)-C(34)	1.521(2)
C(7)-C(8)	1.413(2)	C(34)-H(34A)	0.9800
C(8)-C(9)	1.398(2)	C(34)-H(34B)	0.9800
C(9)-C(10)	1.372(3)	C(34)-H(34C)	0.9800
C(9)-H(9)	0.9500	C(35)-H(35A)	0.9800
C(10)-C(11)	1.397(3)	C(35)-H(35B)	0.9800
C(10)-H(10)	0.9500	C(35)-H(35C)	0.9800
C(11)-C(12)	1.382(3)	C(36)-H(36A)	0.9800
C(11)-H(11)	0.9500	C(36)-H(36B)	0.9800
C(12)-H(12)	0.9500	C(36)-H(36C)	0.9800
C(13)-C(14)	1.410(3)	C(37)-C(39)	1.518(3)
C(13)-C(18)	1.414(3)	C(37)-C(38)	1.522(3)
C(14)-C(15)	1.399(2)	C(37)-C(40)	1.527(3)
C(15)-C(16)	1.378(3)	C(38)-H(38A)	0.9800
C(15)-H(15)	0.9500	C(38)-H(38B)	0.9800
C(16)-C(17)	1.389(3)	C(38)-H(38C)	0.9800
C(16)-H(16)	0.9500	C(39)-H(39A)	0.9800
C(17)-C(18)	1.380(3)	C(39)-H(39B)	0.9800
C(17)-H(17)	0.9500	C(39)-H(39C)	0.9800
C(18)-H(18)	0.9500	C(40)-H(40A)	0.9800
C(19)-C(24)	1.400(2)	C(40)-H(40B)	0.9800
C(19)-C(20)	1.413(2)	C(40)-H(40C)	0.9800
C(20)-C(21)	1.410(2)	N(1)-Cu(1)-N(2)	103.88(5)
C(21)-C(22)	1.380(3)	N(1)-Cu(1)-S(2)	87.36(4)
C(21)-H(21)	0.9500	N(2)-Cu(1)-S(2)	112.76(4)

N(1)-Cu(1)-S(3)	106.53(4)	C(10)-C(9)-H(9)	119.2
N(2)-Cu(1)-S(3)	86.87(4)	C(8)-C(9)-H(9)	119.2
S(2)-Cu(1)-S(3)	152.921(19)	C(9)-C(10)-C(11)	119.18(17)
N(1)-Cu(2)-N(2)	104.59(5)	C(9)-C(10)-H(10)	120.4
N(1)-Cu(2)-S(4)	109.94(4)	C(11)-C(10)-H(10)	120.4
N(2)-Cu(2)-S(4)	86.80(4)	C(12)-C(11)-C(10)	119.65(17)
N(1)-Cu(2)-S(1)	87.87(4)	C(12)-C(11)-H(11)	120.2
N(2)-Cu(2)-S(1)	108.49(4)	C(10)-C(11)-H(11)	120.2
S(4)-Cu(2)-S(1)	153.233(19)	C(11)-C(12)-C(7)	122.42(17)
C(1)-N(1)-C(7)	117.51(14)	C(11)-C(12)-H(12)	118.8
C(1)-N(1)-Cu(2)	114.38(11)	C(7)-C(12)-H(12)	118.8
C(7)-N(1)-Cu(2)	115.46(11)	N(2)-C(13)-C(14)	121.02(16)
C(1)-N(1)-Cu(1)	112.31(11)	N(2)-C(13)-C(18)	121.74(16)
C(7)-N(1)-Cu(1)	113.93(11)	C(14)-C(13)-C(18)	116.92(16)
Cu(2)-N(1)-Cu(1)	76.45(5)	C(15)-C(14)-C(13)	120.74(17)
C(13)-N(2)-C(20)	118.43(14)	C(15)-C(14)-S(3)	119.44(15)
C(13)-N(2)-Cu(1)	114.34(11)	C(13)-C(14)-S(3)	119.71(13)
C(20)-N(2)-Cu(1)	114.60(11)	C(16)-C(15)-C(14)	120.83(19)
C(13)-N(2)-Cu(2)	112.65(10)	C(16)-C(15)-H(15)	119.6
C(20)-N(2)-Cu(2)	114.21(11)	C(14)-C(15)-H(15)	119.6
Cu(1)-N(2)-Cu(2)	74.99(5)	C(15)-C(16)-C(17)	119.21(18)
C(2)-S(1)-C(25)	103.62(9)	C(15)-C(16)-H(16)	120.4
C(2)-S(1)-Cu(2)	96.72(6)	C(17)-C(16)-H(16)	120.4
C(25)-S(1)-Cu(2)	114.49(6)	C(18)-C(17)-C(16)	120.76(19)
C(8)-S(2)-C(29)	104.35(8)	C(18)-C(17)-H(17)	119.6
C(8)-S(2)-Cu(1)	98.12(6)	C(16)-C(17)-H(17)	119.6
C(29)-S(2)-Cu(1)	112.80(6)	C(17)-C(18)-C(13)	121.40(18)
C(14)-S(3)-C(33)	104.44(8)	C(17)-C(18)-H(18)	119.3
C(14)-S(3)-Cu(1)	97.72(6)	C(13)-C(18)-H(18)	119.3
C(33)-S(3)-Cu(1)	110.95(6)	C(24)-C(19)-C(20)	120.70(16)
C(19)-S(4)-C(37)	104.45(8)	C(24)-C(19)-S(4)	119.53(14)
C(19)-S(4)-Cu(2)	98.14(6)	C(20)-C(19)-S(4)	119.71(13)
C(37)-S(4)-Cu(2)	108.17(6)	N(2)-C(20)-C(21)	122.44(16)
N(1)-C(1)-C(6)	121.45(16)	N(2)-C(20)-C(19)	120.65(15)
N(1)-C(1)-C(2)	121.03(16)	C(21)-C(20)-C(19)	116.61(16)
C(6)-C(1)-C(2)	117.12(16)	C(22)-C(21)-C(20)	121.99(17)
C(3)-C(2)-C(1)	120.31(17)	C(22)-C(21)-H(21)	119.0
C(3)-C(2)-S(1)	120.15(14)	C(20)-C(21)-H(21)	119.0
C(1)-C(2)-S(1)	119.47(13)	C(21)-C(22)-C(23)	120.39(18)
C(4)-C(3)-C(2)	121.18(18)	C(21)-C(22)-H(22)	119.8
C(4)-C(3)-H(3)	119.4	C(23)-C(22)-H(22)	119.8
C(2)-C(3)-H(3)	119.4	C(24)-C(23)-C(22)	119.20(17)
C(3)-C(4)-C(5)	119.24(18)	C(24)-C(23)-H(23)	120.4
C(3)-C(4)-H(4)	120.4	C(22)-C(23)-H(23)	120.4
C(5)-C(4)-H(4)	120.4	C(23)-C(24)-C(19)	120.90(18)
C(6)-C(5)-C(4)	120.18(18)	C(23)-C(24)-H(24)	119.5
C(6)-C(5)-H(5)	119.9	C(19)-C(24)-H(24)	119.5
C(4)-C(5)-H(5)	119.9	C(28)-C(25)-C(26)	109.73(16)
C(5)-C(6)-C(1)	121.87(18)	C(28)-C(25)-C(27)	112.27(18)
C(5)-C(6)-H(6)	119.1	C(26)-C(25)-C(27)	110.33(17)
C(1)-C(6)-H(6)	119.1	C(28)-C(25)-S(1)	103.88(13)
N(1)-C(7)-C(12)	121.09(15)	C(26)-C(25)-S(1)	110.75(13)
N(1)-C(7)-C(8)	121.46(15)	C(27)-C(25)-S(1)	109.72(13)
C(12)-C(7)-C(8)	117.17(16)	C(25)-C(26)-H(26A)	109.5
C(9)-C(8)-C(7)	119.94(16)	C(25)-C(26)-H(26B)	109.5
C(9)-C(8)-S(2)	121.01(13)	H(26A)-C(26)-H(26B)	109.5
C(7)-C(8)-S(2)	118.96(13)	C(25)-C(26)-H(26C)	109.5
C(10)-C(9)-C(8)	121.60(16)	H(26A)-C(26)-H(26C)	109.5

H(26B)-C(26)-H(26C)	109.5	C(33)-C(34)-H(34A)	109.5
C(25)-C(27)-H(27A)	109.5	C(33)-C(34)-H(34B)	109.5
C(25)-C(27)-H(27B)	109.5	H(34A)-C(34)-H(34B)	109.5
H(27A)-C(27)-H(27B)	109.5	C(33)-C(34)-H(34C)	109.5
C(25)-C(27)-H(27C)	109.5	H(34A)-C(34)-H(34C)	109.5
H(27A)-C(27)-H(27C)	109.5	H(34B)-C(34)-H(34C)	109.5
H(27B)-C(27)-H(27C)	109.5	C(33)-C(35)-H(35A)	109.5
C(25)-C(28)-H(28A)	109.5	C(33)-C(35)-H(35B)	109.5
C(25)-C(28)-H(28B)	109.5	H(35A)-C(35)-H(35B)	109.5
H(28A)-C(28)-H(28B)	109.5	C(33)-C(35)-H(35C)	109.5
C(25)-C(28)-H(28C)	109.5	H(35A)-C(35)-H(35C)	109.5
H(28A)-C(28)-H(28C)	109.5	H(35B)-C(35)-H(35C)	109.5
H(28B)-C(28)-H(28C)	109.5	C(33)-C(36)-H(36A)	109.5
C(32)-C(29)-C(30)	112.65(17)	C(33)-C(36)-H(36B)	109.5
C(32)-C(29)-C(31)	109.43(16)	H(36A)-C(36)-H(36B)	109.5
C(30)-C(29)-C(31)	110.47(17)	C(33)-C(36)-H(36C)	109.5
C(32)-C(29)-S(2)	103.49(13)	H(36A)-C(36)-H(36C)	109.5
C(30)-C(29)-S(2)	109.87(13)	H(36B)-C(36)-H(36C)	109.5
C(31)-C(29)-S(2)	110.74(13)	C(39)-C(37)-C(38)	111.35(16)
C(29)-C(30)-H(30A)	109.5	C(39)-C(37)-C(40)	110.15(16)
C(29)-C(30)-H(30B)	109.5	C(38)-C(37)-C(40)	110.57(15)
H(30A)-C(30)-H(30B)	109.5	C(39)-C(37)-S(4)	110.11(12)
C(29)-C(30)-H(30C)	109.5	C(38)-C(37)-S(4)	103.29(12)
H(30A)-C(30)-H(30C)	109.5	C(40)-C(37)-S(4)	111.20(13)
H(30B)-C(30)-H(30C)	109.5	C(37)-C(38)-H(38A)	109.5
C(29)-C(31)-H(31A)	109.5	C(37)-C(38)-H(38B)	109.5
C(29)-C(31)-H(31B)	109.5	H(38A)-C(38)-H(38B)	109.5
H(31A)-C(31)-H(31B)	109.5	C(37)-C(38)-H(38C)	109.5
C(29)-C(31)-H(31C)	109.5	H(38A)-C(38)-H(38C)	109.5
H(31A)-C(31)-H(31C)	109.5	H(38B)-C(38)-H(38C)	109.5
H(31B)-C(31)-H(31C)	109.5	C(37)-C(39)-H(39A)	109.5
C(29)-C(32)-H(32A)	109.5	C(37)-C(39)-H(39B)	109.5
C(29)-C(32)-H(32B)	109.5	H(39A)-C(39)-H(39B)	109.5
H(32A)-C(32)-H(32B)	109.5	C(37)-C(39)-H(39C)	109.5
C(29)-C(32)-H(32C)	109.5	H(39A)-C(39)-H(39C)	109.5
H(32A)-C(32)-H(32C)	109.5	H(39B)-C(39)-H(39C)	109.5
H(32B)-C(32)-H(32C)	109.5	C(37)-C(40)-H(40A)	109.5
C(35)-C(33)-C(36)	110.51(16)	C(37)-C(40)-H(40B)	109.5
C(35)-C(33)-C(34)	111.45(16)	H(40A)-C(40)-H(40B)	109.5
C(36)-C(33)-C(34)	109.90(16)	C(37)-C(40)-H(40C)	109.5
C(35)-C(33)-S(3)	103.43(13)	H(40A)-C(40)-H(40C)	109.5
C(36)-C(33)-S(3)	111.30(13)	H(40B)-C(40)-H(40C)	109.5
C(34)-C(33)-S(3)	110.12(13)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2**. 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)	14(1)	15(1)	15(1)	1(1)	0(1)	4(1)
Cu(2)	13(1)	15(1)	15(1)	0(1)	1(1)	4(1)
N(1)	17(1)	18(1)	13(1)	-1(1)	-2(1)	9(1)
N(2)	14(1)	16(1)	13(1)	1(1)	2(1)	6(1)
S(1)	14(1)	19(1)	14(1)	-3(1)	0(1)	4(1)
S(2)	17(1)	16(1)	15(1)	-1(1)	-3(1)	4(1)
S(3)	13(1)	23(1)	17(1)	7(1)	1(1)	4(1)
S(4)	17(1)	14(1)	16(1)	1(1)	5(1)	5(1)
C(1)	13(1)	22(1)	16(1)	1(1)	0(1)	7(1)
C(2)	12(1)	21(1)	17(1)	0(1)	0(1)	4(1)
C(3)	18(1)	30(1)	15(1)	1(1)	1(1)	4(1)
C(4)	25(1)	33(1)	20(1)	10(1)	-1(1)	9(1)
C(5)	29(1)	25(1)	28(1)	6(1)	-3(1)	12(1)
C(6)	28(1)	23(1)	19(1)	-1(1)	-2(1)	13(1)
C(7)	21(1)	14(1)	14(1)	0(1)	1(1)	7(1)
C(8)	18(1)	13(1)	18(1)	1(1)	-1(1)	6(1)
C(9)	28(1)	16(1)	13(1)	0(1)	-1(1)	6(1)
C(10)	29(1)	21(1)	17(1)	0(1)	7(1)	9(1)
C(11)	23(1)	27(1)	25(1)	-1(1)	3(1)	12(1)
C(12)	23(1)	26(1)	18(1)	-3(1)	-3(1)	13(1)
C(13)	9(1)	23(1)	15(1)	-2(1)	-2(1)	4(1)
C(14)	11(1)	25(1)	16(1)	0(1)	-1(1)	4(1)
C(15)	15(1)	37(1)	15(1)	2(1)	0(1)	3(1)
C(16)	19(1)	42(1)	17(1)	-9(1)	2(1)	4(1)
C(17)	17(1)	30(1)	28(1)	-12(1)	1(1)	6(1)
C(18)	15(1)	23(1)	22(1)	-2(1)	1(1)	4(1)
C(19)	18(1)	13(1)	16(1)	0(1)	2(1)	5(1)
C(20)	20(1)	11(1)	16(1)	-1(1)	0(1)	6(1)
C(21)	18(1)	19(1)	22(1)	1(1)	1(1)	6(1)
C(22)	22(1)	20(1)	27(1)	1(1)	-6(1)	9(1)
C(23)	32(1)	18(1)	19(1)	1(1)	-8(1)	6(1)
C(24)	27(1)	15(1)	16(1)	1(1)	1(1)	3(1)
C(25)	14(1)	30(1)	22(1)	-3(1)	-5(1)	-1(1)
C(26)	24(1)	40(1)	24(1)	-1(1)	-9(1)	-1(1)
C(27)	15(1)	54(2)	30(1)	-4(1)	1(1)	5(1)
C(28)	32(1)	28(1)	30(1)	-2(1)	-7(1)	-7(1)
C(29)	27(1)	17(1)	22(1)	-6(1)	-1(1)	-2(1)
C(30)	43(1)	17(1)	33(1)	0(1)	3(1)	3(1)
C(31)	37(1)	27(1)	27(1)	-11(1)	2(1)	-2(1)
C(32)	26(1)	34(1)	28(1)	-7(1)	-2(1)	-6(1)
C(33)	13(1)	28(1)	22(1)	9(1)	1(1)	0(1)
C(34)	18(1)	31(1)	26(1)	7(1)	-5(1)	3(1)
C(35)	27(1)	26(1)	37(1)	12(1)	-1(1)	-1(1)
C(36)	19(1)	48(1)	26(1)	12(1)	5(1)	0(1)
C(37)	23(1)	12(1)	23(1)	1(1)	7(1)	2(1)
C(38)	22(1)	25(1)	29(1)	1(1)	6(1)	-1(1)
C(39)	30(1)	17(1)	28(1)	-4(1)	4(1)	6(1)
C(40)	35(1)	16(1)	31(1)	8(1)	9(1)	4(1)

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

	x	y	z	U_{eq}
H(3)	6029	439	4714	26
H(4)	5861	-1790	4733	31
H(5)	5604	-3106	3693	32
H(6)	5415	-2213	2656	27
H(9)	5151	-969	176	23
H(10)	7459	-813	161	26
H(11)	8769	-324	1201	29
H(12)	7761	67	2221	26
H(15)	1853	1153	4631	29
H(16)	1874	3319	4931	33
H(17)	2328	4857	4095	31
H(18)	2811	4259	2984	25
H(21)	767	2327	2139	23
H(22)	63	2862	1096	27
H(23)	1595	3360	198	28
H(24)	3855	3376	374	24
H(26A)	9074	3394	4732	48
H(26B)	8150	1883	4617	48
H(26C)	7496	2985	4930	48
H(27A)	8376	2743	2889	52
H(27B)	8510	1635	3378	52
H(27C)	9608	3074	3451	52
H(28A)	7230	4727	4169	50
H(28B)	7609	4641	3376	50
H(28C)	8798	5035	3963	50
H(30A)	2630	-2978	1988	48
H(30B)	3783	-3165	1476	48
H(30C)	2283	-4209	1423	48
H(31A)	2015	-3795	152	50
H(31B)	3574	-2884	240	50
H(31C)	2423	-2293	-45	50
H(32A)	279	-3433	944	49
H(32B)	633	-1932	750	49
H(32C)	683	-2252	1538	49
H(34A)	135	-836	2367	39
H(34B)	-223	171	2930	39
H(34C)	-1250	-1292	2780	39
H(35A)	-448	-3240	3126	47
H(35B)	990	-2929	3537	47
H(35C)	955	-2677	2738	47
H(36A)	-1152	-1736	4020	49
H(36B)	-190	-247	4173	49
H(36C)	305	-1449	4409	49
H(38A)	8446	5683	1813	40
H(38B)	8165	4368	1309	40
H(38C)	7934	4262	2116	40
H(39A)	5956	4905	2643	39
H(39B)	4915	5334	2159	39
H(39C)	6431	6307	2319	39
H(40A)	5266	5431	912	41
H(40B)	6502	5006	570	41
H(40C)	6807	6374	1032	41

Table 6. Crystal data and structure refinement for **3**.

Name of Complex	$[(SNS)Cu]_2[B(C_6H_3(CF_3)_2)_4]$	
Empirical formula	$C_{72}H_{64}BCu_2F_{24}N_2S_4 \cdot ½(C_4H_{10}O)$	
Formula weight	1716.478	
Temperature	100 K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Crystal habit	blade	
Crystal color	deep red	
Crystal size	0.34 x 0.28 x 0.14 mm^3	
Space group	P-1 (#2)	
Unit cell dimensions	a = 10.3179(8) Å	α= 74.234(1)°.
	b = 19.3779(14) Å	β= 83.222(1)°.
	c = 19.9116(15) Å	γ = 85.603(1)°.
Volume	3800.4(5) $Å^3$	
Z	2	
Density (calculated)	1.500 g/cm^3	
Absorption coefficient	0.773 mm^{-1}	
F(000)	1748	
Theta range for data collection	1.72 to 28.48°.	
Index ranges	-13<=h<=13, -25<=k<=25, -26<=l<=26	
Reflections collected	79590	
Independent reflections	17675 [R(int) = 0.0552]	
Completeness to theta = 28.48°	91.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17675 / 0 / 1004	
Goodness-of-fit on F^2	1.580	
Final R indices [I>2sigma(I)]	R1 = 0.0393, wR2 = 0.0810	
R indices (all data)	R1 = 0.0597, wR2 = 0.0850	
Largest diff. peak and hole	0.61 and -0.50 $e.Å^{-3}$	

Special Refinement Details

Refinement of F2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F2, conventional R-factors (R) are based on F, with F set to zero for negative F2. The threshold expression of F2 > 2 ∫(F2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

One CF_3 group is disordered and was modeled over 2 locations with one relative population parameter, {F4, F5, and F6} and {F4A, F5A, and F6A; isotropically} in 92.7(4)% and 7.3(4)% respectively. Additionally ½ molecule of diethyl ether is contained in the asymmetric unit with the oxygen atom placed on a center of symmetry (1.0 ,0.5, 0.5) and the alpha carbon split over 2 locations.

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3**. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cu(1)	8093(1)	8303(1)	7388(1)	17(1)
Cu(2)	6977(1)	7654(1)	6728(1)	18(1)
N(1)	6092(2)	8339(1)	7295(1)	17(1)
N(2)	8966(2)	7668(1)	6738(1)	17(1)
S(1)	6133(1)	6726(1)	7604(1)	22(1)
S(2)	8101(1)	9476(1)	6755(1)	18(1)
S(3)	8704(1)	7405(1)	8316(1)	22(1)
S(4)	7230(1)	8278(1)	5575(1)	21(1)
O	10000	5000	5000	195(6)
B(1)	3879(2)	7327(1)	1943(1)	16(1)
C(1)	5340(2)	8007(1)	7922(1)	19(1)
C(2)	5395(2)	7254(1)	8168(1)	22(1)
C(3)	4907(2)	6926(1)	8850(1)	27(1)
C(4)	4281(2)	7324(1)	9280(1)	30(1)
C(5)	4130(2)	8063(1)	9023(1)	25(1)
C(6)	4662(2)	8403(1)	8356(1)	21(1)
C(7)	5602(2)	8995(1)	6870(1)	17(1)
C(8)	6463(2)	9540(1)	6529(1)	18(1)
C(9)	6048(2)	10119(1)	6002(1)	24(1)
C(10)	4777(2)	10184(1)	5828(1)	27(1)
C(11)	3906(2)	9671(1)	6197(1)	26(1)
C(12)	4308(2)	9086(1)	6707(1)	22(1)
C(13)	9565(2)	7011(1)	7095(1)	19(1)
C(14)	9361(2)	6786(1)	7832(1)	22(1)
C(15)	9671(2)	6078(1)	8182(1)	28(1)
C(16)	10267(2)	5606(1)	7821(1)	33(1)
C(17)	10568(2)	5842(1)	7101(1)	30(1)
C(18)	10221(2)	6536(1)	6739(1)	24(1)
C(19)	9619(2)	8084(1)	6120(1)	18(1)
C(20)	8884(2)	8475(1)	5573(1)	20(1)
C(21)	9456(2)	9015(1)	5031(1)	25(1)
C(22)	10757(2)	9144(1)	4998(1)	27(1)
C(23)	11512(2)	8724(1)	5502(1)	26(1)
C(24)	10953(2)	8202(1)	6055(1)	21(1)
C(25)	4710(2)	6392(1)	7303(1)	30(1)
C(26)	5348(2)	5949(1)	6818(2)	44(1)
C(27)	3916(2)	5921(1)	7933(2)	44(1)
C(28)	3870(2)	7017(1)	6917(1)	30(1)
C(29)	8080(2)	10094(1)	7337(1)	24(1)
C(30)	9481(2)	10033(1)	7517(1)	35(1)
C(31)	7106(2)	9858(1)	7979(1)	28(1)
C(32)	7739(3)	10859(1)	6929(1)	34(1)
C(33)	10200(2)	7650(1)	8637(1)	26(1)
C(34)	11171(2)	7980(1)	8013(1)	30(1)
C(35)	10814(2)	6985(1)	9115(1)	36(1)
C(36)	9680(2)	8182(1)	9049(1)	34(1)
C(37)	7366(2)	7681(1)	4965(1)	29(1)
C(38)	7947(3)	8093(1)	4244(1)	40(1)
C(39)	8177(2)	7000(1)	5249(1)	31(1)
C(40)	5946(2)	7528(2)	4945(2)	43(1)
C(41)	4344(2)	6747(1)	1485(1)	17(1)
C(42)	3483(2)	6334(1)	1286(1)	18(1)
C(43)	3899(2)	5848(1)	899(1)	20(1)
C(44)	5218(2)	5750(1)	689(1)	22(1)

C(45)	6100(2)	6150(1)	877(1)	21(1)
C(46)	5672(2)	6635(1)	1264(1)	19(1)
C(47)	2948(2)	5435(1)	674(1)	26(1)
C(48)	7525(2)	6058(1)	652(1)	29(1)
C(49)	4028(2)	6950(1)	2776(1)	17(1)
C(50)	3258(2)	7185(1)	3306(1)	19(1)
C(51)	3404(2)	6892(1)	4014(1)	22(1)
C(52)	4335(2)	6352(1)	4221(1)	21(1)
C(53)	5127(2)	6114(1)	3712(1)	19(1)
C(54)	4966(2)	6400(1)	3005(1)	18(1)
C(55)	2573(2)	7194(2)	4542(1)	36(1)
C(56)	6160(2)	5542(1)	3940(1)	30(1)
C(57)	4826(2)	8013(1)	1663(1)	16(1)
C(58)	5372(2)	8338(1)	2099(1)	17(1)
C(59)	6171(2)	8920(1)	1837(1)	18(1)
C(60)	6452(2)	9209(1)	1123(1)	18(1)
C(61)	5919(2)	8897(1)	677(1)	17(1)
C(62)	5133(2)	8313(1)	940(1)	17(1)
C(63)	6782(2)	9220(1)	2334(1)	24(1)
C(64)	6191(2)	9172(1)	-101(1)	21(1)
C(65)	2352(2)	7583(1)	1829(1)	18(1)
C(66)	1323(2)	7158(1)	2205(1)	20(1)
C(67)	29(2)	7326(1)	2075(1)	21(1)
C(68)	-309(2)	7925(1)	1555(1)	23(1)
C(69)	681(2)	8359(1)	1176(1)	21(1)
C(70)	1975(2)	8194(1)	1319(1)	18(1)
C(71)	-993(2)	6835(1)	2506(1)	30(1)
C(72)	370(2)	9020(1)	621(1)	27(1)
C(73)[c]	9811(12)	5069(7)	5551(6)	87(4)
C(74)[c]	8830(6)	4557(3)	5588(4)	46(2)
C(75)	8491(5)	4747(2)	6130(4)	136(2)
F(1)	1715(1)	5542(1)	919(1)	48(1)
F(2)	3218(1)	4727(1)	864(1)	42(1)
F(3)	2963(1)	5605(1)	-29(1)	40(1)
F(4)[a]	7986(2)	5389(1)	915(1)	77(1)
F(5)[a]	7768(2)	6144(1)	-31(1)	55(1)
F(6)[a]	8264(2)	6488(2)	815(2)	93(1)
F(4A)[b]	8204(17)	5944(11)	1150(9)	22(5)
F(5A)[b]	7929(18)	6628(11)	188(11)	36(6)
F(6A)[b]	7899(19)	5600(12)	391(13)	35(6)
F(7)	2960(2)	7849(1)	4539(1)	56(1)
F(8)	1339(1)	7319(1)	4415(1)	59(1)
F(9)	2627(2)	6805(1)	5194(1)	74(1)
F(10)	5653(2)	4915(1)	4292(1)	49(1)
F(11)	6901(2)	5708(1)	4369(1)	66(1)
F(12)	6950(1)	5398(1)	3411(1)	41(1)
F(13)	6036(1)	9164(1)	2939(1)	44(1)
F(14)	7919(1)	8883(1)	2509(1)	39(1)
F(15)	7034(2)	9913(1)	2074(1)	49(1)
F(16)	6930(1)	9743(1)	-297(1)	33(1)
F(17)	6796(1)	8671(1)	-392(1)	32(1)
F(18)	5087(1)	9374(1)	-419(1)	26(1)
F(19)	-811(2)	6173(1)	2434(1)	63(1)
F(20)	-998(2)	6771(1)	3187(1)	55(1)
F(21)	-2192(1)	7057(1)	2346(1)	61(1)
F(22)	-733(1)	8976(1)	341(1)	37(1)
F(23)	207(2)	9603(1)	861(1)	53(1)
F(24)	1308(1)	9162(1)	82(1)	38(1)

a: population: 0.927(4) / b: population: 0.073(4) / c: population: ½

Table 8. Bond lengths [Å] and angles [°] for **3**.

Cu(1)-Cu(2)	2.4724(4)	C(17)-C(18)	1.385(3)
Cu(1)-N(1)	2.0887(16)	C(17)-H(17)	0.9500
Cu(1)-N(2)	2.1011(17)	C(18)-H(18)	0.9500
Cu(1)-S(2)	2.2805(6)	C(19)-C(24)	1.399(3)
Cu(1)-S(3)	2.2805(6)	C(19)-C(20)	1.411(3)
Cu(2)-N(2)	2.0568(16)	C(20)-C(21)	1.392(3)
Cu(2)-N(1)	2.0641(16)	C(21)-C(22)	1.375(3)
Cu(2)-S(4)	2.2797(6)	C(21)-H(21)	0.9500
Cu(2)-S(1)	2.2834(6)	C(22)-C(23)	1.385(3)
N(1)-C(1)	1.409(2)	C(22)-H(22)	0.9500
N(1)-C(7)	1.416(2)	C(23)-C(24)	1.379(3)
N(2)-C(19)	1.403(2)	C(23)-H(23)	0.9500
N(2)-C(13)	1.415(2)	C(24)-H(24)	0.9500
S(1)-C(2)	1.786(2)	C(25)-C(28)	1.517(3)
S(1)-C(25)	1.870(2)	C(25)-C(26)	1.523(3)
S(2)-C(8)	1.785(2)	C(25)-C(27)	1.526(3)
S(2)-C(29)	1.877(2)	C(26)-H(26A)	0.9800
S(3)-C(14)	1.783(2)	C(26)-H(26B)	0.9800
S(3)-C(33)	1.878(2)	C(26)-H(26C)	0.9800
S(4)-C(20)	1.777(2)	C(27)-H(27A)	0.9800
S(4)-C(37)	1.880(2)	C(27)-H(27B)	0.9800
O-C(73)	1.133(11)	C(27)-H(27C)	0.9800
O-C(73)#1	1.133(11)	C(28)-H(28A)	0.9800
O-C(74)	1.687(6)	C(28)-H(28B)	0.9800
O-C(74)#1	1.687(6)	C(28)-H(28C)	0.9800
B(1)-C(65)	1.638(3)	C(29)-C(31)	1.518(3)
B(1)-C(49)	1.641(3)	C(29)-C(30)	1.519(3)
B(1)-C(41)	1.642(3)	C(29)-C(32)	1.522(3)
B(1)-C(57)	1.643(3)	C(30)-H(30A)	0.9800
C(1)-C(6)	1.399(3)	C(30)-H(30B)	0.9800
C(1)-C(2)	1.406(3)	C(30)-H(30C)	0.9800
C(2)-C(3)	1.386(3)	C(31)-H(31A)	0.9800
C(3)-C(4)	1.377(3)	C(31)-H(31B)	0.9800
C(3)-H(3)	0.9500	C(31)-H(31C)	0.9800
C(4)-C(5)	1.388(3)	C(32)-H(32A)	0.9800
C(4)-H(4)	0.9500	C(32)-H(32B)	0.9800
C(5)-C(6)	1.382(3)	C(32)-H(32C)	0.9800
C(5)-H(5)	0.9500	C(33)-C(36)	1.516(3)
C(6)-H(6)	0.9500	C(33)-C(35)	1.523(3)
C(7)-C(12)	1.398(3)	C(33)-C(34)	1.525(3)
C(7)-C(8)	1.406(3)	C(34)-H(34A)	0.9800
C(8)-C(9)	1.393(3)	C(34)-H(34B)	0.9800
C(9)-C(10)	1.384(3)	C(34)-H(34C)	0.9800
C(9)-H(9)	0.9500	C(35)-H(35A)	0.9800
C(10)-C(11)	1.386(3)	C(35)-H(35B)	0.9800
C(10)-H(10)	0.9500	C(35)-H(35C)	0.9800
C(11)-C(12)	1.375(3)	C(36)-H(36A)	0.9800
C(11)-H(11)	0.9500	C(36)-H(36B)	0.9800
C(12)-H(12)	0.9500	C(36)-H(36C)	0.9800
C(13)-C(18)	1.398(3)	C(37)-C(39)	1.517(3)
C(13)-C(14)	1.407(3)	C(37)-C(38)	1.518(3)
C(14)-C(15)	1.390(3)	C(37)-C(40)	1.524(3)
C(15)-C(16)	1.377(3)	C(38)-H(38A)	0.9800
C(15)-H(15)	0.9500	C(38)-H(38B)	0.9800
C(16)-C(17)	1.386(3)	C(38)-H(38C)	0.9800
C(16)-H(16)	0.9500	C(39)-H(39A)	0.9800

C(39)-H(39B)	0.9800	C(64)-F(18)	1.348(2)
C(39)-H(39C)	0.9800	C(65)-C(70)	1.398(3)
C(40)-H(40A)	0.9800	C(65)-C(66)	1.406(3)
C(40)-H(40B)	0.9800	C(66)-C(67)	1.387(3)
C(40)-H(40C)	0.9800	C(66)-H(66)	0.9500
C(41)-C(42)	1.398(3)	C(67)-C(68)	1.382(3)
C(41)-C(46)	1.408(3)	C(67)-C(71)	1.500(3)
C(42)-C(43)	1.385(3)	C(68)-C(69)	1.388(3)
C(42)-H(42)	0.9500	C(68)-H(68)	0.9500
C(43)-C(44)	1.390(3)	C(69)-C(70)	1.393(3)
C(43)-C(47)	1.492(3)	C(69)-C(72)	1.489(3)
C(44)-C(45)	1.385(3)	C(70)-H(70)	0.9500
C(44)-H(44)	0.9500	C(71)-F(21)	1.325(3)
C(45)-C(46)	1.387(3)	C(71)-F(19)	1.326(3)
C(45)-C(48)	1.498(3)	C(71)-F(20)	1.327(3)
C(46)-H(46)	0.9500	C(72)-F(23)	1.334(3)
C(47)-F(1)	1.329(2)	C(72)-F(24)	1.342(3)
C(47)-F(2)	1.337(2)	C(72)-F(22)	1.344(2)
C(47)-F(3)	1.346(3)	C(73)-C(75)	1.716(13)
C(48)-F(6A)	1.16(2)	C(73)-H(73A)	0.9900
C(48)-F(4A)	1.244(17)	C(73)-H(73B)	0.9900
C(48)-F(5A)	1.293(19)	C(74)-C(75)	1.237(8)
C(48)-F(6)	1.298(3)	C(74)-H(74A)	0.9900
C(48)-F(5)	1.320(3)	C(74)-H(74B)	0.9900
C(48)-F(4)	1.333(3)	C(74)-H(75E)	1.4650
C(49)-C(50)	1.399(3)	C(74)-H(75F)	1.4689
C(49)-C(54)	1.401(3)	C(75)-H(75A)	1.0045
C(50)-C(51)	1.391(3)	C(75)-H(75B)	0.9844
C(50)-H(50)	0.9500	C(75)-H(75C)	0.9865
C(51)-C(52)	1.377(3)	C(75)-H(75D)	1.0401
C(51)-C(55)	1.494(3)	C(75)-H(75E)	0.9524
C(52)-C(53)	1.381(3)	C(75)-H(75F)	0.9543
C(52)-H(52)	0.9500	N(1)-Cu(1)-N(2)	105.53(6)
C(53)-C(54)	1.390(3)	N(1)-Cu(1)-S(2)	87.76(5)
C(53)-C(56)	1.494(3)	N(2)-Cu(1)-S(2)	108.41(5)
C(54)-H(54)	0.9500	N(1)-Cu(1)-S(3)	112.57(5)
C(55)-F(9)	1.318(3)	N(2)-Cu(1)-S(3)	87.25(5)
C(55)-F(8)	1.318(3)	S(2)-Cu(1)-S(3)	150.50(2)
C(55)-F(7)	1.356(3)	N(2)-Cu(2)-N(1)	108.09(6)
C(56)-F(11)	1.328(3)	N(2)-Cu(2)-S(4)	88.22(5)
C(56)-F(12)	1.332(3)	N(1)-Cu(2)-S(4)	108.04(5)
C(56)-F(10)	1.337(3)	N(2)-Cu(2)-S(1)	110.73(5)
C(57)-C(58)	1.391(3)	N(1)-Cu(2)-S(1)	87.69(5)
C(57)-C(62)	1.405(3)	S(4)-Cu(2)-S(1)	150.71(2)
C(58)-C(59)	1.395(3)	C(1)-N(1)-C(7)	118.48(16)
C(58)-H(58)	0.9500	C(1)-N(1)-Cu(2)	115.36(13)
C(59)-C(60)	1.384(3)	C(7)-N(1)-Cu(2)	113.35(12)
C(59)-C(63)	1.494(3)	C(1)-N(1)-Cu(1)	113.92(12)
C(60)-C(61)	1.383(3)	C(7)-N(1)-Cu(1)	114.44(12)
C(60)-H(60)	0.9500	Cu(2)-N(1)-Cu(1)	73.07(5)
C(61)-C(62)	1.390(3)	C(19)-N(2)-C(13)	119.09(16)
C(61)-C(64)	1.494(3)	C(19)-N(2)-Cu(2)	114.69(12)
C(62)-H(62)	0.9500	C(13)-N(2)-Cu(2)	114.79(12)
C(63)-F(13)	1.333(2)	C(19)-N(2)-Cu(1)	111.81(12)
C(63)-F(14)	1.334(2)	C(13)-N(2)-Cu(1)	114.85(13)
C(63)-F(15)	1.336(3)	Cu(2)-N(2)-Cu(1)	72.96(5)
C(64)-F(16)	1.335(2)	C(2)-S(1)-C(25)	103.85(10)
C(64)-F(17)	1.341(2)	C(2)-S(1)-Cu(2)	96.78(7)

C(25)-S(1)-Cu(2)	108.99(8)	C(18)-C(13)-C(14)	118.45(19)
C(8)-S(2)-C(29)	104.32(10)	C(18)-C(13)-N(2)	122.09(19)
C(8)-S(2)-Cu(1)	96.64(7)	C(14)-C(13)-N(2)	119.00(18)
C(29)-S(2)-Cu(1)	111.48(7)	C(15)-C(14)-C(13)	119.8(2)
C(14)-S(3)-C(33)	102.30(10)	C(15)-C(14)-S(3)	120.05(17)
C(14)-S(3)-Cu(1)	97.25(7)	C(13)-C(14)-S(3)	120.15(16)
C(33)-S(3)-Cu(1)	109.99(7)	C(16)-C(15)-C(14)	120.8(2)
C(20)-S(4)-C(37)	102.34(10)	C(16)-C(15)-H(15)	119.6
C(20)-S(4)-Cu(2)	95.40(7)	C(14)-C(15)-H(15)	119.6
C(37)-S(4)-Cu(2)	112.84(8)	C(15)-C(16)-C(17)	119.5(2)
C(73)-O-C(73)#1	180.0(12)	C(15)-C(16)-H(16)	120.2
C(73)-O-C(74)	58.2(8)	C(17)-C(16)-H(16)	120.2
C(73)#1-O-C(74)	121.8(8)	C(18)-C(17)-C(16)	120.5(2)
C(73)-O-C(74)#1	121.8(8)	C(18)-C(17)-H(17)	119.7
C(73)#1-O-C(74)#1	58.2(8)	C(16)-C(17)-H(17)	119.7
C(74)-O-C(74)#1	180.0(4)	C(17)-C(18)-C(13)	120.5(2)
C(65)-B(1)-C(49)	110.28(16)	C(17)-C(18)-H(18)	119.8
C(65)-B(1)-C(41)	108.35(16)	C(13)-C(18)-H(18)	119.8
C(49)-B(1)-C(41)	109.65(16)	C(24)-C(19)-N(2)	122.43(18)
C(65)-B(1)-C(57)	110.87(16)	C(24)-C(19)-C(20)	117.88(19)
C(49)-B(1)-C(57)	109.43(16)	N(2)-C(19)-C(20)	119.17(18)
C(41)-B(1)-C(57)	108.23(16)	C(21)-C(20)-C(19)	120.03(19)
C(6)-C(1)-C(2)	118.20(19)	C(21)-C(20)-S(4)	119.93(16)
C(6)-C(1)-N(1)	121.95(18)	C(19)-C(20)-S(4)	120.04(16)
C(2)-C(1)-N(1)	119.37(18)	C(22)-C(21)-C(20)	120.6(2)
C(3)-C(2)-C(1)	120.0(2)	C(22)-C(21)-H(21)	119.7
C(3)-C(2)-S(1)	120.32(17)	C(20)-C(21)-H(21)	119.7
C(1)-C(2)-S(1)	119.71(16)	C(21)-C(22)-C(23)	119.7(2)
C(4)-C(3)-C(2)	121.0(2)	C(21)-C(22)-H(22)	120.1
C(4)-C(3)-H(3)	119.5	C(23)-C(22)-H(22)	120.1
C(2)-C(3)-H(3)	119.5	C(24)-C(23)-C(22)	120.5(2)
C(3)-C(4)-C(5)	119.4(2)	C(24)-C(23)-H(23)	119.8
C(3)-C(4)-H(4)	120.3	C(22)-C(23)-H(23)	119.8
C(5)-C(4)-H(4)	120.3	C(23)-C(24)-C(19)	120.9(2)
C(6)-C(5)-C(4)	120.4(2)	C(23)-C(24)-H(24)	119.5
C(6)-C(5)-H(5)	119.8	C(19)-C(24)-H(24)	119.5
C(4)-C(5)-H(5)	119.8	C(28)-C(25)-C(26)	111.6(2)
C(5)-C(6)-C(1)	120.7(2)	C(28)-C(25)-C(27)	110.88(19)
C(5)-C(6)-H(6)	119.6	C(26)-C(25)-C(27)	110.7(2)
C(1)-C(6)-H(6)	119.6	C(28)-C(25)-S(1)	110.40(15)
C(12)-C(7)-C(8)	118.23(18)	C(26)-C(25)-S(1)	103.49(15)
C(12)-C(7)-N(1)	121.59(18)	C(27)-C(25)-S(1)	109.56(17)
C(8)-C(7)-N(1)	119.71(17)	C(25)-C(26)-H(26A)	109.5
C(9)-C(8)-C(7)	119.88(19)	C(25)-C(26)-H(26B)	109.5
C(9)-C(8)-S(2)	120.00(16)	H(26A)-C(26)-H(26B)	109.5
C(7)-C(8)-S(2)	120.09(15)	C(25)-C(26)-H(26C)	109.5
C(10)-C(9)-C(8)	120.8(2)	H(26A)-C(26)-H(26C)	109.5
C(10)-C(9)-H(9)	119.6	H(26B)-C(26)-H(26C)	109.5
C(8)-C(9)-H(9)	119.6	C(25)-C(27)-H(27A)	109.5
C(9)-C(10)-C(11)	119.2(2)	C(25)-C(27)-H(27B)	109.5
C(9)-C(10)-H(10)	120.4	H(27A)-C(27)-H(27B)	109.5
C(11)-C(10)-H(10)	120.4	C(25)-C(27)-H(27C)	109.5
C(12)-C(11)-C(10)	120.7(2)	H(27A)-C(27)-H(27C)	109.5
C(12)-C(11)-H(11)	119.6	H(27B)-C(27)-H(27C)	109.5
C(10)-C(11)-H(11)	119.6	C(25)-C(28)-H(28A)	109.5
C(11)-C(12)-C(7)	120.9(2)	C(25)-C(28)-H(28B)	109.5
C(11)-C(12)-H(12)	119.5	H(28A)-C(28)-H(28B)	109.5
C(7)-C(12)-H(12)	119.5	C(25)-C(28)-H(28C)	109.5

H(28A)-C(28)-H(28C)	109.5	H(38A)-C(38)-H(38B)	109.5
H(28B)-C(28)-H(28C)	109.5	C(37)-C(38)-H(38C)	109.5
C(31)-C(29)-C(30)	112.78(19)	H(38A)-C(38)-H(38C)	109.5
C(31)-C(29)-C(32)	110.45(19)	H(38B)-C(38)-H(38C)	109.5
C(30)-C(29)-C(32)	109.98(19)	C(37)-C(39)-H(39A)	109.5
C(31)-C(29)-S(2)	110.45(15)	C(37)-C(39)-H(39B)	109.5
C(30)-C(29)-S(2)	103.21(15)	H(39A)-C(39)-H(39B)	109.5
C(32)-C(29)-S(2)	109.74(15)	C(37)-C(39)-H(39C)	109.5
C(29)-C(30)-H(30A)	109.5	H(39A)-C(39)-H(39C)	109.5
C(29)-C(30)-H(30B)	109.5	H(39B)-C(39)-H(39C)	109.5
H(30A)-C(30)-H(30B)	109.5	C(37)-C(40)-H(40A)	109.5
C(29)-C(30)-H(30C)	109.5	C(37)-C(40)-H(40B)	109.5
H(30A)-C(30)-H(30C)	109.5	H(40A)-C(40)-H(40B)	109.5
H(30B)-C(30)-H(30C)	109.5	C(37)-C(40)-H(40C)	109.5
C(29)-C(31)-H(31A)	109.5	H(40A)-C(40)-H(40C)	109.5
C(29)-C(31)-H(31B)	109.5	H(40B)-C(40)-H(40C)	109.5
H(31A)-C(31)-H(31B)	109.5	C(42)-C(41)-C(46)	115.17(18)
C(29)-C(31)-H(31C)	109.5	C(42)-C(41)-B(1)	123.79(17)
H(31A)-C(31)-H(31C)	109.5	C(46)-C(41)-B(1)	121.04(18)
H(31B)-C(31)-H(31C)	109.5	C(43)-C(42)-C(41)	122.75(19)
C(29)-C(32)-H(32A)	109.5	C(43)-C(42)-H(42)	118.6
C(29)-C(32)-H(32B)	109.5	C(41)-C(42)-H(42)	118.6
H(32A)-C(32)-H(32B)	109.5	C(42)-C(43)-C(44)	120.67(19)
C(29)-C(32)-H(32C)	109.5	C(42)-C(43)-C(47)	121.27(18)
H(32A)-C(32)-H(32C)	109.5	C(44)-C(43)-C(47)	118.03(18)
H(32B)-C(32)-H(32C)	109.5	C(45)-C(44)-C(43)	118.20(19)
C(36)-C(33)-C(35)	110.35(19)	C(45)-C(44)-H(44)	120.9
C(36)-C(33)-C(34)	112.2(2)	C(43)-C(44)-H(44)	120.9
C(35)-C(33)-C(34)	110.66(18)	C(44)-C(45)-C(46)	120.61(19)
C(36)-C(33)-S(3)	103.85(14)	C(44)-C(45)-C(48)	119.16(19)
C(35)-C(33)-S(3)	109.71(16)	C(46)-C(45)-C(48)	120.23(19)
C(34)-C(33)-S(3)	109.80(14)	C(45)-C(46)-C(41)	122.60(19)
C(33)-C(34)-H(34A)	109.5	C(45)-C(46)-H(46)	118.7
C(33)-C(34)-H(34B)	109.5	C(41)-C(46)-H(46)	118.7
H(34A)-C(34)-H(34B)	109.5	F(1)-C(47)-F(2)	106.98(18)
C(33)-C(34)-H(34C)	109.5	F(1)-C(47)-F(3)	105.92(18)
H(34A)-C(34)-H(34C)	109.5	F(2)-C(47)-F(3)	104.86(17)
H(34B)-C(34)-H(34C)	109.5	F(1)-C(47)-C(43)	113.92(18)
C(33)-C(35)-H(35A)	109.5	F(2)-C(47)-C(43)	112.62(18)
C(33)-C(35)-H(35B)	109.5	F(3)-C(47)-C(43)	111.89(18)
H(35A)-C(35)-H(35B)	109.5	F(6A)-C(48)-F(4A)	102.3(14)
C(33)-C(35)-H(35C)	109.5	F(6A)-C(48)-F(5A)	103.0(14)
H(35A)-C(35)-H(35C)	109.5	F(4A)-C(48)-F(5A)	107.8(13)
H(35B)-C(35)-H(35C)	109.5	F(6A)-C(48)-F(6)	125.1(10)
C(33)-C(36)-H(36A)	109.5	F(4A)-C(48)-F(6)	50.5(9)
C(33)-C(36)-H(36B)	109.5	F(5A)-C(48)-F(6)	59.6(10)
H(36A)-C(36)-H(36B)	109.5	F(6A)-C(48)-F(5)	55.6(12)
C(33)-C(36)-H(36C)	109.5	F(4A)-C(48)-F(5)	135.1(8)
H(36A)-C(36)-H(36C)	109.5	F(5A)-C(48)-F(5)	53.1(10)
H(36B)-C(36)-H(36C)	109.5	F(6)-C(48)-F(5)	106.8(2)
C(39)-C(37)-C(38)	111.3(2)	F(6A)-C(48)-F(4)	47.7(12)
C(39)-C(37)-C(40)	111.9(2)	F(4A)-C(48)-F(4)	61.9(9)
C(38)-C(37)-C(40)	110.5(2)	F(5A)-C(48)-F(4)	137.1(9)
C(39)-C(37)-S(4)	110.84(15)	F(6)-C(48)-F(4)	107.6(2)
C(38)-C(37)-S(4)	109.28(16)	F(5)-C(48)-F(4)	102.6(2)
C(40)-C(37)-S(4)	102.74(15)	F(6A)-C(48)-C(45)	120.2(10)
C(37)-C(38)-H(38A)	109.5	F(4A)-C(48)-C(45)	112.2(8)
C(37)-C(38)-H(38B)	109.5	F(5A)-C(48)-C(45)	110.5(9)

F(6)-C(48)-C(45)	114.57(19)	F(16)-C(64)-F(18)	106.07(16)
F(5)-C(48)-C(45)	112.62(19)	F(17)-C(64)-F(18)	105.49(16)
F(4)-C(48)-C(45)	111.8(2)	F(16)-C(64)-C(61)	113.32(17)
C(50)-C(49)-C(54)	115.57(18)	F(17)-C(64)-C(61)	111.99(17)
C(50)-C(49)-B(1)	121.59(17)	F(18)-C(64)-C(61)	112.22(16)
C(54)-C(49)-B(1)	122.77(17)	C(70)-C(65)-C(66)	115.06(18)
C(51)-C(50)-C(49)	122.53(19)	C(70)-C(65)-B(1)	123.42(18)
C(51)-C(50)-H(50)	118.7	C(66)-C(65)-B(1)	121.28(18)
C(49)-C(50)-H(50)	118.7	C(67)-C(66)-C(65)	122.64(19)
C(52)-C(51)-C(50)	120.46(19)	C(67)-C(66)-H(66)	118.7
C(52)-C(51)-C(55)	120.59(19)	C(65)-C(66)-H(66)	118.7
C(50)-C(51)-C(55)	118.90(19)	C(68)-C(67)-C(66)	120.91(19)
C(51)-C(52)-C(53)	118.58(19)	C(68)-C(67)-C(71)	120.80(19)
C(51)-C(52)-H(52)	120.7	C(66)-C(67)-C(71)	118.28(19)
C(53)-C(52)-H(52)	120.7	C(67)-C(68)-C(69)	118.02(19)
C(52)-C(53)-C(54)	120.89(19)	C(67)-C(68)-H(68)	121.0
C(52)-C(53)-C(56)	118.34(19)	C(69)-C(68)-H(68)	121.0
C(54)-C(53)-C(56)	120.77(19)	C(68)-C(69)-C(70)	120.71(19)
C(53)-C(54)-C(49)	121.94(19)	C(68)-C(69)-C(72)	120.33(19)
C(53)-C(54)-H(54)	119.0	C(70)-C(69)-C(72)	118.94(19)
C(49)-C(54)-H(54)	119.0	C(69)-C(70)-C(65)	122.61(19)
F(9)-C(55)-F(8)	109.0(2)	C(69)-C(70)-H(70)	118.7
F(9)-C(55)-F(7)	104.7(2)	C(65)-C(70)-H(70)	118.7
F(8)-C(55)-F(7)	103.4(2)	F(21)-C(71)-F(19)	106.6(2)
F(9)-C(55)-C(51)	113.8(2)	F(21)-C(71)-F(20)	106.43(19)
F(8)-C(55)-C(51)	113.7(2)	F(19)-C(71)-F(20)	105.7(2)
F(7)-C(55)-C(51)	111.4(2)	F(21)-C(71)-C(67)	112.92(19)
F(11)-C(56)-F(12)	107.5(2)	F(19)-C(71)-C(67)	112.57(19)
F(11)-C(56)-F(10)	105.90(19)	F(20)-C(71)-C(67)	112.16(19)
F(12)-C(56)-F(10)	105.07(18)	F(23)-C(72)-F(24)	106.26(19)
F(11)-C(56)-C(53)	111.83(19)	F(23)-C(72)-F(22)	106.36(18)
F(12)-C(56)-C(53)	113.84(18)	F(24)-C(72)-F(22)	105.86(17)
F(10)-C(56)-C(53)	112.12(19)	F(23)-C(72)-C(69)	112.54(18)
C(58)-C(57)-C(62)	115.34(18)	F(24)-C(72)-C(69)	112.81(17)
C(58)-C(57)-B(1)	124.25(17)	F(22)-C(72)-C(69)	112.48(19)
C(62)-C(57)-B(1)	120.41(17)	O-C(73)-C(75)	124.3(11)
C(57)-C(58)-C(59)	122.31(18)	O-C(73)-H(73A)	106.3
C(57)-C(58)-H(58)	118.8	C(75)-C(73)-H(73A)	106.3
C(59)-C(58)-H(58)	118.8	O-C(73)-H(73B)	106.3
C(60)-C(59)-C(58)	121.23(18)	C(75)-C(73)-H(73B)	106.3
C(60)-C(59)-C(63)	119.14(18)	H(73A)-C(73)-H(73B)	106.4
C(58)-C(59)-C(63)	119.58(18)	C(75)-C(74)-O	119.3(5)
C(61)-C(60)-C(59)	117.67(19)	C(75)-C(74)-H(74A)	107.5
C(61)-C(60)-H(60)	121.2	O-C(74)-H(74A)	107.5
C(59)-C(60)-H(60)	121.2	C(75)-C(74)-H(74B)	107.5
C(60)-C(61)-C(62)	120.89(19)	O-C(74)-H(74B)	107.5
C(60)-C(61)-C(64)	120.82(18)	H(74A)-C(74)-H(74B)	107.0
C(62)-C(61)-C(64)	118.28(18)	C(75)-C(74)-H(75E)	40.2
C(61)-C(62)-C(57)	122.55(19)	O-C(74)-H(75E)	127.3
C(61)-C(62)-H(62)	118.7	H(74A)-C(74)-H(75E)	67.7
C(57)-C(62)-H(62)	118.7	H(74B)-C(74)-H(75E)	124.4
F(13)-C(63)-F(14)	105.45(18)	C(75)-C(74)-H(75F)	40.2
F(13)-C(63)-F(15)	106.71(18)	O-C(74)-H(75F)	139.7
F(14)-C(63)-F(15)	105.84(18)	H(74A)-C(74)-H(75F)	112.0
F(13)-C(63)-C(59)	112.62(18)	H(74B)-C(74)-H(75F)	68.1
F(14)-C(63)-C(59)	112.64(17)	H(75E)-C(74)-H(75F)	64.6
F(15)-C(63)-C(59)	113.00(18)	C(74)-C(75)-C(73)	56.2(6)
F(16)-C(64)-F(17)	107.21(16)	C(74)-C(75)-H(75A)	114.0

C(73)-C(75)-H(75A)	167.4	C(74)-C(75)-H(75E)	82.9
C(74)-C(75)-H(75B)	114.3	C(73)-C(75)-H(75E)	112.8
C(73)-C(75)-H(75B)	75.9	H(75A)-C(75)-H(75E)	71.0
H(75A)-C(75)-H(75B)	104.0	H(75B)-C(75)-H(75E)	162.1
C(74)-C(75)-H(75C)	114.1	H(75C)-C(75)-H(75E)	60.8
C(73)-C(75)-H(75C)	88.1	H(75D)-C(75)-H(75E)	103.7
H(75A)-C(75)-H(75C)	103.9	C(74)-C(75)-H(75F)	83.1
H(75B)-C(75)-H(75C)	105.4	C(73)-C(75)-H(75F)	113.7
C(74)-C(75)-H(75D)	167.9	H(75A)-C(75)-H(75F)	54.7
C(73)-C(75)-H(75D)	111.7	H(75B)-C(75)-H(75F)	77.7
H(75A)-C(75)-H(75D)	77.9	H(75C)-C(75)-H(75F)	157.8
H(75B)-C(75)-H(75D)	58.5	H(75D)-C(75)-H(75F)	103.6
H(75C)-C(75)-H(75D)	62.4	H(75E)-C(75)-H(75F)	110.6

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

Table 9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3**. 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)	15(1)	20(1)	16(1)	-3(1)	-2(1)	-2(1)
Cu(2)	16(1)	19(1)	21(1)	-5(1)	-4(1)	0(1)
N(1)	15(1)	16(1)	19(1)	-3(1)	-2(1)	-1(1)
N(2)	14(1)	20(1)	16(1)	-2(1)	-1(1)	-1(1)
S(1)	15(1)	17(1)	33(1)	-2(1)	-3(1)	-2(1)
S(2)	20(1)	19(1)	17(1)	-6(1)	2(1)	-4(1)
S(3)	14(1)	32(1)	17(1)	-1(1)	-2(1)	-2(1)
S(4)	23(1)	24(1)	19(1)	-9(1)	-7(1)	5(1)
O	146(7)	99(5)	302(13)	82(7)	-145(9)	-79(5)
B(1)	16(1)	18(1)	13(1)	-4(1)	-2(1)	1(1)
C(1)	12(1)	23(1)	20(1)	-3(1)	-5(1)	-3(1)
C(2)	12(1)	24(1)	27(1)	-2(1)	-4(1)	-3(1)
C(3)	20(1)	25(1)	31(1)	6(1)	-5(1)	-5(1)
C(4)	23(1)	39(1)	22(1)	2(1)	-2(1)	-10(1)
C(5)	18(1)	38(1)	22(1)	-10(1)	-2(1)	-7(1)
C(6)	17(1)	24(1)	23(1)	-6(1)	-5(1)	-4(1)
C(7)	22(1)	18(1)	13(1)	-7(1)	-1(1)	2(1)
C(8)	21(1)	21(1)	14(1)	-8(1)	-1(1)	1(1)
C(9)	33(1)	22(1)	16(1)	-6(1)	3(1)	-1(1)
C(10)	42(1)	22(1)	17(1)	-7(1)	-9(1)	9(1)
C(11)	28(1)	26(1)	28(1)	-14(1)	-12(1)	9(1)
C(12)	21(1)	22(1)	25(1)	-11(1)	-5(1)	0(1)
C(13)	12(1)	19(1)	24(1)	-2(1)	-5(1)	-3(1)
C(14)	13(1)	27(1)	24(1)	-2(1)	-4(1)	-4(1)
C(15)	21(1)	28(1)	28(1)	6(1)	-6(1)	-4(1)
C(16)	28(1)	23(1)	45(2)	1(1)	-14(1)	1(1)
C(17)	21(1)	24(1)	47(2)	-12(1)	-10(1)	5(1)
C(18)	18(1)	26(1)	27(1)	-6(1)	-5(1)	-1(1)
C(19)	23(1)	16(1)	17(1)	-8(1)	0(1)	-1(1)
C(20)	24(1)	20(1)	17(1)	-9(1)	-2(1)	1(1)
C(21)	37(1)	21(1)	15(1)	-4(1)	-2(1)	5(1)
C(22)	38(1)	22(1)	20(1)	-6(1)	10(1)	-6(1)
C(23)	26(1)	28(1)	25(1)	-13(1)	7(1)	-8(1)
C(24)	20(1)	24(1)	20(1)	-9(1)	-1(1)	0(1)
C(25)	19(1)	26(1)	48(2)	-12(1)	-5(1)	-8(1)
C(26)	34(1)	35(2)	74(2)	-28(2)	-10(1)	-5(1)
C(27)	28(1)	38(2)	61(2)	0(1)	-8(1)	-18(1)
C(28)	20(1)	32(1)	42(2)	-13(1)	-10(1)	0(1)
C(29)	33(1)	21(1)	20(1)	-9(1)	1(1)	-8(1)
C(30)	36(1)	38(2)	37(2)	-18(1)	-2(1)	-14(1)
C(31)	38(1)	29(1)	20(1)	-11(1)	2(1)	-4(1)
C(32)	53(2)	22(1)	28(1)	-10(1)	1(1)	-7(1)
C(33)	14(1)	44(1)	18(1)	-7(1)	-4(1)	-2(1)
C(34)	18(1)	47(2)	26(1)	-13(1)	-2(1)	-9(1)
C(35)	21(1)	57(2)	29(1)	-4(1)	-9(1)	1(1)
C(36)	26(1)	55(2)	26(1)	-17(1)	-6(1)	1(1)
C(37)	31(1)	35(1)	29(1)	-21(1)	-12(1)	6(1)
C(38)	56(2)	47(2)	22(1)	-18(1)	-11(1)	11(1)
C(39)	34(1)	31(1)	35(1)	-19(1)	-7(1)	3(1)
C(40)	37(2)	52(2)	53(2)	-33(1)	-22(1)	9(1)
C(41)	19(1)	17(1)	13(1)	1(1)	-3(1)	0(1)

C(42)	18(1)	17(1)	16(1)	-1(1)	0(1)	0(1)
C(43)	23(1)	16(1)	20(1)	-4(1)	-2(1)	-2(1)
C(44)	25(1)	22(1)	18(1)	-8(1)	0(1)	2(1)
C(45)	18(1)	25(1)	19(1)	-5(1)	0(1)	2(1)
C(46)	18(1)	22(1)	16(1)	-5(1)	-3(1)	-1(1)
C(47)	25(1)	25(1)	31(1)	-13(1)	2(1)	-2(1)
C(48)	22(1)	38(1)	31(1)	-17(1)	-1(1)	3(1)
C(49)	17(1)	15(1)	18(1)	-4(1)	-2(1)	-3(1)
C(50)	19(1)	19(1)	19(1)	-4(1)	-2(1)	0(1)
C(51)	22(1)	25(1)	18(1)	-6(1)	1(1)	-2(1)
C(52)	26(1)	22(1)	14(1)	1(1)	-3(1)	-4(1)
C(53)	22(1)	16(1)	19(1)	-2(1)	-3(1)	-3(1)
C(54)	18(1)	17(1)	19(1)	-5(1)	1(1)	-1(1)
C(55)	34(1)	50(2)	21(1)	-10(1)	0(1)	9(1)
C(56)	40(1)	25(1)	23(1)	-4(1)	-9(1)	9(1)
C(57)	13(1)	18(1)	17(1)	-4(1)	-3(1)	4(1)
C(58)	17(1)	19(1)	14(1)	-3(1)	-2(1)	4(1)
C(59)	16(1)	19(1)	20(1)	-9(1)	-4(1)	3(1)
C(60)	14(1)	17(1)	23(1)	-5(1)	-1(1)	0(1)
C(61)	14(1)	20(1)	16(1)	-4(1)	-2(1)	4(1)
C(62)	16(1)	20(1)	18(1)	-7(1)	-4(1)	1(1)
C(63)	25(1)	27(1)	23(1)	-10(1)	-3(1)	-2(1)
C(64)	20(1)	23(1)	20(1)	-5(1)	-2(1)	-1(1)
C(65)	19(1)	19(1)	16(1)	-8(1)	-1(1)	0(1)
C(66)	23(1)	18(1)	18(1)	-6(1)	-3(1)	2(1)
C(67)	18(1)	24(1)	23(1)	-10(1)	0(1)	-2(1)
C(68)	16(1)	27(1)	27(1)	-12(1)	-5(1)	4(1)
C(69)	23(1)	21(1)	20(1)	-9(1)	-5(1)	4(1)
C(70)	19(1)	19(1)	19(1)	-7(1)	-1(1)	0(1)
C(71)	22(1)	36(1)	31(1)	-7(1)	0(1)	-4(1)
C(72)	26(1)	30(1)	27(1)	-8(1)	-8(1)	6(1)
C(73)	59(6)	48(5)	130(11)	9(6)	-8(6)	28(4)
C(74)	34(3)	40(4)	69(4)	-19(3)	-10(3)	-1(3)
C(75)	87(4)	64(3)	227(7)	35(4)	-59(4)	-22(3)
F(1)	25(1)	59(1)	75(1)	-47(1)	10(1)	-14(1)
F(2)	51(1)	21(1)	57(1)	-9(1)	-16(1)	-6(1)
F(3)	48(1)	44(1)	33(1)	-10(1)	-12(1)	-15(1)
F(4)	34(1)	69(2)	93(2)	24(1)	12(1)	29(1)
F(5)	28(1)	105(2)	28(1)	-17(1)	10(1)	-1(1)
F(6)	19(1)	148(3)	165(3)	-140(2)	21(1)	-24(1)
F(7)	59(1)	62(1)	59(1)	-42(1)	3(1)	10(1)
F(8)	25(1)	112(2)	47(1)	-39(1)	5(1)	12(1)
F(9)	98(1)	88(1)	17(1)	-4(1)	12(1)	44(1)
F(10)	72(1)	22(1)	37(1)	8(1)	11(1)	13(1)
F(11)	72(1)	62(1)	84(1)	-42(1)	-60(1)	38(1)
F(12)	36(1)	43(1)	32(1)	0(1)	1(1)	21(1)
F(13)	39(1)	73(1)	32(1)	-36(1)	7(1)	-17(1)
F(14)	29(1)	56(1)	43(1)	-26(1)	-17(1)	5(1)
F(15)	85(1)	26(1)	43(1)	-10(1)	-26(1)	-16(1)
F(16)	38(1)	38(1)	21(1)	1(1)	0(1)	-20(1)
F(17)	39(1)	34(1)	19(1)	-6(1)	5(1)	9(1)
F(18)	25(1)	33(1)	19(1)	-2(1)	-8(1)	1(1)
F(19)	59(1)	36(1)	90(1)	-22(1)	29(1)	-22(1)
F(20)	47(1)	83(1)	33(1)	-7(1)	8(1)	-30(1)
F(21)	17(1)	69(1)	78(1)	15(1)	-9(1)	-11(1)
F(22)	23(1)	50(1)	33(1)	1(1)	-13(1)	5(1)

F(23)	96(1)	25(1)	42(1)	-11(1)	-30(1)	21(1)
F(24)	28(1)	41(1)	34(1)	10(1)	-6(1)	0(1)

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

	x	y	z	U_{eq}
H(3)	5006	6419	9023	33
H(4)	3955	7094	9747	36
H(5)	3659	8338	9309	30
H(6)	4566	8910	8189	25
H(9)	6646	10475	5758	29
H(10)	4505	10574	5460	32
H(11)	3020	9725	6097	31
H(12)	3697	8738	6952	26
H(15)	9469	5919	8676	34
H(16)	10470	5123	8064	40
H(17)	11017	5524	6854	36
H(18)	10429	6690	6245	28
H(21)	8942	9297	4681	30
H(22)	11137	9519	4631	33
H(23)	12420	8796	5466	31
H(24)	11483	7919	6397	25
H(26A)	4669	5757	6624	67
H(26B)	5883	5551	7083	67
H(26C)	5901	6253	6435	67
H(27A)	3486	6219	8229	66
H(27B)	4498	5555	8206	66
H(27C)	3254	5686	7769	66
H(28A)	4389	7300	6504	46
H(28B)	3555	7321	7229	46
H(28C)	3122	6834	6769	46
H(30A)	9574	10346	7819	52
H(30B)	10069	10179	7084	52
H(30C)	9704	9535	7762	52
H(31A)	7331	9362	8232	43
H(31B)	6225	9885	7832	43
H(31C)	7132	10173	8287	43
H(32A)	6846	10890	6798	51
H(32B)	8350	10996	6504	51
H(32C)	7802	11186	7222	51
H(34A)	10759	8406	7712	45
H(34B)	11436	7628	7745	45
H(34C)	11941	8117	8183	45
H(35A)	11522	7125	9332	55
H(35B)	11166	6652	8840	55
H(35C)	10149	6751	9482	55
H(36A)	9088	7944	9453	52
H(36B)	9205	8583	8748	52
H(36C)	10411	8365	9213	52
H(38A)	8860	8185	4264	60
H(38B)	7451	8550	4092	60
H(38C)	7904	7808	3908	60
H(39A)	8172	6679	4944	47
H(39B)	7807	6760	5724	47
H(39C)	9078	7121	5262	47
H(40A)	5900	7245	4610	64

H(40B)	5438	7982	4800	64
H(40C)	5589	7259	5413	64
H(42)	2575	6388	1422	22
H(44)	5506	5418	422	26
H(46)	6300	6903	1386	23
H(50)	2609	7558	3177	23
H(52)	4431	6146	4705	26
H(54)	5507	6216	2667	22
H(58)	5195	8156	2592	21
H(60)	6991	9607	945	22
H(62)	4789	8109	619	21
H(66)	1522	6738	2562	24
H(68)	-1193	8035	1460	27
H(70)	2627	8509	1059	22
H(73A)	9790	5592	5501	105
H(73B)	10597	4863	5788	105
H(74A)	8041	4583	5342	55
H(74B)	9129	4045	5730	55
H(75A)	7790	4454	6450	203
H(75B)	9198	4716	6431	203
H(75C)	8124	5245	6048	203
H(75D)	8375	4974	6552	203
H(75E)	7684	4868	5929	203
H(75F)	8570	4244	6348	203

Table 11. Crystal data and structure refinement for **4**.

Name of Complex	SNS-CuCl	
Empirical formula	$C_{20}H_{26}ClCuNS_2$	
Formula weight	443.53	
Temperature	96 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Crystal habit	prism	
Crystal color	green	
Crystal size	0.19 x .19 x .19 mm^3	
Space group	pbca (#61)	
Unit cell dimensions	a = 17.0807(13) Å	α= 90°.
	b = 12.3173(10) Å	β= 90°.
	c = 19.5782(15) Å	γ = 90°.
Volume	4119.0(6) $Å^3$	
Z	8	
Density (calculated)	1.430 Mg/m^3	
Absorption coefficient	1.396 mm^{-1}	
F(000)	1848	
Theta range for data collection	2.08 to 28.54°.	
Index ranges	-22<=h<=22, -12<=k<=16, -21<=l<=24	
Reflections collected	24577	
Independent reflections	4901 [R(int) = 0.0698]	
Completeness to theta = 28.54°	93.5 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4901 / 0 / 232	
Goodness-of-fit on F^2	1.235	
Final R indices [I>2sigma(I)]	R1 = 0.0381, wR2 = 0.0694	
R indices (all data)	R1 = 0.0664, wR2 = 0.0753	
Largest diff. peak and hole	0.506 and -0.441 $e.Å^{-3}$	

Special Refinement Details

Refinement of F2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F2, conventional R-factors (R) are based on F, with F set to zero for negative F2. The threshold expression of F2 > 2 $\sqrt{}$(F2) is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table 12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Cu	947(1)	3017(1)	3636(1)	12(1)
N	186(1)	2256(2)	4172(1)	14(1)
S(1)	1844(1)	2552(1)	4497(1)	13(1)
S(2)	-111(1)	3634(1)	2978(1)	12(1)
Cl	1818(1)	3735(1)	2938(1)	17(1)
C(1)	336(1)	2040(2)	4851(1)	12(1)
C(2)	1118(1)	2140(2)	5088(1)	12(1)
C(3)	1315(2)	1985(2)	5771(1)	16(1)
C(4)	752(2)	1704(2)	6245(1)	17(1)
C(5)	-20(2)	1628(2)	6028(1)	17(1)
C(6)	-229(2)	1795(2)	5353(1)	15(1)
C(7)	-538(1)	2030(2)	3870(1)	12(1)
C(8)	-791(1)	2695(2)	3324(1)	12(1)
C(9)	-1490(1)	2519(2)	2985(1)	16(1)
C(10)	-1967(2)	1668(2)	3175(1)	20(1)
C(11)	-1714(2)	964(2)	3685(1)	20(1)
C(12)	-1016(2)	1134(2)	4025(1)	16(1)
C(13)	2309(2)	1248(2)	4214(1)	17(1)
C(14)	1709(2)	516(3)	3878(2)	36(1)
C(15)	2674(2)	701(3)	4831(1)	33(1)
C(16)	2940(2)	1592(2)	3709(1)	21(1)
C(17)	-347(1)	5004(2)	3338(1)	13(1)
C(18)	-70(2)	5098(2)	4072(1)	21(1)
C(19)	-1228(2)	5181(2)	3291(1)	22(1)
C(20)	94(2)	5779(2)	2862(1)	19(1)

Table 13. Bond lengths [Å] and angles [°] for **4**.

Cu-N	1.915(2)	N-Cu-Cl	173.44(7)
Cu-Cl	2.2068(7)	N-Cu-S(2)	86.37(6)
Cu-S(2)	2.3465(7)	Cl-Cu-S(2)	92.80(2)
Cu-S(1)	2.3476(7)	N-Cu-S(1)	86.02(6)
N-C(1)	1.381(3)	Cl-Cu-S(1)	95.89(2)
N-C(7)	1.399(3)	S(2)-Cu-S(1)	167.35(3)
S(1)-C(2)	1.770(2)	C(1)-N-C(7)	122.3(2)
S(1)-C(13)	1.875(3)	C(1)-N-Cu	119.69(16)
S(2)-C(8)	1.773(2)	C(7)-N-Cu	117.76(16)
S(2)-C(17)	1.872(3)	C(2)-S(1)-C(13)	104.15(12)
C(1)-C(6)	1.410(3)	C(2)-S(1)-Cu	94.75(8)
C(1)-C(2)	1.419(3)	C(13)-S(1)-Cu	105.87(8)
C(2)-C(3)	1.391(3)	C(8)-S(2)-C(17)	107.67(11)
C(3)-C(4)	1.380(3)	C(8)-S(2)-Cu	94.73(8)
C(3)-H(3)	0.9500	C(17)-S(2)-Cu	104.55(8)
C(4)-C(5)	1.388(4)	N-C(1)-C(6)	125.8(2)
C(4)-H(4)	0.9500	N-C(1)-C(2)	118.3(2)
C(5)-C(6)	1.385(3)	C(6)-C(1)-C(2)	115.7(2)
C(5)-H(5)	0.9500	C(3)-C(2)-C(1)	122.0(2)
C(6)-H(6)	0.9500	C(3)-C(2)-S(1)	119.94(19)
C(7)-C(12)	1.406(3)	C(1)-C(2)-S(1)	117.97(18)
C(7)-C(8)	1.413(3)	C(4)-C(3)-C(2)	120.8(2)
C(8)-C(9)	1.384(3)	C(4)-C(3)-H(3)	119.6
C(9)-C(10)	1.378(4)	C(2)-C(3)-H(3)	119.6
C(9)-H(11)	0.9500	C(3)-C(4)-C(5)	118.2(2)
C(10)-C(11)	1.391(4)	C(3)-C(4)-H(4)	120.9
C(10)-H(10)	0.9500	C(5)-C(4)-H(4)	120.9
C(11)-C(12)	1.383(3)	C(6)-C(5)-C(4)	121.7(2)
C(11)-H(9)	0.9500	C(6)-C(5)-H(5)	119.1
C(12)-H(8)	0.9500	C(4)-C(5)-H(5)	119.1
C(13)-C(14)	1.516(4)	C(5)-C(6)-C(1)	121.4(2)
C(13)-C(15)	1.518(4)	C(5)-C(6)-H(6)	119.3
C(13)-C(16)	1.522(3)	C(1)-C(6)-H(6)	119.3
C(14)-H(18A)	0.9800	N-C(7)-C(12)	125.2(2)
C(14)-H(18B)	0.9800	N-C(7)-C(8)	118.3(2)
C(14)-H(18C)	0.9800	C(12)-C(7)-C(8)	116.2(2)
C(15)-H(17A)	0.9800	C(9)-C(8)-C(7)	122.4(2)
C(15)-H(17B)	0.9800	C(9)-C(8)-S(2)	118.94(19)
C(15)-H(17C)	0.9800	C(7)-C(8)-S(2)	117.88(18)
C(16)-H(19A)	0.9800	C(10)-C(9)-C(8)	120.0(2)
C(16)-H(19B)	0.9800	C(10)-C(9)-H(11)	120.0
C(16)-H(19C)	0.9800	C(8)-C(9)-H(11)	120.0
C(17)-C(18)	1.519(3)	C(9)-C(10)-C(11)	119.0(2)
C(17)-C(19)	1.523(3)	C(9)-C(10)-H(10)	120.5
C(17)-C(20)	1.532(3)	C(11)-C(10)-H(10)	120.5
C(18)-H(13A)	0.9800	C(12)-C(11)-C(10)	121.3(3)
C(18)-H(13B)	0.9800	C(12)-C(11)-H(9)	119.4
C(18)-H(13C)	0.9800	C(10)-C(11)-H(9)	119.4
C(19)-H(15A)	0.9800	C(11)-C(12)-C(7)	121.0(2)
C(19)-H(15B)	0.9800	C(11)-C(12)-H(8)	119.5
C(19)-H(15C)	0.9800	C(7)-C(12)-H(8)	119.5
C(20)-H(14A)	0.9800	C(14)-C(13)-C(15)	111.1(3)
C(20)-H(14B)	0.9800	C(14)-C(13)-C(16)	111.3(2)
C(20)-H(14C)	0.9800	C(15)-C(13)-C(16)	110.5(2)

C(14)-C(13)-S(1)	110.54(18)	C(19)-C(17)-C(20)	111.1(2)
C(15)-C(13)-S(1)	108.59(18)	C(18)-C(17)-S(2)	110.97(18)
C(16)-C(13)-S(1)	104.67(18)	C(19)-C(17)-S(2)	108.59(18)
C(13)-C(14)-H(18A)	109.5	C(20)-C(17)-S(2)	103.12(17)
C(13)-C(14)-H(18B)	109.5	C(17)-C(18)-H(13A)	109.5
H(18A)-C(14)-H(18B)	109.5	C(17)-C(18)-H(13B)	109.5
C(13)-C(14)-H(18C)	109.5	H(13A)-C(18)-H(13B)	109.5
H(18A)-C(14)-H(18C)	109.5	C(17)-C(18)-H(13C)	109.5
H(18B)-C(14)-H(18C)	109.5	H(13A)-C(18)-H(13C)	109.5
C(13)-C(15)-H(17A)	109.5	H(13B)-C(18)-H(13C)	109.5
C(13)-C(15)-H(17B)	109.5	C(17)-C(19)-H(15A)	109.5
H(17A)-C(15)-H(17B)	109.5	C(17)-C(19)-H(15B)	109.5
C(13)-C(15)-H(17C)	109.5	H(15A)-C(19)-H(15B)	109.5
H(17A)-C(15)-H(17C)	109.5	C(17)-C(19)-H(15C)	109.5
H(17B)-C(15)-H(17C)	109.5	H(15A)-C(19)-H(15C)	109.5
C(13)-C(16)-H(19A)	109.5	H(15B)-C(19)-H(15C)	109.5
C(13)-C(16)-H(19B)	109.5	C(17)-C(20)-H(14A)	109.5
H(19A)-C(16)-H(19B)	109.5	C(17)-C(20)-H(14B)	109.5
C(13)-C(16)-H(19C)	109.5	H(14A)-C(20)-H(14B)	109.5
H(19A)-C(16)-H(19C)	109.5	C(17)-C(20)-H(14C)	109.5
H(19B)-C(16)-H(19C)	109.5	H(14A)-C(20)-H(14C)	109.5
C(18)-C(17)-C(19)	110.8(2)	H(14B)-C(20)-H(14C)	109.5
C(18)-C(17)-C(20)	112.0(2)		

Symmetry transformations used to generate equivalent atoms:

Table 14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. 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	10(1)	14(1)	11(1)	1(1)	0(1)	0(1)
N	11(1)	20(1)	11(1)	2(1)	0(1)	-1(1)
S(1)	12(1)	14(1)	12(1)	1(1)	-1(1)	-1(1)
S(2)	11(1)	14(1)	11(1)	1(1)	0(1)	0(1)
Cl	12(1)	23(1)	17(1)	5(1)	2(1)	-2(1)
C(1)	14(1)	10(1)	12(1)	-2(1)	-2(1)	2(1)
C(2)	11(1)	11(1)	15(1)	-2(1)	2(1)	0(1)
C(3)	15(1)	16(1)	17(1)	-3(1)	-3(1)	2(1)
C(4)	25(2)	18(2)	8(1)	1(1)	-2(1)	2(1)
C(5)	22(2)	17(2)	13(1)	0(1)	4(1)	0(1)
C(6)	14(1)	15(2)	16(1)	0(1)	0(1)	1(1)
C(7)	9(1)	17(1)	9(1)	-2(1)	2(1)	1(1)
C(8)	13(1)	13(1)	11(1)	-2(1)	3(1)	-2(1)
C(9)	13(1)	21(2)	13(1)	2(1)	-1(1)	0(1)
C(10)	13(1)	30(2)	19(2)	0(1)	-3(1)	-6(1)
C(11)	19(1)	24(2)	18(1)	2(1)	3(1)	-9(1)
C(12)	17(1)	18(2)	14(1)	3(1)	2(1)	-1(1)
C(13)	16(1)	15(2)	22(1)	0(1)	5(1)	3(1)
C(14)	22(2)	27(2)	60(2)	-22(2)	12(2)	-3(1)
C(15)	39(2)	33(2)	27(2)	12(1)	13(1)	23(2)
C(16)	16(1)	25(2)	24(2)	3(1)	7(1)	5(1)
C(17)	13(1)	10(1)	17(1)	-1(1)	0(1)	3(1)
C(18)	26(2)	18(2)	19(2)	-4(1)	1(1)	1(1)
C(19)	17(1)	17(2)	33(2)	-3(1)	0(1)	4(1)
C(20)	20(1)	14(2)	24(2)	3(1)	2(1)	-2(1)

Table 15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^{-3}) for **4**.

	x	y	z	U_{eq}
H(3)	1843	2073	5912	19
H(4)	890	1567	6707	21
H(5)	-415	1456	6352	21
H(6)	-764	1744	5225	18
H(11)	-1642	2986	2622	19
H(10)	-2460	1564	2961	24
H(9)	-2028	354	3801	24
H(8)	-856	638	4370	20
H(18A)	1956	-172	3750	54
H(18B)	1502	872	3467	54
H(18C)	1279	376	4198	54
H(17A)	2969	60	4683	50
H(17B)	2261	479	5149	50
H(17C)	3028	1210	5060	50
H(19A)	3338	2022	3947	32
H(19B)	2704	2030	3346	32
H(19C)	3184	946	3510	32
H(13A)	-207	5816	4252	32
H(13B)	500	5003	4090	32
H(13C)	-322	4536	4350	32
H(15A)	-1356	5917	3445	33
H(15B)	-1498	4650	3580	33
H(15C)	-1398	5089	2816	33
H(14A)	-127	5732	2401	29
H(14B)	649	5576	2849	29
H(14C)	43	6524	3032	29