

Table 1. Crystal data and structure refinement for structure9.

Identification code	structure9	
Empirical formula	C12 H10 Cl2 Cu N2 O5	
Formula weight	396.66	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	$a = 7.2504(16) \text{ Å}$	$\alpha = 108.400(3)^\circ$.
	$b = 9.346(2) \text{ Å}$	$\beta = 98.483(3)^\circ$.
	$c = 11.785(3) \text{ Å}$	$\gamma = 108.720(3)^\circ$.
Volume	$689.6(3) \text{ Å}^3$	
Z	2	
Calculated density	1.910 Mg/m^3	
Absorption coefficient	1.996 mm^{-1}	
F(000)	398	
Crystal size	$0.30 \times 0.13 \times 0.12 \text{ mm}^3$	
Theta range for data collection	1.90 to 27.98° .	
Limiting indices	$-9 \leq h \leq 9$, $-12 \leq k \leq 11$, $-15 \leq l \leq 14$	
Reflections collected	7458	
Independent reflections	2962 [$R(\text{int}) = 0.0323$]	
Completeness to $\theta = 27.98^\circ$	88.9%	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.570	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2962 / 4 / 215	
Goodness-of-fit on F^2	1.096	
Final R indices [$I > 2\sigma(I)$]	$R1 = 0.0337$, $wR2 = 0.0933$	
R indices (all data)	$R1 = 0.0364$, $wR2 = 0.0947$	
Largest diff. peak and hole	0.814 and -0.656 e.Å^{-3}	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct9. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	-1896(1)	701(1)	-221(1)	16(1)
Cl(1)	763(1)	-82(1)	-1405(1)	19(1)
Cl(2)	130(1)	3360(1)	828(1)	22(1)
O(1)	-8067(3)	303(2)	-5571(2)	23(1)
O(2)	-5968(3)	2945(2)	-4751(2)	26(1)
O(3)	-10493(3)	-6182(2)	-4149(2)	26(1)
O(4)	-9039(3)	-7345(2)	-3098(2)	25(1)
O(5)	-7864(3)	3540(2)	-6404(2)	37(1)
N(1)	-3382(3)	1091(2)	-1614(2)	16(1)
N(2)	-4170(3)	-1554(2)	-1151(2)	17(1)
C(1)	-2889(4)	2522(3)	-1749(2)	21(1)
C(2)	-3929(4)	2696(3)	-2751(2)	20(1)
C(3)	-5528(3)	1339(3)	-3648(2)	17(1)
C(4)	-6058(3)	-155(3)	-3505(2)	17(1)
C(5)	-4964(3)	-235(3)	-2476(2)	16(1)
C(6)	-5403(3)	-1738(3)	-2213(2)	16(1)
C(7)	-6981(3)	-3216(3)	-2965(2)	18(1)
C(8)	-7317(3)	-4538(3)	-2616(2)	17(1)
C(9)	-6033(4)	-4357(3)	-1531(2)	20(1)
C(10)	-4479(4)	-2852(3)	-833(2)	21(1)
C(11)	-6667(3)	1455(3)	-4757(2)	18(1)
C(12)	-9111(4)	-6096(3)	-3376(2)	19(1)

Table 3. Bond lengths [Å] and angles [°] for struct9.

Cu(1)-N(1)	2.0243(19)
Cu(1)-N(2)	2.0345(19)
Cu(1)-Cl(2)	2.2460(7)
Cu(1)-Cl(1)#1	2.2846(7)
Cu(1)-Cl(1)	2.6930(8)
Cl(1)-Cu(1)#1	2.2846(7)
O(1)-C(11)	1.212(3)
O(2)-C(11)	1.317(3)
O(3)-C(12)	1.214(3)
O(4)-C(12)	1.322(3)
N(1)-C(1)	1.337(3)
N(1)-C(5)	1.353(3)
N(2)-C(10)	1.341(3)
N(2)-C(6)	1.353(3)
C(1)-C(2)	1.388(3)
C(2)-C(3)	1.385(3)
C(3)-C(4)	1.396(3)
C(3)-C(11)	1.494(3)
C(4)-C(5)	1.385(3)
C(5)-C(6)	1.479(3)
C(6)-C(7)	1.384(3)
C(7)-C(8)	1.383(3)
C(8)-C(9)	1.394(3)
C(8)-C(12)	1.494(3)
C(9)-C(10)	1.380(3)
N(1)-Cu(1)-N(2)	79.76(7)
N(1)-Cu(1)-Cl(2)	94.03(6)
N(2)-Cu(1)-Cl(2)	168.99(6)
N(1)-Cu(1)-Cl(1)#1	169.96(6)
N(2)-Cu(1)-Cl(1)#1	93.85(6)
Cl(2)-Cu(1)-Cl(1)#1	90.98(3)
N(1)-Cu(1)-Cl(1)	95.33(6)
N(2)-Cu(1)-Cl(1)	94.20(6)
Cl(2)-Cu(1)-Cl(1)	95.44(3)

Cl (1) #1-Cu (1) -Cl (1)	92.84 (2)
Cu (1) #1-Cl (1) -Cu (1)	87.16 (2)
C (1) -N (1) -C (5)	119.08 (19)
C (1) -N (1) -Cu (1)	125.12 (15)
C (5) -N (1) -Cu (1)	115.78 (15)
C (10) -N (2) -C (6)	118.69 (19)
C (10) -N (2) -Cu (1)	126.06 (16)
C (6) -N (2) -Cu (1)	115.18 (15)
N (1) -C (1) -C (2)	122.3 (2)
C (3) -C (2) -C (1)	119.1 (2)
C (2) -C (3) -C (4)	118.8 (2)
C (2) -C (3) -C (11)	121.1 (2)
C (4) -C (3) -C (11)	120.10 (19)
C (5) -C (4) -C (3)	119.0 (2)
N (1) -C (5) -C (4)	121.7 (2)
N (1) -C (5) -C (6)	114.31 (19)
C (4) -C (5) -C (6)	124.0 (2)
N (2) -C (6) -C (7)	121.9 (2)
N (2) -C (6) -C (5)	114.76 (18)
C (7) -C (6) -C (5)	123.4 (2)
C (8) -C (7) -C (6)	119.1 (2)
C (7) -C (8) -C (9)	119.1 (2)
C (7) -C (8) -C (12)	119.1 (2)
C (9) -C (8) -C (12)	121.7 (2)
C (10) -C (9) -C (8)	118.6 (2)
N (2) -C (10) -C (9)	122.6 (2)
O (1) -C (11) -O (2)	124.1 (2)
O (1) -C (11) -C (3)	123.6 (2)
O (2) -C (11) -C (3)	112.32 (19)
O (3) -C (12) -O (4)	124.2 (2)
O (3) -C (12) -C (8)	122.9 (2)
O (4) -C (12) -C (8)	112.84 (19)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct9.

The anisotropic displacement factor exponent takes the form:

$$-2\pi^2[h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu (1)	15 (1)	11 (1)	17 (1)	3 (1)	-1 (1)	2 (1)
Cl (1)	20 (1)	16 (1)	17 (1)	5 (1)	1 (1)	5 (1)
Cl (2)	22 (1)	12 (1)	22 (1)	2 (1)	-3 (1)	2 (1)
O (1)	24 (1)	13 (1)	23 (1)	4 (1)	-4 (1)	1 (1)
O (2)	30 (1)	13 (1)	24 (1)	8 (1)	-5 (1)	1 (1)
O (3)	26 (1)	17 (1)	25 (1)	7 (1)	-5 (1)	1 (1)
O (4)	21 (1)	12 (1)	33 (1)	8 (1)	-2 (1)	1 (1)
O (5)	48 (1)	23 (1)	25 (1)	3 (1)	-13 (1)	12 (1)
N (1)	16 (1)	12 (1)	17 (1)	4 (1)	1 (1)	3 (1)
N (2)	15 (1)	13 (1)	19 (1)	5 (1)	1 (1)	4 (1)
C (1)	17 (1)	12 (1)	23 (1)	3 (1)	-2 (1)	1 (1)
C (2)	21 (1)	10 (1)	22 (1)	5 (1)	1 (1)	2 (1)
C (3)	15 (1)	15 (1)	17 (1)	4 (1)	3 (1)	5 (1)
C (4)	16 (1)	12 (1)	19 (1)	4 (1)	1 (1)	3 (1)
C (5)	14 (1)	12 (1)	19 (1)	4 (1)	3 (1)	4 (1)
C (6)	16 (1)	13 (1)	16 (1)	5 (1)	3 (1)	4 (1)
C (7)	16 (1)	14 (1)	17 (1)	3 (1)	0 (1)	2 (1)
C (8)	15 (1)	13 (1)	20 (1)	4 (1)	3 (1)	4 (1)
C (9)	19 (1)	16 (1)	24 (1)	8 (1)	2 (1)	6 (1)
C (10)	18 (1)	19 (1)	24 (1)	9 (1)	0 (1)	6 (1)
C (11)	18 (1)	14 (1)	20 (1)	6 (1)	4 (1)	6 (1)
C (12)	21 (1)	14 (1)	19 (1)	5 (1)	5 (1)	4 (1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct9.

	x	y	z	U(eq)
H(1)	-1788	3454	-1137	25
H(2)	-3551	3730	-2820	24
H(4)	-7154	-1102	-4105	21
H(7)	-7822	-3321	-3711	21
H(9)	-6224	-5250	-1276	24
H(10)	-3592	-2730	-98	25
H(2A)	-6640 (40)	3060 (40)	-5330 (20)	39 (9)
H(4A)	-10060 (30)	-8190 (20)	-3510 (30)	37 (9)
H(5A)	-8350 (60)	4250 (40)	-6280 (40)	79 (15)
H(5B)	-8560 (40)	2940 (30)	-7130 (14)	43 (10)

