Table 1. Crystal data and structure refinement for **cr10**

Compound	**cr10**
Formula	$C_{25}H_{36}ClCu_2N_5O_{10}$
Formula weight	729.12
Crystal size (mm^3)	0.52 x 0.40 x 0.36
Crystal color	Blue
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 16.738(1) Å
	b = 13.286(1) Å
	c = 14.082(1) Å
	β = 104.88(1)^o
Volume ($Å^3$)	3026.5(2)
Z	4
Calculated density ($g \cdot cm^{-3}$)	1.600
F(000)	1504
Temperature (K)	293(2)
Wavelength (Å)	0.71073
Absorption coefficient (mm^{-1})	1.556
θ for data collection (^{o})	1.98 to 25.04
Limiting indices	$-19 \leq h \leq 18$, $-7 \leq k \leq 15$, $-13 \leq l \leq 16$
Reflections collected	9793
Unique reflections (R(int))	5279 [R(int) = 0.0210]
Refinement method	Full-matrix least-squares on F^2
Absorption correction	SADABS
Data / restraints / parameters	5279 / 0 / 389
Goodness-of-fit on F^2	1.080
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0512, wR2 = 0.1247
R indices (all data)	R1 = 0.0664, wR2 = 0.1377
Largest diff. peak and hole ($e \cdot Å^3$)	0.804 and -0.489

$R1 = \sum(|F_o| - |F_c|) / \sum|F_o|$, $wR2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{0.5}$.

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **cr10**.

Atom	x	y	z	U(eq)
Cu(1)	6966(1)	5716(1)	121(1)	37(1)
Cu(2)	7659(1)	4024(1)	1790(1)	34(1)
Cl(1)	11361(1)	1555(2)	-1195(1)	81(1)
O(1)	6117(2)	2160(3)	-675(2)	57(1)
O(2)	8746(2)	3135(3)	1373(3)	53(1)
O(3)	6882(2)	3179(2)	864(2)	44(1)
O(4)	6267(2)	4362(3)	-760(3)	54(1)
O(5)	7887(2)	4773(2)	665(2)	36(1)
O(6)	11861(8)	2288(15)	-1203(10)	373(12)
O(7)	10836(5)	1643(8)	-2124(5)	190(4)
O(8)	10932(7)	1686(9)	-548(6)	234(6)
O(9)	11815(10)	773(9)	-933(13)	315(9)
O(10)	5539(3)	5739(4)	2140(3)	80(1)
N(1)	6560(3)	5456(3)	1285(3)	47(1)
N(2)	6083(2)	6800(3)	-483(3)	48(1)
N(3)	8459(2)	4885(3)	2863(3)	44(1)
N(4)	7550(2)	3216(3)	2892(3)	41(1)
N(5)	7508(3)	6167(3)	-863(3)	45(1)
C(1)	6292(3)	1649(4)	204(4)	45(1)
C(2)	7282(3)	2305(4)	2847(3)	46(1)
C(3)	7943(3)	3658(4)	3860(4)	54(1)
C(4)	9652(3)	3705(5)	-684(4)	59(2)

Atom	x	y	z	U(eq)
C(5)	9195(3)	4523(4)	-1063(4)	54(1)
C(6)	7116(4)	7049(5)	-1405(5)	72(2)
C(7)	6709(3)	2242(3)	1016(3)	38(1)
C(8)	6059(3)	5602(4)	1704(4)	47(1)
C(9)	9517(3)	3220(4)	132(4)	52(1)
C(10)	6681(4)	763(4)	2045(4)	59(2)
C(11)	6895(3)	1776(3)	1956(4)	42(1)
C(12)	8581(3)	4906(4)	-637(3)	42(1)
C(13)	5642(4)	1660(5)	-1523(4)	71(2)
C(14)	8441(3)	4426(3)	203(3)	36(1)
C(15)	8131(3)	5763(4)	-1087(4)	49(1)
C(16)	6299(4)	213(4)	1232(5)	70(2)
C(17)	8918(3)	3570(4)	569(3)	42(1)
C(18)	6238(4)	7001(5)	-1472(5)	77(2)
C(19)	8703(4)	4198(5)	3732(4)	68(2)
C(20)	8081(5)	5798(5)	3111(5)	86(2)
C(22)	6099(4)	660(4)	304(5)	59(1)
C(23)	9096(4)	2181(4)	1696(5)	69(2)

C(24)	9233(4)	5164(6)	2611(5)	86(2)
C(25)	6163(5)	7686(5)	148(6)	90(2)
C(26)	5231(3)	6430(5)	-682(5)	69(2)

Table 3. Selected bond lengths [Å] for **cr10**.

Bond	distances
Cu(1)-N(5)	1.936(4)
Cu(1)-N(1)	1.959(4)
Cu(1)-O(5)	1.982(3)
Cu(1)-N(2)	2.082(4)
Cu(1)-O(4)	2.324(3)
Cu(1)-Cu(2)	1.934(4)
Cu(2)-O(3)	1.944(3)
Cu(2)-O(5)	1.989(3)
Cu(2)-N(3)	2.085(4)
Cu(2)-O(2)	2.367(3)
Cl(1)-O(9)	1.284(9)
Cl(1)-O(6)	1.287(12)
Cl(1)-O(8)	1.308(8)
Cl(1)-O(7)	1.381(7)
O(1)-C(1)	1.376(6)
O(1)-C(13)	1.419(6)

Bond	distances

O(2)-C(17)	1.366(6)
O(2)-C(23)	1.422(6)
O(3)-C(7)	1.308(5)
O(5)-C(14)	1.202(6)
N(1)-C(8)	1.459(7)
N(2)-C(26)	1.466(7)
N(2)-C(18)	1.505(7)
N(3)-C(20)	1.451(7)
N(3)-C(24)	1.476(7)
N(3)-C(19)	1.497(7)
N(4)-C(2)	1.287(6)
N(4)-C(3)	1.474(6)
N(5)-C(15)	1.282(6)
N(5)-C(6)	1.459(7)

Bond	distances
C(1)-C(22)	1.370(7)
C(1)-C(7)	1.416(7)
C(2)-C(11)	1.438(7)
C(3)-C(19)	1.511(8)
C(4)-C(5)	1.358(8)
C(4)-C(9)	1.385(8)
C(5)-C(12)	1.412(7)
C(6)-C(18)	1.449(9)
C(7)-C(11)	1.423(6)
C(9)-C(17)	1.383(7)
C(10)-C(16)	1.370(8)
C(10)-C(11)	1.407(7)
C(12)-C(14)	1.415(6)
C(12)-C(15)	1.421(7)
C(14)-C(17)	1.409(7)
C(16)-C(22)	1.395(8)

Table 4. Selected angles [º] for **cr10**

Atom1-atom2-atom3	angles
N(5)-Cu(1)-N(1)	168.62(18)
N(5)-Cu(1)-O(5)	90.65(15)
N(1)-Cu(1)-O(5)	88.16(15)
N(5)-Cu(1)-N(2)	84.68(17)
N(1)-Cu(1)-N(2)	95.82(17)
O(5)-Cu(1)-N(2)	174.42(14)
N(5)-Cu(1)-O(4)	96.94(16)

N(1)-Cu(1)-O(4)	94.31(16)
O(5)-Cu(1)-O(4)	87.25(13)
N(2)-Cu(1)-O(4)	96.33(15)
N(5)-Cu(1)-Cu(2)	125.94(12)
N(1)-Cu(1)-Cu(2)	53.72(12)
O(5)-Cu(1)-Cu(2)	35.29(8)
N(2)-Cu(1)-Cu(2)	149.27(12)
O(4)-Cu(1)-Cu(2)	83.56(9)
N(4)-Cu(2)-O(3)	91.91(15)
N(4)-Cu(2)-O(5)	173.64(14)
O(3)-Cu(2)-O(5)	89.25(13)
N(4)-Cu(2)-N(3)	84.14(16)
O(3)-Cu(2)-N(3)	175.86(15)
O(5)-Cu(2)-N(3)	94.81(14)
N(4)-Cu(2)-O(2)	99.15(14)
O(3)-Cu(2)-O(2)	88.31(14)
O(5)-Cu(2)-O(2)	74.63(12)
N(3)-Cu(2)-O(2)	93.52(15)
N(4)-Cu(2)-Cu(1)	151.21(12)
O(3)-Cu(2)-Cu(1)	82.01(9)
O(5)-Cu(2)-Cu(1)	35.15(8)
N(3)-Cu(2)-Cu(1)	100.88(11)
O(2)-Cu(2)-Cu(1)	108.71(8)
O(9)-Cl(1)-O(6)	106.0(11)
O(9)-Cl(1)-O(8)	107.4(8)

Atom1-atom2-atom3	angles
O(6)-Cl(1)-O(8)	112.3(11)
O(9)-Cl(1)-O(7)	121.7(9)
O(6)-Cl(1)-O(7)	100.6(7)
O(8)-Cl(1)-O(7)	108.6(6)
C(1)-O(1)-C(13)	118.1(4)
C(17)-O(2)-C(23)	119.0(4)
C(17)-O(2)-Cu(2)	109.5(3)
C(23)-O(2)-Cu(2)	130.2(3)
C(7)-O(3)-Cu(2)	125.3(3)
C(14)-O(5)-Cu(1)	126.5(3)
C(14)-O(5)-Cu(2)	120.8(3)
Cu(1)-O(5)-Cu(2)	109.56(13)
C(8)-N(1)-Cu(1)	148.0(4)
C(25)-N(2)-C(26)	108.6(5)
C(25)-N(2)-C(18)	114.2(5)
C(26)-N(2)-C(18)	105.8(5)
C(25)-N(2)-Cu(1)	111.4(4)
C(26)-N(2)-Cu(1)	113.6(3)
C(18)-N(2)-Cu(1)	103.2(3)
C(20)-N(3)-C(24)	108.2(5)
C(20)-N(3)-C(19)	110.9(5)
C(24)-N(3)-C(19)	106.2(5)
C(20)-N(3)-Cu(2)	113.2(3)
C(24)-N(3)-Cu(2)	113.8(4)
C(19)-N(3)-Cu(2)	104.3(3)

C(2)-N(4)-C(3)	119.2(4)
C(2)-N(4)-Cu(2)	125.8(3)
C(3)-N(4)-Cu(2)	114.2(3)
C(15)-N(5)-C(6)	119.5(4)
C(15)-N(5)-Cu(1)	127.4(3)
C(6)-N(5)-Cu(1)	113.1(4)
C(22)-C(1)-O(1)	124.4(5)

Atom1-atom2-atom3	angles
C(22)-C(1)-C(7)	122.2(5)
O(1)-C(1)-C(7)	113.5(4)
N(4)-C(2)-C(11)	125.2(4)
N(4)-C(3)-C(19)	105.5(4)
C(5)-C(4)-C(9)	120.2(5)
C(4)-C(5)-C(12)	121.3(5)
C(18)-C(6)-N(5)	108.1(5)
O(3)-C(7)-C(1)	118.9(4)
O(3)-C(7)-C(11)	124.2(4)
C(1)-C(7)-C(11)	116.9(4)
N(1)-C(8)-O(10)	179.0(6)
C(17)-C(9)-C(4)	120.2(5)
C(16)-C(10)-C(11)	120.7(5)
C(10)-C(11)-C(7)	120.0(5)
C(10)-C(11)-C(2)	117.2(5)
C(7)-C(11)-C(2)	122.7(4)
C(5)-C(12)-C(14)	119.2(5)
C(5)-C(12)-C(15)	117.3(4)
C(14)-C(12)-C(15)	123.5(4)
O(5)-C(14)-C(17)	119.8(4)
O(5)-C(14)-C(12)	122.2(4)
C(17)-C(14)-C(12)	118.0(4)
N(5)-C(15)-C(12)	126.6(4)
C(10)-C(16)-C(22)	120.3(5)
O(2)-C(17)-C(9)	123.8(5)
O(2)-C(17)-C(14)	115.1(4)
C(9)-C(17)-C(14)	121.1(5)
C(6)-C(18)-N(2)	111.1(5)
N(3)-C(19)-C(3)	109.0(5)
C(1)-C(22)-C(16)	119.9(5)

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for **CR10**. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	38(1)	35(1)	37(1)	6(1)	10(1)	4(1)
Cu(2)	39(1)	34(1)	30(1)	1(1)	7(1)	-1(1)
Cl(1)	61(1)	110(1)	68(1)	-19(1)	11(1)	6(1)
O(1)	71(2)	53(2)	39(2)	-5(2)	1(2)	-11(2)
O(2)	59(2)	50(2)	54(2)	13(2)	23(2)	22(2)
O(3)	54(2)	34(2)	38(2)	4(1)	2(2)	-6(1)
O(4)	65(2)	41(2)	48(2)	3(2)	-1(2)	-2(2)
O(5)	38(2)	37(2)	35(2)	6(1)	12(1)	6(1)
O(6)	214(12)	510(30)	291(15)	212(17)	-118(11)	-211(15)
O(7)	165(7)	284(12)	95(5)	-24(6)	-17(5)	-47(8)
O(8)	282(12)	335(14)	110(6)	38(7)	92(7)	188(11)
O(9)	349(17)	197(11)	460(20)	92(12)	216(17)	188(12)
O(10)	73(3)	101(3)	83(3)	-18(3)	48(3)	-3(2)
N(1)	48(2)	52(3)	43(2)	7(2)	14(2)	3(2)
N(2)	45(2)	40(2)	58(3)	12(2)	10(2)	8(2)
N(3)	46(2)	40(2)	42(2)	-3(2)	6(2)	-2(2)
N(4)	45(2)	45(2)	31(2)	2(2)	6(2)	-2(2)
N(5)	52(2)	44(2)	42(2)	13(2)	16(2)	0(2)
C(1)	45(3)	39(3)	49(3)	-5(2)	11(2)	-2(2)
C(2)	55(3)	49(3)	37(3)	15(2)	15(2)	7(2)
C(3)	65(3)	60(3)	32(3)	0(2)	6(2)	-10(3)
C(4)	53(3)	70(4)	63(4)	-16(3)	29(3)	5(3)
C(5)	53(3)	70(4)	46(3)	-5(3)	24(2)	-2(3)
C(6)	84(4)	60(4)	81(4)	33(3)	35(4)	17(3)
C(7)	39(2)	29(2)	47(3)	3(2)	14(2)	3(2)
C(8)	50(3)	45(3)	45(3)	-3(2)	12(2)	-4(2)
C(9)	44(3)	54(3)	57(3)	-12(3)	14(2)	6(2)
C(10)	84(4)	40(3)	58(3)	11(3)	26(3)	-5(3)
C(11)	45(3)	38(2)	45(3)	4(2)	15(2)	1(2)
C(12)	41(2)	48(3)	39(2)	-3(2)	13(2)	-6(2)
C(13)	71(4)	82(4)	52(3)	-16(3)	2(3)	-24(3)
C(14)	30(2)	41(2)	35(2)	-5(2)	7(2)	-3(2)
C(15)	51(3)	57(3)	43(3)	9(2)	19(2)	-8(2)
C(16)	97(5)	33(3)	83(4)	2(3)	31(4)	-16(3)
C(17)	43(3)	45(3)	40(3)	-4(2)	12(2)	4(2)
C(18)	81(5)	76(4)	68(4)	29(3)	12(3)	16(4)
C(19)	73(4)	72(4)	47(3)	-5(3)	-5(3)	-3(3)
C(20)	95(5)	64(4)	79(5)	-29(3)	-12(4)	17(4)
C(22)	66(4)	45(3)	65(4)	-12(3)	19(3)	-12(3)

C(23)	87(4)	57(3)	65(4)	19(3)	23(3)	29(3)
C(24)	65(4)	101(5)	90(5)	-21(4)	19(4)	-29(4)
C(25)	86(5)	44(3)	118(6)	-25(4)	-12(4)	17(3)
C(26)	44(3)	70(4)	84(4)	1(3)	-1(3)	13(3)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **cr10**.

x	y	z	U(eq)
H(4A)	5833	4559	-1130	65
H(4B)	6495	3767	-668	65
H(2A)	7343	1961	3436	55
H(3A)	8094	3136	4355	64
H(3B)	7570	4126	4057	64
H(4A)	10057	3469	-972	71
H(5A)	9288	4838	-1615	65
H(6A)	7350	7658	-1066	87
H(6B)	7208	7056	-2057	87
H(9A)	9829	2658	387	62
H(10A)	6799	463	2663	71
H(13A)	5532	2115	-2072	107
H(13B)	5129	1439	-1408	107
H(13C)	5944	1089	-1665	107
H(15A)	8308	6063	-1594	59
H(16A)	6173	-461	1299	83

H(18A)	5989	6470	-1925	92
H(18B)	5981	7632	-1729	92
H(19A)	8952	4584	4318	81
H(19B)	9106	3712	3631	81
H(20A)	8472	6150	3622	129
H(20B)	7603	5627	3335	129
H(20C)	7920	6219	2541	129
H(22A)	5835	286	-246	70
H(23A)	9538	2040	1395	103
H(23B)	8679	1670	1514	103
H(23C)	9308	2188	2397	103
H(24A)	9572	5556	3134	128
H(24B)	9106	5552	2016	128
H(24C)	9525	4565	2519	128
H(25A)	5750	8172	-150	135
H(25B)	6703	7974	231	135
H(25C)	6090	7493	777	135
H(26A)	4856	6963	-962	104
H(26B)	5119	6210	-80	104
H(26C)	5159	5878	-1135	104

Table 7. Selected Hydrogen Bonds Lengths (Å)

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A
O4-H4A	0.820	2.404	151.45	3.148	O10 [-x+1, -y+1, -z]
O4-H4B	0.872	2.226	139.10	2.941	O1
O4-H4B	0.872	2.229	117.97	2.748	O3

Figure:

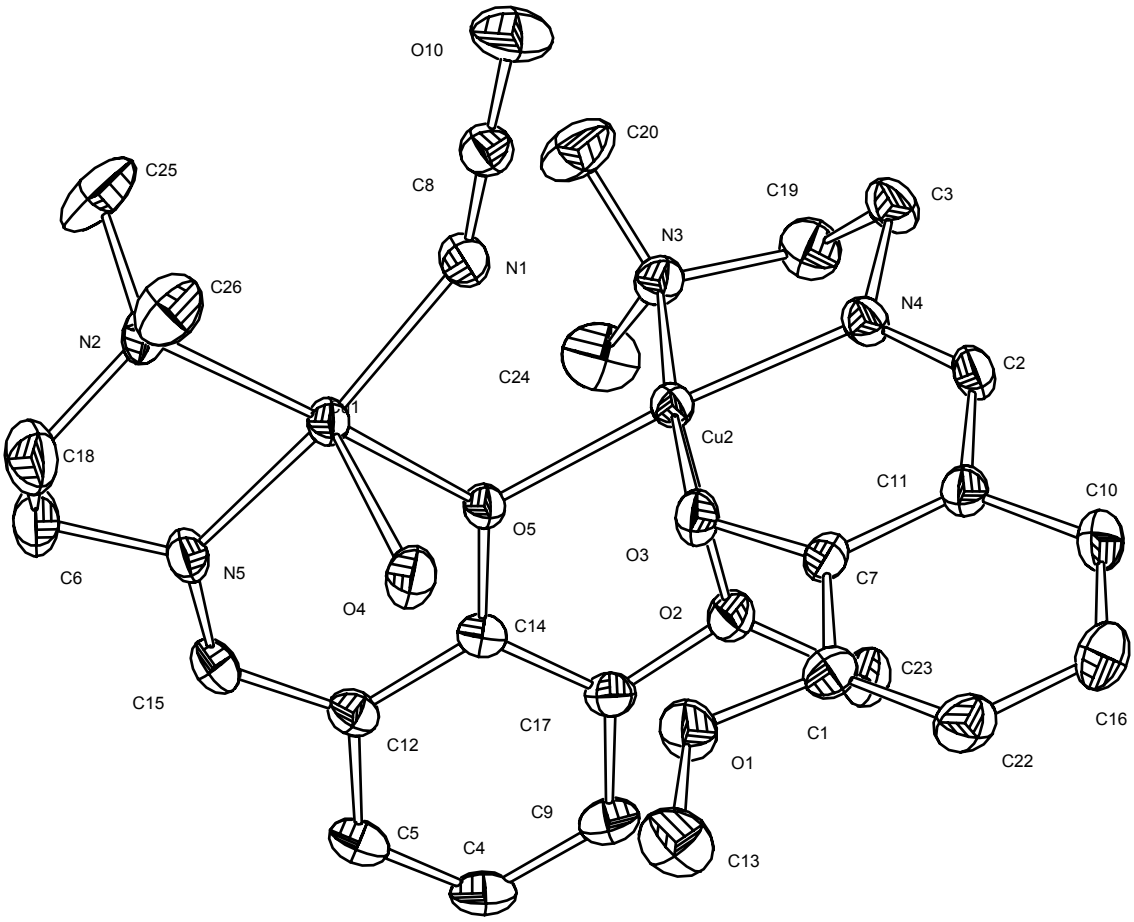

Figure 1. ORTEP representations of the symmetry expanded local structure in **cr10**.