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Table S1.

STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_6 H_{10} Cl_4 Cu N_2$
Color; Habit	Green, rectangular
Crystal size (mm)	0.23 x 0.23 x 0.45
Crystal System	Orthorhombic
Space Group	$Pna2_1$
Unit Cell Dimensions	a = 7.747(2) Å
	b = 24.966(5) Å
	c = 17.041(3) Å
Volume	3295.9(12) $Å^3$
Z	12
Formula weight	315.5
Density(calc.)	1.907 Mg/m^3
Absorption Coefficient	2.915 mm^{-1}
F(000)	1884

Table S1.

Data Collection

Diffractometer Used	Siemens R3m/V
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	294
Monochromator	Highly oriented graphite crystal
2θ Range	3.0 to 55.0°
Scan Type	ω
Scan Speed	Constant; 3.00°/min. in ω
Scan Range (ω)	0.90°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 50% of total scan time
Standard Reflections	3 measured every 100 reflections
Index Ranges	$-1 \leq h \leq 9$, $-29 \leq k \leq 1$ $-1 \leq l \leq 20$
Reflections Collected	3908
Independent Reflections	3224 (R_{int} = 3.92%)
Observed Reflections	2823 ($F > 3.0\sigma(F)$)
Absorption Correction	Empirical; Tmax/Tmin=0.823/0.365

Table S1.

Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o-F_c)^2$
Absolute Structure	n=0.00(1)
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0029F^2$
Number of Parameters Refined	352
Final R Indices (obs. data)	R = 5.21 %, wR = 6.38 %
R Indices (all data)	R = 5.92 %, wR = 6.67 %
Goodness-of-Fit	0.97
Largest and Mean Δ/σ	0.142, 0.026
Data-to-Parameter Ratio	8.0:1
Largest Difference Peak	0.96 $eÅ^{-3}$
Largest Difference Hole	-1.50 $eÅ^{-3}$

Table S2.

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
Cu(1)	1206(1)	3213(1)	39	30(1)
Cu(2)	-3761(1)	4791(1)	159(1)	32(1)
Cu(3)	2283(1)	6542(1)	61(1)	33(1)
Cl(9)	1195(4)	6573(1)	1315(2)	37(1)
Cl(10)	1221(4)	6588(1)	-1153(2)	45(1)
Cl(5)	-5926(3)	4143(1)	170(2)	34(1)
Cl(8)	-3505(4)	4694(1)	-1175(2)	41(1)
Cl(7)	-1753(3)	5454(1)	148(2)	39(1)
Cl(11)	3560(3)	7348(1)	93(2)	40(1)
Cl(6)	-3853(4)	4803(1)	1495(2)	53(1)
Cl(1)	-963(3)	3814(1)	266(2)	37(1)
Cl(2)	1159(4)	3391(1)	-1276(2)	45(1)
Cl(3)	3394(3)	2605(1)	-156(2)	42(1)
Cl(4)	1428(4)	3059(1)	1380(2)	43(1)
Cl(12)	3213(3)	5682(1)	97(2)	48(1)
N(1)	-964(14)	8225(4)	6229(6)	45(3)
C(1)	-1644(19)	8359(6)	7000(8)	57(5)
C(2)	-354(16)	8362(5)	7645(6)	37(4)
C(3)	235(16)	8866(5)	7963(7)	48(4)
C(4)	1324(16)	8845(5)	8590(8)	49(4)
C(5)	1837(17)	8395(5)	8915(8)	45(4)
N(2)	1271(13)	7922(4)	8619(6)	46(4)
C(6)	184(15)	7904(4)	7994(7)	41(4)
N(3)	1125(14)	1603(4)	8961(6)	43(3)
C(7)	1708(18)	1844(6)	8206(7)	51(4)
C(8)	360(16)	1752(4)	7549(6)	32(3)
C(9)	-368(15)	2187(5)	7169(7)	40(4)
C(10)	-1419(14)	2108(4)	6566(6)	35(4)
C(11)	-1810(19)	1634(6)	6313(8)	52(5)
N(4)	-1110(13)	1162(4)	6675(6)	52(4)
C(12)	-45(15)	1235(4)	7297(6)	33(3)
N(5)	5958(11)	277(3)	9216(5)	39(3)
C(13)	6781(18)	126(7)	8476(7)	60(5)
C(15)	5576(11)	28(4)	7827(6)	34(3)
C(18)	4941(18)	-478(4)	7667(8)	50(4)
C(17)	3873(18)	-557(5)	7014(9)	62(5)
C(16)	3375(18)	-149(6)	6571(8)	62(5)
N(6)	3978(12)	340(3)	6753(6)	46(3)
C(14)	5018(16)	440(5)	7330(6)	37(3)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table S3.

Table 2. Bond lengths (Å)

Cu(1)-Cl(1)	2.285 (3)	Cu(1)-Cl(2)	2.283 (3)
Cu(1)-Cl(3)	2.300 (3)	Cu(1)-Cl(4)	2.325 (3)
Cu(2)-Cl(5)	2.330 (2)	Cu(2)-Cl(8)	2.294 (4)
Cu(2)-Cl(7)	2.271 (2)	Cu(2)-Cl(6)	2.278 (4)
Cu(3)-Cl(9)	2.298 (4)	Cu(3)-Cl(10)	2.230 (4)
Cu(3)-Cl(11)	2.245 (2)	Cu(3)-Cl(12)	2.264 (2)
N(1)-C(1)	1.454 (17)	C(1)-C(2)	1.485 (18)
C(2)-C(3)	1.443 (18)	C(2)-C(6)	1.356 (16)
C(3)-C(4)	1.363 (18)	C(4)-C(5)	1.314 (18)
C(5)-N(2)	1.356 (16)	N(2)-C(6)	1.358 (15)
N(3)-C(7)	1.490 (16)	C(7)-C(8)	1.548 (17)
C(8)-C(9)	1.386 (16)	C(8)-C(12)	1.396 (15)
C(9)-C(10)	1.327 (16)	C(10)-C(11)	1.295 (18)
C(11)-N(4)	1.435 (18)	N(4)-C(12)	1.356 (15)
N(5)-C(13)	1.463 (16)	C(13)-C(15)	1.467 (16)
C(15)-C(18)	1.383 (16)	C(15)-C(14)	1.400 (15)
C(18)-C(17)	1.402 (20)	C(17)-C(16)	1.324 (20)
C(16)-N(6)	1.345 (18)	N(6)-C(14)	1.295 (15)

Table S4.

Table 3. Bond angles (°)

Cl(1)-Cu(1)-Cl(2)	91.5(1)	Cl(1)-Cu(1)-Cl(3)	178.5(1)
Cl(2)-Cu(1)-Cl(3)	90.0(1)	Cl(1)-Cu(1)-Cl(4)	89.8(1)
Cl(2)-Cu(1)-Cl(4)	176.3(1)	Cl(3)-Cu(1)-Cl(4)	88.7(1)
Cl(5)-Cu(2)-Cl(8)	89.8(1)	Cl(5)-Cu(2)-Cl(7)	177.2(1)
Cl(8)-Cu(2)-Cl(7)	90.6(1)	Cl(5)-Cu(2)-Cl(6)	88.7(1)
Cl(8)-Cu(2)-Cl(6)	173.7(1)	Cl(7)-Cu(2)-Cl(6)	91.2(1)
Cl(9)-Cu(3)-Cl(10)	136.5(1)	Cl(9)-Cu(3)-Cl(11)	96.2(1)
Cl(10)-Cu(3)-Cl(11)	98.0(1)	Cl(9)-Cu(3)-Cl(12)	97.1(1)
Cl(10)-Cu(3)-Cl(12)	101.0(1)	Cl(11)-Cu(3)-Cl(12)	135.2(1)
N(1)-C(1)-C(2)	115.2(12)	C(1)-C(2)-C(3)	119.7(11)
C(1)-C(2)-C(6)	121.8(11)	C(3)-C(2)-C(6)	118.2(11)
C(2)-C(3)-C(4)	117.2(12)	C(3)-C(4)-C(5)	123.4(13)
C(4)-C(5)-N(2)	119.3(12)	C(5)-N(2)-C(6)	121.4(10)
C(2)-C(6)-N(2)	120.4(10)	N(3)-C(7)-C(8)	111.0(10)
C(7)-C(8)-C(9)	119.7(10)	C(7)-C(8)-C(12)	120.8(10)
C(9)-C(8)-C(12)	119.3(10)	C(8)-C(9)-C(10)	119.6(11)
C(9)-C(10)-C(11)	122.6(11)	C(10)-C(11)-N(4)	121.2(12)
C(11)-N(4)-C(12)	117.2(11)	C(8)-C(12)-N(4)	120.1(10)
N(5)-C(13)-C(15)	114.5(10)	C(13)-C(15)-C(18)	121.8(11)
C(13)-C(15)-C(14)	122.0(11)	C(18)-C(15)-C(14)	116.2(10)
C(15)-C(18)-C(17)	119.6(11)	C(18)-C(17)-C(16)	121.2(12)
C(17)-C(16)-N(6)	117.7(13)	C(16)-N(6)-C(14)	124.5(11)
C(15)-C(14)-N(6)	120.7(10)		

Table S5.

Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu(1)	34(1)	23(1)	33(1)	6(1)	-1(1)	2(1)
Cu(2)	35(1)	28(1)	32(1)	-8(1)	-4(1)	0(1)
Cu(3)	40(1)	23(1)	36(1)	-1(1)	-1(1)	-3(1)
Cl(9)	48(2)	26(1)	38(1)	1(1)	3(1)	1(1)
Cl(10)	57(2)	39(2)	38(2)	-6(1)	0(1)	-7(1)
Cl(5)	32(1)	25(1)	45(1)	-1(1)	0(1)	-2(1)
Cl(8)	51(2)	37(1)	34(1)	-10(1)	0(1)	-3(1)
Cl(7)	37(1)	31(1)	48(1)	-7(1)	1(1)	-6(1)
Cl(11)	41(1)	32(1)	48(1)	-10(1)	0(1)	-2(1)
Cl(6)	65(2)	61(2)	34(1)	-22(2)	-15(1)	11(1)
Cl(1)	37(1)	26(1)	49(2)	5(1)	5(1)	3(1)
Cl(2)	60(2)	41(1)	34(1)	2(1)	1(1)	0(1)
Cl(3)	39(1)	30(1)	59(2)	11(1)	-3(1)	-7(1)
Cl(4)	62(2)	27(1)	38(1)	3(1)	-7(1)	2(1)
Cl(12)	50(1)	29(1)	66(2)	7(1)	1(2)	-6(2)
N(1)	56(6)	46(6)	34(5)	5(5)	-15(5)	8(5)
C(1)	42(7)	83(10)	45(7)	-9(7)	1(6)	-21(7)
C(2)	36(6)	49(7)	28(6)	8(5)	5(5)	3(5)
C(3)	51(7)	46(7)	46(7)	-5(6)	0(6)	3(6)
C(4)	61(8)	42(7)	45(7)	-4(7)	-10(6)	-1(6)
C(5)	42(7)	56(8)	37(6)	-5(6)	-2(6)	2(6)
N(2)	60(7)	37(6)	43(6)	0(5)	-8(5)	13(5)
C(6)	47(7)	31(6)	44(7)	10(5)	0(5)	-12(5)
N(3)	58(6)	35(5)	37(5)	2(4)	-7(5)	2(4)
C(7)	47(7)	78(10)	29(6)	-21(7)	-5(6)	7(6)
C(8)	43(7)	26(6)	25(5)	-7(4)	-3(5)	5(4)
C(9)	45(6)	27(5)	48(7)	3(5)	14(5)	-4(5)
C(10)	42(6)	30(6)	34(6)	11(5)	-7(5)	12(5)
C(11)	46(7)	76(11)	33(7)	2(7)	-11(6)	11(7)
N(4)	57(7)	45(7)	54(6)	-8(6)	7(5)	-2(5)
C(12)	41(6)	24(5)	36(6)	-2(5)	-6(5)	2(4)
N(5)	53(5)	30(4)	34(5)	-11(4)	-10(4)	1(4)
C(13)	53(8)	88(12)	40(7)	30(8)	-13(6)	5(7)
C(15)	26(5)	39(6)	36(5)	2(5)	4(4)	-2(5)
C(18)	65(8)	20(6)	65(9)	8(6)	21(7)	13(6)
C(17)	77(9)	29(6)	79(10)	-25(6)	16(8)	-13(7)
C(16)	62(8)	81(12)	44(8)	-38(8)	5(7)	-19(7)
N(6)	64(6)	26(5)	47(6)	-3(4)	-1(5)	12(4)
C(14)	52(7)	32(6)	25(5)	1(6)	2(5)	0(4)

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table S6.

Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(1A)	-1875	8230	5847	80
H(1B)	-452	7875	6245	80
H(1C)	-103	8484	6089	80
H(1D)	-2163	8708	6971	80
H(1E)	-2511	8098	7127	80
H(3)	-297	9139	7649	80
H(4A)	1543	9217	8693	80
H(5)	2580	8299	9343	80
H(2)	1459	7552	8742	80
H(6A)	-387	7627	7701	80
H(3A)	1975	1659	9362	80
H(3B)	953	1226	8885	80
H(3C)	56	1766	9116	80
H(7A)	1880	2222	8282	80
H(7B)	2777	1681	8051	80
H(9)	62	2494	7447	80
H(10)	-1737	2463	6409	80
H(11)	-2517	1494	5898	80
H(4)	-1196	782	6598	80
H(12)	562	994	7638	80
H(5A)	6800	353	9614	80
H(5B)	5265	-23	9377	80
H(5C)	5233	584	9140	80
H(13A)	7476	426	8320	80
H(13B)	7508	-180	8557	80
H(18)	5069	-822	7912	80
H(17)	3648	-935	7007	80
H(16)	2611	-296	6182	80
H(6)	3827	691	6532	80
H(14)	5592	749	7539	80

STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_6 H_{10} Br_4 Cu N_2$
Color; Habit	Dark Brown, rectangular
Crystal size (mm)	0.23 x 0.30 x 0.25
Crystal System	Orthorhombic
Space Group	Pna2(1)
Unit Cell Dimensions	a = 8.133(2) Å
	b = 26.129(5) Å
	c = 17.148(3) Å
Volume	3644(2) $Å^3$
Z	12
Formula weight	493.3
Density(calc.)	2.698 Mg/m^3
Absorption Coefficient	17.638 mm^{-1}
F(000)	2748

Table S7.

Data Collection

Diffractometer Used	Siemens R3m/V
Radiation	CuKα (λ = 1.54180 Å)
Temperature (K)	294
Monochromator	Highly oriented graphite crystal
2θ Range	3.50 to 113.5°
Scan Type	ω
Scan Speed	Variable; 2.00 to 29.30°/min. in ω
Scan Range (ω)	0.9°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 50% of total scan time
Standard Reflections	3 measured every 100 reflections
Index Ranges	$-1 \leq h \leq 8$, $-28 \leq k \leq 1$ $-1 \leq l \leq 18$
Reflections Collected	3333
Independent Reflections	2728 (R_{int} = 3.48%)
Observed Reflections	2575 ($F > 3.0\sigma(F)$)
Absorption Correction	Empirical;Tmax/Tmin=0.986/0.349

Table S7.

Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\Sigma w(F_o-F_c)^2$
Absolute Structure	η = 0.0(2)
Extinction Correction	χ = 0.00127(9), where $F^* = F\,[\,1 + 0.002\chi F^2/\sin(2\theta)\,]^{-1/4}$
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0069F^2$
Number of Parameters Refined	353
Final R Indices (obs. data)	R = 4.47 %, wR = 6.00 %
R Indices (all data)	R = 4.76 %, wR = 6.30 %
Goodness-of-Fit	0.68
Largest and Mean Δ/σ	.0.003, 0.001
Data-to-Parameter Ratio	7.3:1
Largest Difference Peak	1.32 eÅ^{-3}
Largest Difference Hole	-1.53 eÅ^{-3}

Table S8.

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
Cu(1)	1147(2)	3223(1)	38	26(1)
Cu(2)	-3785(2)	4814(1)	149(2)	28(1)
Cu(3)	2275(3)	6549(1)	52(2)	28(1)
Br(9)	1143(2)	6573(1)	1348(2)	33(1)
Br(10)	1157(2)	6604(1)	-1231(2)	36(1)
Br(5)	-5957(2)	4141(1)	172(2)	29(1)
Br(6)	-3580(2)	4718(1)	-1271(2)	36(1)
Br(7)	-1706(2)	5474(1)	115(2)	32(1)
Br(11)	3635(2)	7352(1)	82(2)	34(1)
Br(8)	-3918(2)	4854(1)	1547(2)	44(1)
Br(1)	-1023(2)	3841(1)	278(2)	32(1)
Br(2)	1066(2)	3401(1)	-1363(2)	39(1)
Br(3)	3326(2)	2600(1)	-184(2)	37(1)
Br(4)	1370(2)	3072(1)	1449(2)	40(1)
Br(12)	3247(2)	5683(1)	52(2)	39(1)
N(1)	-959(18)	8214(6)	6252(9)	52(6)
C(1)	-1575(23)	8373(8)	6960(12)	55(7)
C(2)	-281(19)	8383(5)	7622(8)	26(5)
C(3)	268(22)	8826(6)	7920(10)	41(6)
C(4)	1351(21)	8834(5)	8549(10)	41(6)
C(5)	1857(21)	8387(6)	8879(10)	40(6)
N(2)	1336(19)	7939(6)	8572(10)	54(6)
C(6)	268(22)	7934(6)	7965(10)	45(6)
N(3)	1057(21)	1593(5)	8925(8)	55(6)
C(7)	1598(27)	1812(8)	8178(10)	60(7)
C(8)	287(21)	1756(6)	7535(8)	34(5)
C(9)	-393(19)	2161(5)	7204(9)	34(5)
C(10)	-1431(18)	2101(5)	6600(9)	26(5)
C(11)	-1810(19)	1653(6)	6317(10)	38(6)
N(4)	-1162(20)	1230(7)	6638(9)	59(6)
C(12)	-52(20)	1280(6)	7256(9)	38(5)
N(5)	5925(14)	287(5)	9159(7)	33(4)
C(13)	6753(23)	140(9)	8411(10)	58(8)
C(15)	5558(15)	43(6)	7794(9)	29(5)
C(18)	4935(30)	-452(6)	7638(12)	64(8)
C(17)	3848(23)	-531(7)	6997(14)	57(8)
C(16)	3423(21)	-126(8)	6572(11)	47(7)
N(6)	3958(12)	321(5)	6731(8)	31(4)
C(14)	5031(22)	419(5)	7321(9)	36(5)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Table S9.

Table 2. Bond lengths (Å)

Cu(1)-Br(1)	2.427 (3)	Cu(1)-Br(2)	2.448 (3)
Cu(1)-Br(3)	2.436 (3)	Cu(1)-Br(4)	2.458 (3)
Cu(2)-Br(5)	2.492 (3)	Cu(2)-Br(6)	2.454 (4)
Cu(2)-Br(7)	2.416 (3)	Cu(2)-Br(8)	2.402 (4)
Cu(3)-Br(9)	2.407 (4)	Cu(3)-Br(10)	2.386 (4)
Cu(3)-Br(11)	2.371 (2)	Cu(3)-Br(12)	2.397 (2)
N(1)-C(1)	1.377 (26)	C(1)-C(2)	1.548 (25)
C(2)-C(3)	1.343 (21)	C(2)-C(6)	1.384 (21)
C(3)-C(4)	1.393 (24)	C(4)-C(5)	1.363 (22)
C(5)-N(2)	1.351 (22)	N(2)-C(6)	1.355 (24)
N(3)-C(7)	1.471 (24)	C(7)-C(8)	1.541 (25)
C(8)-C(9)	1.323 (22)	C(8)-C(12)	1.361 (22)
C(9)-C(10)	1.346 (22)	C(10)-C(11)	1.304 (21)
C(11)-N(4)	1.344 (24)	N(4)-C(12)	1.398 (22)
N(5)-C(13)	1.499 (22)	C(13)-C(15)	1.459 (23)
C(15)-C(18)	1.414 (23)	C(15)-C(14)	1.345 (21)
C(18)-C(17)	1.425 (31)	C(17)-C(16)	1.331 (28)
C(16)-N(6)	1.277 (24)	N(6)-C(14)	1.359 (20)

Table S10.

Table 3. Bond angles (°)

Br(1)-Cu(1)-Br(2)	91.2(1)	Br(1)-Cu(1)-Br(3)	179.2(1)
Br(2)-Cu(1)-Br(3)	89.6(1)	Br(1)-Cu(1)-Br(4)	89.6(1)
Br(2)-Cu(1)-Br(4)	176.8(1)	Br(3)-Cu(1)-Br(4)	89.6(1)
Br(5)-Cu(2)-Br(6)	89.5(1)	Br(5)-Cu(2)-Br(7)	179.1(1)
Br(6)-Cu(2)-Br(7)	90.1(1)	Br(5)-Cu(2)-Br(8)	89.0(1)
Br(6)-Cu(2)-Br(8)	176.4(1)	Br(7)-Cu(2)-Br(8)	91.4(1)
Br(9)-Cu(3)-Br(10)	134.8(1)	Br(9)-Cu(3)-Br(11)	97.8(1)
Br(10)-Cu(3)-Br(11)	98.3(1)	Br(9)-Cu(3)-Br(12)	98.7(1)
Br(10)-Cu(3)-Br(12)	100.5(1)	Br(11)-Cu(3)-Br(12)	132.9(1)
N(1)-C(1)-C(2)	113.8(15)	C(1)-C(2)-C(3)	121.3(14)
C(1)-C(2)-C(6)	121.1(14)	C(3)-C(2)-C(6)	117.4(14)
C(2)-C(3)-C(4)	121.2(14)	C(3)-C(4)-C(5)	119.9(14)
C(4)-C(5)-N(2)	119.1(16)	C(5)-N(2)-C(6)	120.6(15)
C(2)-C(6)-N(2)	121.7(15)	N(3)-C(7)-C(8)	112.3(16)
C(7)-C(8)-C(9)	121.3(16)	C(7)-C(8)-C(12)	118.6(15)
C(9)-C(8)-C(12)	119.8(15)	C(8)-C(9)-C(10)	120.0(14)
C(9)-C(10)-C(11)	122.6(14)	C(10)-C(11)-N(4)	119.6(15)
C(11)-N(4)-C(12)	119.1(15)	C(8)-C(12)-N(4)	118.8(15)
N(5)-C(13)-C(15)	111.5(14)	C(13)-C(15)-C(18)	122.3(17)
C(13)-C(15)-C(14)	121.5(16)	C(18)-C(15)-C(14)	116.1(15)
C(15)-C(18)-C(17)	120.0(16)	C(18)-C(17)-C(16)	118.0(17)
C(17)-C(16)-N(6)	121.4(17)	C(16)-N(6)-C(14)	123.4(14)
C(15)-C(14)-N(6)	121.1(14)		

Table S11.

Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu(1)	32(1)	28(1)	20(1)	7(1)	-2(1)	1(1)
Cu(2)	37(1)	31(1)	16(1)	-9(1)	-2(1)	1(1)
Cu(3)	42(1)	23(1)	20(1)	-2(1)	0(1)	-1(1)
Br(9)	47(1)	26(1)	26(1)	2(1)	6(1)	1(1)
Br(10)	46(1)	38(1)	24(1)	-4(1)	-4(1)	-7(1)
Br(5)	30(1)	25(1)	33(1)	-3(1)	0(1)	-2(1)
Br(6)	48(1)	40(1)	19(1)	-11(1)	2(1)	-4(1)
Br(7)	30(1)	33(1)	34(1)	-8(1)	-1(1)	-3(1)
Br(11)	36(1)	32(1)	35(1)	-10(1)	2(1)	-5(1)
Br(8)	60(1)	53(1)	19(1)	-19(1)	-10(1)	9(1)
Br(1)	32(1)	33(1)	32(1)	6(1)	4(1)	1(1)
Br(2)	55(1)	41(1)	22(1)	5(1)	-1(1)	0(1)
Br(3)	35(1)	30(1)	46(1)	9(1)	-5(1)	-5(1)
Br(4)	69(1)	32(1)	20(1)	2(1)	-6(1)	4(1)
Br(12)	43(1)	29(1)	46(1)	6(1)	3(1)	-5(1)
N(1)	79(12)	42(8)	34(9)	0(8)	-11(8)	16(7)
C(1)	32(10)	88(16)	44(11)	6(10)	-10(9)	-26(11)
C(2)	21(8)	37(8)	19(8)	1(6)	-4(6)	-4(6)
C(3)	61(11)	29(8)	34(9)	-15(8)	-5(8)	9(7)
C(4)	71(12)	12(7)	40(10)	-15(7)	-17(9)	0(7)
C(5)	40(10)	54(12)	25(9)	-6(8)	8(8)	-2(8)
N(2)	67(11)	54(10)	42(9)	9(8)	4(8)	2(8)
C(6)	55(12)	42(10)	38(11)	3(9)	-3(9)	3(8)
N(3)	106(14)	42(9)	16(8)	-15(7)	12(8)	3(6)
C(7)	78(14)	81(15)	20(9)	-18(12)	0(9)	21(10)
C(8)	40(10)	47(9)	16(8)	-9(8)	1(7)	14(7)
C(9)	27(9)	26(8)	50(11)	-11(7)	19(8)	-4(7)
C(10)	35(9)	16(7)	28(8)	1(6)	-3(7)	8(7)
C(11)	29(9)	62(11)	22(8)	-17(8)	-12(7)	27(8)
N(4)	81(12)	72(12)	24(8)	-40(10)	4(8)	-1(8)
C(12)	25(8)	32(9)	55(11)	-1(7)	-10(8)	4(7)
N(5)	35(7)	49(8)	15(6)	2(6)	1(5)	3(6)
C(13)	51(12)	104(17)	19(10)	18(11)	9(8)	3(10)
C(15)	7(7)	58(10)	22(7)	2(7)	-1(6)	-9(8)
C(18)	109(18)	21(8)	63(14)	18(10)	29(13)	31(9)
C(17)	52(12)	35(10)	85(17)	-12(9)	18(12)	-15(11)
C(16)	38(10)	72(14)	29(10)	-10(10)	-15(8)	8(10)
N(6)	13(6)	46(8)	34(8)	-7(5)	-13(5)	13(6)
C(14)	56(11)	21(7)	31(9)	-1(7)	7(8)	2(6)

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Table S12.

Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(1A)	-1758	8204	5889	80
H(1B)	-183	8440	6105	80
H(1C)	-504	7902	6301	80
H(1D)	-2415	8134	7111	80
H(1E)	-2076	8704	6904	80
H(3D)	-81	9144	7692	80
H(4A)	1717	9155	8760	80
H(5D)	2598	8394	9315	80
H(2A)	1717	7643	8770	80
H(6A)	-170	7616	7780	80
H(3A)	1860	1631	9281	80
H(3B)	146	1757	9088	80
H(3C)	835	1258	8864	80
H(7A)	2582	1641	8011	80
H(7B)	1854	2168	8247	80
H(9A)	-116	2498	7386	80
H(10A)	-1943	2400	6382	80
H(11A)	-2547	1628	5881	80
H(4B)	-1411	918	6447	80
H(12A)	435	984	7495	80
H(5A)	6671	357	9531	80
H(5B)	5286	563	9079	80
H(5C)	5295	22	9313	80
H(13A)	7444	-153	8496	80
H(13B)	7435	420	8247	80
H(15A)	5315	-733	7950	80
H(16A)	3398	-865	6902	80
H(17A)	2709	-175	6132	80
H(6B)	3616	586	6438	80
H(18A)	5412	762	7410	80

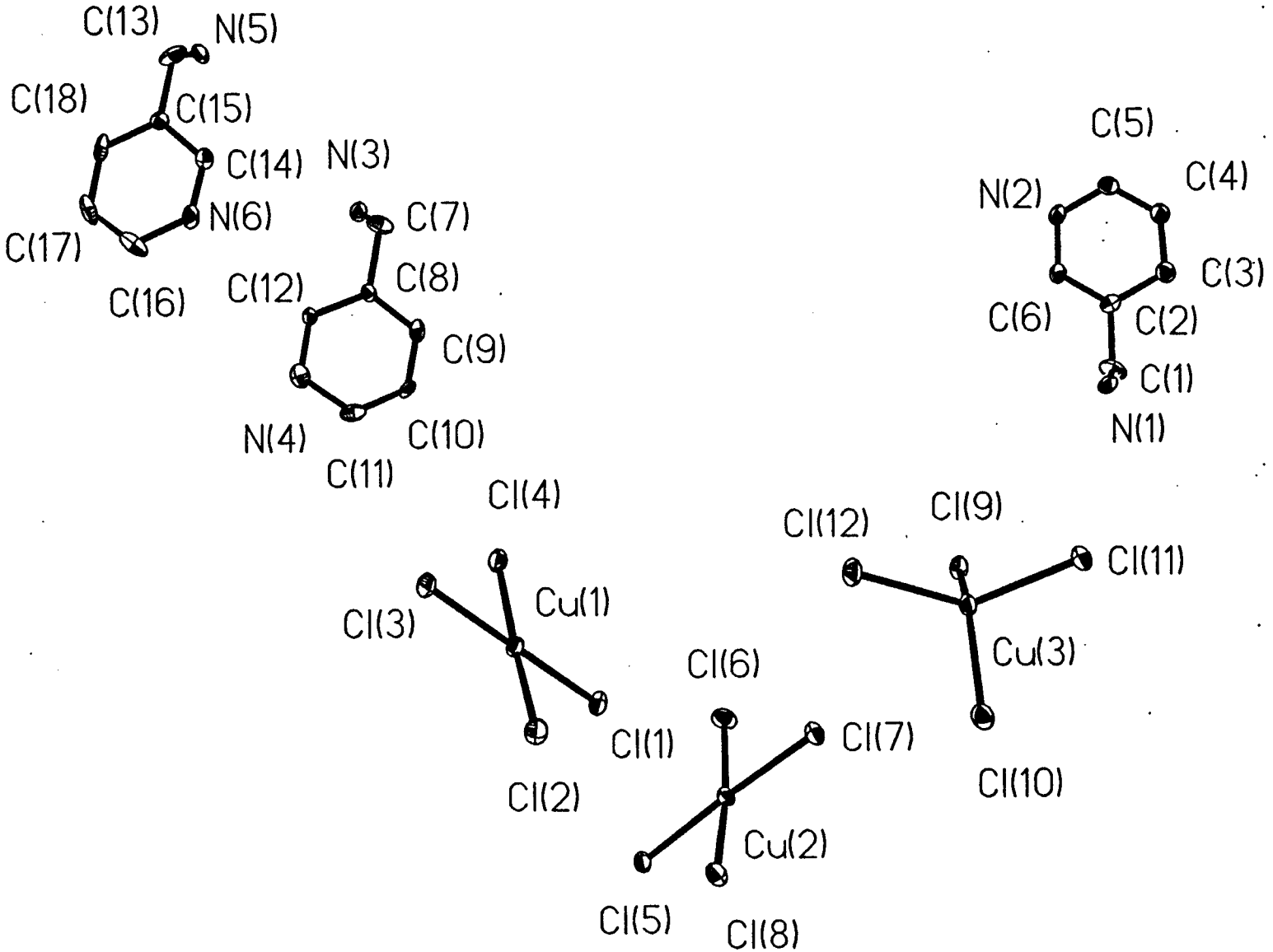

Figure S1. Illustration of the Asymmetric Unit Cell (The *a* axis is vertical and the *b* axis is horizontal)