Table 1. Crystal data and structure refinement for **cr11a**

Compound	**cr11a**
Formula	$C_{24}H_{36}ClCu_2N_7O_9$
Formula weight	729.13
Crystal size (mm^3)	0.50 × 0.44 × 0.36
Crystal color	Blue
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 16.675(1) Å
	b = 13.319(1) Å
	c = 14.064(1) Å
	β = 104.699(1)°
Volume ($Å^3$)	3021.2(1)
Z	4
Calculated density ($g·cm^{-3}$)	1.603
F(000)	1504
Temperature (K)	293(2)
Wavelength (Å)	0.71073
Absorption coefficient (mm^{-1})	1.558
θ for data collection (°)	1.98 to 25.10
Limiting indices	$-13 \le h \le 19$, $-9 \le k \le 15$, $-16 \le l \le 14$
Reflections collected	9445
Unique reflections (R(int))	5272 [R(int) = 0.0240]
Refinement method	Full-matrix least-squares on F^2
Absorption correction	SADABS
Data / restraints / parameters	5272 / 0 / 389
Goodness-of-fit on F^2	1.148
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0556, wR2 = 0.1227
R indices (all data)	R1 = 0.0731, wR2 = 0.1372
Largest diff. peak and hole ($e·Å^3$)	0.665 and -0.496

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

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **cr11a**.

Atom	x	y	z	U(eq)
Cu(1)	6959(1)	5680(1)	124(1)	36(1)
Cu(2)	7655(1)	3989(1)	1789(1)	33(1)
Cl(1)	11370(1)	1558(2)	-1199(2)	83(1)
O(1)	6133(3)	2120(3)	-689(3)	55(1)
O(2)	8768(2)	3138(3)	1373(3)	51(1)
O(3)	6904(2)	3129(3)	857(2)	41(1)
O(4)	6291(2)	4318(3)	-761(3)	49(1)
O(5)	7890(2)	4757(2)	666(2)	34(1)
O(6)	11867(8)	2286(16)	-1254(11)	362(13)
O(7)	10835(6)	1607(10)	-2112(6)	214(5)
O(8)	10960(8)	1724(10)	-535(7)	239(7)
O(9)	11836(11)	807(10)	-898(13)	311(9)
N(1)	6596(3)	5326(4)	1311(3)	44(1)
N(2)	6062(3)	6732(3)	-461(3)	45(1)
N(3)	8447(3)	4856(3)	2870(3)	42(1)
N(4)	7553(3)	3159(3)	2892(3)	40(1)
N(5)	7511(3)	6164(3)	-849(3)	42(1)
N(6)	6069(3)	5626(3)	1666(3)	43(1)
N(7)	5559(3)	5894(5)	2038(4)	68(2)
C(1)	6296(3)	1611(4)	186(4)	42(1)
C(2)	7286(3)	2257(4)	2829(4)	44(1)
C(3)	7946(4)	3600(5)	3855(4)	51(2)
C(4)	9669(4)	3716(5)	-697(5)	58(2)
C(5)	9202(4)	4531(5)	-1067(4)	53(2)
C(6)	7108(4)	7056(5)	-1366(5)	65(2)

C(7)	6720(3)	2195(4)	1003(4)	36(1)
C(9)	9539(3)	3228(5)	124(4)	50(1)
C(10)	6686(4)	718(4)	2019(5)	56(2)
C(11)	6897(3)	1734(4)	1939(4)	39(1)
C(12)	8586(3)	4899(4)	-637(4)	40(1)
C(13)	5656(4)	1625(6)	-1546(5)	68(2)
C(14)	8444(3)	4422(4)	205(4)	35(1)
C(15)	8133(3)	5770(4)	-1070(4)	46(1)
C(16)	6294(4)	182(5)	1215(5)	65(2)
C(17)	8934(3)	3574(4)	562(4)	41(1)
C(18)	6209(4)	6961(5)	-1444(5)	64(2)
C(19)	8698(4)	4164(5)	3730(5)	65(2)
C(20)	8043(5)	5751(5)	3127(6)	83(2)
C(22)	6093(4)	622(4)	288(5)	54(2)
C(23)	9121(5)	2185(5)	1688(5)	70(2)
C(24)	9209(4)	5172(6)	2614(6)	80(2)
C(25)	6149(5)	7629(5)	167(6)	74(2)
C(26)	5207(3)	6355(5)	-647(5)	58(2)

Table S3. Selected bond lengths [Å] for **cr11a**.

Bond	distances	
Cu(1)-N(5)		1.944(4)
Cu(1)-N(1)	1.971(4)	
Cu(1)-O(5)	1.975(3)	
Cu(1)-N(2)	2.064(4)	
Cu(1)-O(4)	2.318(4)	
Cu(1)-Cu(2)	3.244(1)	
Cu(2)-O(3)	1.941(3)	
Cu(2)-N(4)	1.946(4)	
Cu(2)-O(5)	2.003(3)	
Cu(2)-N(3)	2.090(4)	
Cu(2)-O(2)	2.370(4)	
Cu(2)-N(1)	2.479(4)	
Cl(1)-O(9)	1.272(10)	
Cl(1)-O(6)	1.290(13)	
Cl(1)-O(8)	1.308(9)	
Cl(1)-O(7)	1.366(8)	
O(1)-C(1)	1.370(6)	

Bond	distances

O(1)-C(13)	1.426(7)
O(2)-C(17)	1.371(6)
O(2)-C(23)	1.422(7)
O(3)-C(7)	1.310(6)
O(5)-C(14)	1.332(6)
N(1)-N(6)	1.184(6)
N(2)-C(26)	1.470(7)
N(2)-C(25)	1.471(8)
N(2)-C(18)	1.496(8)
N(3)-C(20)	1.459(8)
N(3)-C(24)	1.468(8)
N(3)-C(19)	1.493(8)
N(4)-C(2)	1.277(7)
N(4)-C(3)	1.469(7)
N(5)-C(15)	1.269(7)
N(5)-C(6)	1.463(7)
N(6)-N(7)	1.163(7)

Bond	distances
C(1)-C(22)	1.376(8)
C(1)-C(7)	1.419(7)
C(2)-C(11)	1.435(7)
C(3)-C(19)	1.511(9)
C(4)-C(5)	1.360(9)
C(4)-C(9)	1.389(9)
C(5)-C(12)	1.405(7)
C(6)-C(18)	1.480(9)
C(7)-C(11)	1.414(7)
C(9)-C(17)	1.386(7)
C(10)-C(16)	1.356(9)
C(10)-C(11)	1.410(8)
C(12)-C(14)	1.417(7)
C(12)-C(15)	1.433(8)
C(14)-C(17)	1.410(7)

C(16)-C(22)	1.391(9)

Table 4. Selected angles [º] for **cr11a**

Atom1-atom2-atom3	angles	Atom1-atom2-atom3	angles	Atom1-atom2-atom3	angles
N(5)-Cu(1)-N(1)	167.88(19)	O(2)-Cu(2)-Cu(1)	108.24(9)	C(15)-N(5)-C(6)	121.0(5)
N(5)-Cu(1)-O(5)	90.67(16)	N(1)-Cu(2)-Cu(1)	37.37(10)	C(15)-N(5)-Cu(1)	126.6(4)
N(1)-Cu(1)-O(5)	84.58(16)	O(9)-Cl(1)-O(6)	105.3(11)	C(6)-N(5)-Cu(1)	112.3(4)
N(5)-Cu(1)-N(2)	85.32(19)	O(9)-Cl(1)-O(8)	106.3(8)	N(7)-N(6)-N(1)	177.6(6)
N(1)-Cu(1)-N(2)	98.77(19)	O(6)-Cl(1)-O(8)	112.1(12)	O(1)-C(1)-C(22)	124.7(5)
O(5)-Cu(1)-N(2)	175.01(16)	O(9)-Cl(1)-O(7)	123.3(10)	O(1)-C(1)-C(7)	113.6(5)
N(5)-Cu(1)-O(4)	97.49(17)	O(6)-Cl(1)-O(7)	100.6(8)	C(22)-C(1)-C(7)	121.7(5)
N(1)-Cu(1)-O(4)	93.38(17)	O(8)-Cl(1)-O(7)	109.1(7)	N(4)-C(2)-C(11)	126.1(5)
O(5)-Cu(1)-O(4)	86.81(14)	C(1)-O(1)-C(13)	118.1(5)	N(4)-C(3)-C(19)	106.2(5)
N(2)-Cu(1)-O(4)	96.65(16)	C(17)-O(2)-C(23)	118.8(5)	C(5)-C(4)-C(9)	119.8(5)
N(5)-Cu(1)-Cu(2)	126.33(13)	C(17)-O(2)-Cu(2)	109.9(3)	C(4)-C(5)-C(12)	121.6(6)
N(1)-Cu(1)-Cu(2)	49.74(13)	C(23)-O(2)-Cu(2)	129.7(4)	N(5)-C(6)-C(18)	107.3(5)
O(5)-Cu(1)-Cu(2)	35.66(9)	C(7)-O(3)-Cu(2)	126.2(3)	O(3)-C(7)-C(11)	123.8(5)
N(2)-Cu(1)-Cu(2)	148.23(13)	C(14)-O(5)-Cu(1)	126.5(3)	O(3)-C(7)-C(1)	118.8(5)
O(4)-Cu(1)-Cu(2)	83.11(9)	C(14)-O(5)-Cu(2)	120.7(3)	C(11)-C(7)-C(1)	117.4(5)
O(3)-Cu(2)-N(4)	91.81(16)	Cu(1)-O(5)-Cu(2)	109.27(15)	C(17)-C(9)-C(4)	119.9(6)
O(3)-Cu(2)-O(5)	89.44(14)	N(6)-N(1)-Cu(1)	134.1(4)	C(16)-C(10)-C(11)	121.1(6)
N(4)-Cu(2)-O(5)	173.09(16)	N(6)-N(1)-Cu(2)	133.0(4)	C(10)-C(11)-C(7)	119.5(5)
O(3)-Cu(2)-N(3)	176.10(16)	Cu(1)-N(1)-Cu(2)	92.89(17)	C(10)-C(11)-C(2)	117.6(5)
N(4)-Cu(2)-N(3)	84.31(18)	C(26)-N(2)-C(25)	109.2(5)	C(7)-C(11)-C(2)	122.9(5)
O(5)-Cu(2)-N(3)	94.45(16)	C(26)-N(2)-C(18)	106.6(5)	C(5)-C(12)-C(14)	119.9(5)
O(3)-Cu(2)-O(2)	87.83(15)	C(25)-N(2)-C(18)	112.0(5)	C(5)-C(12)-C(15)	117.6(5)
N(4)-Cu(2)-O(2)	99.05(16)	C(26)-N(2)-Cu(1)	114.3(4)	C(14)-C(12)-C(15)	122.4(5)
O(5)-Cu(2)-O(2)	74.21(13)	C(25)-N(2)-Cu(1)	111.1(4)	O(5)-C(14)-C(17)	120.5(4)
N(3)-Cu(2)-O(2)	93.12(16)	C(18)-N(2)-Cu(1)	103.6(3)	O(5)-C(14)-C(12)	122.7(5)
O(3)-Cu(2)-N(1)	86.99(15)	C(20)-N(3)-C(24)	108.0(6)	C(17)-C(14)-C(12)	116.8(5)
N(4)-Cu(2)-N(1)	115.07(17)	C(20)-N(3)-C(19)	110.9(5)	N(5)-C(15)-C(12)	127.4(5)
O(5)-Cu(2)-N(1)	71.78(14)	C(24)-N(3)-C(19)	107.1(5)	C(10)-C(16)-C(22)	120.6(6)
N(3)-Cu(2)-N(1)	94.32(17)	C(20)-N(3)-Cu(2)	112.7(4)	O(2)-C(17)-C(9)	123.6(5)
O(2)-Cu(2)-N(1)	145.62(14)	C(24)-N(3)-Cu(2)	114.0(4)	O(2)-C(17)-C(14)	114.4(4)
O(3)-Cu(2)-Cu(1)	82.56(10)	C(19)-N(3)-Cu(2)	104.1(3)	C(9)-C(17)-C(14)	122.0(5)
N(4)-Cu(2)-Cu(1)	151.83(13)	C(2)-N(4)-C(3)	120.4(5)	C(6)-C(18)-N(2)	110.4(5)
O(5)-Cu(2)-Cu(1)	35.07(9)	C(2)-N(4)-Cu(2)	125.3(4)	N(3)-C(19)-C(3)	109.3(5)
N(3)-Cu(2)-Cu(1)	100.70(12)	C(3)-N(4)-Cu(2)	113.6(3)	C(1)-C(22)-C(16)	119.7(6)

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for **CR11a**. 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)	37(1)	35(1)	36(1)	6(1)	9(1)	3(1)
Cu(2)	36(1)	33(1)	30(1)	1(1)	7(1)	-1(1)

Cl(1)	60(1)	114(2)	70(1)	-22(1)	10(1)	10(1)
O(1)	67(3)	53(2)	37(2)	-2(2)	1(2)	-12(2)
O(2)	51(2)	51(2)	54(2)	14(2)	20(2)	23(2)
O(3)	49(2)	35(2)	35(2)	2(2)	2(2)	-7(2)
O(4)	57(2)	38(2)	48(2)	3(2)	4(2)	1(2)
O(5)	35(2)	37(2)	34(2)	4(2)	13(1)	4(2)
O(6)	198(12)	500(30)	296(17)	203(18)	-103(12)	-191(16)
O(7)	170(9)	350(16)	98(6)	-52(8)	-11(6)	-58(10)
O(8)	290(14)	334(16)	116(7)	33(8)	92(8)	185(13)
O(9)	362(19)	209(12)	430(20)	113(14)	223(18)	198(13)
N(1)	40(2)	50(3)	44(3)	8(2)	17(2)	7(2)
N(2)	45(3)	38(2)	50(3)	8(2)	8(2)	7(2)
N(3)	42(2)	42(3)	39(2)	-2(2)	5(2)	-1(2)
N(4)	44(2)	44(3)	31(2)	2(2)	5(2)	-3(2)
N(5)	44(3)	40(3)	43(2)	10(2)	13(2)	-4(2)
N(6)	42(3)	45(3)	38(2)	-5(2)	6(2)	-2(2)
N(7)	56(3)	86(4)	67(4)	-15(3)	28(3)	7(3)
C(1)	43(3)	37(3)	44(3)	-4(2)	9(2)	-3(2)
C(2)	52(3)	47(3)	36(3)	10(2)	15(2)	2(3)
C(3)	60(4)	62(4)	29(3)	1(3)	6(3)	-8(3)
C(4)	47(3)	75(5)	56(4)	-15(3)	22(3)	6(3)
C(5)	48(3)	74(4)	45(3)	-9(3)	24(3)	-9(3)
C(6)	78(5)	54(4)	68(4)	28(3)	25(4)	7(3)
C(7)	32(3)	30(3)	47(3)	0(2)	11(2)	3(2)
C(9)	41(3)	54(4)	57(4)	-10(3)	16(3)	12(3)
C(10)	78(4)	41(3)	55(4)	9(3)	25(3)	-2(3)
C(11)	42(3)	34(3)	41(3)	4(2)	12(2)	0(2)
C(12)	38(3)	47(3)	36(3)	-6(2)	11(2)	-6(2)
C(13)	71(4)	77(5)	47(4)	-16(3)	1(3)	-20(4)
C(14)	32(3)	41(3)	32(3)	-7(2)	8(2)	-4(2)
C(15)	45(3)	55(4)	42(3)	8(3)	15(3)	-12(3)
C(16)	89(5)	36(3)	70(4)	-2(3)	23(4)	-18(3)
C(17)	38(3)	43(3)	39(3)	-1(2)	7(2)	1(2)
C(18)	64(4)	62(4)	61(4)	24(3)	9(3)	11(3)
C(19)	67(4)	71(5)	49(4)	-1(3)	1(3)	-4(3)
C(20)	93(6)	56(4)	84(5)	-25(4)	-8(4)	17(4)

C(22)	55(4)	44(3)	65(4)	-13(3)	16(3)	-11(3)
C(23)	85(5)	61(4)	64(4)	16(3)	20(4)	28(4)
C(24)	65(5)	93(6)	79(5)	-18(4)	14(4)	-32(4)
C(25)	76(5)	41(4)	93(5)	-6(4)	-3(4)	11(3)
C(26)	37(3)	58(4)	72(4)	2(3)	1(3)	11(3)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for **cr11a**.

	x	y	z	U(eq)
H(4A)	5855	4505	-1134	59
H(4B)	6519	3724	-669	59
H(2A)	7350	1905	3415	53
H(3A)	8108	3077	4347	62
H(3B)	7565	4052	4060	62
H(4A)	10074	3486	-993	69
H(5A)	9293	4852	-1617	64
H(6A)	7208	7097	-2015	78
H(6B)	7326	7658	-1003	78
H(9A)	9857	2670	379	60
H(10A)	6817	411	2633	68
H(13A)	5548	2083	-2091	102
H(13B)	5141	1402	-1434	102
H(13C)	5960	1057	-1691	102
H(15A)	8316	6081	-1568	56
H(16A)	6159	-487	1285	78
H(18A)	5979	6428	-1903	76
H(18B)	5932	7582	-1695	76
H(19A)	8940	4546	4320	77
H(19B)	9111	3693	3624	77

H(20A)	8426	6113	3637	125
H(20B)	7569	5557	3354	125
H(20C)	7868	6172	2558	125
H(22A)	5822	251	-259	65
H(23A)	9563	2049	1382	105
H(23B)	8704	1675	1504	105
H(23C)	9335	2187	2389	105
H(24A)	9543	5563	3141	120
H(24B)	9069	5570	2026	120
H(24C)	9515	4590	2507	120
H(25A)	5736	8114	-131	111
H(25B)	6691	7913	242	111
H(25C)	6078	7445	801	111
H(26A)	4827	6881	-927	87
H(26B)	5102	6138	-39	87
H(26C)	5135	5800	-1096	87

Table S5. Selected Hydrogen Bonds Lengths (Å)

D-H	d(D-H)	d(H..A)	<DHA	d(D..A)	A

O4-H4A	0.820	2.437	148.30	3.164	N7 [-x+1, -y+1, -z]
O4-H4B	0.874	2.223	118.35	2.748	O3
O4-H4B	0.874	2.229	138.92	2.944	O1

Figure:

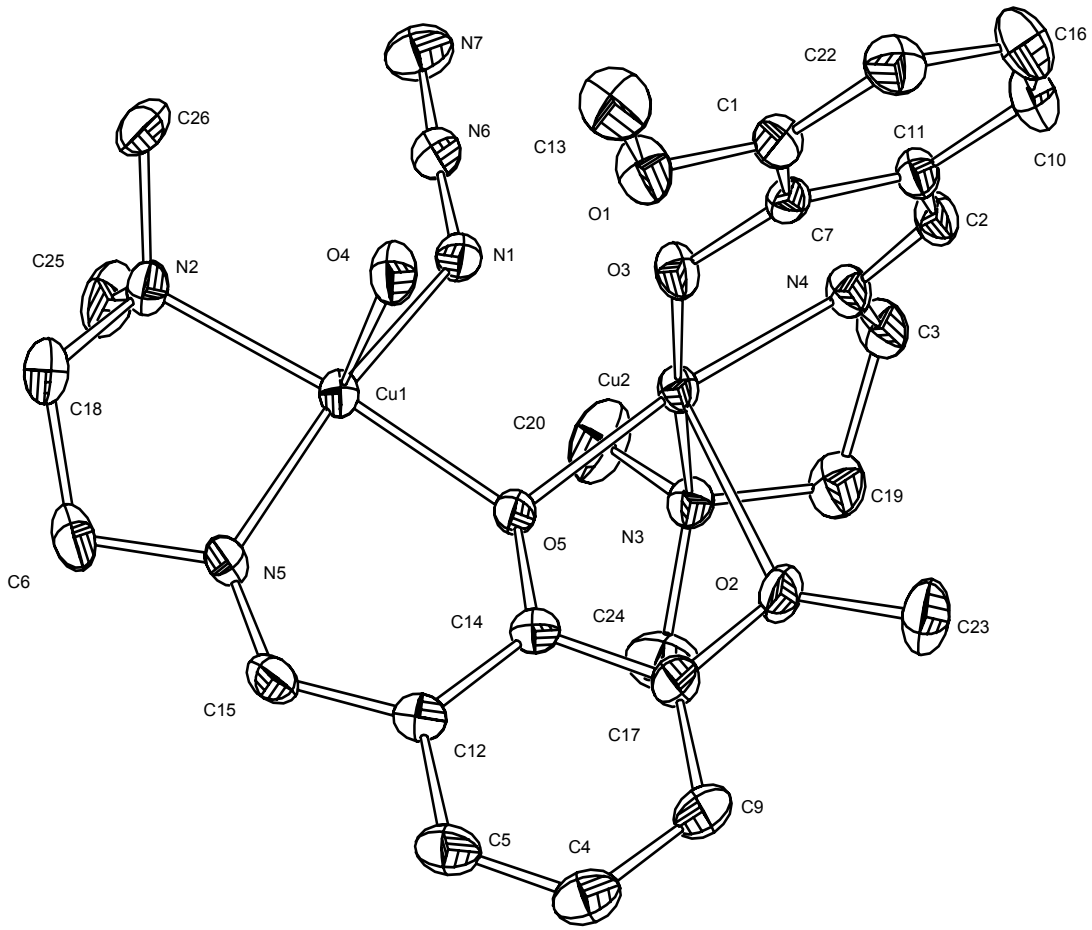
N7
C16
C22
C26
N6
C1
C13
C11
C10
O1
C7
C2
C25
N2
O4
N1
O3
N4
C3
Cu1
Cu2
C18
C20
C19
O5
N3
C6
N5
O2
C14
C24
C23
C15
C12
C17
C9
C5
C4

Figure 1. ORTEP representations of the symmetry expanded local structure in **cr11a**.