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The first tris(imidazolylbenzothiazole) copper(II) complex

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Table S1 Crystal data and structure refinement for complex **2**.

Empirical formula	C30 H21 Cl2 Cu N9 O8 S3	
Formula weight	866.18	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 13.0454(14) Å	α= 90°.
	b = 14.3302(14) Å	β= 90°.
	c = 18.4226(18) Å	γ = 90°.
Volume	3444.0(6) $Å^3$	
Z	4	
Density (calculated)	1.671 Mg/m^3	
Absorption coefficient	1.037 mm^{-1}	
F(000)	1756	
Crystal size	0.30 x 0.25 x 0.05 mm^3	
Theta range for data collection	1.80 to 29.00°.	
Index ranges	-17<=h<=17, -18<=k<=19, -20<=l<=25	
Reflections collected	27616	
Independent reflections	9131 [R(int) = 0.0931]	
Completeness to theta = 29.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.950 and 0.742	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9131 / 0 / 481	
Goodness-of-fit on F^2	1.040	
Final R indices [for 6191 rfln with I>2sigma(I)]	R1 = 0.0548, wR2 = 0.0983	
R indices (all data)	R1 = 0.0991, wR2 = 0.1147	
Absolute structure parameter	-0.021(15)	
Largest diff. peak and hole	0.699 and -0.602 e. $Å^{-3}$	

Table S2 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)	1594(1)	409(1)	1186(1)	24(1)
S(1)	1963(1)	3661(1)	760(1)	33(1)
N(1)	1466(3)	1912(3)	629(2)	25(1)
N(2)	3057(3)	2567(3)	2176(2)	34(1)
N(3)	2475(3)	1214(3)	1793(2)	26(1)
C(1)	1967(3)	2494(3)	1045(2)	27(1)
C(2)	1187(4)	3333(3)	39(3)	29(1)
C(3)	771(4)	3896(4)	-513(3)	35(1)
C(4)	168(4)	3463(4)	-1030(3)	40(1)
C(5)	0(4)	2500(4)	-1010(3)	39(1)
C(6)	406(4)	1944(4)	-481(3)	32(1)
C(7)	1012(3)	2367(3)	58(3)	25(1)
C(8)	2493(3)	2117(3)	1661(2)	28(1)
C(9)	3432(4)	1902(4)	2628(3)	38(1)
C(10)	3070(4)	1073(4)	2402(2)	32(1)
S(1A)	-1671(1)	160(1)	1981(1)	35(1)
N(1A)	210(3)	672(3)	1787(2)	25(1)
N(2A)	-993(3)	-596(3)	300(2)	32(1)
N(3A)	609(3)	-252(3)	554(2)	26(1)
C(1A)	-547(3)	208(3)	1487(2)	28(1)
C(2A)	-1104(3)	862(3)	2635(3)	29(1)
C(3A)	-1550(4)	1243(3)	3252(2)	35(1)
C(4A)	-968(4)	1836(4)	3676(3)	35(1)
C(5A)	50(4)	2043(4)	3490(3)	34(1)
C(6A)	495(4)	1665(3)	2882(2)	29(1)
C(7A)	-86(4)	1072(3)	2438(2)	25(1)
C(8A)	-355(3)	-223(3)	794(2)	26(1)
C(9A)	-414(4)	-888(4)	-275(3)	38(1)
C(10A)	577(4)	-670(3)	-108(3)	32(1)
S(1B)	3598(1)	-2068(1)	2092(1)	36(1)
N(1B)	2100(3)	-904(3)	1897(2)	30(1)
N(2B)	4146(3)	-1019(3)	530(2)	30(1)

N(3B)	2799(3)	-112(3)	623(2)	26(1)
C(1B)	2978(4)	-1204(3)	1623(3)	30(1)
C(2B)	2618(4)	-2043(3)	2733(3)	33(1)
C(3B)	2508(4)	-2573(4)	3353(3)	44(1)
C(4B)	1645(4)	-2421(3)	3780(3)	40(1)
C(5B)	926(4)	-1762(4)	3594(3)	41(1)
C(6B)	1027(4)	-1228(4)	2971(3)	38(1)
C(7B)	1889(4)	-1372(3)	2532(2)	30(1)
C(8B)	3322(3)	-789(3)	949(2)	26(1)
C(9B)	4124(3)	-483(4)	-69(3)	33(1)
C(10B)	3294(3)	87(3)	-7(2)	32(1)
Cl(1)	4358(1)	4903(1)	2244(1)	28(1)
Cl(2)	1925(1)	6920(1)	-631(1)	29(1)
O(3)	4168(3)	5875(2)	2244(2)	56(1)
O(7)	888(2)	7210(2)	-807(2)	35(1)
O(6)	2380(3)	7587(3)	-162(2)	42(1)
O(4)	3466(3)	4447(3)	1934(2)	56(1)
O(5)	2517(2)	6816(2)	-1278(2)	41(1)
O(2)	5225(3)	4692(3)	1813(2)	47(1)
O(1)	4508(3)	4573(3)	2960(2)	50(1)
O(8)	1874(3)	6028(2)	-267(2)	38(1)

Table S3 Bond lengths [Å] and angles [°] for **2**.

Cu(1)-N(3A)	1.976(4)	N(2A)-H(2NA)	0.8600
Cu(1)-N(3)	1.976(4)	N(3A)-C(8A)	1.335(5)
Cu(1)-N(3B)	2.025(4)	N(3A)-C(10A)	1.359(6)
Cu(1)-N(1A)	2.150(4)	C(1A)-C(8A)	1.440(6)
Cu(1)-N(1B)	2.387(4)	C(2A)-C(3A)	1.390(6)
Cu(1)-N(1)	2.391(4)	C(2A)-C(7A)	1.409(6)
S(1)-C(2)	1.735(5)	C(3A)-C(4A)	1.381(7)
S(1)-C(1)	1.752(5)	C(3A)-H(3AA)	0.9500
N(1)-C(1)	1.307(6)	C(4A)-C(5A)	1.403(7)
N(1)-C(7)	1.373(6)	C(4A)-H(4AA)	0.9500
N(2)-C(9)	1.358(6)	C(5A)-C(6A)	1.372(7)
N(2)-C(8)	1.362(6)	C(5A)-H(5AA)	0.9500
N(2)-H(2N)	0.9377	C(6A)-C(7A)	1.403(6)
N(3)-C(8)	1.317(6)	C(6A)-H(6AA)	0.9500
N(3)-C(10)	1.379(6)	C(9A)-C(10A)	1.366(7)
C(1)-C(8)	1.433(6)	C(9A)-H(9AA)	0.9500
C(2)-C(7)	1.403(7)	C(10A)-H(10B)	0.9500
C(2)-C(3)	1.407(7)	S(1B)-C(1B)	1.713(5)
C(3)-C(4)	1.383(7)	S(1B)-C(2B)	1.740(5)
C(3)-H(3A)	0.9500	N(1B)-C(1B)	1.323(6)
C(4)-C(5)	1.398(7)	N(1B)-C(7B)	1.376(6)
C(4)-H(4A)	0.9500	N(2B)-C(9B)	1.345(6)
C(5)-C(6)	1.367(7)	N(2B)-C(8B)	1.364(6)
C(5)-H(5A)	0.9500	N(2B)-H(2NB)	0.9541
C(6)-C(7)	1.407(7)	N(3B)-C(8B)	1.330(6)
C(6)-H(6A)	0.9500	N(3B)-C(10B)	1.359(6)
C(9)-C(10)	1.344(7)	C(1B)-C(8B)	1.448(6)
C(9)-H(9A)	0.9500	C(2B)-C(3B)	1.379(7)
C(10)-H(10A)	0.9500	C(2B)-C(7B)	1.403(6)
S(1A)-C(1A)	1.727(4)	C(3B)-C(4B)	1.391(8)
S(1A)-C(2A)	1.734(5)	C(3B)-H(3BA)	0.9500
N(1A)-C(1A)	1.313(6)	C(4B)-C(5B)	1.375(7)
N(1A)-C(7A)	1.385(6)	C(4B)-H(4BA)	0.9500
N(2A)-C(8A)	1.343(6)	C(5B)-C(6B)	1.386(7)
N(2A)-C(9A)	1.366(6)	C(5B)-H(5BA)	0.9500

C(6B)-C(7B)	1.400(7)	C(10)-N(3)-Cu(1)	134.6(3)
C(6B)-H(6BA)	0.9500	N(1)-C(1)-C(8)	117.6(4)
C(9B)-C(10B)	1.361(7)	N(1)-C(1)-S(1)	115.6(4)
C(9B)-H(9BA)	0.9500	C(8)-C(1)-S(1)	126.7(4)
C(10B)-H(10C)	0.9500	C(7)-C(2)-C(3)	121.4(5)
Cl(1)-O(2)	1.414(3)	C(7)-C(2)-S(1)	110.1(4)
Cl(1)-O(3)	1.414(4)	C(3)-C(2)-S(1)	128.6(4)
Cl(1)-O(1)	1.416(4)	C(4)-C(3)-C(2)	117.4(5)
Cl(1)-O(4)	1.451(4)	C(4)-C(3)-H(3A)	121.3
Cl(2)-O(6)	1.419(4)	C(2)-C(3)-H(3A)	121.3
Cl(2)-O(5)	1.428(3)	C(3)-C(4)-C(5)	121.0(5)
Cl(2)-O(8)	1.445(3)	C(3)-C(4)-H(4A)	119.5
Cl(2)-O(7)	1.452(3)	C(5)-C(4)-H(4A)	119.5
N(3A)-Cu(1)-N(3)	172.74(16)	C(6)-C(5)-C(4)	122.2(5)
N(3A)-Cu(1)-N(3B)	91.49(14)	C(6)-C(5)-H(5A)	118.9
N(3)-Cu(1)-N(3B)	93.06(15)	C(4)-C(5)-H(5A)	118.9
N(3A)-Cu(1)-N(1A)	80.91(15)	C(5)-C(6)-C(7)	118.0(5)
N(3)-Cu(1)-N(1A)	95.42(15)	C(5)-C(6)-H(6A)	121.0
N(3B)-Cu(1)-N(1A)	168.31(15)	C(7)-C(6)-H(6A)	121.0
N(3A)-Cu(1)-N(1B)	97.22(14)	N(1)-C(7)-C(2)	114.7(4)
N(3)-Cu(1)-N(1B)	89.31(15)	N(1)-C(7)-C(6)	125.3(4)
N(3B)-Cu(1)-N(1B)	77.03(14)	C(2)-C(7)-C(6)	120.0(4)
N(1A)-Cu(1)-N(1B)	95.02(13)	N(3)-C(8)-N(2)	110.2(4)
N(3A)-Cu(1)-N(1)	97.68(14)	N(3)-C(8)-C(1)	120.6(4)
N(3)-Cu(1)-N(1)	75.99(14)	N(2)-C(8)-C(1)	129.2(5)
N(3B)-Cu(1)-N(1)	99.59(14)	C(10)-C(9)-N(2)	107.6(4)
N(1A)-Cu(1)-N(1)	90.27(13)	C(10)-C(9)-H(9A)	126.2
N(1B)-Cu(1)-N(1)	164.80(13)	N(2)-C(9)-H(9A)	126.2
C(2)-S(1)-C(1)	88.4(2)	C(9)-C(10)-N(3)	108.7(4)
C(1)-N(1)-C(7)	111.2(4)	C(9)-C(10)-H(10A)	125.7
C(1)-N(1)-Cu(1)	106.8(3)	N(3)-C(10)-H(10A)	125.7
C(7)-N(1)-Cu(1)	141.9(3)	C(1A)-S(1A)-C(2A)	88.9(2)
C(9)-N(2)-C(8)	106.9(4)	C(1A)-N(1A)-C(7A)	111.4(4)
C(9)-N(2)-H(2N)	124.2	C(1A)-N(1A)-Cu(1)	109.0(3)
C(8)-N(2)-H(2N)	126.5	C(7A)-N(1A)-Cu(1)	138.9(3)
C(8)-N(3)-C(10)	106.5(4)	C(8A)-N(2A)-C(9A)	107.8(4)
C(8)-N(3)-Cu(1)	118.6(3)	C(8A)-N(2A)-H(2NA)	127.6

C(9A)-N(2A)-H(2NA)	124.2	C(7B)-N(1B)-Cu(1)	142.7(3)
C(8A)-N(3A)-C(10A)	106.4(4)	C(9B)-N(2B)-C(8B)	108.0(4)
C(8A)-N(3A)-Cu(1)	113.7(3)	C(9B)-N(2B)-H(2NB)	125.3
C(10A)-N(3A)-Cu(1)	139.5(3)	C(8B)-N(2B)-H(2NB)	125.7
N(1A)-C(1A)-C(8A)	117.4(4)	C(8B)-N(3B)-C(10B)	107.1(4)
N(1A)-C(1A)-S(1A)	115.9(3)	C(8B)-N(3B)-Cu(1)	115.9(3)
C(8A)-C(1A)-S(1A)	126.7(4)	C(10B)-N(3B)-Cu(1)	136.8(3)
C(3A)-C(2A)-C(7A)	121.4(5)	N(1B)-C(1B)-C(8B)	117.5(4)
C(3A)-C(2A)-S(1A)	128.2(4)	N(1B)-C(1B)-S(1B)	116.8(4)
C(7A)-C(2A)-S(1A)	110.3(4)	C(8B)-C(1B)-S(1B)	125.7(4)
C(4A)-C(3A)-C(2A)	118.3(5)	C(3B)-C(2B)-C(7B)	121.7(5)
C(4A)-C(3A)-H(3AA)	120.9	C(3B)-C(2B)-S(1B)	128.8(4)
C(2A)-C(3A)-H(3AA)	120.9	C(7B)-C(2B)-S(1B)	109.4(4)
C(3A)-C(4A)-C(5A)	120.8(5)	C(2B)-C(3B)-C(4B)	117.8(5)
C(3A)-C(4A)-H(4AA)	119.6	C(2B)-C(3B)-H(3BA)	121.1
C(5A)-C(4A)-H(4AA)	119.6	C(4B)-C(3B)-H(3BA)	121.1
C(6A)-C(5A)-C(4A)	121.1(5)	C(5B)-C(4B)-C(3B)	121.3(5)
C(6A)-C(5A)-H(5AA)	119.5	C(5B)-C(4B)-H(4BA)	119.4
C(4A)-C(5A)-H(5AA)	119.5	C(3B)-C(4B)-H(4BA)	119.4
C(5A)-C(6A)-C(7A)	119.1(4)	C(4B)-C(5B)-C(6B)	121.4(5)
C(5A)-C(6A)-H(6AA)	120.5	C(4B)-C(5B)-H(5BA)	119.3
C(7A)-C(6A)-H(6AA)	120.5	C(6B)-C(5B)-H(5BA)	119.3
N(1A)-C(7A)-C(6A)	127.2(4)	C(5B)-C(6B)-C(7B)	118.2(5)
N(1A)-C(7A)-C(2A)	113.4(4)	C(5B)-C(6B)-H(6BA)	120.9
C(6A)-C(7A)-C(2A)	119.3(4)	C(7B)-C(6B)-H(6BA)	120.9
N(3A)-C(8A)-N(2A)	110.3(4)	N(1B)-C(7B)-C(6B)	125.4(4)
N(3A)-C(8A)-C(1A)	118.1(4)	N(1B)-C(7B)-C(2B)	115.0(4)
N(2A)-C(8A)-C(1A)	131.6(4)	C(6B)-C(7B)-C(2B)	119.6(4)
N(2A)-C(9A)-C(10A)	106.2(4)	N(3B)-C(8B)-N(2B)	109.0(4)
N(2A)-C(9A)-H(9AA)	126.9	N(3B)-C(8B)-C(1B)	121.9(4)
C(10A)-C(9A)-H(9AA)	126.9	N(2B)-C(8B)-C(1B)	129.0(4)
N(3A)-C(10A)-C(9A)	109.3(4)	N(2B)-C(9B)-C(10B)	107.0(4)
N(3A)-C(10A)-H(10B)	125.3	N(2B)-C(9B)-H(9BA)	126.5
C(9A)-C(10A)-H(10B)	125.3	C(10B)-C(9B)-H(9BA)	126.5
C(1B)-S(1B)-C(2B)	88.9(2)	N(3B)-C(10B)-C(9B)	108.9(4)
C(1B)-N(1B)-C(7B)	109.8(4)	N(3B)-C(10B)-H(10C)	125.6
C(1B)-N(1B)-Cu(1)	106.6(3)	C(9B)-C(10B)-H(10C)	125.6

O(2)-Cl(1)-O(3)	110.6(3)	O(6)-Cl(2)-O(5)	110.7(2)
O(2)-Cl(1)-O(1)	109.9(2)	O(6)-Cl(2)-O(8)	109.4(2)
O(3)-Cl(1)-O(1)	110.7(2)	O(5)-Cl(2)-O(8)	108.7(2)
O(2)-Cl(1)-O(4)	108.9(2)	O(6)-Cl(2)-O(7)	109.5(2)
O(3)-Cl(1)-O(4)	107.6(2)	O(5)-Cl(2)-O(7)	110.3(2)
O(1)-Cl(1)-O(4)	109.0(3)	O(8)-Cl(2)-O(7)	108.3(2)

Symmetry transformations used to generate equivalent atoms:

Table S4 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)	18(1)	27(1)	27(1)	-1(1)	1(1)	3(1)
S(1)	34(1)	27(1)	38(1)	-4(1)	4(1)	-5(1)
N(1)	24(2)	29(2)	24(2)	1(2)	0(2)	-1(2)
N(2)	20(2)	47(3)	36(2)	-7(2)	2(2)	-8(2)
N(3)	17(2)	33(2)	29(2)	-1(2)	0(2)	3(2)
C(1)	21(2)	32(3)	29(3)	-2(2)	9(2)	-4(2)
C(2)	25(2)	30(3)	32(3)	3(2)	8(2)	3(2)
C(3)	35(3)	30(3)	42(3)	8(2)	9(2)	8(2)
C(4)	31(3)	47(3)	41(3)	13(3)	4(2)	12(2)
C(5)	31(3)	52(4)	35(3)	3(3)	-8(2)	1(3)
C(6)	29(2)	32(3)	34(3)	1(2)	-3(2)	-5(2)
C(7)	22(2)	26(3)	28(3)	2(2)	5(2)	3(2)
C(8)	16(2)	40(3)	26(3)	-10(2)	4(2)	-3(2)
C(9)	21(2)	69(4)	25(3)	-10(3)	-3(2)	0(3)
C(10)	24(2)	51(3)	22(3)	-4(2)	-5(2)	9(2)
S(1A)	21(1)	42(1)	41(1)	-5(1)	7(1)	-4(1)
N(1A)	19(2)	27(2)	31(2)	2(2)	5(2)	3(2)
N(2A)	23(2)	35(3)	38(3)	1(2)	-2(2)	-5(2)
N(3A)	24(2)	25(2)	29(2)	-5(2)	3(2)	1(2)
C(1A)	19(2)	32(3)	32(3)	7(2)	0(2)	4(2)

C(2A)	20(2)	31(3)	37(3)	5(2)	5(2)	2(2)
C(3A)	28(2)	43(3)	33(3)	2(2)	5(2)	3(3)
C(4A)	38(3)	39(3)	29(3)	2(2)	9(2)	11(2)
C(5A)	38(3)	37(3)	27(3)	1(2)	-3(2)	2(3)
C(6A)	27(2)	37(3)	21(3)	4(2)	0(2)	-1(2)
C(7A)	24(2)	26(3)	26(3)	4(2)	1(2)	3(2)
C(8A)	24(2)	23(3)	31(3)	-1(2)	3(2)	0(2)
C(9A)	36(3)	39(3)	38(3)	-8(2)	-1(2)	3(2)
C(10A)	33(3)	28(3)	34(3)	-5(2)	5(2)	-1(2)
S(1B)	23(1)	31(1)	56(1)	12(1)	-5(1)	1(1)
N(1B)	27(2)	30(2)	31(2)	2(2)	3(2)	8(2)
N(2B)	22(2)	30(2)	38(3)	-9(2)	3(2)	1(2)
N(3B)	20(2)	29(2)	29(2)	-3(2)	1(2)	1(2)
C(1B)	26(2)	31(3)	35(3)	-3(2)	-6(2)	-4(2)
C(2B)	31(2)	33(3)	35(3)	5(2)	-7(2)	-10(2)
C(3B)	39(3)	42(3)	50(4)	15(3)	-19(3)	-12(3)
C(4B)	51(3)	40(3)	30(3)	13(2)	-13(3)	-14(3)
C(5B)	47(3)	47(4)	29(3)	0(2)	3(2)	-10(3)
C(6B)	44(3)	35(3)	33(3)	4(2)	2(2)	4(3)
C(7B)	37(3)	23(2)	31(3)	1(2)	-4(2)	-2(2)
C(8B)	18(2)	29(2)	33(3)	-8(2)	-1(2)	2(2)
C(9B)	26(2)	40(3)	32(3)	-6(2)	7(2)	-4(2)
C(10B)	27(2)	44(3)	24(2)	0(2)	1(2)	-5(2)
Cl(1)	25(1)	24(1)	36(1)	-3(1)	-4(1)	-1(1)
Cl(2)	22(1)	34(1)	31(1)	0(1)	3(1)	0(1)
O(3)	64(3)	27(2)	76(3)	-1(2)	-22(2)	3(2)
O(7)	21(2)	41(2)	42(2)	1(2)	3(2)	2(2)
O(6)	39(2)	46(2)	41(2)	-9(2)	-3(2)	-10(2)
O(4)	32(2)	52(2)	85(3)	-24(2)	-16(2)	-9(2)
O(5)	28(2)	61(2)	33(2)	9(2)	12(2)	9(2)
O(2)	36(2)	67(3)	39(2)	-12(2)	7(2)	0(2)
O(1)	53(2)	58(2)	40(2)	16(2)	7(2)	22(2)
O(8)	34(2)	40(2)	39(2)	8(2)	8(2)	0(2)

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

	x	y	z	U(eq)
H(2N)	3310	3178	2149	80(20)
H(3A)	899	4548	-530	42
H(4A)	-137	3826	-1404	48
H(5A)	-411	2223	-1378	47
H(6A)	283	1291	-477	38
H(9A)	3871	2003	3032	46
H(10A)	3203	487	2624	39
H(2NA)	-1638	-703	346	40(15)
H(3AA)	-2238	1100	3380	42
H(4AA)	-1260	2107	4099	42
H(5AA)	437	2452	3789	41
H(6AA)	1188	1803	2764	34
H(9AA)	-654	-1184	-704	45
H(10B)	1154	-790	-409	38
H(2NB)	4584	-1544	603	70(20)
H(3BA)	3006	-3027	3485	52
H(4BA)	1549	-2780	4209	48
H(5BA)	348	-1670	3900	49
H(6BA)	525	-776	2845	45
H(9BA)	4597	-500	-460	39
H(10C)	3094	548	-349	38

Table S6 Torsion angles [°] for **2**.

N(3A)-Cu(1)-N(1)-C(1)	171.1(3)	C(1)-N(1)-C(7)-C(6)	-179.0(4)
N(3)-Cu(1)-N(1)-C(1)	-5.3(3)	Cu(1)-N(1)-C(7)-C(6)	-4.0(8)
N(3B)-Cu(1)-N(1)-C(1)	-96.0(3)	C(3)-C(2)-C(7)-N(1)	-179.9(4)
N(1A)-Cu(1)-N(1)-C(1)	90.3(3)	S(1)-C(2)-C(7)-N(1)	0.9(5)
N(1B)-Cu(1)-N(1)-C(1)	-20.3(7)	C(3)-C(2)-C(7)-C(6)	-0.3(7)
N(3A)-Cu(1)-N(1)-C(7)	-4.0(5)	S(1)-C(2)-C(7)-C(6)	-179.5(4)
N(3)-Cu(1)-N(1)-C(7)	179.6(5)	C(5)-C(6)-C(7)-N(1)	179.3(4)
N(3B)-Cu(1)-N(1)-C(7)	88.8(5)	C(5)-C(6)-C(7)-C(2)	-0.3(7)
N(1A)-Cu(1)-N(1)-C(7)	-84.9(5)	C(10)-N(3)-C(8)-N(2)	-1.6(5)
N(1B)-Cu(1)-N(1)-C(7)	164.5(5)	Cu(1)-N(3)-C(8)-N(2)	173.9(3)
N(3A)-Cu(1)-N(3)-C(8)	-23.7(14)	C(10)-N(3)-C(8)-C(1)	178.2(4)
N(3B)-Cu(1)-N(3)-C(8)	105.1(3)	Cu(1)-N(3)-C(8)-C(1)	-6.3(5)
N(1A)-Cu(1)-N(3)-C(8)	-82.9(3)	C(9)-N(2)-C(8)-N(3)	2.3(5)
N(1B)-Cu(1)-N(3)-C(8)	-177.9(3)	C(9)-N(2)-C(8)-C(1)	-177.5(4)
N(1)-Cu(1)-N(3)-C(8)	6.0(3)	N(1)-C(1)-C(8)-N(3)	0.7(6)
N(3A)-Cu(1)-N(3)-C(10)	150.3(11)	S(1)-C(1)-C(8)-N(3)	-176.4(3)
N(3B)-Cu(1)-N(3)-C(10)	-80.9(4)	N(1)-C(1)-C(8)-N(2)	-179.5(4)
N(1A)-Cu(1)-N(3)-C(10)	91.1(4)	S(1)-C(1)-C(8)-N(2)	3.4(7)
N(1B)-Cu(1)-N(3)-C(10)	-3.9(4)	C(8)-N(2)-C(9)-C(10)	-2.0(5)
N(1)-Cu(1)-N(3)-C(10)	180.0(4)	N(2)-C(9)-C(10)-N(3)	1.0(5)
C(7)-N(1)-C(1)-C(8)	-179.3(4)	C(8)-N(3)-C(10)-C(9)	0.4(5)
Cu(1)-N(1)-C(1)-C(8)	3.9(5)	Cu(1)-N(3)-C(10)-C(9)	-174.1(3)
C(7)-N(1)-C(1)-S(1)	-1.9(5)	N(3A)-Cu(1)-N(1A)-C(1A)	5.8(3)
Cu(1)-N(1)-C(1)-S(1)	-178.7(2)	N(3)-Cu(1)-N(1A)-C(1A)	179.5(3)
C(2)-S(1)-C(1)-N(1)	2.0(4)	N(3B)-Cu(1)-N(1A)-C(1A)	-44.2(9)
C(2)-S(1)-C(1)-C(8)	179.2(4)	N(1B)-Cu(1)-N(1A)-C(1A)	-90.7(3)
C(1)-S(1)-C(2)-C(7)	-1.5(3)	N(1)-Cu(1)-N(1A)-C(1A)	103.5(3)
C(1)-S(1)-C(2)-C(3)	179.3(4)	N(3A)-Cu(1)-N(1A)-C(7A)	174.4(5)
C(7)-C(2)-C(3)-C(4)	1.1(7)	N(3)-Cu(1)-N(1A)-C(7A)	-11.9(5)
S(1)-C(2)-C(3)-C(4)	-179.9(4)	N(3B)-Cu(1)-N(1A)-C(7A)	124.5(7)
C(2)-C(3)-C(4)-C(5)	-1.4(7)	N(1B)-Cu(1)-N(1A)-C(7A)	77.9(5)
C(3)-C(4)-C(5)-C(6)	0.9(8)	N(1)-Cu(1)-N(1A)-C(7A)	-87.8(5)
C(4)-C(5)-C(6)-C(7)	0.0(8)	N(3)-Cu(1)-N(3A)-C(8A)	-60.7(13)
C(1)-N(1)-C(7)-C(2)	0.6(5)	N(3B)-Cu(1)-N(3A)-C(8A)	170.4(3)
Cu(1)-N(1)-C(7)-C(2)	175.7(3)	N(1A)-Cu(1)-N(3A)-C(8A)	-0.6(3)

N(1B)-Cu(1)-N(3A)-C(8A)	93.3(3)	S(1A)-C(1A)-C(8A)-N(3A)	-168.2(4)
N(1)-Cu(1)-N(3A)-C(8A)	-89.7(3)	N(1A)-C(1A)-C(8A)-N(2A)	-167.0(5)
N(3)-Cu(1)-N(3A)-C(10A)	110.8(12)	S(1A)-C(1A)-C(8A)-N(2A)	14.6(8)
N(3B)-Cu(1)-N(3A)-C(10A)	-18.1(5)	C(8A)-N(2A)-C(9A)-C(10A)	-0.5(6)
N(1A)-Cu(1)-N(3A)-C(10A)	170.8(5)	C(8A)-N(3A)-C(10A)-C(9A)	0.6(6)
N(1B)-Cu(1)-N(3A)-C(10A)	-95.2(5)	Cu(1)-N(3A)-C(10A)-C(9A)	-171.3(4)
N(1)-Cu(1)-N(3A)-C(10A)	81.8(5)	N(2A)-C(9A)-C(10A)-N(3A)	0.0(6)
C(7A)-N(1A)-C(1A)-C(8A)	178.2(4)	N(3A)-Cu(1)-N(1B)-C(1B)	98.8(3)
Cu(1)-N(1A)-C(1A)-C(8A)	-9.8(5)	N(3)-Cu(1)-N(1B)-C(1B)	-84.4(3)
C(7A)-N(1A)-C(1A)-S(1A)	-3.1(5)	N(3B)-Cu(1)-N(1B)-C(1B)	8.9(3)
Cu(1)-N(1A)-C(1A)-S(1A)	168.8(2)	N(1A)-Cu(1)-N(1B)-C(1B)	-179.7(3)
C(2A)-S(1A)-C(1A)-N(1A)	2.5(4)	N(1)-Cu(1)-N(1B)-C(1B)	-69.8(6)
C(2A)-S(1A)-C(1A)-C(8A)	-179.0(4)	N(3A)-Cu(1)-N(1B)-C(7B)	-93.5(5)
C(1A)-S(1A)-C(2A)-C(3A)	174.8(5)	N(3)-Cu(1)-N(1B)-C(7B)	83.3(5)
C(1A)-S(1A)-C(2A)-C(7A)	-1.1(4)	N(3B)-Cu(1)-N(1B)-C(7B)	176.6(5)
C(7A)-C(2A)-C(3A)-C(4A)	-0.3(7)	N(1A)-Cu(1)-N(1B)-C(7B)	-12.1(5)
S(1A)-C(2A)-C(3A)-C(4A)	-175.8(4)	N(1)-Cu(1)-N(1B)-C(7B)	97.9(7)
C(2A)-C(3A)-C(4A)-C(5A)	-0.4(7)	N(3A)-Cu(1)-N(3B)-C(8B)	-105.4(3)
C(3A)-C(4A)-C(5A)-C(6A)	0.1(8)	N(3)-Cu(1)-N(3B)-C(8B)	80.3(3)
C(4A)-C(5A)-C(6A)-C(7A)	0.9(7)	N(1A)-Cu(1)-N(3B)-C(8B)	-56.2(9)
C(1A)-N(1A)-C(7A)-C(6A)	-175.5(5)	N(1B)-Cu(1)-N(3B)-C(8B)	-8.3(3)
Cu(1)-N(1A)-C(7A)-C(6A)	16.1(8)	N(1)-Cu(1)-N(3B)-C(8B)	156.6(3)
C(1A)-N(1A)-C(7A)-C(2A)	2.2(5)	N(3A)-Cu(1)-N(3B)-C(10B)	80.5(4)
Cu(1)-N(1A)-C(7A)-C(2A)	-166.2(3)	N(3)-Cu(1)-N(3B)-C(10B)	-93.9(4)
C(5A)-C(6A)-C(7A)-N(1A)	176.0(4)	N(1A)-Cu(1)-N(3B)-C(10B)	129.6(7)
C(5A)-C(6A)-C(7A)-C(2A)	-1.5(7)	N(1B)-Cu(1)-N(3B)-C(10B)	177.6(5)
C(3A)-C(2A)-C(7A)-N(1A)	-176.6(4)	N(1)-Cu(1)-N(3B)-C(10B)	-17.6(5)
S(1A)-C(2A)-C(7A)-N(1A)	-0.4(5)	C(7B)-N(1B)-C(1B)-C(8B)	179.7(4)
C(3A)-C(2A)-C(7A)-C(6A)	1.3(7)	Cu(1)-N(1B)-C(1B)-C(8B)	-8.2(5)
S(1A)-C(2A)-C(7A)-C(6A)	177.5(3)	C(7B)-N(1B)-C(1B)-S(1B)	0.9(5)
C(10A)-N(3A)-C(8A)-N(2A)	-0.9(5)	Cu(1)-N(1B)-C(1B)-S(1B)	172.9(2)
Cu(1)-N(3A)-C(8A)-N(2A)	173.3(3)	C(2B)-S(1B)-C(1B)-N(1B)	-0.6(4)
C(10A)-N(3A)-C(8A)-C(1A)	-178.7(4)	C(2B)-S(1B)-C(1B)-C(8B)	-179.4(4)
Cu(1)-N(3A)-C(8A)-C(1A)	-4.5(5)	C(1B)-S(1B)-C(2B)-C(3B)	180.0(5)
C(9A)-N(2A)-C(8A)-N(3A)	0.9(5)	C(1B)-S(1B)-C(2B)-C(7B)	0.2(4)
C(9A)-N(2A)-C(8A)-C(1A)	178.3(5)	C(7B)-C(2B)-C(3B)-C(4B)	-0.1(7)
N(1A)-C(1A)-C(8A)-N(3A)	10.2(6)	S(1B)-C(2B)-C(3B)-C(4B)	-179.8(4)

C(2B)-C(3B)-C(4B)-C(5B)	-0.4(8)	Cu(1)-N(3B)-C(8B)-N(2B)	-175.7(3)
C(3B)-C(4B)-C(5B)-C(6B)	0.6(8)	C(10B)-N(3B)-C(8B)-C(1B)	-177.0(4)
C(4B)-C(5B)-C(6B)-C(7B)	-0.4(8)	Cu(1)-N(3B)-C(8B)-C(1B)	7.1(5)
C(1B)-N(1B)-C(7B)-C(6B)	179.5(5)	C(9B)-N(2B)-C(8B)-N(3B)	-0.8(5)
Cu(1)-N(1B)-C(7B)-C(6B)	12.0(8)	C(9B)-N(2B)-C(8B)-C(1B)	176.1(4)
C(1B)-N(1B)-C(7B)-C(2B)	-0.7(6)	N(1B)-C(1B)-C(8B)-N(3B)	2.0(6)
Cu(1)-N(1B)-C(7B)-C(2B)	-168.1(4)	S(1B)-C(1B)-C(8B)-N(3B)	-179.2(3)
C(5B)-C(6B)-C(7B)-N(1B)	179.8(5)	N(1B)-C(1B)-C(8B)-N(2B)	-174.6(4)
C(5B)-C(6B)-C(7B)-C(2B)	-0.1(7)	S(1B)-C(1B)-C(8B)-N(2B)	4.2(7)
C(3B)-C(2B)-C(7B)-N(1B)	-179.6(4)	C(8B)-N(2B)-C(9B)-C(10B)	1.2(5)
S(1B)-C(2B)-C(7B)-N(1B)	0.2(5)	C(8B)-N(3B)-C(10B)-C(9B)	0.6(5)
C(3B)-C(2B)-C(7B)-C(6B)	0.3(7)	Cu(1)-N(3B)-C(10B)-C(9B)	175.1(3)
S(1B)-C(2B)-C(7B)-C(6B)	-179.9(4)	N(2B)-C(9B)-C(10B)-N(3B)	-1.1(5)
C(10B)-N(3B)-C(8B)-N(2B)	0.2(5)		

Symmetry transformations used to generate equivalent atoms:

Table S7 Hydrogen bonds for **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2A)-H(2NA)...O(5)#1	0.86	2.59	3.176(5)	126
N(2A)-H(2NA)...O(8)#1	0.86	2.00	2.851(6)	170
N(2)-H(2N)...O(4)#2	0.94	1.87	2.782(6)	163
N(2B)-H(2NB)...O(7)#3	0.95	1.99	2.888(5)	157

Symmetry transformations used to generate equivalent atoms:

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