

Table 1. Crystal data and structure refinement for structure11.

Identification code	structure11	
Empirical formula	C12 H10 Cu N4 O11	
Formula weight	449.78	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 6.4404(4) Å	$\alpha = 76.3390(10)^\circ$.
	b = 9.7045(6) Å	$\beta = 84.2050(10)^\circ$.
	c = 13.6309(8) Å	$\gamma = 78.8940(10)^\circ$.
Volume	810.96(9) Å ³	
Z	2	
Calculated density	1.842 Mg/m ³	
Absorption coefficient	1.421 mm ⁻¹	
F(000)	454	
Crystal size	0.48 x 0.08 x 0.07 mm ³	
Theta range for data collection	1.54 to 29.98°.	
Limiting indices	-9<=h<=8, -13<=k<=13, -18<=l<=18	
Reflections collected	8948	
Independent reflections	4456 [R(int) = 0.0324]	
Completeness to theta = 29.98°	94.6%	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.770	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4456 / 2 / 261	
Goodness-of-fit on F ²	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0478, wR2 = 0.1221	
R indices (all data)	R1 = 0.0547, wR2 = 0.1255	
Largest diff. peak and hole	3.024 and -0.405 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct11. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Cu(1)	1991(1)	8769(1)	2882(1)	18(1)
O(10)	800(3)	10835(2)	2388(2)	25(1)
O(11)	4112(3)	9300(2)	3618(2)	25(1)
O(2)	-5295(3)	6666(2)	383(2)	28(1)
N(1)	178(4)	8026(2)	2105(2)	20(1)
N(2)	3493(4)	6741(2)	3113(2)	18(1)
O(9)	1597(4)	12646(2)	1231(2)	30(1)
O(3)	5814(3)	1658(2)	2780(2)	25(1)
O(4)	7627(3)	1810(2)	4068(2)	27(1)
O(7)	-448(3)	9157(2)	4117(2)	24(1)
N(3)	-1291(4)	8147(3)	4715(2)	22(1)
O(1)	-2660(4)	4747(2)	490(2)	30(1)
O(8)	3381(4)	10483(2)	1278(2)	35(1)
N(4)	1956(4)	11345(3)	1605(2)	23(1)
O(6)	-2675(4)	8481(3)	5355(2)	34(1)
C(12)	6296(4)	2325(3)	3346(2)	20(1)
C(11)	-3440(4)	5975(3)	620(2)	21(1)
C(8)	5352(4)	3883(3)	3278(2)	19(1)
C(6)	2670(4)	5886(3)	2662(2)	18(1)
C(1)	-1553(5)	8784(3)	1631(2)	23(1)
C(4)	-372(4)	5923(3)	1611(2)	20(1)
C(5)	760(4)	6616(3)	2098(2)	18(1)
O(5)	-670(4)	6893(2)	4635(2)	38(1)
C(10)	5207(5)	6181(3)	3650(2)	22(1)
C(7)	3556(4)	4458(3)	2727(2)	19(1)
C(9)	6200(4)	4753(3)	3750(2)	22(1)
C(3)	-2164(4)	6719(3)	1122(2)	19(1)
C(2)	-2757(5)	8170(3)	1133(2)	23(1)

Table 3. Bond lengths [Å] and angles [°] for struct11.

Cu(1)-O(11)	1.983(2)
Cu(1)-O(10)	1.984(2)
Cu(1)-N(1)	1.985(2)
Cu(1)-N(2)	1.986(2)
Cu(1)-O(7)	2.231(2)
O(10)-N(4)	1.293(3)
O(2)-C(11)	1.284(3)
N(1)-C(1)	1.344(3)
N(1)-C(5)	1.349(3)
N(2)-C(10)	1.339(3)
N(2)-C(6)	1.351(3)
O(9)-N(4)	1.230(3)
O(3)-C(12)	1.213(3)
O(4)-C(12)	1.314(3)
O(7)-N(3)	1.287(3)
N(3)-O(5)	1.232(3)
N(3)-O(6)	1.235(3)
O(1)-C(11)	1.247(3)
O(8)-N(4)	1.240(3)
C(12)-C(8)	1.502(4)
C(11)-C(3)	1.497(4)
C(8)-C(9)	1.389(4)
C(8)-C(7)	1.394(4)
C(6)-C(7)	1.378(4)
C(6)-C(5)	1.484(4)
C(1)-C(2)	1.376(4)
C(4)-C(5)	1.387(4)
C(4)-C(3)	1.394(4)
C(10)-C(9)	1.391(4)
C(3)-C(2)	1.389(4)
O(11)-Cu(1)-O(10)	90.23(9)
O(11)-Cu(1)-N(1)	172.21(9)
O(10)-Cu(1)-N(1)	95.94(9)
O(11)-Cu(1)-N(2)	91.25(9)

O(10)-Cu(1)-N(2)	168.69(9)
N(1)-Cu(1)-N(2)	81.78(9)
O(11)-Cu(1)-O(7)	89.41(9)
O(10)-Cu(1)-O(7)	78.57(8)
N(1)-Cu(1)-O(7)	96.46(9)
N(2)-Cu(1)-O(7)	112.66(8)
N(4)-O(10)-Cu(1)	108.21(16)
C(1)-N(1)-C(5)	119.4(2)
C(1)-N(1)-Cu(1)	125.93(19)
C(5)-N(1)-Cu(1)	114.69(18)
C(10)-N(2)-C(6)	119.0(2)
C(10)-N(2)-Cu(1)	126.27(18)
C(6)-N(2)-Cu(1)	114.70(18)
N(3)-O(7)-Cu(1)	123.23(16)
O(5)-N(3)-O(6)	122.8(3)
O(5)-N(3)-O(7)	119.0(2)
O(6)-N(3)-O(7)	118.2(2)
O(9)-N(4)-O(8)	123.8(3)
O(9)-N(4)-O(10)	118.7(2)
O(8)-N(4)-O(10)	117.5(2)
O(3)-C(12)-O(4)	125.9(3)
O(3)-C(12)-C(8)	121.2(2)
O(4)-C(12)-C(8)	112.8(2)
O(1)-C(11)-O(2)	125.8(3)
O(1)-C(11)-C(3)	118.5(2)
O(2)-C(11)-C(3)	115.7(2)
C(9)-C(8)-C(7)	119.5(2)
C(9)-C(8)-C(12)	122.2(2)
C(7)-C(8)-C(12)	118.3(2)
N(2)-C(6)-C(7)	122.0(2)
N(2)-C(6)-C(5)	114.3(2)
C(7)-C(6)-C(5)	123.7(2)
N(1)-C(1)-C(2)	122.1(2)
C(5)-C(4)-C(3)	118.3(2)
N(1)-C(5)-C(4)	121.9(2)
N(1)-C(5)-C(6)	114.5(2)
C(4)-C(5)-C(6)	123.6(2)

N (2) -C (10) -C (9)	122.6 (2)
C (6) -C (7) -C (8)	118.9 (2)
C (8) -C (9) -C (10)	118.0 (3)
C (2) -C (3) -C (4)	119.5 (2)
C (2) -C (3) -C (11)	121.5 (2)
C (4) -C (3) -C (11)	119.0 (2)
C (1) -C (2) -C (3)	118.9 (3)

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct11.

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)	12 (1)	21 (1)	-5 (1)	-3 (1)	-1 (1)
O (10)	29 (1)	18 (1)	27 (1)	-4 (1)	4 (1)	-2 (1)
O (11)	28 (1)	20 (1)	29 (1)	-8 (1)	-2 (1)	-7 (1)
O (2)	20 (1)	34 (1)	33 (1)	-14 (1)	-5 (1)	-2 (1)
N (1)	21 (1)	16 (1)	21 (1)	-5 (1)	-4 (1)	1 (1)
N (2)	20 (1)	15 (1)	19 (1)	-4 (1)	-3 (1)	-2 (1)
O (9)	41 (1)	15 (1)	30 (1)	0 (1)	-2 (1)	-1 (1)
O (3)	25 (1)	19 (1)	32 (1)	-9 (1)	-5 (1)	-2 (1)
O (4)	30 (1)	20 (1)	30 (1)	-7 (1)	-11 (1)	6 (1)
O (7)	26 (1)	16 (1)	26 (1)	-3 (1)	1 (1)	-1 (1)
N (3)	22 (1)	22 (1)	24 (1)	-7 (1)	-1 (1)	-5 (1)
O (1)	30 (1)	22 (1)	39 (1)	-11 (1)	-11 (1)	-1 (1)
O (8)	42 (1)	25 (1)	33 (1)	-8 (1)	8 (1)	5 (1)
N (4)	28 (1)	17 (1)	23 (1)	-5 (1)	-5 (1)	-1 (1)
O (6)	33 (1)	32 (1)	37 (1)	-13 (1)	14 (1)	-9 (1)
C (12)	19 (1)	16 (1)	24 (1)	-3 (1)	1 (1)	-3 (1)
C (11)	19 (1)	22 (1)	21 (1)	-5 (1)	-3 (1)	-3 (1)
C (8)	18 (1)	16 (1)	21 (1)	-3 (1)	-1 (1)	-2 (1)
C (6)	19 (1)	15 (1)	17 (1)	-3 (1)	-2 (1)	-3 (1)
C (1)	28 (1)	15 (1)	26 (1)	-7 (1)	-6 (1)	3 (1)
C (4)	21 (1)	16 (1)	21 (1)	-5 (1)	-2 (1)	-1 (1)
C (5)	19 (1)	15 (1)	18 (1)	-3 (1)	-2 (1)	1 (1)
O (5)	45 (1)	20 (1)	51 (2)	-13 (1)	5 (1)	-6 (1)
C (10)	25 (1)	18 (1)	25 (1)	-6 (1)	-5 (1)	-5 (1)
C (7)	21 (1)	15 (1)	21 (1)	-6 (1)	-3 (1)	-2 (1)
C (9)	23 (1)	17 (1)	24 (1)	-3 (1)	-5 (1)	-2 (1)
C (3)	18 (1)	20 (1)	20 (1)	-6 (1)	-1 (1)	-2 (1)
C (2)	22 (1)	20 (1)	26 (1)	-7 (1)	-6 (1)	3 (1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct11.

	x	y	z	U(eq)
H(2A)	-5898	6175	107	42
H(4A)	8113	939	4077	41
H(1)	-1959	9775	1641	28
H(4)	63	4930	1611	24
H(10)	5767	6783	3975	27
H(7)	2954	3877	2402	23
H(9)	7422	4383	4130	26
H(2)	-3974	8728	803	28
H(11B)	3530 (50)	9610 (40)	4123 (18)	31 (10)
H(11A)	4790 (60)	9930 (30)	3280 (30)	41 (11)

