

Table 1. Crystal data and structure refinement for structure7.

Identification code	structure7	
Empirical formula	C22 H25 Cu N4 O9.50	
Formula weight	561.00	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	$a = 23.117(5)$ Å	$\alpha = 90^\circ$.
	$b = 12.426(2)$ Å	$\beta = 95.574(3)^\circ$.
	$c = 17.652(3)$ Å	$\gamma = 90^\circ$.
Volume	$5046.8(17)$ Å ³	
Z	8	
Calculated density	1.477 Mg/m ³	
Absorption coefficient	0.925 mm ⁻¹	
F(000)	2320	
Crystal size	0.43 x 0.20 x 0.13 mm ³	
Theta range for data collection	1.86 to 28.25°.	
Limiting indices	$-30 \leq h \leq 30$, $-16 \leq k \leq 15$, $-23 \leq l \leq 23$	
Reflections collected	27592	
Independent reflections	5817 [R(int) = 0.0493]	
Completeness to theta = 28.25°	93.0%	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.713	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5817 / 26 / 363	
Goodness-of-fit on F ²	0.983	
Final R indices [I>2sigma(I)]	R1 = 0.0422, wR2 = 0.1062	
R indices (all data)	R1 = 0.0541, wR2 = 0.1108	
Largest diff. peak and hole	0.624 and -0.351 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct7. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	2115(1)	-188(1)	1188(1)	19(1)
N(1)	2181(1)	-177(1)	66(1)	17(1)
N(2)	2755(1)	-1271(1)	1150(1)	19(1)
N(3)	1640(1)	1172(1)	1175(1)	22(1)
N(4)	-121(1)	5802(2)	1228(2)	65(1)
C(1)	1842(1)	380(2)	-457(1)	21(1)
C(2)	1928(1)	356(2)	-1218(1)	21(1)
C(3)	2371(1)	-274(2)	-1457(1)	18(1)
C(4)	2715(1)	-866(2)	-915(1)	18(1)
C(5)	2611(1)	-791(2)	-160(1)	15(1)
C(6)	2943(1)	-1405(2)	458(1)	16(1)
C(7)	3402(1)	-2079(2)	343(1)	19(1)
C(8)	3673(1)	-2654(2)	955(1)	21(1)
C(9)	3471(1)	-2519(2)	1659(1)	26(1)
C(10)	3017(1)	-1825(2)	1740(1)	25(1)
C(11)	2478(1)	-332(2)	-2286(1)	23(1)
C(12)	4171(1)	-3419(2)	847(2)	29(1)
C(13)	1097(1)	1135(2)	1367(1)	26(1)
C(14)	745(1)	2029(2)	1368(1)	30(1)
C(17)	12(1)	3964(2)	879(2)	56(1)
C(18)	-324(2)	4876(2)	918(3)	69(1)
C(19)	433(1)	5830(2)	1507(2)	59(1)
C(20)	802(1)	4958(2)	1496(2)	50(1)
C(21)	1525(1)	3052(2)	973(2)	39(1)
C(22)	1848(1)	2121(2)	982(1)	31(1)
C(15)	958(1)	3016(2)	1169(2)	33(1)
C(16)	586(1)	3992(2)	1179(2)	42(1)
O(1)	2873(1)	-886(2)	-2475(1)	46(1)
O(2)	2129(1)	241(1)	-2717(1)	25(1)
O(3)	4320(1)	-3524(2)	186(1)	44(1)
O(4)	4394(1)	-3885(2)	1422(1)	51(1)

O(5)	1423(1)	-1415(1)	1128(1)	28(1)
O(6)	383(1)	-907(2)	4596(1)	56(1)
O(7)	798(1)	-1721(2)	2307(1)	49(1)
O(8)	1836(1)	-3826(2)	3993(1)	43(1)
O(9)	0	-95(2)	2500	43(1)
O(10)	871(1)	-2469(1)	3798(1)	38(1)

Table 3. Bond lengths [Å] and angles [°] for struct7.

Cu(1)-O(2) #1	1.9307(15)
Cu(1)-N(1)	2.0025(18)
Cu(1)-N(2)	2.0066(18)
Cu(1)-N(3)	2.0139(18)
Cu(1)-O(5)	2.2036(16)
N(1)-C(1)	1.344(3)
N(1)-C(5)	1.344(3)
N(2)-C(10)	1.342(3)
N(2)-C(6)	1.347(3)
N(3)-C(22)	1.330(3)
N(3)-C(13)	1.334(3)
N(4)-C(19)	1.328(4)
N(4)-C(18)	1.338(4)
C(1)-C(2)	1.376(3)
C(2)-C(3)	1.388(3)
C(3)-C(4)	1.394(3)
C(3)-C(11)	1.508(3)
C(4)-C(5)	1.380(3)
C(5)-C(6)	1.482(3)
C(6)-C(7)	1.383(3)
C(7)-C(8)	1.393(3)
C(8)-C(9)	1.380(3)
C(8)-C(12)	1.519(3)
C(9)-C(10)	1.377(3)
C(11)-O(1)	1.217(3)
C(11)-O(2)	1.271(3)
C(12)-O(4)	1.236(3)
C(12)-O(3)	1.256(3)
C(13)-C(14)	1.378(3)
C(14)-C(15)	1.380(3)
C(17)-C(18)	1.380(4)
C(17)-C(16)	1.382(4)
C(19)-C(20)	1.381(4)
C(20)-C(16)	1.396(4)
C(21)-C(22)	1.377(3)

C (21) -C (15)	1.387 (4)
C (15) -C (16)	1.488 (3)
O (2) -Cu (1) #2	1.9307 (15)

O (2) #1 -Cu (1) -N (1)	174.43 (7)
O (2) #1 -Cu (1) -N (2)	94.00 (7)
N (1) -Cu (1) -N (2)	81.02 (7)
O (2) #1 -Cu (1) -N (3)	89.82 (7)
N (1) -Cu (1) -N (3)	94.37 (7)
N (2) -Cu (1) -N (3)	164.83 (7)
O (2) #1 -Cu (1) -O (5)	88.13 (6)
N (1) -Cu (1) -O (5)	94.67 (6)
N (2) -Cu (1) -O (5)	93.95 (7)
N (3) -Cu (1) -O (5)	100.85 (7)
C (1) -N (1) -C (5)	119.20 (18)
C (1) -N (1) -Cu (1)	126.02 (14)
C (5) -N (1) -Cu (1)	114.79 (13)
C (10) -N (2) -C (6)	118.66 (18)
C (10) -N (2) -Cu (1)	126.64 (15)
C (6) -N (2) -Cu (1)	114.65 (13)
C (22) -N (3) -C (13)	117.9 (2)
C (22) -N (3) -Cu (1)	122.50 (16)
C (13) -N (3) -Cu (1)	119.57 (15)
C (19) -N (4) -C (18)	117.5 (3)
N (1) -C (1) -C (2)	122.0 (2)
C (1) -C (2) -C (3)	119.34 (19)
C (2) -C (3) -C (4)	118.53 (19)
C (2) -C (3) -C (11)	121.15 (19)
C (4) -C (3) -C (11)	120.32 (19)
C (5) -C (4) -C (3)	119.09 (18)
N (1) -C (5) -C (4)	121.86 (18)
N (1) -C (5) -C (6)	114.79 (17)
C (4) -C (5) -C (6)	123.30 (18)
N (2) -C (6) -C (7)	121.85 (18)
N (2) -C (6) -C (5)	114.50 (17)
C (7) -C (6) -C (5)	123.65 (18)
C (6) -C (7) -C (8)	119.41 (19)

C (9) -C (8) -C (7)	118.09 (19)
C (9) -C (8) -C (12)	121.03 (19)
C (7) -C (8) -C (12)	120.9 (2)
C (10) -C (9) -C (8)	119.79 (19)
N (2) -C (10) -C (9)	122.2 (2)
O (1) -C (11) -O (2)	127.0 (2)
O (1) -C (11) -C (3)	119.4 (2)
O (2) -C (11) -C (3)	113.58 (19)
O (4) -C (12) -O (3)	125.7 (2)
O (4) -C (12) -C (8)	116.8 (2)
O (3) -C (12) -C (8)	117.5 (2)
N (3) -C (13) -C (14)	123.0 (2)
C (13) -C (14) -C (15)	119.3 (2)
C (18) -C (17) -C (16)	119.0 (3)
N (4) -C (18) -C (17)	123.4 (3)
N (4) -C (19) -C (20)	123.3 (3)
C (19) -C (20) -C (16)	118.8 (3)
C (22) -C (21) -C (15)	119.7 (2)
N (3) -C (22) -C (21)	122.6 (2)
C (14) -C (15) -C (21)	117.5 (2)
C (14) -C (15) -C (16)	120.0 (2)
C (21) -C (15) -C (16)	122.5 (2)
C (17) -C (16) -C (20)	118.0 (3)
C (17) -C (16) -C (15)	120.6 (2)
C (20) -C (16) -C (15)	121.4 (2)
C (11) -O (2) -Cu (1) #2	121.91 (14)

Symmetry transformations used to generate equivalent atoms:

#1 $x, -y, z+1/2$ #2 $x, -y, z-1/2$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct7.

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)	21 (1)	25 (1)	10 (1)	-2 (1)	2 (1)	5 (1)
N (1)	18 (1)	20 (1)	12 (1)	-1 (1)	1 (1)	2 (1)
N (2)	24 (1)	21 (1)	13 (1)	1 (1)	0 (1)	1 (1)
N (3)	24 (1)	26 (1)	17 (1)	-5 (1)	3 (1)	1 (1)
N (4)	43 (2)	30 (1)	120 (3)	-9 (1)	7 (2)	7 (1)
C (1)	20 (1)	25 (1)	18 (1)	-1 (1)	2 (1)	7 (1)
C (2)	22 (1)	24 (1)	16 (1)	3 (1)	-1 (1)	4 (1)
C (3)	19 (1)	21 (1)	13 (1)	1 (1)	3 (1)	-2 (1)
C (4)	16 (1)	21 (1)	17 (1)	-1 (1)	3 (1)	1 (1)
C (5)	16 (1)	17 (1)	14 (1)	0 (1)	1 (1)	0 (1)
C (6)	17 (1)	17 (1)	13 (1)	-1 (1)	0 (1)	-1 (1)
C (7)	18 (1)	22 (1)	17 (1)	-3 (1)	1 (1)	1 (1)
C (8)	19 (1)	18 (1)	25 (1)	-1 (1)	-5 (1)	-1 (1)
C (9)	28 (1)	26 (1)	21 (1)	5 (1)	-6 (1)	2 (1)
C (10)	32 (1)	29 (1)	14 (1)	2 (1)	0 (1)	1 (1)
C (11)	24 (1)	31 (1)	14 (1)	0 (1)	2 (1)	-3 (1)
C (12)	18 (1)	19 (1)	49 (2)	-2 (1)	-8 (1)	0 (1)
C (13)	27 (1)	25 (1)	27 (1)	-2 (1)	6 (1)	1 (1)
C (14)	23 (1)	29 (1)	39 (1)	-6 (1)	4 (1)	3 (1)
C (17)	37 (2)	30 (2)	99 (3)	-2 (2)	-6 (2)	0 (1)
C (18)	39 (2)	35 (2)	130 (4)	-1 (2)	-9 (2)	6 (1)
C (19)	48 (2)	28 (2)	101 (3)	-17 (2)	6 (2)	-1 (1)
C (20)	36 (2)	34 (2)	80 (2)	-12 (1)	2 (2)	0 (1)
C (21)	32 (1)	24 (1)	61 (2)	-2 (1)	7 (1)	-3 (1)
C (22)	25 (1)	31 (1)	39 (1)	-3 (1)	7 (1)	0 (1)
C (15)	28 (1)	24 (1)	47 (2)	-8 (1)	-2 (1)	1 (1)
C (16)	34 (2)	28 (1)	63 (2)	-3 (1)	2 (1)	1 (1)
O (1)	46 (1)	73 (1)	20 (1)	3 (1)	11 (1)	30 (1)
O (2)	31 (1)	33 (1)	11 (1)	4 (1)	3 (1)	1 (1)
O (3)	29 (1)	56 (1)	45 (1)	-22 (1)	-8 (1)	20 (1)
O (4)	31 (1)	52 (1)	68 (1)	30 (1)	-4 (1)	14 (1)

O (5)	27 (1)	33 (1)	23 (1)	-5 (1)	3 (1)	-4 (1)
O (6)	57 (1)	36 (1)	82 (2)	-3 (1)	42 (1)	-4 (1)
O (7)	54 (1)	47 (1)	48 (1)	4 (1)	25 (1)	4 (1)
O (8)	39 (1)	60 (1)	30 (1)	1 (1)	4 (1)	17 (1)
O (9)	56 (2)	33 (1)	35 (2)	0	-20 (1)	0
O (10)	31 (1)	29 (1)	54 (1)	-4 (1)	12 (1)	-3 (1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct7.

	x	y	z	U(eq)
H(1)	1533	802	-298	25
H(2)	1686	768	-1575	25
H(4)	3018	-1314	-1063	21
H(7)	3532	-2148	-149	23
H(9)	3645	-2905	2087	31
H(10)	2885	-1734	2229	30
H(13)	946	462	1509	31
H(14)	358	1967	1505	37
H(17)	-149	3326	649	67
H(18)	-720	4846	715	83
H(19)	583	6484	1726	71
H(20)	1197	5014	1701	60
H(21)	1689	3715	833	46
H(22)	2235	2157	845	38
H(5A)	1210(8)	-1540(20)	1477(9)	42
H(5B)	1157(7)	-1410(20)	769(9)	42
H(6B)	183(12)	-730(30)	4193(10)	84
H(6A)	96(8)	-980(30)	4850(15)	84
H(7A)	571(12)	-1204(18)	2355(17)	73
H(7B)	813(15)	-1930(20)	2760(6)	73
H(8A)	1586(10)	-3337(18)	4003(16)	64
H(8B)	1849(14)	-3810(30)	3519(3)	64
H(9A)	158(13)	358(6)	2807(11)	64
H(10A)	716(11)	-2106(18)	4125(13)	57
H(10B)	636(10)	-2986(15)	3794(16)	57

