

Table 1. Crystal data and structure refinement for struct1.

Identification code	struct1
Empirical formula	C12 H14 Cu N2 O8
Formula weight	377.79
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pnna
Unit cell dimensions	a = 14.7685(9) Å α = 90°. b = 10.8176(7) Å β = 90°. c = 9.0272(5) Å γ = 90°.
Volume	1442.18(15) Å ³
Calculated density	1.740 Mg/m ³
Z	4
Absorption coefficient	1.560 mm ⁻¹
F(000)	772
Crystal size	0.2 x 0.15 x 0.1 mm ³
Theta range for data collection	2.64 to 25.00°.
Limiting indices	-17<=h<=17, -12<=k<=12, -10<=l<=10
Reflections collected	10531
Independent reflections	1276 [R(int) = 0.0555]
Completeness to theta = 25.00°	99.9 %
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.787
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1276 / 6 / 123
Goodness-of-fit on F ²	1.274
Final R indices [I>2sigma(I)]	R1 = 0.0532, wR2 = 0.1059
R indices (all data)	R1 = 0.0585, wR2 = 0.1076
Largest diff. peak and hole	0.428 and -0.538 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Cu(1)	3322(1)	2500	7500	15(1)
N(1)	2290(2)	1987(4)	6200(4)	16(1)
C(1)	1457(3)	2243(4)	6730(5)	12(1)
C(2)	687(3)	2048(4)	5908(5)	14(1)
C(3)	780(3)	1544(4)	4485(5)	13(1)
C(4)	1632(3)	1291(4)	3946(5)	17(1)
C(5)	2376(3)	1539(4)	4844(5)	18(1)
C(6)	-63(3)	1281(4)	3551(5)	15(1)
O(1)	3341(3)	591(4)	8946(4)	27(1)
O(2)	-752(2)	1924(3)	3895(3)	17(1)
O(3)	-9(2)	493(3)	2556(4)	24(1)
O(4)	1306(3)	-1293(4)	1883(5)	38(1)

Table 3. Bond lengths [Å] and angles [°] for struct1.

Cu(1)-O(2)#1	1.960(3)
Cu(1)-O(2)#2	1.960(3)
Cu(1)-N(1)	2.002(4)
Cu(1)-N(1)#3	2.002(4)
N(1)-C(5)	1.323(6)
N(1)-C(1)	1.349(5)
C(1)-C(2)	1.374(6)
C(1)-C(1)#3	1.497(9)
C(2)-C(3)	1.402(6)
C(3)-C(4)	1.377(7)
C(3)-C(6)	1.530(6)
C(4)-C(5)	1.392(7)
C(6)-O(3)	1.241(6)
C(6)-O(2)	1.270(6)
O(2)-Cu(1)#4	1.960(3)
O(2)#1-Cu(1)-O(2)#2	91.55(19)
O(2)#1-Cu(1)-N(1)	174.60(15)
O(2)#2-Cu(1)-N(1)	93.81(14)
O(2)#1-Cu(1)-N(1)#3	93.81(14)
O(2)#2-Cu(1)-N(1)#3	174.60(15)
N(1)-Cu(1)-N(1)#3	80.8(2)
C(5)-N(1)-C(1)	119.4(4)
C(5)-N(1)-Cu(1)	124.8(3)
C(1)-N(1)-Cu(1)	115.4(3)
N(1)-C(1)-C(2)	122.1(4)
N(1)-C(1)-C(1)#3	113.9(3)
C(2)-C(1)-C(1)#3	124.0(3)
C(1)-C(2)-C(3)	118.3(4)
C(4)-C(3)-C(2)	119.4(4)
C(4)-C(3)-C(6)	120.8(4)
C(2)-C(3)-C(6)	119.9(4)

C (3) -C (4) -C (5)	118.5 (4)
N (1) -C (5) -C (4)	122.3 (4)
O (3) -C (6) -O (2)	127.2 (4)
O (3) -C (6) -C (3)	118.3 (4)
O (2) -C (6) -C (3)	114.5 (4)
C (6) -O (2) -Cu (1) #4	125.1 (3)

Symmetry transformations used to generate equivalent atoms:

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

#3 $x, -y+1/2, -z+3/2$ #4 $x-1/2, y, -z+1$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct1.

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)	8 (1)	24 (1)	13 (1)	0 (1)	0	0
N (1)	8 (2)	23 (2)	16 (2)	3 (2)	3 (2)	1 (2)
C (1)	9 (2)	13 (2)	15 (2)	3 (2)	0 (2)	-1 (2)
C (2)	12 (2)	16 (2)	13 (2)	0 (2)	1 (2)	2 (2)
C (3)	14 (2)	11 (2)	15 (2)	4 (2)	-3 (2)	-2 (2)
C (4)	16 (2)	23 (3)	14 (2)	-2 (2)	-1 (2)	0 (2)
C (5)	13 (2)	21 (3)	19 (3)	2 (2)	3 (2)	0 (2)
C (6)	13 (2)	17 (2)	14 (2)	4 (2)	-1 (2)	0 (2)
O (1)	17 (2)	39 (2)	25 (2)	6 (2)	3 (2)	-2 (2)
O (2)	12 (2)	27 (2)	13 (2)	-2 (2)	-3 (1)	3 (2)
O (3)	21 (2)	29 (2)	23 (2)	-9 (2)	-6 (2)	5 (2)
O (4)	43 (2)	43 (3)	27 (2)	-9 (2)	-11 (2)	22 (2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct1.

	x	y	z	U(eq)
H(2)	107	2249	6294	16
H(4)	1710	955	2982	21
H(5)	2966	1381	4470	21
H(1A)	3830(20)	380(60)	8560(60)	40
H(1B)	2830(40)	280(110)	8760(120)	40
H(1C)	3430(90)	650(110)	9860(30)	40
H(4A)	920(30)	-760(50)	2100(80)	56
H(4B)	1310(90)	-1960(70)	2340(150)	56
H(4C)	1340(100)	-1200(130)	970(30)	56

