Table S1. Crystal data and structure refinement for $[Cu(bbtmp)NO_3]NO_3$ **(1)**

Empirical formula	$C_{21}H_{17}CuN_7O_6S_2$
Formula weight	591.08
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 9.2339(5) Å, α = 90.000° b = 14.2902(8) Å, β = 108.808(2)° c = 9.3986(5) Å, γ = 90.000°
Volume	1173.96(11) A^3
Z	4
Density (calculated)	1.672 Mg/m^3
Absorption coefficient	1.163 mm^{-1}
F(000)	602
Crystal size	0.3 x 0.15 x 0.3 mm
Theta range for data collection	2.29 to 23.28 deg.
Index ranges	$-10 \le h \le 10, -15 \le k \le 15, -10 \le l \le 5$
Reflections collected	4967
Independent reflections	3156 [R(int) = 0.0469]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3156 / 1 / 335
Goodness-of-fit on F^2	0.992
Final R indices [I>2sigma(I)]	R1 = 0.0403, wR2 = 0.0998
R indices (all data)	R1 = 0.0647, wR2 = 0.1098
Absolute structure parameter	0.98(2)
Largest diff. peak and hole	0.332 and -0.365 $e.A^{-3}$

$$R = \sum||F_o| - |F_c|| / \sum|F_o|; \quad wR2 = \{\sum[w(F_o^2 - F_c^2)^2 / \sum[w(F_o^2)^2]\}^{1/2}$$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 X 10^3) for $[Cu(bbtmp)NO_3]NO_3$

atom	x	y	z	U_{eq}*
Cu(1)	4165(1)	1577(1)	331(1)	36(1)
S(2)	3616(2)	870(2)	-3717(2)	53(1)
S(3)	7748(2)	2252(2)	3501(2)	50(1)
O(1)	2314(4)	1521(4)	928(5)	40(1)
N(3)	6072(5)	1628(6)	-233(6)	35(1)
N(5)	7161(6)	585(4)	4395(6)	38(2)
N(1)	2983(6)	2113(4)	-1688(6)	34(1)
N(4)	5368(6)	989(4)	2283(6)	35(2)
C(14)	6907(8)	2812(5)	1697(9)	44(2)
N(2)	1867(7)	2377(5)	-4107(7)	44(2)
C(6)	1378(8)	3075(5)	-3387(8)	38(2)
C(21)	4973(8)	124(5)	2797(8)	36(2)
C(1)	2072(8)	2917(5)	-1857(9)	37(2)
C(8)	4960(9)	416(6)	-2036(9)	46(2)
N(6)	2441(8)	1964(5)	2176(7)	48(2)
O(2)	3465(7)	2557(4)	2599(7)	69(2)
C(16)	6114(7)	-134(5)	4116(8)	36(2)
C(15)	6701(7)	1229(5)	3328(8)	37(2)
C(7)	2825(7)	1818(5)	-3077(8)	35(2)
C(17)	6003(9)	-941(6)	4893(8)	46(2)
C(13)	7187(8)	2263(5)	469(8)	40(2)
C(9)	6260(7)	1066(5)	-1305(9)	39(2)
C(12)	8492(8)	2314(6)	83(9)	47(2)
O(3)	1539(6)	1779(5)	2845(6)	70(2)
C(10)	7549(8)	1090(6)	-1707(9)	52(2)
C(2)	1870(8)	3528(6)	-788(9)	43(2)
C(18)	4773(10)	-1493(6)	4312(9)	51(2)
C(4)	195(9)	4429(6)	-2886(11)	56(2)
C(5)	410(9)	3839(6)	-3905(10)	53(2)
C(11)	8687(8)	1748(7)	-989(9)	56(2)
C(19)	3620(9)	-1234(6)	2991(10)	57(2)
C(3)	896(10)	4296(6)	-1354(11)	60(2)
C(20)	3695(9)	-440(5)	2182(8)	45(2)
O(4)	10032(5)	637(4)	-3327(6)	51(2)
N(7)	10451(7)	-52(5)	-2468(8)	45(2)
O(5)	11738(7)	-76(4)	-1507(7)	60(2)
O(6)	9577(7)	-724(5)	-2570(7)	77(2)

Table S3. Bond Distances (Å) and Angles (deg) for $[Cu(bbtmp)NO_3]NO_3$

Cu(1)-O(1)	1.966(4)	C(9)-C(10)	1.361(10)
Cu(1)-N(3)	1.997(5)	C(12)-C(11)	1.347(11)
Cu(1)-N(4)	1.999(5)	C(12)-H(10)	0.972(8)
Cu(1)-N(1)	2.011(5)	C(10)-C(11)	1.410(12)
S(2)-C(7)	1.737(7)	C(10)-H(8)	0.966(9)
S(2)-C(8)	1.787(8)	C(2)-C(3)	1.410(12)
S(3)-C(15)	1.730(7)	C(2)-H(1)	1.082(8)
S(3)-C(14)	1.809(8)	C(18)-C(19)	1.400(11)
O(1)-N(6)	1.304(8)	C(18)-H(15)	0.906(8)
N(3)-C(9)	1.342(10)	C(4)-C(5)	1.336(12)
N(3)-C(13)	1.371(10)	C(4)-C(3)	1.389(12)
N(5)-C(15)	1.327(9)	C(4)-H(3)	1.098(8)
N(5)-C(16)	1.376(9)	C(5)-H(4)	0.729(8)
N(5)-H(13)	0.959(5)	C(11)-H(9)	0.864(7)
N(1)-C(7)	1.334(8)	C(19)-C(20)	1.381(11)
N(1)-C(1)	1.403(9)	C(19)-H(16)	0.729(8)
N(4)-C(15)	1.348(8)	C(3)-H(2)	0.977(9)
N(4)-C(21)	1.417(9)	C(20)-H(17)	1.063(7)
C(14)-C(13)	1.485(11)	O(4)-N(7)	1.253(8)
C(14)-H(11)	0.879(7)	N(7)-O(6)	1.238(8)
C(14)-H(12)	1.111(8)	N(7)-O(5)	1.239(7)
N(2)-C(7)	1.344(9)	O(1)-Cu(1)-N(3)	178.8(2)
N(2)-C(6)	1.360(9)	O(1)-Cu(1)-N(4)	89.8(2)
N(2)-H(5)	0.996(6)	N(3)-Cu(1)-N(4)	89.0(2)
C(6)-C(1)	1.392(10)	O(1)-Cu(1)-N(1)	91.6(2)
C(6)-C(5)	1.396(11)	N(3)-Cu(1)-N(1)	89.6(2)
C(21)-C(20)	1.392(10)	N(4)-Cu(1)-N(1)	177.1(3)
C(21)-C(16)	1.393(9)	C(7)-S(2)-C(8)	103.1(3)
C(1)-C(2)	1.388(11)	C(15)-S(3)-C(14)	103.2(3)
C(8)-C(9)	1.498(10)	N(6)-O(1)-Cu(1)	113.7(4)
C(8)-H(7)	0.860(8)	C(9)-N(3)-C(13)	119.9(6)
C(8)-H(6)	1.047(8)	C(9)-N(3)-Cu(1)	121.1(5)
N(6)-O(3)	1.223(8)	C(13)-N(3)-Cu(1)	119.1(6)
N(6)-O(2)	1.236(8)	C(15)-N(5)-C(16)	109.9(6)
C(16)-C(17)	1.388(11)	C(15)-N(5)-H(13)	131.6(7)
C(17)-C(18)	1.345(10)	C(16)-N(5)-H(13)	115.9(6)
C(17)-H(14)	0.979(7)	C(7)-N(1)-C(1)	105.9(6)
C(13)-C(12)	1.368(10)	C(7)-N(1)-Cu(1)	131.2(5)

C(1)-N(1)-Cu(1)	122.9(5)	C(18)-C(17)-H(14)	130.4(8)
C(15)-N(4)-C(21)	104.4(6)	C(16)-C(17)-H(14)	111.4(8)
C(15)-N(4)-Cu(1)	131.9(5)	C(12)-C(13)-N(3)	119.8(7)
C(21)-N(4)-Cu(1)	123.5(4)	C(12)-C(13)-C(14)	124.6(7)
C(13)-C(14)-S(3)	111.4(5)	N(3)-C(13)-C(14)	115.5(6)
C(13)-C(14)-H(11)	113.3(8)	N(3)-C(9)-C(10)	122.0(7)
S(3)-C(14)-H(11)	95.8(6)	N(3)-C(9)-C(8)	115.9(6)
C(13)-C(14)-H(12)	117.6(6)	C(10)-C(9)-C(8)	122.1(7)
S(3)-C(14)-H(12)	108.0(6)	C(11)-C(12)-C(13)	120.5(7)
H(11)-C(14)-H(12)	108.4(7)	C(11)-C(12)-H(10)	129.0(8)
C(7)-N(2)-C(6)	108.9(6)	C(13)-C(12)-H(10)	110.3(8)
C(7)-N(2)-H(5)	117.1(7)	C(9)-C(10)-C(11)	117.9(8)
C(6)-N(2)-H(5)	133.4(7)	C(9)-C(10)-H(8)	111.5(8)
N(2)-C(6)-C(1)	106.2(6)	C(11)-C(10)-H(8)	130.6(8)
N(2)-C(6)-C(5)	132.7(8)	C(1)-C(2)-C(3)	115.7(7)
C(1)-C(6)-C(5)	121.1(8)	C(1)-C(2)-H(1)	126.2(7)
C(20)-C(21)-C(16)	120.8(7)	C(3)-C(2)-H(1)	117.8(8)
C(20)-C(21)-N(4)	129.8(6)	C(17)-C(18)-C(19)	120.4(7)
C(16)-C(21)-N(4)	109.3(6)	C(17)-C(18)-H(15)	133.0(9)
C(2)-C(1)-C(6)	121.4(7)	C(19)-C(18)-H(15)	102.8(8)
C(2)-C(1)-N(1)	130.4(7)	C(5)-C(4)-C(3)	121.9(8)
C(6)-C(1)-N(1)	108.1(7)	C(5)-C(4)-H(3)	114.1(8)
C(9)-C(8)-S(2)	114.0(6)	C(3)-C(4)-H(3)	122.5(9)
C(9)-C(8)-H(7)	117.1(7)	C(4)-C(5)-C(6)	118.0(8)
S(2)-C(8)-H(7)	105.6(6)	C(4)-C(5)-H(4)	129.5(11)
C(9)-C(8)-H(6)	105.8(7)	C(6)-C(5)-H(4)	112.5(11)
S(2)-C(8)-H(6)	110.4(6)	C(12)-C(11)-C(10)	119.9(7)
H(7)-C(8)-H(6)	103.4(8)	C(12)-C(11)-H(9)	127.0(10)
O(3)-N(6)-O(2)	124.1(7)	C(10)-C(11)-H(9)	112.9(10)
O(3)-N(6)-O(1)	118.5(7)	C(20)-C(19)-C(18)	123.2(7)
O(2)-N(6)-O(1)	117.4(7)	C(20)-C(19)-H(16)	120.5(10)
N(5)-C(16)-C(17)	133.4(7)	C(18)-C(19)-H(16)	115.1(10)
N(5)-C(16)-C(21)	104.8(6)	C(4)-C(3)-C(2)	121.7(8)
C(17)-C(16)-C(21)	121.8(7)	C(4)-C(3)-H(2)	134.9(9)
N(5)-C(15)-N(4)	111.6(7)	C(2)-C(3)-H(2)	103.3(9)
N(5)-C(15)-S(3)	118.9(5)	C(19)-C(20)-C(21)	115.7(7)
N(4)-C(15)-S(3)	129.4(6)	C(19)-C(20)-H(17)	123.0(8)
N(1)-C(7)-N(2)	110.9(6)	C(21)-C(20)-H(17)	120.5(7)
N(1)-C(7)-S(2)	131.2(6)	O(6)-N(7)-O(5)	118.8(7)
N(2)-C(7)-S(2)	117.9(5)	O(6)-N(7)-O(4)	120.1(6)
C(18)-C(17)-C(16)	118.0(7)	O(5)-N(7)-O(4)	121.1(7)

Table S4. Anisotropic displacement parameters* ($A^2 \times 10^3$) for $[Cu(Bbtmp)NO_3]NO_3$

	U11	U22	U33	U23	U13	U12
Cu(1)	28(1)	44(1)	33(1)	0(1)	7(1)	3(1)
S(2)	41(1)	73(2)	42(1)	-16(1)	9(1)	6(1)
S(3)	47(1)	55(1)	42(1)	-4(1)	4(1)	-13(1)
O(1)	28(2)	58(3)	29(3)	-6(3)	5(2)	0(3)
N(3)	22(3)	46(4)	37(3)	10(4)	8(2)	5(4)
N(5)	23(3)	53(4)	31(4)	11(3)	0(3)	5(3)
N(1)	29(3)	41(4)	32(4)	0(3)	10(3)	3(3)
N(4)	31(3)	39(4)	31(3)	5(3)	3(3)	6(3)
C(14)	40(5)	29(4)	57(6)	-4(4)	10(4)	-13(4)
N(2)	43(4)	52(4)	34(4)	-2(3)	8(3)	-6(3)
C(6)	33(4)	44(5)	39(5)	9(4)	15(4)	1(4)
C(21)	34(4)	37(4)	37(5)	-3(4)	12(4)	-2(4)
C(1)	30(4)	34(5)	49(5)	1(4)	15(4)	-6(3)
C(8)	55(5)	46(5)	43(5)	1(4)	22(4)	9(4)
N(6)	41(4)	66(5)	32(4)	3(4)	6(3)	18(4)
O(2)	54(4)	71(4)	67(4)	-31(4)	0(3)	-4(3)
C(16)	26(4)	46(5)	34(4)	6(4)	7(4)	10(4)
C(15)	25(4)	55(5)	31(4)	-3(4)	8(3)	4(3)
C(7)	28(4)	45(5)	34(4)	-5(4)	12(3)	-11(3)
C(17)	41(5)	54(5)	37(5)	10(4)	5(4)	5(4)
C(13)	26(4)	45(5)	43(5)	15(4)	1(3)	4(4)
C(9)	25(4)	39(4)	52(5)	5(4)	13(4)	-1(4)
C(12)	27(4)	62(6)	48(5)	2(4)	6(4)	-7(4)
O(3)	62(3)	108(6)	50(3)	8(4)	33(3)	20(4)
C(10)	33(4)	69(6)	51(5)	-2(5)	11(4)	1(4)
C(2)	35(4)	48(5)	42(5)	2(4)	9(4)	1(4)
C(18)	52(5)	47(5)	54(6)	5(4)	18(5)	-5(4)
C(4)	42(5)	49(6)	71(7)	8(5)	10(5)	0(4)
C(5)	41(5)	67(6)	47(5)	10(5)	8(4)	-5(4)
C(11)	33(4)	80(7)	58(5)	20(6)	21(4)	8(5)
C(19)	44(5)	60(6)	65(6)	0(5)	13(5)	-13(4)
C(3)	60(6)	48(6)	78(7)	-23(5)	30(5)	-1(5)
C(20)	50(5)	41(5)	41(5)	9(4)	9(4)	4(4)
O(4)	36(3)	56(4)	54(4)	15(3)	7(3)	9(3)
N(7)	35(4)	60(5)	39(4)	-3(4)	10(4)	0(4)
O(5)	54(4)	59(4)	50(4)	1(3)	-5(3)	9(3)
O(6)	61(4)	74(4)	82(5)	13(4)	1(4)	-13(4)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for $[Cu(bbtmp)NO_3]NO_3$

	x	y	z	U(eq)
H(4)	75	3845	-4721	50
H(2)	861	4616	-446	50
H(8)	7539	607	-2430	50
H(16)	2904	-1491	2836	50
H(11)	7459	3325	1924	50
H(9)	9435	1759	-1354	50
H(1)	2301	3434	419	50
H(3)	-761	4917	-3340	50
H(10)	9203	2760	723	50
H(7)	5189	-135	-2263	50
H(13)	8148	452	5104	50
H(5)	1759	2258	-5180	50
H(15)	4297	-1918	4723	50
H(14)	6837	-982	5850	50
H(6)	4424	289	-1229	50
H(12)	5703	2990	1579	50
H(17)	2768	-204	1251	50

Table S6. Possible hydrogen bonding interactions for $[Cu(bbtmp)NO_3]NO_3$ (distance in Å, angles in deg)

D	H	A	D-H	H·····A	D·····A	D-H·····A
N2	H5	O3	0.9955	1.9267	2.910(8)	169.01
N5	H13	O4	0.9587	1.9018	2.821(8)	159.77
C2	H1	O2	1.0827	2.3460	3.347(10)	153.06
C8	H6	Cu1	1.0465	2.4127	3.048(8)	118.07
C8	H6	O5	1.0465	2.4645	3.248(11)	130.90
C14	H11	O5	0.8790	2.4722	3.294(9)	155.85
C14	H12	Cu1	1.1106	2.5286	3.012(8)	104.94
C17	H14	O6	0.9792	2.5139	3.406(10)	151.34
C20	H17	Cu1	1.0626	3.1004	3.466(7)	101.13
C20	H17	O1	1.0626	2.5025	3.146(9)	118.13
C20	H17	O5	1.0626	2.4632	3.394(10)	145.62

Table S7. Crystal data and structure refinement for [Cu(bbtmp)NO_3] **(2)**

Empirical formula	$C_{21}H_{17}CuN_6O_3S_2$
Formula weight	529.07
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 8.7099(2) Å, α = 90° b = 10.9708(2) Å, β = 90° c = 22.1656(3) Å, γ = 90°
Volume	2118.02(7) A^3
Z	4
Density (calculated)	1.659 Mg/m^3
Absorption coefficient	1.267 mm^{-1}
F(000)	1080
Crystal size	0.22 x 0.12 x 0.22 mm
Theta range for data collection	1.84 to 23.25°
Index ranges	$-9 \le h \le 9, -12 \le k \le 11, -14 \le l \le 24$
Reflections collected	8819
Independent reflections	3030 [R(int) = 0.0341]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3030 / 0 / 299
Goodness-of-fit on F^2	1.081
Final R indices [I>2sigma(I)]	R1 = 0.0289, wR2 = 0.0833
R indices (all data)	R1 = 0.0321, wR2 = 0.0850
Absolute structure parameter	-0.01(2)
Largest diff. peak and hole	0.263 and -0.610 $e.A^{-3}$

$R = \Sigma||F_o|-|F_c||/\Sigma|F_o|$; $wR2 = \{\Sigma[w(F_o^2-F_c^2)^2/\Sigma[w(F_o^2)^2]\}^{1/2}$

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 X 10^3) for [Cu(bbtmp)NO_3]

atom	x	y	z	U_{eq}*
Cu(1)	7318(1)	8384(1)	815(1)	36(1)
S(2)	7637(1)	5296(1)	45(1)	39(1)
S(3)	6043(1)	11343(1)	254(1)	36(1)
O(3)	9408(3)	12448(2)	1060(1)	43(1)
N(3)	7344(3)	8662(3)	-114(1)	29(1)
N(2)	9350(4)	5011(2)	1029(1)	31(1)
N(5)	4420(4)	11107(3)	1281(1)	35(1)
N(4)	6270(4)	9698(3)	1204(1)	31(1)
N(6)	10720(4)	11969(3)	1087(1)	34(1)
O(1)	10848(4)	10844(3)	1110(2)	50(1)
O(2)	11889(3)	12639(3)	1079(2)	52(1)
C(9)	7360(4)	7643(3)	-461(2)	30(1)
C(8)	6478(4)	6583(3)	-207(2)	34(1)
C(5)	10851(5)	5241(4)	2011(2)	38(1)
C(1)	9361(4)	6799(3)	1493(2)	30(1)
C(11)	8790(5)	8644(4)	-1223(2)	45(1)
C(16)	5489(4)	9539(3)	1759(2)	28(1)
C(2)	9759(5)	7682(3)	1921(2)	37(1)
C(13)	8009(4)	9685(3)	-328(2)	31(1)
C(6)	9928(4)	5618(3)	1537(2)	32(1)
N(1)	8452(3)	6914(2)	968(1)	28(1)
C(21)	4312(4)	10394(3)	1803(2)	33(1)
C(18)	4722(5)	8723(4)	2707(2)	46(1)
C(20)	3315(5)	10439(4)	2294(2)	41(1)
C(17)	5697(4)	8671(4)	2208(2)	39(1)
C(10)	8093(4)	7607(4)	-1016(2)	37(1)
C(15)	5606(4)	10649(3)	943(2)	30(1)
C(12)	8742(4)	9714(4)	-881(2)	38(1)
C(7)	8492(4)	5807(3)	716(2)	30(1)
C(4)	11192(5)	6102(4)	2444(2)	45(1)
C(3)	10679(5)	7312(4)	2400(2)	41(1)
C(14)	7979(4)	10772(3)	91(2)	34(1)
C(19)	3550(5)	9596(4)	2740(2)	46(1)

* U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table S9. Bond Distances (Å) and Angles (deg) for [Cu(bbtmp)NO_3]

Cu(1)-N(4)	1.912(3)	C(20)-C(19)	1.369(6)
Cu(1)-N(1)	1.921(3)	C(4)-C(3)	1.405(6)
Cu(1)-N(3)	2.082(3)		
S(2)-C(7)	1.755(4)	N(4)-Cu(1)-N(1)	143.03(13)
S(2)-C(8)	1.823(4)	N(4)-Cu(1)-N(3)	109.93(12)
S(3)-C(15)	1.749(4)	N(1)-Cu(1)-N(3)	106.96(12)
S(3)-C(14)	1.835(4)	C(7)-S(2)-C(8)	104.4(2)
O(3)-N(6)	1.259(4)	C(15)-S(3)-C(14)	102.9(2)
N(3)-C(13)	1.349(4)	C(13)-N(3)-C(9)	118.8(3)
N(3)-C(9)	1.358(4)	C(13)-N(3)-Cu(1)	118.3(2)
N(2)-C(7)	1.343(5)	C(9)-N(3)-Cu(1)	116.1(2)
N(2)-C(6)	1.401(5)	C(7)-N(2)-C(6)	107.8(3)
N(5)-C(15)	1.371(5)	C(15)-N(5)-C(21)	107.3(3)
N(5)-C(21)	1.400(5)	C(15)-N(4)-C(16)	105.5(3)
N(4)-C(15)	1.325(5)	C(15)-N(4)-Cu(1)	127.2(2)
N(4)-C(16)	1.415(5)	C(16)-N(4)-Cu(1)	121.9(2)
N(6)-O(1)	1.241(4)	O(1)-N(6)-O(2)	120.6(3)
N(6)-O(2)	1.256(4)	O(1)-N(6)-O(3)	119.9(4)
C(9)-C(10)	1.386(5)	O(2)-N(6)-O(3)	119.4(3)
C(9)-C(8)	1.503(5)	N(3)-C(9)-C(10)	122.0(3)
C(5)-C(4)	1.379(6)	N(3)-C(9)-C(8)	114.8(3)
C(5)-C(6)	1.386(5)	C(10)-C(9)-C(8)	123.1(3)
C(1)-C(6)	1.390(5)	C(9)-C(8)-S(2)	115.5(2)
C(1)-C(2)	1.400(5)	C(4)-C(5)-C(6)	116.7(4)
C(1)-N(1)	1.414(5)	C(6)-C(1)-C(2)	120.7(4)
C(11)-C(10)	1.369(6)	C(6)-C(1)-N(1)	109.9(3)
C(11)-C(12)	1.399(6)	C(2)-C(1)-N(1)	129.4(3)
C(16)-C(17)	1.390(5)	C(10)-C(11)-C(12)	120.1(3)
C(16)-C(21)	1.394(5)	C(17)-C(16)-C(21)	120.4(4)
C(2)-C(3)	1.391(6)	C(17)-C(16)-N(4)	130.1(3)
C(13)-C(12)	1.382(6)	C(21)-C(16)-N(4)	109.4(3)
C(13)-C(14)	1.511(5)	C(3)-C(2)-C(1)	117.2(4)
N(1)-C(7)	1.338(4)	N(3)-C(13)-C(12)	121.9(3)
C(21)-C(20)	1.393(6)	N(3)-C(13)-C(14)	115.7(3)
C(18)-C(17)	1.396(6)	C(12)-C(13)-C(14)	122.3(3)
C(18)-C(19)	1.402(6)	C(5)-C(6)-C(1)	122.5(4)

C(5)-C(6)-N(2)	132.5(3)	N(4)-C(15)-N(5)	112.3(3)
C(1)-C(6)-N(2)	105.1(3)	N(4)-C(15)-S(3)	129.0(3)
C(7)-N(1)-C(1)	104.3(3)	N(5)-C(15)-S(3)	118.8(3)
C(7)-N(1)-Cu(1)	134.6(2)	C(13)-C(12)-C(11)	118.4(4)
C(1)-N(1)-Cu(1)	120.6(2)	N(1)-C(7)-N(2)	112.9(3)
C(20)-C(21)-C(16)	122.5(4)	N(1)-C(7)-S(2)	129.2(3)
C(20)-C(21)-N(5)	131.9(4)	N(2)-C(7)-S(2)	117.8(3)
C(16)-C(21)-N(5)	105.5(3)	C(5)-C(4)-C(3)	122.0(4)
C(17)-C(18)-C(19)	120.7(4)	C(2)-C(3)-C(4)	120.9(4)
C(19)-C(20)-C(21)	116.5(4)	C(13)-C(14)-S(3)	114.0(3)
C(16)-C(17)-C(18)	117.5(4)	C(20)-C(19)-C(18)	122.3(4)
C(11)-C(10)-C(9)	118.6(3)		

Table S10. Anisotropic displacement parameters* (A^2 x 10^3) for [Cu(bbtmp)NO_3]

	U11	U22	U33	U23	U13	U12
Cu(1)	41(1)	29(1)	37(1)	-2(1)	2(1)	8(1)
S(2)	49(1)	28(1)	40(1)	-8(1)	-8(1)	9(1)
S(3)	41(1)	30(1)	35(1)	2(1)	-3(1)	7(1)
O(3)	42(2)	32(1)	55(2)	-7(1)	-7(1)	8(1)
N(3)	28(2)	33(2)	27(2)	-1(1)	-4(1)	0(1)
N(2)	39(2)	21(2)	32(2)	1(1)	3(2)	7(1)
N(5)	37(2)	32(2)	36(2)	-5(2)	-1(2)	11(1)
N(4)	34(2)	23(2)	36(2)	-4(1)	0(1)	8(1)
N(6)	47(2)	27(2)	29(2)	-3(1)	-5(2)	8(2)
O(1)	59(2)	26(2)	66(2)	-1(2)	-11(2)	6(1)
O(2)	45(2)	34(2)	78(2)	6(2)	-4(2)	-1(1)
C(9)	28(2)	32(2)	31(2)	-6(2)	-6(2)	7(2)
C(8)	29(2)	31(2)	43(2)	-2(2)	-4(2)	1(2)
C(5)	41(2)	34(2)	39(2)	8(2)	3(2)	2(2)
C(1)	29(2)	33(2)	27(2)	2(2)	6(2)	0(2)
C(11)	41(2)	63(3)	32(2)	2(2)	6(2)	11(2)
C(16)	28(2)	27(2)	30(2)	-3(2)	-5(2)	-1(2)
C(2)	41(2)	30(2)	39(2)	-6(2)	1(2)	1(2)
C(13)	30(2)	31(2)	33(2)	2(2)	-6(2)	1(2)
C(6)	31(2)	32(2)	33(2)	4(2)	6(2)	4(2)
N(1)	30(2)	25(2)	29(2)	-4(1)	-1(1)	2(1)
C(21)	34(2)	32(2)	32(2)	-5(2)	-6(2)	1(2)
C(18)	52(3)	50(2)	35(2)	5(2)	-4(2)	-3(2)
C(20)	37(2)	44(2)	41(2)	-8(2)	3(2)	5(2)
C(17)	36(2)	42(2)	40(2)	3(2)	-6(2)	6(2)
C(10)	39(2)	38(2)	34(2)	-3(2)	-2(2)	11(2)
C(15)	34(2)	24(2)	32(2)	-6(2)	-6(2)	1(2)
C(12)	37(2)	41(2)	35(2)	6(2)	6(2)	3(2)
C(7)	26(2)	33(2)	30(2)	2(2)	5(2)	4(2)
C(4)	42(2)	60(3)	33(2)	5(2)	-10(2)	2(2)
C(3)	46(2)	40(2)	38(2)	-6(2)	0(2)	-1(2)
C(14)	34(2)	31(2)	38(2)	2(2)	1(2)	-4(2)
C(19)	44(3)	56(3)	37(2)	-7(2)	7(2)	-7(2)

* taken form $-2\pi^2[h^2 a^{*2} U11 + ... + 2 hk a^* b^* U12]$

Table S11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [Cu(bbtmp)NO_3]

	x	y	z	U(eq)
H(20)	2425	11089	2325	50
H(19)	2934	9539	3108	50
H(3)	10775	7993	2737	50
H(4)	11935	5833	2766	50
H(18)	4907	8064	3007	50
H(11)	9351	8599	-1590	50
H(5)	11289	4451	2045	50
H(2)	9498	8640	1933	50
H(17)	6563	8112	2237	50
H(12)	9260	10536	-1053	50
H(14B)	8561	11448	-117	50
H(5A)	3599	11637	1195	50
H(10)	7972	6816	-1259	50
H(2A)	9514	4202	993	50
H(14A)	8458	10755	514	50
H(8A)	5731	6758	157	50
H(8B)	5768	6156	-512	50

Table S12. Possible hydrogen bonding interactions for [Cu(bbtmp)NO_3] (distance in Å, angles in deg)

D	H	A	D-H	H·····A	D·····A	D-H·····A
N2	H2A	O3	0.903(2)	1.932(2)	2.813(3)	164.8(2)
N5	H5A	O1	0.941(3)	2.556(3)	3.147(5)	121.1(2)
N5	H5A	O2	0.941(3)	1.869(3)	2.808(4)	175.4(2)
C8	H8A	Cu1	1.054(4)	2.6870(4)	3.094(4)	102.64(19)
C8	H8B	Cu1	1.029(4)	3.1202(4)	3.866(4)	130.3(2)
C8	H8B	O1	1.029(4)	2.564(4)	3.376(5)	135.5(2)
C14	H14A	O1	1.026(4)	2.467(4)	3.369(6)	146.2(2)
C14	H14A	O3	1.026(4)	2.366(3)	3.090(5)	126.5(2)

Table S13. Crystal data and structure refinement for [Cu(bbtmp)Cl] **(3)**

Empirical formula	$C_{42}H_{34}Cl_2Cu_2N_{10}S_4$
Formula weight	1005.01
Temperature	293(2) K
Wavelength	1.54180 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 8.4268(14) Å, α = 99.03(2)° b = 13.525(2) Å, β = 94.65(2)° c = 18.850(4) Å, γ = 89.872(14)°
Volume	2114.6(6) A^3
Z	2
Density (calculated)	1.578 Mg/m^3
Absorption coefficient	4.618 mm^{-1}
F(000)	1024
Crystal size	0.15 x 0.08 x 0.08 mm
Theta range for data collection	2.38 to 67.95°
Index ranges	$0 \le h \le 10$, $-16 \le k \le 16$, $-22 \le l \le 22$
Reflections collected	8026
Independent reflections	7478 [R(int) = 0.0803]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7452 / 0 / 541
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0579, wR2 = 0.1549
R indices (all data)	R1 = 0.0764, wR2 = 0.2054
Largest diff. peak and hole	0.751 and -0.607 $e.A^{-3}$

$$R = \Sigma||F_o| - |F_c||/\Sigma|F_o|; \quad wR2 = \{\Sigma[w(F_o^2-F_c^2)^2/\Sigma[w(F_o^2)^2]\}^{1/2}$$

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 X 10^3) for [Cu(bbtmp)Cl]

atom	x	y	z	U_{eq}*
Cu(1)	4800(1)	9450(1)	2839(1)	47(1)
Cu(2)	-181(1)	4629(1)	2820(1)	48(1)
Cl(1)	7816(1)	9667(1)	2950(1)	45(1)
Cl(2)	2854(1)	4480(1)	2970(1)	44(1)
S(1)	5427(2)	6930(1)	3520(1)	54(1)
S(2)	2794(2)	11741(1)	3559(1)	52(1)
S(3)	-2183(2)	2638(1)	3526(1)	53(1)
S(4)	353(2)	7444(1)	3514(1)	55(1)
N(6)	-577(4)	3194(3)	2425(2)	38(1)
N(7)	-988(5)	1557(3)	2391(2)	46(1)
N(8)	-1076(4)	5126(3)	3836(2)	38(1)
N(9)	-743(5)	5903(3)	2421(2)	40(1)
N(10)	-1474(5)	7446(3)	2298(2)	49(1)
N(5)	3613(5)	6391(3)	2308(2)	49(1)
N(4)	4224(5)	8016(3)	2452(2)	41(1)
N(1)	4340(5)	10709(3)	2436(2)	39(1)
N(2)	4031(5)	12344(3)	2436(2)	42(1)
N(3)	3922(4)	9389(3)	3855(2)	39(1)
C(1)	5715(7)	10403(4)	1278(3)	53(1)
C(2)	6237(8)	10885(5)	746(3)	65(2)
C(3)	6073(8)	11914(5)	767(4)	69(2)
C(4)	5383(7)	12488(4)	1314(4)	59(2)
C(5)	4827(6)	12001(4)	1840(3)	44(1)
C(6)	5001(6)	10976(3)	1830(3)	39(1)
C(7)	3764(5)	11541(3)	2767(3)	39(1)
C(8)	1839(6)	10534(4)	3542(3)	50(1)
C(9)	2638(6)	9911(4)	4066(3)	44(1)
C(10)	2063(7)	9879(4)	4727(3)	58(2)
C(11)	2745(8)	9259(5)	5166(3)	62(2)
C(12)	3999(7)	8676(4)	4939(3)	55(1)
C(13)	4573(6)	8761(4)	4279(3)	41(1)
C(14)	5962(6)	8165(4)	4009(3)	46(1)

C(15)	4396(6)	7173(3)	2726(3)	40(1)
C(16)	2851(6)	6740(4)	1721(3)	44(1)
C(17)	1860(7)	6282(4)	1142(3)	58(1)
C(18)	1263(7)	6877(5)	664(3)	64(2)
C(19)	1609(7)	7909(5)	755(3)	61(2)
C(20)	2607(7)	8349(4)	1334(3)	50(1)
C(21)	3241(6)	7756(3)	1822(3)	40(1)
C(22)	895(7)	2998(4)	1292(3)	52(1)
C(23)	1435(7)	2293(5)	766(3)	61(2)
C(24)	1191(8)	1280(5)	755(4)	69(2)
C(25)	396(7)	930(4)	1270(4)	61(2)
C(26)	-151(6)	1637(4)	1801(3)	45(1)
C(27)	83(5)	2666(3)	1828(3)	39(1)
C(28)	-1212(5)	2488(3)	2735(3)	40(1)
C(29)	-3120(6)	3845(4)	3521(3)	53(1)
C(30)	-2344(6)	4673(4)	4045(3)	42(1)
C(31)	-2922(7)	4986(4)	4712(3)	58(2)
C(32)	-2236(8)	5786(5)	5155(3)	63(2)
C(33)	-992(7)	6287(4)	4931(3)	52(1)
C(34)	-429(6)	5931(3)	4270(3)	41(1)
C(35)	941(6)	6421(4)	4009(3)	48(1)
C(36)	-662(6)	6852(3)	2716(3)	42(1)
C(37)	-2151(6)	6843(4)	1697(3)	44(1)
C(38)	-1696(6)	5881(3)	1778(3)	42(1)
C(39)	-3096(7)	7059(4)	1104(4)	60(2)
C(40)	-3556(8)	6269(5)	595(4)	67(2)
C(41)	-3119(8)	5290(5)	661(3)	65(2)
C(42)	-2187(7)	5083(4)	1252(3)	53(1)

* U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Table S15. Bond Distances (Å) and Angles (deg) for [Cu(bbtmp)Cl]

Cu(1)-N(1)	1.996(4)	C(1)-C(6)	1.375(7)
Cu(1)-N(4)	2.008(4)	C(1)-C(2)	1.378(8)
Cu(1)-N(3)	2.123(4)	C(2)-C(3)	1.393(9)
Cu(1)-Cl(1)	2.547(2)	C(3)-C(4)	1.360(9)
Cu(2)-N(6)	1.986(4)	C(4)-C(5)	1.385(7)
Cu(2)-N(9)	2.026(4)	C(5)-C(6)	1.391(6)
Cu(2)-N(8)	2.125(4)	C(8)-C(9)	1.513(7)
Cu(2)-Cl(2)	2.562(2)	C(9)-C(10)	1.380(7)
S(1)-C(15)	1.746(5)	C(10)-C(11)	1.362(9)
S(1)-C(14)	1.815(6)	C(11)-C(12)	1.373(9)
S(2)-C(7)	1.743(5)	C(12)-C(13)	1.392(7)
S(2)-C(8)	1.816(6)	C(13)-C(14)	1.498(7)
S(3)-C(28)	1.743(5)	C(16)-C(17)	1.383(8)
S(3)-C(29)	1.812(6)	C(16)-C(21)	1.393(7)
S(4)-C(36)	1.746(6)	C(17)-C(18)	1.365(9)
S(4)-C(35)	1.833(5)	C(18)-C(19)	1.407(9)
N(6)-C(28)	1.329(6)	C(19)-C(20)	1.378(8)
N(6)-C(27)	1.390(6)	C(20)-C(21)	1.388(7)
N(7)-C(28)	1.343(6)	C(22)-C(23)	1.368(8)
N(7)-C(26)	1.382(7)	C(22)-C(27)	1.394(7)
N(8)-C(34)	1.343(6)	C(23)-C(24)	1.383(9)
N(8)-C(30)	1.349(6)	C(24)-C(25)	1.367(9)
N(9)-C(36)	1.316(6)	C(25)-C(26)	1.378(8)
N(9)-C(38)	1.394(7)	C(26)-C(27)	1.399(7)
N(10)-C(36)	1.358(6)	C(29)-C(30)	1.486(8)
N(10)-C(37)	1.371(7)	C(30)-C(31)	1.390(7)
N(5)-C(15)	1.353(7)	C(31)-C(32)	1.357(9)
N(5)-C(16)	1.381(7)	C(32)-C(33)	1.379(9)
N(4)-C(15)	1.326(6)	C(33)-C(34)	1.384(7)
N(4)-C(21)	1.389(6)	C(34)-C(35)	1.487(7)
N(1)-C(7)	1.311(6)	C(37)-C(38)	1.384(6)
N(1)-C(6)	1.407(6)	C(37)-C(39)	1.387(8)
N(2)-C(7)	1.362(6)	C(38)-C(42)	1.386(8)
N(2)-C(5)	1.373(6)	C(39)-C(40)	1.354(9)
N(3)-C(13)	1.342(6)	C(40)-C(41)	1.395(9)
N(3)-C(9)	1.343(6)	C(41)-C(42)	1.375(8)

N(1)-Cu(1)-N(4)	131.4(2)	C(4)-C(3)-C(2)	121.2(5)
N(1)-Cu(1)-N(3)	115.4(2)	C(3)-C(4)-C(5)	117.0(5)
N(4)-Cu(1)-N(3)	93.7(2)	N(2)-C(5)-C(4)	131.6(5)
N(1)-Cu(1)-Cl(1)	95.55(12)	N(2)-C(5)-C(6)	106.1(4)
N(4)-Cu(1)-Cl(1)	109.53(12)	C(4)-C(5)-C(6)	122.3(5)
N(3)-Cu(1)-Cl(1)	111.39(12)	C(1)-C(6)-C(5)	120.3(5)
N(6)-Cu(2)-N(9)	132.2(2)	C(1)-C(6)-N(1)	130.9(4)
N(6)-Cu(2)-N(8)	115.4(2)	C(5)-C(6)-N(1)	108.8(4)
N(9)-Cu(2)-N(8)	94.5(2)	N(1)-C(7)-N(2)	112.7(4)
N(6)-Cu(2)-Cl(2)	95.19(12)	N(1)-C(7)-S(2)	129.1(4)
N(9)-Cu(2)-Cl(2)	109.04(12)	N(2)-C(7)-S(2)	118.1(3)
N(8)-Cu(2)-Cl(2)	110.06(11)	C(9)-C(8)-S(2)	114.0(4)
C(15)-S(1)-C(14)	103.9(2)	N(3)-C(9)-C(10)	121.8(5)
C(7)-S(2)-C(8)	101.9(2)	N(3)-C(9)-C(8)	116.9(4)
C(28)-S(3)-C(29)	102.3(2)	C(10)-C(9)-C(8)	121.2(5)
C(36)-S(4)-C(35)	104.5(2)	C(11)-C(10)-C(9)	119.8(5)
C(28)-N(6)-C(27)	104.2(4)	C(10)-C(11)-C(12)	119.0(5)
C(28)-N(6)-Cu(2)	128.6(3)	C(11)-C(12)-C(13)	119.1(5)
C(27)-N(6)-Cu(2)	125.7(3)	N(3)-C(13)-C(12)	121.8(5)
C(28)-N(7)-C(26)	107.6(4)	N(3)-C(13)-C(14)	116.6(4)
C(34)-N(8)-C(30)	118.6(4)	C(12)-C(13)-C(14)	121.6(5)
C(34)-N(8)-Cu(2)	120.3(3)	C(13)-C(14)-S(1)	113.9(4)
C(30)-N(8)-Cu(2)	121.1(3)	N(4)-C(15)-N(5)	112.5(5)
C(36)-N(9)-C(38)	105.2(4)	N(4)-C(15)-S(1)	130.8(4)
C(36)-N(9)-Cu(2)	132.1(4)	N(5)-C(15)-S(1)	116.7(3)
C(38)-N(9)-Cu(2)	121.2(3)	N(5)-C(16)-C(17)	132.6(5)
C(36)-N(10)-C(37)	107.9(4)	N(5)-C(16)-C(21)	104.7(4)
C(15)-N(5)-C(16)	107.8(4)	C(17)-C(16)-C(21)	122.7(5)
C(15)-N(4)-C(21)	104.6(4)	C(18)-C(17)-C(16)	116.7(5)
C(15)-N(4)-Cu(1)	133.1(4)	C(17)-C(18)-C(19)	122.2(6)
C(21)-N(4)-Cu(1)	121.5(3)	C(20)-C(19)-C(18)	120.1(5)
C(7)-N(1)-C(6)	105.2(4)	C(19)-C(20)-C(21)	118.6(5)
C(7)-N(1)-Cu(1)	127.3(3)	C(20)-C(21)-N(4)	129.9(5)
C(6)-N(1)-Cu(1)	125.1(3)	C(20)-C(21)-C(16)	119.7(5)
C(7)-N(2)-C(5)	107.1(4)	N(4)-C(21)-C(16)	110.4(4)
C(13)-N(3)-C(9)	118.3(4)	C(23)-C(22)-C(27)	118.0(5)
C(13)-N(3)-Cu(1)	120.0(3)	C(22)-C(23)-C(24)	121.9(5)
C(9)-N(3)-Cu(1)	121.5(3)	C(25)-C(24)-C(23)	121.6(5)
C(6)-C(1)-C(2)	117.4(5)	C(24)-C(25)-C(26)	116.8(5)
C(1)-C(2)-C(3)	121.8(5)	C(25)-C(26)-N(7)	132.3(5)

C(25)-C(26)-C(27)	122.9(5)	N(8)-C(34)-C(35)	116.7(4)
N(7)-C(26)-C(27)	104.8(4)	C(33)-C(34)-C(35)	121.3(5)
N(6)-C(27)-C(22)	131.0(4)	C(34)-C(35)-S(4)	113.3(3)
N(6)-C(27)-C(26)	110.2(4)	N(9)-C(36)-N(10)	111.9(5)
C(22)-C(27)-C(26)	118.9(5)	N(9)-C(36)-S(4)	130.9(4)
N(6)-C(28)-N(7)	113.2(4)	N(10)-C(36)-S(4)	117.1(4)
N(6)-C(28)-S(3)	128.0(4)	N(10)-C(37)-C(38)	105.3(4)
N(7)-C(28)-S(3)	118.7(3)	N(10)-C(37)-C(39)	131.8(5)
C(30)-C(29)-S(3)	114.4(4)	C(38)-C(37)-C(39)	123.0(5)
N(8)-C(30)-C(31)	121.3(5)	C(37)-C(38)-C(42)	119.8(5)
N(8)-C(30)-C(29)	117.0(4)	C(37)-C(38)-N(9)	109.7(4)
C(31)-C(30)-C(29)	121.6(5)	C(42)-C(38)-N(9)	130.4(4)
C(32)-C(31)-C(30)	119.6(5)	C(40)-C(39)-C(37)	116.2(5)
C(31)-C(32)-C(33)	119.5(5)	C(39)-C(40)-C(41)	122.2(6)
C(32)-C(33)-C(34)	118.8(5)	C(42)-C(41)-C(40)	121.2(6)
N(8)-C(34)-C(33)	122.1(5)	C(41)-C(42)-C(38)	117.6(5)

Table S16. Anisotropic displacement parameters* ($A^2 \times 10^3$) for [Cu(Bbtmp)Cl]

	U11	U22	U33	U23	U13	U12
Cu(1)	64(1)	31(1)	52(1)	14(1)	15(1)	7(1)
Cu(2)	65(1)	29(1)	52(1)	8(1)	17(1)	-1(1)
Cl(1)	45(1)	29(1)	64(1)	14(1)	16(1)	2(1)
Cl(2)	45(1)	27(1)	62(1)	11(1)	15(1)	6(1)
S(1)	66(1)	39(1)	61(1)	23(1)	5(1)	9(1)
S(2)	63(1)	40(1)	54(1)	6(1)	17(1)	14(1)
S(3)	60(1)	46(1)	60(1)	22(1)	16(1)	-5(1)
S(4)	71(1)	32(1)	62(1)	2(1)	12(1)	-4(1)
N(6)	40(2)	27(2)	47(2)	9(2)	4(2)	-4(2)
N(7)	47(2)	27(2)	67(3)	16(2)	3(2)	-6(2)
N(8)	37(2)	37(2)	40(2)	7(2)	8(2)	6(2)
N(9)	48(2)	27(2)	48(2)	9(2)	16(2)	3(2)
N(10)	61(3)	28(2)	61(3)	10(2)	23(2)	6(2)
N(5)	63(3)	27(2)	61(3)	11(2)	21(2)	-3(2)
N(4)	47(2)	33(2)	46(2)	13(2)	11(2)	5(2)
N(1)	45(2)	27(2)	48(2)	9(2)	7(2)	4(2)
N(2)	47(2)	25(2)	56(3)	8(2)	1(2)	7(2)
N(3)	39(2)	40(2)	40(2)	10(2)	10(2)	-1(2)
C(1)	59(3)	46(3)	55(3)	11(2)	13(3)	11(2)
C(2)	66(4)	80(4)	53(3)	14(3)	21(3)	11(3)
C(3)	65(4)	78(4)	77(4)	38(4)	25(3)	8(3)
C(4)	61(3)	46(3)	79(4)	30(3)	15(3)	2(3)
C(5)	41(2)	36(2)	57(3)	16(2)	5(2)	4(2)
C(6)	43(2)	33(2)	42(3)	9(2)	4(2)	3(2)
C(7)	36(2)	34(2)	46(3)	8(2)	2(2)	7(2)
C(8)	30(2)	54(3)	68(3)	16(3)	7(2)	2(2)
C(9)	36(2)	44(3)	53(3)	8(2)	13(2)	-6(2)
C(10)	53(3)	58(3)	68(4)	10(3)	30(3)	-9(3)
C(11)	74(4)	66(4)	48(3)	8(3)	27(3)	-16(3)
C(12)	67(4)	54(3)	46(3)	19(3)	8(3)	-11(3)
C(13)	40(2)	41(3)	45(3)	12(2)	8(2)	-7(2)
C(14)	44(3)	45(3)	54(3)	22(2)	1(2)	1(2)
C(15)	43(2)	32(2)	50(3)	14(2)	18(2)	6(2)

C(16)	49(3)	36(2)	51(3)	12(2)	18(2)	-3(2)
C(17)	61(3)	51(3)	61(4)	6(3)	13(3)	-14(3)
C(18)	60(4)	81(4)	49(3)	5(3)	4(3)	-15(3)
C(19)	57(3)	74(4)	56(3)	26(3)	8(3)	2(3)
C(20)	59(3)	44(3)	50(3)	17(2)	12(2)	6(2)
C(21)	42(2)	38(2)	45(3)	10(2)	20(2)	4(2)
C(22)	57(3)	50(3)	54(3)	21(3)	11(2)	3(2)
C(23)	55(3)	81(4)	51(3)	15(3)	13(3)	11(3)
C(24)	66(4)	71(4)	65(4)	-8(3)	13(3)	16(3)
C(25)	62(3)	42(3)	75(4)	-2(3)	0(3)	13(3)
C(26)	43(3)	35(2)	57(3)	9(2)	-1(2)	0(2)
C(27)	38(2)	35(2)	45(3)	12(2)	5(2)	1(2)
C(28)	36(2)	35(2)	51(3)	13(2)	4(2)	-4(2)
C(29)	35(3)	57(3)	69(4)	14(3)	10(2)	0(2)
C(30)	41(2)	42(3)	48(3)	16(2)	13(2)	14(2)
C(31)	58(3)	56(3)	67(4)	19(3)	34(3)	22(3)
C(32)	81(4)	66(4)	48(3)	15(3)	26(3)	29(3)
C(33)	61(3)	51(3)	43(3)	3(2)	4(2)	15(3)
C(34)	45(3)	36(2)	44(3)	9(2)	6(2)	14(2)
C(35)	45(3)	40(3)	56(3)	0(2)	4(2)	7(2)
C(36)	46(3)	32(2)	51(3)	10(2)	18(2)	3(2)
C(37)	51(3)	35(2)	50(3)	12(2)	19(2)	6(2)
C(38)	42(3)	36(3)	52(3)	12(2)	19(2)	3(2)
C(39)	65(4)	49(3)	72(4)	24(3)	15(3)	12(3)
C(40)	67(4)	70(4)	68(4)	23(3)	0(3)	6(3)
C(41)	69(4)	62(4)	59(4)	3(3)	-3(3)	-3(3)
C(42)	58(3)	42(3)	60(3)	8(3)	10(3)	4(2)

* taken form $-2\pi^2[h^2 a^{*2} U11 + ... + 2 hk a^* b^* U12]$

Table S17. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for [Cu(bbtmp)Cl]

	x	y	z	U(eq)
H(1)	5733	9737	1242	50
H(2)	6551	10566	307	50
H(3)	6505	12229	379	50
H(4)	5325	13170	1342	50
H(5)	3745	12900	2608	50
H(6)	741	10652	3696	50
H(7)	1845	10140	3113	50
H(8)	1285	10333	4875	50
H(9)	2536	9301	5601	50
H(10)	4571	8225	5236	50
H(11)	6615	7979	4384	50
H(12)	6634	8528	3748	50
H(13)	3517	5903	2417	50
H(14)	1590	5547	1068	50
H(15)	587	6606	288	50
H(16)	1092	8265	391	50
H(17)	2802	9016	1438	50
H(18)	1112	3664	1341	50
H(19)	1850	2451	433	50
H(20)	1540	881	382	50
H(21)	168	218	1227	50
H(22)	-1435	1006	2467	50
H(23)	-3171	3985	3021	50
H(24)	-4140	3729	3653	50
H(25)	-3803	4604	4875	50
H(26)	-2673	5910	5573	50
H(27)	-472	6906	5218	50
H(28)	1546	6845	4336	50
H(29)	1494	5905	3715	50
H(30)	-1457	8025	2446	50
H(31)	-3374	7716	1084	50
H(32)	-4123	6360	185	50
H(33)	-3405	4747	290	50
H(34)	-1925	4500	1272	50

Table S18. Possible hydrogen bonding interactions for [Cu(bbtmp)Cl] (distance in Å, angles in deg)

D	H	A	D-H	H·····A	D·····A	D-H·····A
N2	H5	Cl2	0.8149	2.2837	3.095(4)	174.01
N5	H13	Cl2	0.7279	2.4148	3.130(4)	167.61
N7	H22	Cl1	0.8725	2.2631	3.113(4)	164.48
N10	H30	Cl1	0.7887	2.3737	3.137(4)	163.27
C1	H1	Cu1	0.8928	3.2525	3.532(6)	100.89
C8	H7	Cu1	0.8963	2.7175	3.169(5)	112.38
C14	H12	Cu1	0.9623	2.6675	3.113(6)	108.76
C14	H12	Cl1	0.9623	2.5704	3.514(6)	166.73
C20	H17	Cu1	0.9051	2.9908	3.393(6)	108.82
C22	H18	Cu2	0.9084	3.1634	3.522(6)	105.88
C29	H23	Cu2	0.9876	2.7419	3.160(5)	106.00
C35	H29	Cu2	0.9646	2.5551	3.123(6)	117.75
C35	H29	Cl2	0.9646	2.5299	3.493(6)	176.82
C42	H34	Cu2	0.8241	3.1383	3.424(6)	103.36