Supporting Information For

**Synthesis, Characterization, and Computational Study of
Three-Coordinate SNS-Copper(I) Complexes Based on
Bis-Thione Precursors**

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Supporting Information:

The ESI-MS, UV-Vis, ATR-IR, and EPR spectra of **4-6** are provided. Crystallographic details of **5 and 6** are also given. The Cartesian coordinates of all the optimized structures provided by density functional theory are also provided.

Figure 1: ESI-MS (positive ion mode) of **4**.

Figure 2: IR bands (reflectance, solid crystal), $\nu_{\text{max}}/\text{cm}^{-1}$ (intensity) 3125.98 (br), 3082.50 (br), 3050.56 (br), 2970.64 (br), 1603.64 (m), 1560.98 (m), 1447.50 (m), 1413.81 (s), 1365.84 (m), 1322.09 (w), 1306.71 (w), 1279.89 (w), 1242.24 (m), 1228.55 (m), 1181.47 (m), 1133.67 (w), 1112.41 (w), 1076.94 (w), 1014.53 (w), 985.24 (w), 916.65 (w), 878.46 (w), 835.45 (w), 795.96 (m), 760.48 (s), 722.18 (m), 688.28 (m), 643.69 (m), 635.94 (m)

Figure 2: ATR-IR of 4.

Figure 3: EPR Spectrum of 4.

Figure 4: UV-Vis Spectrum of 4.

Electronic absorption, λ_{max} (MeCN)/nm ($\epsilon/\text{M}^{-1} \text{cm}^{-1}$): 462 (260), 265 (36000), 204 (46000).

Figure 5: ESI-MS (positive ion mode) of **5**.

IR bands (reflectance, solid crystal), $\nu_{\max}/\text{cm}^{-1}$ (intensity) 3107.21 (br), 3034.61 (br), 2983.51 (br), 2971.02 (br), 2940.92 (br), 1738.29 (m), 1603.74 (w), 1539.94 (w), 1464.59 (w), 1429.55 (s), 1365.39 (s), 1288.62 (m), 1267.92 (m), 1228.06 (m), 1217.51 (m), 1167.77 (m), 1133.75 (m), 1115.38 (w), 1001.75 (s), 916.77 (w), 882.52 (w), 865.89 (w), 769.14 (m), 728.45 (m), 689.79 (w), 655.80 (m), 640.80 (m).

Figure 6: ATR-IR of 5.

Figure 7: EPR of **5** in methanol at 10K.

Figure 8: UV-Vis of **5** in acetonitrile

Electronic absorption, λ_{max} (MeCN)/nm ($\epsilon/\text{M}^{-1} \text{cm}^{-1}$): 461 (1200), 299 (5100), 258 (34000).

Table 1: X-ray crystallographic and refinement data for **5**.

Formula	$C_{34}H_{46}Cl_4Cu_3N_{14}S_4$
FW (g/mol)	1111.58
CCDC code	835944
Wavelength (Å)	0.71073
Temperature (K)	203(2)
Crystal System	Triclinic
Space group	P-1
a (Å)	9.6763(19)
b (Å)	12.338(3)
c (Å)	21.048(4)
α (°)	88.48(3)
β (°)	77.41(3)
γ (°)	74.00(3)
Volume (Å)³	2355.8(8)
Z	2
ρ (calc) (g/cm³)	1.567
Abs (mm⁻¹)	1.789
F(000)	1134
Crystal Size (mm³)	0.35 x 0.27 x 0.15
Theta range (°)	1.72 to 23.41
Refl/Uniq	20435/6866
R (int)	0.0414
Abs Correction	Multi-Scan
Max./Min.	0.765/0.566
Ref Method	Full Matrix least squares on F ²
Data / restr / par	6866 / 0 / 572
GOF on F²	1.024
R1 Indices (I>2s)	0.0490
wR2	0.1345
Peak/hole (e/Å⁻³)	2.04 and -0.46

Table 2. Bond lengths [Å] and angles [°] for **5**.

Cu(1)-S(1)	2.1989(17)
Cu(1)-S(2)	2.2003(17)
Cu(1)-N(4)	2.005(4)
Cu(2)-S(3)	2.2123(16)
Cu(2)-S(4)	2.2139(17)
Cu(2)-N(11)	2.032(4)
Cu(3)-Cl(1)	2.2343(17)
Cu(3)-Cl(2)	2.2606(16)
Cu(3)-Cl(3)	2.2750(15)
Cu(3)-Cl(4)	2.2507(16)
S(1)-C(4)	1.695(6)
S(2)-C(14)	1.696(5)
S(3)-C(21)	1.699(5)
S(4)-C(31)	1.678(5)
N(1)-N(2)	1.376(6)
N(1)-C(2)	1.466(7)
N(1)-C(4)	1.341(6)
N(2)-C(5)	1.293(7)
N(3)-C(4)	1.356(7)
N(3)-C(5)	1.362(7)

N(3)-C(6)	1.462(6)
N(4)-C(7)	1.356(7)
N(4)-C(11)	1.343(7)
N(5)-C(12)	1.462(7)
N(5)-C(13)	1.363(7)
N(5)-C(14)	1.356(7)
N(6)-N(7)	1.372(6)
N(6)-C(13)	1.286(8)
N(7)-C(14)	1.324(7)
N(7)-C(16)	1.456(8)
N(8)-N(9)	1.375(6)
N(8)-C(19)	1.456(7)
N(8)-C(21)	1.326(7)
N(9)-C(22)	1.291(7)
N(10)-C(21)	1.355(7)
N(10)-C(22)	1.358(7)
N(10)-C(23)	1.458(7)
N(11)-C(24)	1.354(6)
N(11)-C(28)	1.342(6)
N(12)-C(29)	1.455(6)
N(12)-C(30)	1.370(7)

N(12)-C(31)	1.372(6)
N(13)-N(14)	1.363(6)
N(13)-C(30)	1.273(7)
N(14)-C(31)	1.347(6)
N(14)-C(33)	1.475(7)
C(1)-C(2)	1.522(8)
C(2)-C(3)	1.498(8)
C(6)-C(7)	1.503(7)
C(7)-C(8)	1.364(8)
C(8)-C(9)	1.383(9)
C(9)-C(10)	1.354(9)
C(10)-C(11)	1.385(8)
C(11)-C(12)	1.504(8)
C(15)-C(16)	1.490(11)
C(16)-C(17)	1.523(9)
C(18)-C(19)	1.478(8)
C(19)-C(20)	1.493(9)
C(23)-C(24)	1.508(7)
C(24)-C(25)	1.369(7)
C(25)-C(26)	1.378(7)
C(26)-C(27)	1.379(7)

C(27)-C(28)	1.375(7)
C(28)-C(29)	1.496(7)
C(32)-C(33)	1.485(9)
C(33)-C(34)	1.503(10)
S(1)-Cu(1)-S(2)	123.63(7)
S(1)-Cu(1)-N(4)	118.86(15)
S(2)-Cu(1)-N(4)	117.49(15)
S(3)-Cu(2)-S(4)	121.60(7)
S(3)-Cu(2)-N(11)	118.67(12)
S(4)-Cu(2)-N(11)	119.40(12)
Cl(1)-Cu(3)-Cl(4)	98.70(7)
Cl(2)-Cu(3)-Cl(3)	101.02(6)
Cl(2)-Cu(3)-Cl(4)	130.93(7)
Cl(3)-Cu(3)-Cl(4)	98.87(7)
Cl(1)-Cu(3)-Cl(2)	97.12(6)
Cl(1)-Cu(3)-Cl(3)	136.07(6)
Cu(1)-S(1)-C(4)	103.7(2)
Cu(1)-S(2)-C(14)	101.0(2)
Cu(2)-S(3)-C(21)	100.88(16)
Cu(2)-S(4)-C(31)	103.30(19)
C(2)-N(1)-C(4)	127.9(5)

N(2)-N(1)-C(4)	112.3(4)
N(2)-N(1)-C(2)	119.7(5)
N(1)-N(2)-C(5)	103.5(5)
C(4)-N(3)-C(5)	107.3(5)
C(5)-N(3)-C(6)	125.6(5)
C(4)-N(3)-C(6)	127.1(5)
Cu(1)-N(4)-C(11)	121.9(4)
C(7)-N(4)-C(11)	117.9(5)
Cu(1)-N(4)-C(7)	120.0(4)
C(12)-N(5)-C(13)	126.2(5)
C(12)-N(5)-C(14)	126.7(5)
C(13)-N(5)-C(14)	107.0(5)
N(7)-N(6)-C(13)	103.9(5)
N(6)-N(7)-C(14)	112.3(5)
N(6)-N(7)-C(16)	120.0(5)
C(14)-N(7)-C(16)	127.3(5)
N(9)-N(8)-C(19)	119.9(4)
C(19)-N(8)-C(21)	126.8(5)
N(9)-N(8)-C(21)	113.3(4)
N(8)-N(9)-C(22)	102.9(5)
C(21)-N(10)-C(23)	126.0(5)

C(22)-N(10)-C(23)	126.5(5)
C(21)-N(10)-C(22)	107.5(4)
C(24)-N(11)-C(28)	117.6(4)
Cu(2)-N(11)-C(24)	122.4(3)
Cu(2)-N(11)-C(28)	120.0(3)
C(29)-N(12)-C(31)	126.5(4)
C(30)-N(12)-C(31)	107.2(4)
C(29)-N(12)-C(30)	126.0(4)
N(14)-N(13)-C(30)	105.2(4)
C(31)-N(14)-C(33)	126.1(4)
N(13)-N(14)-C(33)	121.3(4)
N(13)-N(14)-C(31)	112.3(4)
C(1)-C(2)-C(3)	112.4(5)
N(1)-C(2)-C(1)	108.7(5)
N(1)-C(2)-C(3)	110.3(5)
N(1)-C(4)-N(3)	104.5(5)
S(1)-C(4)-N(1)	126.4(5)
S(1)-C(4)-N(3)	129.0(5)
N(2)-C(5)-N(3)	112.3(5)
N(3)-C(6)-C(7)	111.7(5)
N(4)-C(7)-C(6)	117.2(5)

C(6)-C(7)-C(8)	120.7(6)
N(4)-C(7)-C(8)	122.1(6)
C(7)-C(8)-C(9)	119.5(6)
C(8)-C(9)-C(10)	118.9(6)
C(9)-C(10)-C(11)	119.7(6)
C(10)-C(11)-C(12)	121.2(6)
N(4)-C(11)-C(10)	121.9(6)
N(4)-C(11)-C(12)	116.8(5)
N(5)-C(12)-C(11)	111.2(5)
N(5)-C(13)-N(6)	111.8(5)
S(2)-C(14)-N(7)	127.3(5)
N(5)-C(14)-N(7)	104.9(5)
S(2)-C(14)-N(5)	127.8(5)
N(7)-C(16)-C(15)	109.6(6)
C(15)-C(16)-C(17)	111.0(6)
N(7)-C(16)-C(17)	111.3(6)
C(18)-C(19)-C(20)	112.9(6)
N(8)-C(19)-C(18)	110.2(5)
N(8)-C(19)-C(20)	110.2(5)
S(3)-C(21)-N(10)	128.3(4)
S(3)-C(21)-N(8)	127.5(4)

N(8)-C(21)-N(10)	104.1(4)
N(9)-C(22)-N(10)	112.2(5)
N(10)-C(23)-C(24)	111.5(5)
C(23)-C(24)-C(25)	119.7(5)
N(11)-C(24)-C(23)	117.2(4)
N(11)-C(24)-C(25)	123.2(4)
C(24)-C(25)-C(26)	118.6(5)
C(25)-C(26)-C(27)	118.9(5)
C(26)-C(27)-C(28)	119.7(5)
C(27)-C(28)-C(29)	120.6(4)
N(8)-C(19)-C(20)	110.2(5)
S(3)-C(21)-N(10)	128.3(4)
S(3)-C(21)-N(8)	127.5(4)
N(8)-C(21)-N(10)	104.1(4)
N(9)-C(22)-N(10)	112.2(5)
N(10)-C(23)-C(24)	111.5(5)
C(23)-C(24)-C(25)	119.7(5)
N(11)-C(24)-C(23)	117.2(4)
N(11)-C(24)-C(25)	123.2(4)
C(24)-C(25)-C(26)	118.6(5)
C(25)-C(26)-C(27)	118.9(5)

C(26)-C(27)-C(28)	119.7(5)
C(27)-C(28)-C(29)	120.6(4)
N(11)-C(28)-C(27)	122.1(5)
N(11)-C(28)-C(29)	117.4(4)
N(12)-C(29)-C(28)	113.6(5)
N(12)-C(30)-N(13)	111.6(5)
N(12)-C(31)-N(14)	103.6(4)
S(4)-C(31)-N(14)	127.7(4)
S(4)-C(31)-N(12)	128.8(4)
C(32)-C(33)-C(34)	113.4(6)
N(14)-C(33)-C(32)	110.4(5)
<u>N(14)-C(33)-C(34)</u>	<u>108.2(6)</u>

Symmetry transformations used to generate equivalent atoms:

Table 3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Atom	x	y	z	U(eq)
S(1)	839(17)	7693(14)	5205(7)	53(5)
S(2)	2823(18)	9863(14)	5572(7)	54(6)
N(1)	-1546(5)	6870(4)	5483(2)	39(14)
N(2)	-2383(5)	6418(4)	5976(2)	44(2)
N(3)	-647(5)	6927(3)	6317(2)	39(2)
N(4)	15(5)	9119(4)	6781(2)	39(2)
N(5)	1509(5)	11000(4)	6747(2)	42(2)
N(6)	3388(6)	11121(4)	7138(2)	54(2)
N(7)	3847(5)	10586(4)	6535(2)	46(2)
C(1)	-3484(7)	7422(5)	4878(3)	57(2)
C(2)	-1839(6)	6913(5)	4827(3)	46(2)
C(3)	-1285(7)	5760(5)	4504(3)	56(2)
C(4)	-475(6)	7178(4)	5679(3)	38(2)
C(5)	-1809(6)	6476(5)	6470(3)	41(2)
C(6)	239(6)	7100(4)	6766(3)	45(2)
C(7)	-375(6)	8245(5)	7103(3)	42(2)
C(8)	-1312(8)	8389(6)	7700(3)	65(3)
C(9)	-1891(9)	9457(7)	7991(3)	79(3)

C(10)	-1490(8)	10333(6)	7679(3)	65(3)
C(11)	-531(6)	10148(5)	7074(3)	43(2)
C(12)	-18(6)	11092(5)	6723(3)	45(2)
C(13)	1974(7)	11361(5)	7248(3)	51(2)
C(14)	2732(6)	10483(4)	6295(3)	43(2)
C(15)	6004(8)	9142(6)	6670(5)	10(4)
C(16)	5412(7)	10094(6)	6266(4)	62(3)
C(17)	6261(7)	10976(6)	6221(4)	66(3)
Cu(2)	34347(8)	7339(6)	8352(3)	48(3)
S(3)	3619(18)	6900(12)	7319(7)	49(5)
S(4)	3635(2)	8984(12)	8654(7)	60(6)
N(8)	4457(5)	4668(4)	6973(2)	40(2)
N(9)	4126(5)	3666(4)	7129(2)	44(2)
N(10)	2677(5)	5065(4)	7793(2)	39(2)
N(11)	2850(4)	6270(3)	9044(19)	35(1)
N(12)	3383(5)	8113(3)	9878(2)	37(1)
N(13)	2223(5)	9607(4)	10514(2)	46(2)

N(14)	2412(5)	9892(3)	9878(2)	42(2)
C(18)	5177(8)	4657(8)	5804(3)	78(3)
C(19)	5650(6)	4703(5)	6422(3)	48(2)
C(20)	7004(7)	3784(6)	6460(3)	63(3)
C(21)	3607(6)	5526(4)	7369(2)	38(2)

C(22)	3044(6)	3948(5)	7630(3)	42(2)
C(23)	1506(6)	5662(5)	8329(2)	41(2)
C(24)	2025(5)	5583(4)	8959(2)	36(2)
C(25)	1668(6)	4827(4)	9409(2)	39(2)
C(26)	2162(6)	4766(4)	9979(3)	39(2)
C(27)	3008(6)	5458(4)	10072(2)	39(2)
C(28)	3336(5)	6194(4)	9599(2)	32(2)
C(29)	4246(6)	6956(4)	9691(3)	40(2)
C(30)	2792(7)	8544(5)	10502(3)	44(2)
C(32)	616(7)	11720(5)	10149(3)	63(2)
C(33)	1985(7)	11080(5)	9694(3)	51(2)
C(34)	3268(9)	11555(6)	9670(5)	99(4)
Cu(3)	8248(7)	4188(5)	8133(3)	40(2)
Cl(1)	9924(15)	4190(12)	7216(6)	47(4)
Cl(2)	9741(15)	2919(12)	8656(6)	48(4)
Cl(3)	6136(14)	3649(12)	8416(6)	42(4)
Cl(4)	7276(18)	6065(11)	8299(7)	59(5)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**. The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	44(4)	46(4)	47(4)	-58(3)	-10(1)	-19(1)
S(1)	55(9)	66(1)	44(1)	-14(1)	-1(1)	-33(1)
S(2)	59(1)	67(1)	45(1)	-7(1)	-8(1)	-36(1)
N(1)	45(3)	39(2)	38(2)	0(2)	-12(2)	-17(2)
N(2)	50(3)	3(3)	44(3)	4(2)	-10(2)	-24(2)
N(3)	44(3)	36(2)	41(3)	2(2)	-15(2)	-14(2)
N(4)	42(3)	37(3)	42(3)	-4(2)	-17(2)	-12(2)
N(5)	44(3)	33(2)	50(3)	-1(2)	-11(2)	-11(2)
N(6)	53(3)	51(3)	58(3)	-21(2)	-15(2)	-12(2)
N(7)	38(3)	47(3)	55(3)	-12(2)	-13(2)	-14(2)
C(1)	65(4)	51(4)	66(4)	0(3)	-35(3)	-17(3)
C(2)	52(4)	54(4)	42(3)	6(3)	-16(3)	-29(3)
C(3)	65(4)	62(4)	35(3)	-7(3)	-7(3)	-11(3)
C(4)	37(3)	35(3)	41(3)	-8(2)	-9(2)	-7(2)
C(5)	48(4)	42(3)	37(3)	6(3)	-16(3)	-16(3)
C(6)	57(4)	40(3)	51(3)	11(3)	-30(3)	-20(3)
C(7)	49(3)	45(3)	43(3)	-3(3)	-24(3)	-19(3)
C(8)	104(6)	76(5)	32(3)	6(3)	-16(3)	-54(4)
C(9)	115(6)	91(6)	38(4)	-16(4)	7(4)	-56(5)
C(10)	84(5)	64(4)	50(4)	-19(3)	1(3)	-36(4)

C(11)	42(3)	44(3)	49(3)	-7(3)	-11(3)	-19(3)
C(12)	35(3)	39(3)	60(4)	-7(3)	-9(3)	-7(2)
C(13)	52(4)	41(3)	58(4)	-15(3)	-10(3)	-12(3)
C(14)	44(3)	37(3)	48(3)	-4(3)	-8(3)	-12(3)
C(15)	61(5)	48(4)	192(10)	8(5)	-30(6)	-4(4)
C(16)	44(4)	63(4)	77(5)	-25(4)	-11(3)	-11(3)
C(17)	52(4)	63(4)	84(5)	4(4)	-16(3)	-19(3)
Cu(2)	69(5)	40(4)	37(4)	-19(3)	-8(1)	-22(1)
S(3)	73(1)	46(1)	34(1)	5(1)	14(1)	-27(1)
S(4)	104(14)	41(1)	37(1)	-1(1)	-4(1)	-31(1)
N(8)	39(3)	50(3)	35(2)	-1(2)	-7(2)	-21(2)
N(9)	51(3)	45(3)	43(3)	-3(2)	-7(2)	-25(2)
N(10)	41(3)	45(3)	37(2)	-1(2)	-7(2)	-21(2)
N(11)	36(2)	30(2)	36(2)	-3(2)	-4(2)	10(2)
N(12)	44(3)	32(2)	36(2)	-3(2)	-10(2)	-11(2)
N(13)	69(3)	36(3)	33(3)	0(2)	-12(2)	-14(2)
N(14)	56(3)	32(2)	40(3)	-3(2)	-13(2)	-14(2)
C(18)	70(5)	136(7)	38(4)	11(4)	-15(3)	-41(5)
C(19)	53(4)	56(4)	40(3)	-8(3)	-3(3)	-27(3)
C(20)	53(4)	79(5)	56(4)	-4(3)	-2(3)	-25(4)
C(21)	44(3)	46(3)	29(3)	-1(2)	-13(2)	-19(3)
C(22)	44(3)	46(3)	45(3)	0(3)	-13(3)	-23(3)

C(23)	38(3)	51(3)	36(3)	-5(2)	-7(2)	-14(3)
C(24)	32(3)	40(3)	34(3)	-10(2)	-2(2)	-9(2)
C(25)	38(3)	37(3)	38(3)	-6(2)	0(2)	-11(2)
C(26)	40(3)	35(3)	38(3)	0(2)	1(2)	-11(2)
C(27)	45(3)	31(3)	36(3)	-3(2)	-7(2)	-4(2)
C(28)	30(3)	30(3)	35(3)	-4(2)	-5(2)	-6(2)
C(29)	41(3)	34(3)	45(3)	-1(2)	-10(3)	-9(2)
C(30)	66(4)	36(3)	32(3)	5(3)	-18(3)	-14(3)
C(31)	48(3)	31(3)	39(3)	-1(2)	-10(3)	-14(2)
C(32)	68(4)	50(4)	65(4)	2(3)	-19(3)	-3(3)
C(33)	68(4)	30(3)	50(4)	0(3)	-15(3)	-6(3)
C(34)	82(6)	43(4)	167(9)	-4(5)	-4(1)	-29(4)
Cu(3)	43(4)	39(4)	35(4)	2(3)	-7(1)	-10(1)
Cl(1)	47(8)	52(1)	38(7)	4(1)	-5(1)	-11(1)
Cl(2)	48(8)	50(1)	37(1)	6(1)	-9(1)	-1(1)
Cl(3)	42(8)	59(1)	36(1)	13(6)	-16(1)	-26(1)
Cl(4)	71(10)	31(1)	55(1)	1(1)	16(1)	-5(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **5**.

Atom	x	y	z	U(eq)
H(1A)	14023	3493	4858	86
H(1B)	13690	2534	5554	86
H(1C)	13787	1827	4920	86
H(2)	11200	2602	5398	63
H(3A)	10236	4529	5517	84
H(3B)	11462	4196	5933	84
H(3C)	11798	4740	5247	84
H(5)	12061	3733	3117	45
H(6A)	8750	2978	3476	55
H(6B)	9731	3482	2907	55
H(8)	11563	2233	2088	78
H(9)	12552	427	1601	95
H(10)	11862	-1064	2128	78
H(12A)	10100	-1071	3732	54
H(12B)	10653	-1817	3076	54
H(13)	8721	-1688	2331	56
H(15A)	4158	586	2885	153
H(15B)	2948	1172	3503	153
H(15C)	4496	1438	3340	153

H(16)	4460	169	4128	107
H(17A)	4102	-1560	4067	98
H(17B)	2699	-621	3950	98
H(17C)	3876	-1307	3350	98
H(18A)	5068	6047	4233	117
H(18B)	4029	5299	4559	117
H(18C)	5681	4715	4202	117
H(19)	4227	4587	3515	41
H(20A)	2749	6159	3122	95
H(20B)	2186	6144	3886	95
H(20C)	3175	6943	3587	95
H(22)	7532	6614	2130	47
H(23A)	9330	4660	1618	49
H(23B)	8833	3543	1775	49
H(25)	8901	5641	669	47
H(26)	8074	5739	-299	47
H(27)	6642	4573	-457	47
H(29A)	5208	3345	-27	48
H(29B)	5034	3043	716	48
H(30)	7094	1862	-807	15
H(32A)	10114	-1303	-202	95

H(32B)	9764	-2450	27	95
H(32C)	9168	-1827	-568	95
H(33)	8111	-954	723	56
H(34A)	6606	-1641	-110	148
H(34B)	6918	-2285	528	148
H(34C)	5845	-1047	586	148

Table 6. Torsion angles [°] for **5**.

S(2)-Cu(1)-S(1)-C(4)	179.8(2)
N(4)-Cu(1)-S(1)-C(4)	-2.0(3)
S(1)-Cu(1)-S(2)-C(14)	-174.3(2)
N(4)-Cu(1)-S(2)-C(14)	7.5(3)
S(2)-Cu(1)-N(4)-C(7)	-145.7(4)
S(1)-Cu(1)-N(4)-C(11)	-138.4(4)
S(1)-Cu(1)-N(4)-C(7)	36.0(5)
S(2)-Cu(1)-N(4)-C(11)	39.9(5)
S(3)-Cu(2)-N(11)-C(24)	-27.1(4)
S(4)-Cu(2)-S(3)-C(21)	173.0(2)
N(11)-Cu(2)-S(4)-C(31)	-2.6(3)
S(4)-Cu(2)-N(11)-C(28)	-36.4(4)
S(4)-Cu(2)-N(11)-C(24)	146.4(3)
S(3)-Cu(2)-N(11)-C(28)	150.1(3)
S(3)-Cu(2)-S(4)-C(31)	170.7(2)
N(11)-Cu(2)-S(3)-C(21)	-13.7(3)
Cu(1)-S(1)-C(4)-N(3)	-37.1(5)
Cu(1)-S(1)-C(4)-N(1)	146.8(4)
Cu(1)-S(2)-C(14)-N(5)	-45.6(5)
Cu(1)-S(2)-C(14)-N(7)	135.9(5)

Cu(2)-S(3)-C(21)-N(10)	47.6(5)
Cu(2)-S(3)-C(21)-N(8)	-136.9(5)
Cu(2)-S(4)-C(31)-N(14)	-146.2(5)
Cu(2)-S(4)-C(31)-N(12)	35.2(6)
N(2)-N(1)-C(4)-N(3)	-0.7(6)
C(2)-N(1)-N(2)-C(5)	177.9(5)
C(4)-N(1)-C(2)-C(3)	102.2(7)
C(4)-N(1)-C(2)-C(1)	-134.2(6)
C(2)-N(1)-C(4)-S(1)	-0.6(8)
C(2)-N(1)-C(4)-N(3)	-177.4(5)
N(2)-N(1)-C(4)-S(1)	176.1(4)
N(2)-N(1)-C(2)-C(3)	-74.3(7)
C(4)-N(1)-N(2)-C(5)	0.9(6)
N(2)-N(1)-C(2)-C(1)	49.4(7)
N(1)-N(2)-C(5)-N(3)	-0.7(6)
C(4)-N(3)-C(5)-N(2)	0.3(6)
C(5)-N(3)-C(4)-N(1)	-179.8(4)
C(6)-N(3)-C(4)-N(1)	0.3(6)
C(5)-N(3)-C(4)-S(1)	-176.5(4)

C(5)-N(3)-C(6)-C(7)	-90.4(6)
C(6)-N(3)-C(4)-S(1)	3.5(7)
C(4)-N(3)-C(6)-C(7)	89.7(6)
C(6)-N(3)-C(5)-N(2)	-179.7(5)
Cu(1)-N(4)-C(7)-C(8)	-173.4(5)
C(11)-N(4)-C(7)-C(8)	1.2(9)
C(11)-N(4)-C(7)-C(6)	179.6(5)
C(7)-N(4)-C(11)-C(10)	-1.5(9)
Cu(1)-N(4)-C(7)-C(6)	5.0(7)
Cu(1)-N(4)-C(11)-C(12)	-8.6(7)
Cu(1)-N(4)-C(11)-C(10)	173.1(5)
C(7)-N(4)-C(11)-C(12)	176.8(5)
C(13)-N(5)-C(14)-S(2)	179.5(4)
C(13)-N(5)-C(12)-C(11)	-82.4(7)
C(14)-N(5)-C(12)-C(11)	93.4(6)
C(12)-N(5)-C(14)-S(2)	3.0(8)
C(12)-N(5)-C(14)-N(7)	-178.1(5)
C(14)-N(5)-C(13)-N(6)	0.8(7)
C(12)-N(5)-C(13)-N(6)	177.3(5)
C(13)-N(5)-C(14)-N(7)	-1.7(6)

C(13)-N(6)-N(7)-C(14)	-1.5(6)
N(7)-N(6)-C(13)-N(5)	0.4(6)
C(13)-N(6)-N(7)-C(16)	-174.6(5)
N(6)-N(7)-C(16)-C(15)	65.5(7)
N(6)-N(7)-C(14)-S(2)	-179.2(4)
C(16)-N(7)-C(14)-S(2)	-6.7(9)
C(14)-N(7)-C(16)-C(15)	-106.5(7)
N(6)-N(7)-C(16)-C(17)	-57.7(8)
C(16)-N(7)-C(14)-N(5)	174.5(5)
N(6)-N(7)-C(14)-N(5)	2.0(6)
C(14)-N(7)-C(16)-C(17)	130.3(7)
C(21)-N(8)-N(9)-C(22)	0.3(6)
C(19)-N(8)-N(9)-C(22)	179.8(5)
C(19)-N(8)-C(21)-S(3)	3.4(9)

N(9)-N(8)-C(21)-N(10)	179.7(5)
N(9)-N(8)-C(21)-S(3)	-177.1(4)
C(21)-N(8)-C(19)-C(20)	130.2(6)
N(9)-N(8)-C(19)-C(20)	-49.2(7)
N(9)-N(8)-C(19)-C(18)	76.0(7)
C(21)-N(8)-C(19)-C(18)	-104.6(7)
C(19)-N(8)-C(21)-N(10)	179.7(5)
N(8)-N(9)-C(22)-N(10)	0.3(6)
C(21)-N(10)-C(22)-N(9)	-0.8(7)
C(22)-N(10)-C(21)-N(8)	0.9(6)
C(23)-N(10)-C(21)-S(3)	-3.3(8)
C(23)-N(10)-C(21)-N(8)	-179.6(5)
C(21)-N(10)-C(23)-C(24)	-94.0(6)
C(22)-N(10)-C(23)-C(24)	85.4(7)
C(22)-N(10)-C(21)-S(3)	177.2(5)
C(23)-N(10)-C(22)-N(9)	179.7(5)
Cu(2)-N(11)-C(24)-C(25)	177.4(4)
Cu(2)-N(11)-C(28)-C(27)	-177.9(4)
Cu(2)-N(11)-C(24)-C(23)	-1.8(6)
C(28)-N(11)-C(24)-C(23)	-179.0(4)
C(28)-N(11)-C(24)-C(25)	0.2(7)

Cu(2)-N(11)-C(28)-C(29)	2.8(6)
C(24)-N(11)-C(28)-C(29)	-179.9(4)
C(24)-N(11)-C(28)-C(27)	-0.6(7)
C(31)-N(12)-C(29)-C(28)	-96.5(7)
C(29)-N(12)-C(31)-S(4)	4.7(9)
C(29)-N(12)-C(31)-N(14)	-174.2(5)
C(30)-N(12)-C(31)-N(14)	-0.1(6)
C(29)-N(12)-C(30)-N(13)	173.4(6)
C(30)-N(12)-C(31)-S(4)	178.8(5)
C(31)-N(12)-C(30)-N(13)	-0.8(8)
C(30)-N(12)-C(29)-C(28)	90.5(7)
N(14)-N(13)-C(30)-N(12)	1.3(7)
C(30)-N(13)-N(14)-C(31)	-1.3(7)
C(30)-N(13)-N(14)-C(33)	-175.5(6)
N(13)-N(14)-C(33)-C(32)	-36.9(8)
N(13)-N(14)-C(33)-C(34)	87.7(7)
C(33)-N(14)-C(31)-N(12)	174.7(5)
C(33)-N(14)-C(31)-S(4)	-178.1(5)
C(31)-N(14)-C(33)-C(34)	-85.6(8)
C(31)-N(14)-C(33)-C(32)	149.8(6)

N(13)-N(14)-C(31)-N(12)	0.8(6)
N(13)-N(14)-C(31)-S(4)	-4.2(9)
N(3)-C(6)-C(7)-N(4)	-84.1(6)
N(3)-C(6)-C(7)-C(8)	94.3(7)
C(6)-C(7)-C(8)-C(9)	-178.3(7)
N(4)-C(7)-C(8)-C(9)	0.1(11)
C(7)-C(8)-C(9)-C(10)	-1.2(12)
C(8)-C(9)-C(10)-C(11)	0.9(12)
C(9)-C(10)-C(11)-N(4)	0.4(11)
C(9)-C(10)-C(11)-C(12)	-177.8(7)
N(4)-C(11)-C(12)-N(5)	-72.7(7)
C(10)-C(11)-C(12)-N(5)	105.6(7)
N(10)-C(23)-C(24)-C(25)	-100.9(6)
N(10)-C(23)-C(24)-N(11)	78.4(6)
N(11)-C(24)-C(25)-C(26)	0.5(8)
C(23)-C(24)-C(25)-C(26)	179.6(5)
C(24)-C(25)-C(26)-C(27)	-0.7(8)
C(25)-C(26)-C(27)-C(28)	0.3(8)
C(26)-C(27)-C(28)-N(11)	0.4(8)
C(26)-C(27)-C(28)-C(29)	179.7(5)
N(11)-C(28)-C(29)-N(12)	77.3(6)

C(27)-C(28)-C(29)-N(12) -102.0(6)

Symmetry transformations used to generate equivalent atoms:

Figure 9: ESI-MS (positive ion mode) of **6**.

Figure 10: ATR-IR of **6**.

Figure 11: UV-Vis Spectrum of **6** in acetonitrile

Electronic absorption, λ_{max} (MeCN)/nm ($\epsilon/\text{M}^{-1} \text{cm}^{-1}$): 461 (790), 307 (3200), 258 (22000).

Table 7. Crystal data and structure refinement for **6**.

Identification code	aed-20	
Empirical formula	C38 H54 Cl4 Cu3 N14 S4	
Formula weight	1167.61	
Temperature	173(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 8.7628(6) Å	$\alpha = 102.099(6)^\circ$.
	b = 14.7735(10) Å	$\beta = 90.808(5)^\circ$.
	c = 19.8970(13) Å	$\gamma = 90.228(5)^\circ$.
Volume	2518.3(3) Å ³	
Z	2	
Density (calculated)	1.540 Mg/m ³	
Absorption coefficient	5.331 mm ⁻¹	
F(000)	1198	
Crystal size	0.12 x 0.10 x 0.06 mm ³	
Theta range for data collection	3.41 to 71.49°.	
Index ranges	-9<=h<=10, -17<=k<=18, -24<=l<=20	
Reflections collected	16392	
Independent reflections	9552 [R(int) = 0.0351]	
Completeness to theta = 67.50°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.39117	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9552 / 0 / 573	
Goodness-of-fit on F ²	1.068	
Final R indices [I>2sigma(I)]	R1 = 0.0881, wR2 = 0.2502	
R indices (all data)	R1 = 0.1028, wR2 = 0.2699	
Largest diff. peak and hole	3.078 and -1.223 e.Å ⁻³	

Table 8. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **6**. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	2749(1)	5434(1)	7377(1)	35(1)
Cu(2)	7355(1)	410(1)	7402(1)	35(1)
Cu(3)	14776(1)	2268(1)	9838(1)	36(1)
Cl(1)	16463(2)	2743(1)	9163(1)	41(1)
Cl(2)	12547(3)	2922(2)	10290(1)	58(1)
Cl(3)	16143(3)	2387(2)	10810(1)	47(1)
Cl(4)	13689(2)	1108(2)	9059(1)	46(1)
S(1)	2040(3)	6702(1)	7049(1)	46(1)
S(2)	3806(3)	4286(1)	6626(1)	42(1)
S(3)	8036(3)	1679(1)	7066(1)	45(1)
S(4)	6266(3)	-772(1)	6667(1)	41(1)
N(1)	1325(8)	8319(4)	7911(3)	34(1)
N(2)	571(9)	8670(5)	8503(4)	40(2)
N(3)	525(7)	7145(4)	8287(3)	28(1)
N(4)	2392(7)	5283(4)	8344(3)	31(1)
N(5)	2990(9)	2581(5)	6848(4)	40(2)
N(6)	3017(9)	2062(5)	7348(4)	44(2)
N(7)	3989(8)	3456(4)	7743(3)	36(1)
N(8)	8896(8)	3303(5)	7909(4)	39(2)
N(9)	9725(9)	3659(5)	8489(4)	44(2)
N(10)	9694(7)	2138(4)	8285(3)	34(1)
N(11)	7802(7)	261(4)	8370(3)	32(1)
N(12)	7135(8)	-2446(5)	6919(4)	39(2)
N(13)	7163(10)	-2955(5)	7427(4)	46(2)
N(14)	6213(8)	-1569(4)	7801(3)	36(1)
C(1)	1314(9)	7393(5)	7765(4)	34(2)
C(2)	112(9)	7954(5)	8723(4)	36(2)
C(3)	118(9)	6208(5)	8342(4)	34(2)
C(4)	1262(9)	5740(5)	8721(4)	31(2)
C(5)	1133(9)	5763(5)	9411(4)	36(2)
C(6)	2116(10)	5276(5)	9734(4)	40(2)

C(7)	3257(10)	4782(6)	9353(4)	41(2)
C(8)	3371(8)	4798(5)	8668(4)	32(2)
C(9)	4604(9)	4262(5)	8236(4)	38(2)
C(10)	3577(9)	3428(6)	7078(4)	38(2)
C(11)	3624(10)	2617(6)	7877(4)	41(2)
C(12)	1946(10)	8916(5)	7483(4)	38(2)
C(13)	848(9)	8990(6)	6897(4)	38(2)
C(14)	1515(11)	9595(6)	6436(5)	46(2)
C(15)	473(13)	9632(8)	5829(5)	60(3)
C(16)	2465(12)	2169(7)	6154(5)	49(2)
C(17)	3680(14)	1545(11)	5757(6)	79(4)
C(18)	5198(17)	1902(10)	5734(6)	79(4)
C(19)	6235(18)	1164(13)	5338(7)	101(6)
C(20)	8877(9)	2375(5)	7766(4)	35(2)
C(21)	10171(10)	2947(6)	8705(4)	42(2)
C(22)	10079(9)	1199(5)	8341(4)	36(2)
C(23)	8958(9)	748(5)	8730(4)	32(2)
C(24)	9128(10)	824(5)	9436(4)	38(2)
C(25)	8129(11)	372(6)	9778(4)	41(2)
C(26)	6948(10)	-162(5)	9411(4)	37(2)
C(27)	6813(9)	-193(5)	8711(4)	33(2)
C(28)	5578(10)	-760(5)	8284(4)	38(2)
C(29)	6540(9)	-1601(5)	7139(4)	35(2)
C(30)	6599(11)	-2394(6)	7957(4)	41(2)
C(31)	8223(10)	3887(6)	7474(5)	43(2)
C(32)	9286(10)	3963(6)	6887(5)	41(2)
C(33)	8557(12)	4545(7)	6423(5)	52(2)
C(34)	9554(14)	4610(9)	5810(6)	64(3)
C(35)	7631(11)	-2864(7)	6225(5)	49(2)
C(36)	6419(14)	-3515(10)	5821(6)	76(4)
C(37)	4936(15)	-3112(8)	5767(6)	68(3)
C(38)	3808(16)	-3844(10)	5362(6)	81(4)

Table 9. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for **6**.

Cu(1)-N(4)	2.012(6)
Cu(1)-S(1)	2.198(2)
Cu(1)-S(2)	2.225(2)
Cu(2)-N(11)	2.018(6)
Cu(2)-S(3)	2.201(2)
Cu(2)-S(4)	2.230(2)
Cu(3)-Cl(1)	2.219(2)
Cu(3)-Cl(3)	2.235(2)
Cu(3)-Cl(4)	2.255(2)
Cu(3)-Cl(2)	2.293(2)
S(1)-C(1)	1.702(8)
S(2)-C(10)	1.714(8)
S(3)-C(20)	1.705(8)
S(4)-C(29)	1.709(8)
N(1)-C(1)	1.338(9)
N(1)-N(2)	1.365(10)
N(1)-C(12)	1.457(10)
N(2)-C(2)	1.292(11)
N(3)-C(1)	1.367(10)
N(3)-C(2)	1.374(9)
N(3)-C(3)	1.456(9)
N(4)-C(4)	1.347(10)
N(4)-C(8)	1.360(10)
N(5)-C(10)	1.337(11)
N(5)-N(6)	1.378(10)
N(5)-C(16)	1.454(12)
N(6)-C(11)	1.296(12)
N(7)-C(10)	1.359(11)
N(7)-C(11)	1.359(11)
N(7)-C(9)	1.470(11)
N(8)-C(20)	1.340(10)
N(8)-N(9)	1.362(10)
N(8)-C(31)	1.463(11)
N(9)-C(21)	1.277(12)

N(10)-C(20)	1.355(10)
N(10)-C(21)	1.368(10)
N(10)-C(22)	1.454(10)
N(11)-C(23)	1.347(10)
N(11)-C(27)	1.365(10)
N(12)-C(29)	1.344(10)
N(12)-N(13)	1.379(10)
N(12)-C(35)	1.464(11)
N(13)-C(30)	1.302(12)
N(14)-C(29)	1.342(11)
N(14)-C(30)	1.363(10)
N(14)-C(28)	1.484(10)
C(2)-H(2)	0.9300
C(3)-C(4)	1.501(10)
C(3)-H(3A)	0.9700
C(3)-H(3B)	0.9700
C(4)-C(5)	1.372(11)
C(5)-C(6)	1.363(12)
C(5)-H(5)	0.9300
C(6)-C(7)	1.380(13)
C(6)-H(6)	0.9300
C(7)-C(8)	1.373(11)
C(7)-H(7)	0.9300
C(8)-C(9)	1.510(11)
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(11)-H(11)	0.9300
C(12)-C(13)	1.524(11)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(13)-C(14)	1.528(11)
C(13)-H(13A)	0.9700
C(13)-H(13B)	0.9700
C(14)-C(15)	1.514(13)
C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700

C(15)-H(15A)	0.9600
C(15)-H(15B)	0.9600
C(15)-H(15C)	0.9600
C(16)-C(17)	1.529(15)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(17)-C(18)	1.43(2)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(18)-C(19)	1.517(18)
C(18)-H(18A)	0.9700
C(18)-H(18B)	0.9700
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(21)-H(21)	0.9300
C(22)-C(23)	1.498(11)
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-C(24)	1.391(11)
C(24)-C(25)	1.371(13)
C(24)-H(24)	0.9300
C(25)-C(26)	1.399(12)
C(25)-H(25)	0.9300
C(26)-C(27)	1.387(11)
C(26)-H(26)	0.9300
C(27)-C(28)	1.505(11)
C(28)-H(28A)	0.9700
C(28)-H(28B)	0.9700
C(30)-H(30)	0.9300
C(31)-C(32)	1.527(12)
C(31)-H(31A)	0.9700
C(31)-H(31B)	0.9700
C(32)-C(33)	1.523(12)
C(32)-H(32A)	0.9700
C(32)-H(32B)	0.9700

C(33)-C(34)	1.531(14)
C(33)-H(33A)	0.9700
C(33)-H(33B)	0.9700
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600
C(35)-C(36)	1.530(14)
C(35)-H(35A)	0.9700
C(35)-H(35B)	0.9700
C(36)-C(37)	1.444(18)
C(36)-H(36A)	0.9700
C(36)-H(36B)	0.9700
C(37)-C(38)	1.550(15)
C(37)-H(37A)	0.9700
C(37)-H(37B)	0.9700
C(38)-H(38A)	0.9600
C(38)-H(38B)	0.9600
C(38)-H(38C)	0.9600
N(4)-Cu(1)-S(1)	120.54(19)
N(4)-Cu(1)-S(2)	119.51(18)
S(1)-Cu(1)-S(2)	119.92(9)
N(11)-Cu(2)-S(3)	120.74(19)
N(11)-Cu(2)-S(4)	118.30(19)
S(3)-Cu(2)-S(4)	120.88(9)
Cl(1)-Cu(3)-Cl(3)	101.20(9)
Cl(1)-Cu(3)-Cl(4)	98.66(9)
Cl(3)-Cu(3)-Cl(4)	136.07(9)
Cl(1)-Cu(3)-Cl(2)	130.91(10)
Cl(3)-Cu(3)-Cl(2)	99.22(10)
Cl(4)-Cu(3)-Cl(2)	96.58(10)
C(1)-S(1)-Cu(1)	105.1(3)
C(10)-S(2)-Cu(1)	98.0(3)
C(20)-S(3)-Cu(2)	105.8(3)
C(29)-S(4)-Cu(2)	97.8(3)
C(1)-N(1)-N(2)	112.0(7)

C(1)-N(1)-C(12)	126.2(7)
N(2)-N(1)-C(12)	121.7(6)
C(2)-N(2)-N(1)	105.0(6)
C(1)-N(3)-C(2)	106.7(6)
C(1)-N(3)-C(3)	126.3(6)
C(2)-N(3)-C(3)	126.9(6)
C(4)-N(4)-C(8)	117.1(6)
C(4)-N(4)-Cu(1)	121.0(5)
C(8)-N(4)-Cu(1)	121.6(5)
C(10)-N(5)-N(6)	111.8(7)
C(10)-N(5)-C(16)	127.8(7)
N(6)-N(5)-C(16)	120.2(7)
C(11)-N(6)-N(5)	103.7(7)
C(10)-N(7)-C(11)	106.8(7)
C(10)-N(7)-C(9)	126.4(7)
C(11)-N(7)-C(9)	126.6(7)
C(20)-N(8)-N(9)	112.2(7)
C(20)-N(8)-C(31)	125.1(7)
N(9)-N(8)-C(31)	122.5(7)
C(21)-N(9)-N(8)	104.2(7)
C(20)-N(10)-C(21)	106.5(7)
C(20)-N(10)-C(22)	125.7(6)
C(21)-N(10)-C(22)	127.6(7)
C(23)-N(11)-C(27)	118.3(6)
C(23)-N(11)-Cu(2)	119.3(5)
C(27)-N(11)-Cu(2)	121.4(5)
C(29)-N(12)-N(13)	112.2(7)
C(29)-N(12)-C(35)	127.6(8)
N(13)-N(12)-C(35)	120.1(7)
C(30)-N(13)-N(12)	103.8(7)
C(29)-N(14)-C(30)	108.6(7)
C(29)-N(14)-C(28)	125.6(7)
C(30)-N(14)-C(28)	125.8(7)
N(1)-C(1)-N(3)	105.0(7)
N(1)-C(1)-S(1)	126.0(6)
N(3)-C(1)-S(1)	128.8(6)

N(2)-C(2)-N(3)	111.4(7)
N(2)-C(2)-H(2)	124.3
N(3)-C(2)-H(2)	124.3
N(3)-C(3)-C(4)	115.0(6)
N(3)-C(3)-H(3A)	108.5
C(4)-C(3)-H(3A)	108.5
N(3)-C(3)-H(3B)	108.5
C(4)-C(3)-H(3B)	108.5
H(3A)-C(3)-H(3B)	107.5
N(4)-C(4)-C(5)	122.3(7)
N(4)-C(4)-C(3)	116.3(7)
C(5)-C(4)-C(3)	121.4(7)
C(6)-C(5)-C(4)	120.4(7)
C(6)-C(5)-H(5)	119.8
C(4)-C(5)-H(5)	119.8
C(5)-C(6)-C(7)	118.2(8)
C(5)-C(6)-H(6)	120.9
C(7)-C(6)-H(6)	120.9
C(8)-C(7)-C(6)	119.5(8)
C(8)-C(7)-H(7)	120.3
C(6)-C(7)-H(7)	120.3
N(4)-C(8)-C(7)	122.5(7)
N(4)-C(8)-C(9)	116.7(7)
C(7)-C(8)-C(9)	120.8(7)
N(7)-C(9)-C(8)	112.2(7)
N(7)-C(9)-H(9A)	109.2
C(8)-C(9)-H(9A)	109.2
N(7)-C(9)-H(9B)	109.2
C(8)-C(9)-H(9B)	109.2
H(9A)-C(9)-H(9B)	107.9
N(5)-C(10)-N(7)	105.3(7)
N(5)-C(10)-S(2)	127.5(7)
N(7)-C(10)-S(2)	127.2(6)
N(6)-C(11)-N(7)	112.4(7)
N(6)-C(11)-H(11)	123.8
N(7)-C(11)-H(11)	123.8

N(1)-C(12)-C(13)	111.2(7)
N(1)-C(12)-H(12A)	109.4
C(13)-C(12)-H(12A)	109.4
N(1)-C(12)-H(12B)	109.4
C(13)-C(12)-H(12B)	109.4
H(12A)-C(12)-H(12B)	108.0
C(12)-C(13)-C(14)	111.3(7)
C(12)-C(13)-H(13A)	109.4
C(14)-C(13)-H(13A)	109.4
C(12)-C(13)-H(13B)	109.4
C(14)-C(13)-H(13B)	109.4
H(13A)-C(13)-H(13B)	108.0
C(15)-C(14)-C(13)	111.9(8)
C(15)-C(14)-H(14A)	109.2
C(13)-C(14)-H(14A)	109.2
C(15)-C(14)-H(14B)	109.2
C(13)-C(14)-H(14B)	109.2
H(14A)-C(14)-H(14B)	107.9
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
N(5)-C(16)-C(17)	111.4(8)
N(5)-C(16)-H(16A)	109.3
C(17)-C(16)-H(16A)	109.3
N(5)-C(16)-H(16B)	109.3
C(17)-C(16)-H(16B)	109.3
H(16A)-C(16)-H(16B)	108.0
C(18)-C(17)-C(16)	119.0(11)
C(18)-C(17)-H(17A)	107.6
C(16)-C(17)-H(17A)	107.6
C(18)-C(17)-H(17B)	107.6
C(16)-C(17)-H(17B)	107.6
H(17A)-C(17)-H(17B)	107.0

C(17)-C(18)-C(19)	110.6(13)
C(17)-C(18)-H(18A)	109.5
C(19)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
C(19)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	108.1
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
N(8)-C(20)-N(10)	104.6(7)
N(8)-C(20)-S(3)	126.2(6)
N(10)-C(20)-S(3)	129.2(6)
N(9)-C(21)-N(10)	112.4(8)
N(9)-C(21)-H(21)	123.8
N(10)-C(21)-H(21)	123.8
N(10)-C(22)-C(23)	114.8(7)
N(10)-C(22)-H(22A)	108.6
C(23)-C(22)-H(22A)	108.6
N(10)-C(22)-H(22B)	108.6
C(23)-C(22)-H(22B)	108.6
H(22A)-C(22)-H(22B)	107.6
N(11)-C(23)-C(24)	121.8(7)
N(11)-C(23)-C(22)	117.6(7)
C(24)-C(23)-C(22)	120.7(7)
C(25)-C(24)-C(23)	119.8(8)
C(25)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1
C(24)-C(25)-C(26)	119.3(8)
C(24)-C(25)-H(25)	120.3
C(26)-C(25)-H(25)	120.3
C(27)-C(26)-C(25)	118.2(8)
C(27)-C(26)-H(26)	120.9
C(25)-C(26)-H(26)	120.9

N(11)-C(27)-C(26)	122.5(7)
N(11)-C(27)-C(28)	116.6(7)
C(26)-C(27)-C(28)	120.9(7)
N(14)-C(28)-C(27)	111.6(7)
N(14)-C(28)-H(28A)	109.3
C(27)-C(28)-H(28A)	109.3
N(14)-C(28)-H(28B)	109.3
C(27)-C(28)-H(28B)	109.3
H(28A)-C(28)-H(28B)	108.0
N(14)-C(29)-N(12)	104.4(7)
N(14)-C(29)-S(4)	128.8(6)
N(12)-C(29)-S(4)	126.8(7)
N(13)-C(30)-N(14)	111.1(7)
N(13)-C(30)-H(30)	124.5
N(14)-C(30)-H(30)	124.5
N(8)-C(31)-C(32)	110.7(7)
N(8)-C(31)-H(31A)	109.5
C(32)-C(31)-H(31A)	109.5
N(8)-C(31)-H(31B)	109.5
C(32)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	108.1
C(33)-C(32)-C(31)	110.4(7)
C(33)-C(32)-H(32A)	109.6
C(31)-C(32)-H(32A)	109.6
C(33)-C(32)-H(32B)	109.6
C(31)-C(32)-H(32B)	109.6
H(32A)-C(32)-H(32B)	108.1
C(32)-C(33)-C(34)	112.4(9)
C(32)-C(33)-H(33A)	109.1
C(34)-C(33)-H(33A)	109.1
C(32)-C(33)-H(33B)	109.1
C(34)-C(33)-H(33B)	109.1
H(33A)-C(33)-H(33B)	107.9
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5

C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
N(12)-C(35)-C(36)	112.1(8)
N(12)-C(35)-H(35A)	109.2
C(36)-C(35)-H(35A)	109.2
N(12)-C(35)-H(35B)	109.2
C(36)-C(35)-H(35B)	109.2
H(35A)-C(35)-H(35B)	107.9
C(37)-C(36)-C(35)	115.5(10)
C(37)-C(36)-H(36A)	108.4
C(35)-C(36)-H(36A)	108.4
C(37)-C(36)-H(36B)	108.4
C(35)-C(36)-H(36B)	108.4
H(36A)-C(36)-H(36B)	107.5
C(36)-C(37)-C(38)	110.4(11)
C(36)-C(37)-H(37A)	109.6
C(38)-C(37)-H(37A)	109.6
C(36)-C(37)-H(37B)	109.6
C(38)-C(37)-H(37B)	109.6
H(37A)-C(37)-H(37B)	108.1
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 10. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **6**. The anisotropic displacement factor exponent takes the form: $-2p^2[h^2 a^{*2}U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	40(1)	28(1)	40(1)	12(1)	8(1)	8(1)
Cu(2)	40(1)	28(1)	38(1)	10(1)	-8(1)	-2(1)
Cu(3)	27(1)	42(1)	45(1)	20(1)	2(1)	4(1)
Cl(1)	31(1)	46(1)	50(1)	18(1)	6(1)	2(1)
Cl(2)	44(1)	75(2)	65(1)	35(1)	19(1)	26(1)
Cl(3)	45(1)	50(1)	49(1)	19(1)	-6(1)	-10(1)
Cl(4)	38(1)	44(1)	58(1)	17(1)	-11(1)	-2(1)
S(1)	70(2)	32(1)	42(1)	16(1)	17(1)	17(1)
S(2)	54(1)	34(1)	43(1)	16(1)	16(1)	15(1)
S(3)	63(1)	31(1)	43(1)	14(1)	-15(1)	-9(1)
S(4)	50(1)	34(1)	39(1)	10(1)	-12(1)	-5(1)
N(1)	40(4)	21(3)	41(3)	10(2)	-5(3)	6(2)
N(2)	48(4)	29(3)	42(4)	3(3)	-6(3)	6(3)
N(3)	27(3)	23(3)	33(3)	7(2)	5(2)	6(2)
N(4)	34(3)	27(3)	35(3)	9(2)	1(3)	4(2)
N(5)	45(4)	33(3)	45(4)	13(3)	7(3)	9(3)
N(6)	52(4)	34(3)	50(4)	15(3)	8(3)	8(3)
N(7)	39(4)	31(3)	41(3)	11(3)	6(3)	9(3)
N(8)	45(4)	30(3)	44(4)	11(3)	10(3)	-1(3)
N(9)	48(4)	35(4)	46(4)	5(3)	8(3)	-11(3)
N(10)	30(3)	34(3)	38(3)	6(3)	1(3)	-6(3)
N(11)	30(3)	29(3)	37(3)	8(2)	-3(3)	4(2)
N(12)	39(4)	32(3)	45(4)	5(3)	-5(3)	2(3)
N(13)	58(5)	36(4)	46(4)	11(3)	-6(3)	5(3)
N(14)	39(4)	30(3)	40(3)	8(3)	-6(3)	-1(3)
C(1)	40(4)	23(3)	40(4)	11(3)	0(3)	5(3)
C(2)	38(4)	28(4)	40(4)	2(3)	2(3)	8(3)
C(3)	33(4)	28(4)	43(4)	10(3)	2(3)	2(3)
C(4)	34(4)	19(3)	41(4)	9(3)	4(3)	-1(3)
C(5)	38(4)	30(4)	38(4)	4(3)	9(3)	2(3)
C(6)	51(5)	33(4)	38(4)	16(3)	6(3)	-4(3)

C(7)	48(5)	32(4)	45(4)	13(3)	-3(4)	1(3)
C(8)	22(3)	28(3)	45(4)	8(3)	1(3)	1(3)
C(9)	31(4)	34(4)	52(5)	13(3)	1(3)	10(3)
C(10)	36(4)	33(4)	45(4)	8(3)	11(3)	10(3)
C(11)	50(5)	33(4)	45(4)	19(3)	8(4)	9(3)
C(12)	38(4)	30(4)	51(5)	17(3)	-5(3)	3(3)
C(13)	36(4)	34(4)	48(4)	16(3)	0(3)	3(3)
C(14)	46(5)	44(5)	51(5)	20(4)	1(4)	3(4)
C(15)	65(7)	68(7)	52(5)	25(5)	0(5)	8(5)
C(16)	58(6)	44(5)	47(5)	14(4)	-1(4)	4(4)
C(17)	59(7)	107(10)	54(6)	-21(6)	3(5)	3(7)
C(18)	90(9)	89(9)	59(7)	17(6)	-2(6)	23(8)
C(19)	83(10)	151(15)	57(7)	-9(8)	7(7)	54(10)
C(20)	34(4)	27(3)	46(4)	12(3)	3(3)	-3(3)
C(21)	39(4)	48(5)	36(4)	4(3)	3(3)	-14(4)
C(22)	32(4)	36(4)	41(4)	9(3)	-6(3)	4(3)
C(23)	32(4)	25(3)	40(4)	6(3)	-2(3)	6(3)
C(24)	42(4)	30(4)	43(4)	12(3)	-11(3)	5(3)
C(25)	52(5)	34(4)	37(4)	8(3)	-5(4)	9(4)
C(26)	41(4)	33(4)	39(4)	13(3)	2(3)	7(3)
C(27)	32(4)	28(4)	39(4)	7(3)	-1(3)	2(3)
C(28)	43(4)	32(4)	41(4)	10(3)	-4(3)	1(3)
C(29)	30(4)	31(4)	42(4)	3(3)	-7(3)	-3(3)
C(30)	51(5)	35(4)	41(4)	16(3)	-6(4)	0(4)
C(31)	39(4)	30(4)	61(5)	17(4)	13(4)	3(3)
C(32)	41(4)	35(4)	52(5)	18(4)	7(4)	3(3)
C(33)	55(6)	43(5)	66(6)	27(4)	-2(5)	3(4)
C(34)	69(7)	75(7)	57(6)	36(5)	-2(5)	-8(6)
C(35)	43(5)	50(5)	50(5)	-1(4)	2(4)	3(4)
C(36)	59(7)	95(9)	57(6)	-28(6)	-4(5)	2(6)
C(37)	79(8)	61(6)	61(6)	10(5)	-16(6)	-8(6)
C(38)	72(8)	105(10)	58(7)	2(7)	-5(6)	-43(8)

Table 11. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for **6**.

	x	y	z	U(eq)
H(2)	-430	7982	9125	44
H(3A)	-23	5835	7882	41
H(3B)	-853	6226	8573	41
H(5)	369	6114	9660	43
H(6)	2021	5276	10199	47
H(7)	3944	4440	9558	49
H(9A)	5124	4668	7987	46
H(9B)	5348	4054	8535	46
H(11)	3790	2459	8300	49
H(12A)	2910	8668	7296	46
H(12B)	2139	9528	7763	46
H(13A)	-106	9253	7085	46
H(13B)	634	8376	6625	46
H(14A)	1677	10217	6704	55
H(14B)	2497	9351	6270	55
H(15A)	277	9014	5573	89
H(15B)	954	9987	5538	89
H(15C)	-473	9917	5991	89
H(16A)	2214	2657	5913	59
H(16B)	1546	1809	6176	59
H(17A)	3748	995	5950	94
H(17B)	3313	1347	5287	94
H(18A)	5595	2110	6198	95
H(18B)	5176	2429	5514	95
H(19A)	6183	620	5531	152
H(19B)	7266	1393	5370	152
H(19C)	5911	1011	4865	152
H(21)	10756	2976	9103	50
H(22A)	11072	1211	8565	44
H(22B)	10165	822	7881	44

H(24)	9918	1180	9675	45
H(25)	8234	420	10250	49
H(26)	6272	-488	9630	44
H(28A)	4863	-975	8585	46
H(28B)	5024	-375	8026	46
H(30)	6476	-2538	8386	50
H(31A)	8035	4499	7749	51
H(31B)	7252	3623	7287	51
H(32A)	10244	4246	7074	49
H(32B)	9501	3350	6621	49
H(33A)	8376	5164	6690	63
H(33B)	7577	4275	6256	63
H(34A)	10538	4858	5972	96
H(34B)	9077	5008	5546	96
H(34C)	9674	4004	5526	96
H(35A)	8562	-3208	6254	59
H(35B)	7856	-2378	5980	59
H(36A)	6791	-3747	5360	92
H(36B)	6301	-4041	6037	92
H(37A)	5025	-2599	5534	81
H(37B)	4547	-2873	6224	81
H(38A)	4232	-4114	4923	121
H(38B)	2857	-3554	5294	121
H(38C)	3638	-4319	5617	121

Table 12. Torsion angles [°] for **6**.

N(4)-Cu(1)-S(1)-C(1)	2.3(4)
S(2)-Cu(1)-S(1)-C(1)	-179.6(3)
N(4)-Cu(1)-S(2)-C(10)	14.8(4)
S(1)-Cu(1)-S(2)-C(10)	-163.3(3)
N(11)-Cu(2)-S(3)-C(20)	-0.9(4)
S(4)-Cu(2)-S(3)-C(20)	-177.7(3)
N(11)-Cu(2)-S(4)-C(29)	-13.5(4)
S(3)-Cu(2)-S(4)-C(29)	163.4(3)
C(1)-N(1)-N(2)-C(2)	0.7(9)
C(12)-N(1)-N(2)-C(2)	176.4(7)
S(1)-Cu(1)-N(4)-C(4)	25.6(6)
S(2)-Cu(1)-N(4)-C(4)	-152.6(5)
S(1)-Cu(1)-N(4)-C(8)	-147.4(5)
S(2)-Cu(1)-N(4)-C(8)	34.5(6)
C(10)-N(5)-N(6)-C(11)	0.2(9)
C(16)-N(5)-N(6)-C(11)	176.1(8)
C(20)-N(8)-N(9)-C(21)	-1.6(9)
C(31)-N(8)-N(9)-C(21)	-177.0(7)
S(3)-Cu(2)-N(11)-C(23)	-24.1(6)
S(4)-Cu(2)-N(11)-C(23)	152.7(5)
S(3)-Cu(2)-N(11)-C(27)	144.5(5)
S(4)-Cu(2)-N(11)-C(27)	-38.7(6)
C(29)-N(12)-N(13)-C(30)	-1.0(10)
C(35)-N(12)-N(13)-C(30)	-177.4(8)
N(2)-N(1)-C(1)-N(3)	-0.2(9)
C(12)-N(1)-C(1)-N(3)	-175.8(7)
N(2)-N(1)-C(1)-S(1)	176.2(6)
C(12)-N(1)-C(1)-S(1)	0.7(12)
C(2)-N(3)-C(1)-N(1)	-0.3(8)
C(3)-N(3)-C(1)-N(1)	176.0(7)
C(2)-N(3)-C(1)-S(1)	-176.6(6)
C(3)-N(3)-C(1)-S(1)	-0.3(12)
Cu(1)-S(1)-C(1)-N(1)	150.4(7)
Cu(1)-S(1)-C(1)-N(3)	-34.0(8)

N(1)-N(2)-C(2)-N(3)	-0.8(9)
C(1)-N(3)-C(2)-N(2)	0.7(9)
C(3)-N(3)-C(2)-N(2)	-175.5(7)
C(1)-N(3)-C(3)-C(4)	91.1(9)
C(2)-N(3)-C(3)-C(4)	-93.3(9)
C(8)-N(4)-C(4)-C(5)	3.4(10)
Cu(1)-N(4)-C(4)-C(5)	-169.9(6)
C(8)-N(4)-C(4)-C(3)	-175.2(6)
Cu(1)-N(4)-C(4)-C(3)	11.6(9)
N(3)-C(3)-C(4)-N(4)	-87.4(8)
N(3)-C(3)-C(4)-C(5)	94.0(9)
N(4)-C(4)-C(5)-C(6)	-3.5(12)
C(3)-C(4)-C(5)-C(6)	175.0(7)
C(4)-C(5)-C(6)-C(7)	1.5(12)
C(5)-C(6)-C(7)-C(8)	0.2(12)
C(4)-N(4)-C(8)-C(7)	-1.6(11)
Cu(1)-N(4)-C(8)-C(7)	171.7(6)
C(4)-N(4)-C(8)-C(9)	178.1(6)
Cu(1)-N(4)-C(8)-C(9)	-8.7(9)
C(6)-C(7)-C(8)-N(4)	-0.2(12)
C(6)-C(7)-C(8)-C(9)	-179.8(7)
C(10)-N(7)-C(9)-C(8)	94.0(9)
C(11)-N(7)-C(9)-C(8)	-80.9(10)
N(4)-C(8)-C(9)-N(7)	-70.7(9)
C(7)-C(8)-C(9)-N(7)	109.0(8)
N(6)-N(5)-C(10)-N(7)	-0.2(9)
C(16)-N(5)-C(10)-N(7)	-175.7(8)
N(6)-N(5)-C(10)-S(2)	178.4(6)
C(16)-N(5)-C(10)-S(2)	2.9(13)
C(11)-N(7)-C(10)-N(5)	0.0(9)
C(9)-N(7)-C(10)-N(5)	-175.8(7)
C(11)-N(7)-C(10)-S(2)	-178.6(6)
C(9)-N(7)-C(10)-S(2)	5.6(12)
Cu(1)-S(2)-C(10)-N(5)	130.4(7)
Cu(1)-S(2)-C(10)-N(7)	-51.3(7)
N(5)-N(6)-C(11)-N(7)	-0.2(10)

C(10)-N(7)-C(11)-N(6)	0.2(10)
C(9)-N(7)-C(11)-N(6)	175.9(7)
C(1)-N(1)-C(12)-C(13)	78.9(10)
N(2)-N(1)-C(12)-C(13)	-96.3(9)
N(1)-C(12)-C(13)-C(14)	-178.5(7)
C(12)-C(13)-C(14)-C(15)	176.9(8)
C(10)-N(5)-C(16)-C(17)	98.4(11)
N(6)-N(5)-C(16)-C(17)	-76.8(12)
N(5)-C(16)-C(17)-C(18)	-51.3(16)
C(16)-C(17)-C(18)-C(19)	177.9(12)
N(9)-N(8)-C(20)-N(10)	1.5(9)
C(31)-N(8)-C(20)-N(10)	176.8(7)
N(9)-N(8)-C(20)-S(3)	-177.0(6)
C(31)-N(8)-C(20)-S(3)	-1.7(12)
C(21)-N(10)-C(20)-N(8)	-0.8(9)
C(22)-N(10)-C(20)-N(8)	-176.2(7)
C(21)-N(10)-C(20)-S(3)	177.6(7)
C(22)-N(10)-C(20)-S(3)	2.3(12)
Cu(2)-S(3)-C(20)-N(8)	-150.3(7)
Cu(2)-S(3)-C(20)-N(10)	31.6(8)
N(8)-N(9)-C(21)-N(10)	1.1(9)
C(20)-N(10)-C(21)-N(9)	-0.2(10)
C(22)-N(10)-C(21)-N(9)	175.0(8)
C(20)-N(10)-C(22)-C(23)	-91.6(9)
C(21)-N(10)-C(22)-C(23)	94.0(9)
C(27)-N(11)-C(23)-C(24)	-2.4(10)
Cu(2)-N(11)-C(23)-C(24)	166.6(5)
C(27)-N(11)-C(23)-C(22)	176.8(6)
Cu(2)-N(11)-C(23)-C(22)	-14.2(8)
N(10)-C(22)-C(23)-N(11)	90.2(8)
N(10)-C(22)-C(23)-C(24)	-90.7(8)
N(11)-C(23)-C(24)-C(25)	2.0(11)
C(22)-C(23)-C(24)-C(25)	-177.1(7)
C(23)-C(24)-C(25)-C(26)	0.1(12)
C(24)-C(25)-C(26)-C(27)	-1.7(12)
C(23)-N(11)-C(27)-C(26)	0.7(11)

Cu(2)-N(11)-C(27)-C(26)	-168.0(6)
C(23)-N(11)-C(27)-C(28)	-177.5(6)
Cu(2)-N(11)-C(27)-C(28)	13.7(9)
C(25)-C(26)-C(27)-N(11)	1.3(11)
C(25)-C(26)-C(27)-C(28)	179.5(7)
C(29)-N(14)-C(28)-C(27)	-95.9(9)
C(30)-N(14)-C(28)-C(27)	82.2(10)
N(11)-C(27)-C(28)-N(14)	67.2(9)
C(26)-C(27)-C(28)-N(14)	-111.0(8)
C(30)-N(14)-C(29)-N(12)	-0.7(9)
C(28)-N(14)-C(29)-N(12)	177.7(7)
C(30)-N(14)-C(29)-S(4)	178.8(6)
C(28)-N(14)-C(29)-S(4)	-2.8(12)
N(13)-N(12)-C(29)-N(14)	1.1(9)
C(35)-N(12)-C(29)-N(14)	177.2(8)
N(13)-N(12)-C(29)-S(4)	-178.5(6)
C(35)-N(12)-C(29)-S(4)	-2.4(12)
Cu(2)-S(4)-C(29)-N(14)	50.2(7)
Cu(2)-S(4)-C(29)-N(12)	-130.4(7)
N(12)-N(13)-C(30)-N(14)	0.5(10)
C(29)-N(14)-C(30)-N(13)	0.1(10)
C(28)-N(14)-C(30)-N(13)	-178.3(8)
C(20)-N(8)-C(31)-C(32)	-80.5(10)
N(9)-N(8)-C(31)-C(32)	94.2(9)
N(8)-C(31)-C(32)-C(33)	178.1(7)
C(31)-C(32)-C(33)-C(34)	-177.7(8)
C(29)-N(12)-C(35)-C(36)	-98.6(11)
N(13)-N(12)-C(35)-C(36)	77.3(11)
N(12)-C(35)-C(36)-C(37)	55.5(15)
C(35)-C(36)-C(37)-C(38)	-178.7(11)

Symmetry transformations used to generate equivalent atoms:

Table 13. Hydrogen bonds for **6** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2)...Cl(2)#1	0.93	2.70	3.483(9)	142.8
C(3)-H(3B)...Cl(2)#1	0.97	2.80	3.640(8)	145.7
C(9)-H(9B)...Cl(1)#2	0.97	2.70	3.574(8)	150.9
C(28)-H(28A)...Cl(3)#3	0.97	2.76	3.627(9)	148.6
C(11)-H(11)...Cl(4)#2	0.93	2.74	3.563(8)	147.4
C(22)-H(22A)...Cl(4)	0.97	2.50	3.467(8)	174.6
C(30)-H(30)...Cl(3)#3	0.93	2.80	3.455(10)	128.6

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+2 #2 x-1,y,z #3 -x+2,-y,-z+2

Table 14. Optimized (Gaussian 03; B3LYP functional; 6-31G(d) basis sets for H, C, N, and S; 6-311G(d,p) basis set for Cu) structure of bis-[(η^3 -S,S,N)(2,6-bis){[N-methyl-N'-methylene]imidazole-1-ylidene-2-thione} pyridine copper(I)

Cu	0.000000	0.000000	0.861789
S	0.059612	1.946241	1.968002
S	-0.059612	-1.946241	1.968002
N	-0.490272	4.333703	0.766311
N	0.700858	3.034911	-0.515904
N	0.000000	0.000000	-1.129657
N	-0.700858	-3.034911	-0.515904
N	0.490272	-4.333703	0.766311
C	0.080695	3.099499	0.705837
C	0.500939	4.227375	-1.206032
C	1.509913	1.912399	-0.991235
C	0.726337	0.909674	-1.818112
C	0.751414	0.933923	-3.212248
C	0.000000	0.000000	-3.922959
C	-0.751414	-0.933923	-3.212248
C	-0.726337	-0.909674	-1.818112
C	-1.509913	-1.912399	-0.991235
C	-0.500939	-4.227375	-1.206032
C	-0.080695	-3.099499	0.705837
H	0.903685	4.392759	-2.192661
H	1.353066	1.672592	-3.732371
H	0.000000	0.000000	-5.008478
H	-1.353066	-1.672592	-3.732371
H	-0.903685	-4.392759	-2.192661
H	1.931405	1.421767	-0.110141
H	2.332819	2.327734	-1.577823
H	-2.332819	-2.327734	-1.577823
H	-1.931405	-1.421767	-0.110141
C	-1.232792	4.838060	1.919826
C	1.232792	-4.838060	1.919826
H	-0.549990	5.047433	2.747443
H	-1.748250	5.753153	1.625170
H	-1.957592	4.087593	2.241173
H	1.957592	-4.087593	2.241173
H	0.549990	-5.047433	2.747443
H	1.748250	-5.753153	1.625170
C	-0.235759	5.033164	-0.404304
C	0.235759	-5.033164	-0.404304
H	-0.600274	6.036671	-0.558077
H	0.600274	-6.036671	-0.558077

Table 15. Optimized (Gaussian 03; B3LYP functional; 6-31G(d) basis sets for H, C, N, and S; 6-311G(d,p) basis set for Cu) structure of bis-[(η^3 -S,S,N)(2,6-bis){[N-methyl-N'-methylene]imidazole-1-ylidene-2-thione} pyridine copper(II)

Cu	0.000000	0.000000	0.989383
S	-0.664620	1.971660	1.712774
S	0.664620	-1.971660	1.712774
N	-0.594958	4.453399	0.623109
N	0.759691	3.098489	-0.428035
N	0.000000	0.000000	-0.988649
N	-0.759691	-3.098489	-0.428035
N	0.594958	-4.453399	0.623109
C	-0.145352	3.174446	0.594789
C	0.862823	4.341829	-1.035375
C	1.524263	1.911248	-0.823835
C	0.729344	0.917357	-1.658649
C	0.752963	0.937948	-3.052269
C	0.000000	0.000000	-3.758867
C	-0.752963	-0.937948	-3.052269
C	-0.729344	-0.917357	-1.658649
C	-1.524263	-1.911248	-0.823835
C	-0.862823	-4.341829	-1.035375
C	0.145352	-3.174446	0.594789
H	1.524122	4.522738	-1.868697
H	1.355398	1.672089	-3.577290
H	0.000000	0.000000	-4.844469
H	-1.355398	-1.672089	-3.577290
H	-1.524122	-4.522738	-1.868697
H	1.908282	1.432295	0.082469
H	2.389041	2.265012	-1.387975
H	-2.389041	-2.265012	-1.387975
H	-1.908282	-1.432295	0.082469
C	-1.563000	4.989590	1.592858
C	1.563000	-4.989590	1.592858
H	-1.098590	5.067292	2.578623
H	-1.873262	5.977092	1.251754
H	-2.429236	4.327719	1.645206
H	2.429236	-4.327719	1.645206
H	1.098590	-5.067292	2.578623
H	1.873262	-5.977092	1.251754
C	0.024061	5.182389	-0.372238
C	-0.024061	-5.182389	-0.372238
H	-0.177400	6.232473	-0.520717
H	0.177400	-6.232473	-0.520717

Table 16. Optimized (Gaussian 03; B3LYP functional; 6-31G(d) basis sets for H, C, N, and S; 6-311G(d,p) basis set for Cu) structure of bis-[(η^3 -S,S,N)(2,6-bis){[N-methyl-N'-methylene]triazole-1-ylidene-2-thione} pyridine copper(I)

Cu	0.000000	0.000000	0.876947
S	0.009500	1.942824	1.995754
S	-0.009500	-1.942824	1.995754
N	-0.496005	4.323533	0.759106
N	-0.235955	5.040042	-0.378514
N	0.690345	3.029372	-0.484289
N	0.000000	0.000000	-1.113266
N	-0.690345	-3.029372	-0.484289
N	0.235955	-5.040042	-0.378514
N	0.496005	-4.323533	0.759106
C	0.052411	3.088991	0.738033
C	0.476714	4.237470	-1.110422
C	1.505417	1.916787	-0.977698
C	0.722144	0.912274	-1.802829
C	0.747041	0.937439	-3.196797
C	0.000000	0.000000	-3.907689
C	-0.747041	-0.937439	-3.196797
C	-0.722144	-0.912274	-1.802829
C	-1.505417	-1.916787	-0.977698
C	-0.476714	-4.237470	-1.110422
C	-0.052411	-3.088991	0.738033
H	0.861864	4.481939	-2.089680
H	1.344870	1.678787	-3.717534
H	0.000000	0.000000	-4.993098
H	-1.344870	-1.678787	-3.717534
H	-0.861864	-4.481939	-2.089680
H	1.941303	1.427946	-0.102276
H	2.318312	2.344721	-1.568679
H	-2.318312	-2.344721	-1.568679
H	-1.941303	-1.427946	-0.102276
C	-1.257152	4.922071	1.850191
C	1.257152	-4.922071	1.850191
H	-0.583607	5.228987	2.654959
H	-1.776867	5.788877	1.443804
H	-1.967912	4.188196	2.234581
H	1.967912	-4.188196	2.234581
H	0.583607	-5.228987	2.654959
H	1.776867	-5.788877	1.443804

Table 17. Optimized (Gaussian 03; B3LYP functional; 6-31G(d) basis sets for H, C, N, and S; 6-311G(d,p) basis set for Cu) structure of bis-[(η^3 -S,S,N)(2,6-bis){[N-methyl-N'-methylene]triazole-1-ylidene-2-thione} pyridine copper(II)

Cu	0.000000	0.000000	0.996018
S	-0.767930	1.956945	1.677099
S	0.767930	-1.956945	1.677099
N	-0.558298	4.449291	0.623554
N	0.094131	5.195770	-0.309487
N	0.767813	3.087670	-0.395160
N	0.000000	0.000000	-0.973201
N	-0.767813	-3.087670	-0.395160
N	-0.094131	-5.195770	-0.309487
N	0.558298	-4.449291	0.623554
C	-0.169092	3.162759	0.604882
C	0.883797	4.359670	-0.917202
C	1.533964	1.907245	-0.812502
C	0.732682	0.915991	-1.643536
C	0.754818	0.936384	-3.036981
C	0.000000	0.000000	-3.743963
C	-0.754818	-0.936384	-3.036981
C	-0.732682	-0.915991	-1.643536
C	-1.533964	-1.907245	-0.812502
C	-0.883797	-4.359670	-0.917202
C	0.169092	-3.162759	0.604882
H	1.553923	4.621680	-1.724070
H	1.357688	1.670204	-3.562149
H	0.000000	0.000000	-4.829624
H	-1.357688	-1.670204	-3.562149
H	-1.553923	-4.621680	-1.724070
H	1.939610	1.426467	0.084045
H	2.386977	2.272299	-1.387713
H	-2.386977	-2.272299	-1.387713
H	-1.939610	-1.426467	0.084045
C	-1.520530	5.087260	1.530924
C	1.520530	-5.087260	1.530924
H	-1.059338	5.239343	2.509921
H	-1.785364	6.045828	1.086894
H	-2.401502	4.449946	1.626023
H	2.401502	-4.449946	1.626023
H	1.059338	-5.239343	2.509921
H	1.785364	-6.045828	1.086894

Table 18. Cartesian coordinates of structure used to model tetrachlorocuprate anion.

Cu	0.00000000	0.00000000	0.00000000
Cl	0.00000000	1.76487337	1.45921966
Cl	0.00000000	-1.74943943	1.44649980
Cl	1.76485300	0.00000000	-1.45924429
Cl	-1.74943943	0.00000000	-1.44649980

Figure 12. Calculated (Gaussian 03) IR spectrum for C_2 -symmetric N-methyl-substituted model for **4**. The blue vertical lines indicate individually calculated IR-active modes and the black line is the composite calculated IR spectrum.

Table 19. Comparison of calculated (N-methyl-substituted) and experimental (N-isopropyl-substituted) IR features above 200 cm^{-1} for **4**.

Calculated wavenumber (cm^{-1}); model N-methyl-substituted system	Experimental wavenumber (cm^{-1}); N-isopropyl-substituted system (4)	Calculated Relative Intensity	Motion (symmetry)
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3322.80	3200-2900	1.85	imidazolyl C-H stretch (a)
3322.80		4.71	imidazolyl C-H stretch (b)
3303.76		4.16	imidazolyl C-H stretch (a)
3303.76		9.43	imidazolyl C-H stretch (b)
3232.56		1.20	pyridinyl C-H stretch (a)
3220.09		3.37	pyridinyl C-H stretch (b)
3213.22		0.01	pyridinyl C-H stretch (a)
3186.16		0.00	methyl C-H stretch (a)
3186.15		8.09	methyl C-H stretch (b)
3164.76		1.01	methyl C-H stretch (a)
3164.76		4.79	methyl C-H stretch (b)
3147.81		0.00	methylene C-H stretch (a)
3147.73		2.06	methylene C-H stretch (b)
3095.62		14.77	methylene C-H stretch (b)
3095.53		6.87	methylene C-H stretch (a)
3088.19		8.11	methyl C-H stretch (a)
3088.16		23.44	methyl C-H stretch (b)
1655.72	1560-1605	19.44	pyridinyl C-C stretch (a)
1624.91		4.61	pyridinyl and imidazolyl C-C stretch (a)
1624.82		39.66	pyridinyl and imidazolyl C-C stretch (b)
1624.07		7.32	pyridinyl and imidazolyl C-C stretch (b)

1536.50	1447	12.42	methyl C-H scissoring (a)
1535.72		87.54	methyl C-H scissoring (b)
1514.86		80.54	overall C-H scissoring and wagging (b)
1513.71		24.27	overall C-H scissoring and wagging (a)
1510.12		12.39	overall C-H scissoring and wagging (b)
1502.02		2.05	overall C-H scissoring and wagging (a)
1501.92		78.87	overall C-H scissoring and wagging (b)
1498.13		2.66	overall C-H scissoring and wagging (a)
1496.19		34.28	overall C-H scissoring and wagging (b)
1482.86		0.70	pyridinyl N-C stretching and C-H wagging and twisting (a)
1462.00	1413	1.90	imidazolyl N-C stretching and C-H wagging (b)
1461.71		65.01	imidazolyl N-C stretching and C-H scissoring (a)
1450.39		193.27	imidazolyl N-C stretching and C-H twisting and wagging (b)
1447.74		47.46	imidazolyl N-C stretching and C-H wagging and twisting (a)
1411.11		20.63	methylene C-H wagging (a)

1405.84		18.13	methylene C-H wagging (b)
1388.73	1365-1306	50.98	imidazolyl N-C stretching and C-H wagging (b)
1380.73		0.74	imidazolyl N-C stretching and C-H wagging (a)
1359.65		13.06	imidazolyl N-C stretching (a)
1358.01		2.91	imidazolyl N-C stretching (b)
1331.02		2.58	pyridinyl N-C and C-C stretching and C-H wagging and twisting (b)
1287.52	1279-1242	7.58	pyridinyl N-C and C-C stretching and C-H wagging and twisting (a)
1269.96		13.75	pyridinyl N-C and C-C stretching and C-H wagging and twisting (b)
1268.99		39.52	pyridinyl N-C and C-C stretching and C-H wagging and twisting (a)
1257.30		49.69	pyridinyl N-C and C-C stretching and C-H wagging (b)
1229.75		2.45	imidazolyl C-S and C-N stretching and C-H wagging and twisting (a)
1221.72		62.15	imidazolyl C-S and C-N stretching and C-H wagging and twisting (b)
1199.03	1200-500	4.01	pyridinyl C-H rocking (b)
1164.73		10.36	C-H rocking and twisting (a)
1163.97		2.72	C-H rocking and twisting (b)

1159.91		2.11	C-H rocking and twisting (a)
1159.43		2.38	C-H rocking and twisting (b)
1133.90		6.06	C-H rocking and twisting (a)
1117.43		5.56	C-H rocking and twisting (b)
1117.23		20.60	C-H rocking and twisting (a)
1072.93		11.82	C-H rocking and twisting (b)
1072.27		0.64	C-H rocking and twisting (a)
1035.64		0.42	C-H rocking and twisting (a)
1035.25		0.24	C-H rocking and twisting (b)
1033.27		2.47	Cu-N stretching (a)
1019.62		0.22	pyridinyl C-H twisting (b)
1002.17		4.16	C-H rocking and twisting (b)
949.03		0.14	C-C, C-N, and C-H wagging and twisting (a)
932.94		0.26	C-C, C-N, and C-H wagging and twisting (a)
924.93		20.66	C-C, C-N, and C-H wagging and twisting (b)
851.94		4.39	C-C, C-N, and C-H wagging and twisting (b)
818.72		0.60	C-C, C-N, and C-H wagging and twisting (a)
818.55		1.25	C-C, C-N, and C-H wagging and twisting (b)
806.00		2.84	C-C, C-N, and C-H wagging and twisting (a)
781.79		39.50	C-C, C-N, and C-H

			wagging and twisting (b)
774.51		13.98	C-C, C-N, and C-H wagging and twisting (a)
753.16		26.75	C-C, C-N, and C-H wagging and twisting (b)
712.74		1.38	C-C, C-N, and C-H wagging and twisting (a)
712.37		35.62	C-C, C-N, and C-H wagging and twisting (b)
702.02		13.00	C-C, C-N, and C-H wagging and twisting (a)
678.41		58.82	C-C, C-N, and C-H wagging and twisting (b)
671.30		4.79	C-C, C-N, and C-H wagging and twisting (a)
660.48		3.07	C-C, C-N, and C-H wagging and twisting; S-Cu-S rocking (b)
633.75		0.61	C-C, C-N, and C-H wagging and twisting; Cu-N stretching; S-Cu-S scissoring (a)
615.24		1.27	C-C, C-N, and C-H wagging and twisting (b)
605.91		0.02	C-C, C-N, and C-H wagging and twisting (a)
584.73		8.37	C-C, C-N, and C-H wagging and twisting (b)
552.49		1.17	C-C, C-N, and C-H wagging and twisting; S-Cu-S scissoring (a)

516.83		11.25	C-C, C-N, and C-H wagging and twisting; S-Cu-S rocking (b)
498.55	Below the window of the experimental spectrum	6.60	S-Cu-S scissoring (a)
488.44		5.94	overall rocking (b)
487.87		1.89	overall rocking (a)
451.53		1.42	overall twisting (b)
426.25		4.88	overall rocking (b)
358.11		2.11	Cu-N stretching and overall rocking (a)
327.72		7.88	Cu-S stretching and overall rocking (b)
315.88		6.43	Cu-S stretching and overall rocking (b)
310.72		0.17	Cu-S stretching and overall rocking (a)
291.21		2.49	Cu-S and Cu-N stretching (a)
272.68		2.36	overall rocking (b)
246.64		0.28	Cu-N stretching and S-Cu-S scissoring (a)
239.60		3.82	overall rocking (b)
233.91		9.68	overall rocking (b)
226.39		1.19	Cu-N stretching (a)
201.11		0.26	Cu-N stretching and pyridinyl twisting (a)

Figure 13. Calculated (Gaussian 03) IR spectrum for C_2 -symmetric N-methyl-substituted model for **5** and **6**. The blue vertical lines indicate individually calculated IR-active modes and the black line is the composite calculated IR spectrum.

Table 20. Comparison of calculated (N-methyl-substituted) and experimental IR features above 500 cm^{-1} for **5** (N-isopropyl-substituted) and **6** (N-butyl-substituted).

Calculated wavenumber (cm^{-1}); model N-methyl-substituted system	Experimental wavenumber (cm^{-1}); N-isopropyl- (5) and N-butyl- (6) substituted systems	Calculated Relative Intensity	Motion (symmetry)
3301.69	3200-2900	1.27	triazolyl C-H stretch (b)
3301.69		5.97	triazolyl C-H stretch (a)
3234.49		0.31	pyridinyl C-H stretch (a)
3221.13		2.12	pyridinyl C-H stretch (b)
3215.12		0.00	pyridinyl C-H

			stretch (a)
3206.16		0.12	methyl C-H stretch (a)
3206.16		0.26	methyl C-H stretch (b)
3167.67		0.63	methyl C-H stretch (a)
3167.67		3.72	methyl C-H stretch (b)
3150.84		0.02	methylene C-H stretch (a)
3150.76		1.28	methylene C-H stretch (b)
3096.99		9.86	methylene C-H stretch (b)
3096.91		5.29	methylene C-H stretch (a)
3091.00		6.73	methyl C-H stretch (a)
3090.99		9.51	methyl C-H stretch (b)
1655.62	1603	19.79	pyridinyl C-C stretch stretch (a)
1624.03		16.90	pyridinyl C-C stretch stretch (b)
1597.34	1539	31.95	triazolyl C-N stretch (a)
1596.57		29.93	triazolyl C-N stretch (b)
1532.20	1430-1330	6.73	methyl C-H scissoring (a)
1531.36		178.53	methyl C-H scissoring (b)
1512.16		25.51	pyridinyl C-C stretch and C-H rocking (b)
1510.39		0.08	methyl C-H wagging (a)
1510.15		22.79	methyl C-H wagging (b)
1498.40		5.34	methyl and methylene C-H wagging and scissoring (a)
1496.56		0.02	methyl and

			methylene C-H wagging and scissoring (a)
1496.46		106.72	methyl and methylene C-H wagging and scissoring (b)
1495.48		65.90	methyl and methylene C-H wagging and scissoring (b)
1480.81		1.65	pyridinyl C-N stretching (a)
1448.35		179.13	triazolyl C-N stretching and methyl C-H wagging (b)
1447.40		16.51	triazolyl C-N stretching and methyl C-H wagging (a)
1427.89		12.03	triazolyl C-N stretching and overall C-H wagging (b)
1425.89		34.65	triazolyl C-N stretching and overall C-H wagging (a)
1414.03		39.16	triazolyl C-N stretching and overall C-H wagging (a)
1413.05		5.67	triazolyl C-N stretching and overall C-H wagging (b)
1389.92		50.78	triazolyl and pyridinyl C-N stretching and overall C-H wagging (a)
1386.87		2.09	triazolyl and pyridinyl C-N stretching and

			overall C-H wagging (b)
1346.13	1200-500	28.04	triazolyl C-N and C-S stretching; pyridinyl C-N stretching; overall C-H wagging (b)
1320.91		6.37	triazolyl C-N and C-S stretching; pyridinyl C-N stretching; overall C-H wagging (a)
1305.06		1.72	triazolyl C-N and C-S stretching; pyridinyl C-N stretching; overall C-H wagging (b)
1284.98		1.21	triazolyl C-N-C scissoring (a)
1262.99		8.46	pyridinyl rocking (b)
1251.40		34.40	overall rocking and scissoring (a)
1245.20		9.20	overall rocking and scissoring (b)
1211.97		9.98	overall rocking and scissoring (a)
1208.44		94.68	overall rocking and scissoring (b)
1199.52		4.40	overall rocking and scissoring (b)
1165.07		6.42	overall rocking and scissoring (a)
1163.65		2.90	overall rocking and scissoring (b)
1158.74		2.06	overall rocking and scissoring (a)
1157.03		2.75	overall rocking and scissoring (b)
1131.75		3.12	overall rocking and scissoring (a)
1088.67		2.97	overall rocking and scissoring (a)
1087.90		1.44	overall rocking and scissoring (b)

1033.81		2.75	Cu-N stretching (a)
1022.64		0.14	overall wagging and twisting (b)
1005.04		40.42	overall wagging and twisting (b)
1004.20		0.10	overall wagging and twisting (a)
1000.89		8.18	overall wagging and twisting (b)
950.86		0.00	overall wagging and twisting (a)
933.72		1.77	overall wagging and twisting (a)
925.94		34.11	overall wagging and twisting (b)
856.86		0.56	overall wagging and twisting (b)
830.74		2.55	overall wagging and twisting (a)
829.55		18.79	overall wagging and twisting (b)
814.97		6.89	overall wagging and twisting (a)
787.18		73.99	overall wagging and twisting (b)
782.20		14.95	overall wagging and twisting (a)
765.74		24.16	overall wagging and twisting (b)
712.34		8.74	overall wagging and twisting (a)
688.61		14.17	overall wagging and twisting (b)
677.87		0.07	overall wagging and twisting (a)
664.08		5.55	overall wagging and twisting (b)
647.14		2.11	overall wagging and twisting (a)
645.99		10.88	overall wagging and twisting (b)
632.28		0.13	overall wagging and twisting and Cu-N stretching(a)
592.63		7.53	overall wagging

			and twisting (b)
551.37		0.24	overall wagging and twisting and S-Cu-S scissoring (a)
519.67		7.71	overall wagging and twisting and S-Cu-S rocking (b)
505.88		7.72	overall wagging and twisting and S-Cu-S scissoring (a)
494.12	Below the window of the experimental spectrum	9.03	overall rocking (b)
489.69		0.06	overall rocking (a)
451.28		0.97	pyridinyl twisting (b)
422.33		4.87	overall rocking (b)
350.10		2.71	overall rocking (a)
331.48		3.89	Cu-S stretching and overall rocking (b)
311.39		7.91	Cu-S stretching and overall rocking (b)
309.50		0.95	Cu-S stretching and overall rocking (a)
293.73		0.70	Cu-S and Cu-N stretching and overall twisting (a)
269.13		3.36	overall rocking (b)
250.39		0.29	overall twisting (a)
244.18		4.48	overall rocking (b)
237.26		13.48	overall rocking (b)
229.47		2.12	Cu-N stretching (a)
200.26		0.17	Cu-N stretching (a)

Figure 14. UV-Vis absorption spectrum of **4** (0.060 mM) in acetonitrile.

Figure 15. UV-Vis absorption spectrum of **5** (0.053 mM) in acetonitrile.

Figure 16. UV-Vis spectrum of K_2CuCl_4 (0.018 mM) in acetonitrile.

Figure 17. Cyclic voltammogram of **4** in DMSO (5.6 mM) with 0.2 M TBAF. The scan rate was 100 mV/s with ferrocene ($E_{1/2} = 400$ mV) used as an internal standard.

Figure 18. Cyclic voltammogram of **5** in DMSO (5.6 mM) with 0.2 M TBAF. The scan rate was 100 mV/s with ferrocene ($E_{1/2} = 400$ mV) used as an internal standard.