

Table 1. Crystal data and structure refinement for Struct14.

Identification code	Struct14
Empirical formula	C ₂₈ H ₃₈ Cu N ₆ O ₁₃
Formula weight	730.18
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 31.125(10) Å α = 90°. b = 7.174(2) Å β = 108.528(6)°. c = 14.457(5) Å γ = 90°.
Volume	3060.8(17) Å ³
Z	4
Calculated density	1.585 Mg/m ³
Absorption coefficient	0.793 mm ⁻¹
F(000)	1524
Crystal size	0.23 x 0.11 x 0.01 mm ³
Theta range for data collection	2.76 to 22.50°.
Limiting indices	-33<=h<=33, -7<=k<=7, -15<=l<=15
Reflections collected	10898
Independent reflections	2000 [R(int) = 0.0865]
Completeness to theta = 22.50°	99.7 %
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.770
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	2000 / 18 / 235
Goodness-of-fit on F ²	1.053
Final R indices [I>2sigma(I)]	R1 = 0.0598, wR2 = 0.1323
R indices (all data)	R1 = 0.0859, wR2 = 0.1442
Largest diff. peak and hole	0.575 and -0.479 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Struct14. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	0	3949(2)	2500	23(1)
C(1)	735(2)	1968(8)	1870(4)	24(1)
C(2)	917(2)	1252(8)	1193(4)	25(1)
C(3)	668(2)	1315(8)	208(4)	21(1)
C(4)	233(2)	2006(8)	-51(4)	19(1)
C(5)	66(2)	2693(7)	668(4)	18(1)
C(6)	-402(2)	3441(7)	453(4)	19(1)
C(7)	-720(2)	3530(7)	-464(4)	20(1)
C(8)	-1145(2)	4221(8)	-574(4)	23(1)
C(9)	-1240(2)	4885(8)	239(4)	25(1)
C(10)	-911(2)	4772(8)	1137(4)	26(1)
C(11)	866(2)	622(8)	-572(4)	28(2)
C(12)	-1494(2)	4235(10)	-1582(4)	36(2)
C(13)	2855(4)	-1779(17)	1356(8)	113(4)
C(14)	2186(3)	8(19)	1409(7)	114(4)
N(1)	320(1)	2708(6)	1623(3)	20(1)
N(2)	-501(1)	4045(7)	1254(3)	23(1)
N(3)	2657(3)	51(13)	1342(5)	89(2)
O(1)	619(1)	764(6)	-1444(3)	38(1)
O(2)	1258(1)	-13(6)	-284(3)	39(1)
O(3)	-1377(1)	3752(7)	-2291(3)	45(1)
O(4)	-1890(2)	4676(10)	-1628(3)	79(2)
O(5)	0	6882(8)	2500	39(2)
O(6)	1698(2)	576(9)	-1605(4)	66(2)
O(7)	2583(2)	963(12)	-600(4)	111(3)

Table 3. Bond lengths [Å] and angles [°] for Struct14.

Cu(1)-N(2)	1.974(4)
Cu(1)-N(2)#1	1.974(4)
Cu(1)-N(1)#1	2.048(4)
Cu(1)-N(1)	2.048(4)
Cu(1)-O(5)	2.104(6)
C(1)-N(1)	1.336(7)
C(1)-C(2)	1.375(7)
C(2)-C(3)	1.389(7)
C(3)-C(4)	1.378(7)
C(3)-C(11)	1.531(8)
C(4)-C(5)	1.390(7)
C(5)-N(1)	1.356(7)
C(5)-C(6)	1.491(7)
C(6)-N(2)	1.361(7)
C(6)-C(7)	1.380(7)
C(7)-C(8)	1.376(7)
C(8)-C(9)	1.385(8)
C(8)-C(12)	1.516(8)
C(9)-C(10)	1.377(7)
C(10)-N(2)	1.337(7)
C(11)-O(2)	1.241(7)
C(11)-O(1)	1.255(7)
C(12)-O(3)	1.240(7)
C(12)-O(4)	1.255(7)
C(13)-N(3)	1.448(12)
C(14)-N(3)	1.499(11)
N(2)-Cu(1)-N(2)#1	176.0(3)
N(2)-Cu(1)-N(1)#1	100.43(17)
N(2)#1-Cu(1)-N(1)#1	81.34(17)
N(2)-Cu(1)-N(1)	81.34(17)
N(2)#1-Cu(1)-N(1)	100.43(17)
N(1)#1-Cu(1)-N(1)	128.5(2)
N(2)-Cu(1)-O(5)	87.99(14)
N(2)#1-Cu(1)-O(5)	87.99(14)
N(1)#1-Cu(1)-O(5)	115.76(12)
N(1)-Cu(1)-O(5)	115.76(12)
N(1)-C(1)-C(2)	122.7(5)
C(1)-C(2)-C(3)	119.7(5)
C(4)-C(3)-C(2)	118.0(5)
C(4)-C(3)-C(11)	120.6(5)
C(2)-C(3)-C(11)	121.4(5)
C(3)-C(4)-C(5)	119.5(5)
N(1)-C(5)-C(4)	121.9(5)
N(1)-C(5)-C(6)	115.1(5)
C(4)-C(5)-C(6)	123.0(5)
N(2)-C(6)-C(7)	121.1(5)
N(2)-C(6)-C(5)	114.1(5)
C(7)-C(6)-C(5)	124.8(5)
C(8)-C(7)-C(6)	119.8(5)
C(7)-C(8)-C(9)	118.9(5)
C(7)-C(8)-C(12)	118.9(5)
C(9)-C(8)-C(12)	122.3(5)
C(10)-C(9)-C(8)	119.0(5)
N(2)-C(10)-C(9)	122.5(5)
O(2)-C(11)-O(1)	126.1(5)
O(2)-C(11)-C(3)	117.0(5)

O(1)-C(11)-C(3)	116.9(5)
O(3)-C(12)-O(4)	124.6(6)
O(3)-C(12)-C(8)	118.9(5)
O(4)-C(12)-C(8)	116.4(5)
C(1)-N(1)-C(5)	118.0(5)
C(1)-N(1)-Cu(1)	128.8(4)
C(5)-N(1)-Cu(1)	113.2(3)
C(10)-N(2)-C(6)	118.7(4)
C(10)-N(2)-Cu(1)	125.1(4)
C(6)-N(2)-Cu(1)	116.0(4)
C(13)-N(3)-C(14)	113.6(10)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y,-z+1/2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Struct14.
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)	19(1)	40(1)	11(1)	0	5(1)	0
C(1)	26(3)	29(4)	17(3)	3(3)	5(3)	2(3)
C(2)	24(3)	24(4)	30(3)	3(3)	13(3)	2(3)
C(3)	26(3)	16(3)	23(3)	1(3)	11(3)	0(3)
C(4)	24(3)	21(3)	14(3)	-3(2)	8(3)	0(3)
C(5)	17(3)	18(3)	20(3)	1(3)	6(3)	-3(2)
C(6)	27(3)	16(3)	18(3)	0(2)	13(3)	-4(3)
C(7)	30(3)	19(4)	12(3)	1(2)	8(2)	-7(3)
C(8)	18(3)	28(4)	22(3)	-2(3)	6(2)	-10(3)
C(9)	19(3)	33(4)	27(3)	1(3)	11(3)	1(3)
C(10)	22(3)	42(4)	18(3)	-3(3)	11(3)	3(3)
C(11)	33(4)	26(4)	32(4)	-1(3)	19(3)	3(3)
C(12)	26(4)	50(5)	31(4)	3(3)	6(3)	-4(3)
C(13)	138(10)	116(10)	88(8)	-9(7)	38(7)	3(9)
C(14)	51(6)	216(14)	72(7)	-2(8)	17(5)	0(7)
N(1)	17(3)	27(3)	17(3)	5(2)	8(2)	2(2)
N(2)	23(3)	33(3)	14(2)	-1(2)	7(2)	-2(2)
N(3)	82(6)	112(7)	54(5)	0(5)	-3(4)	10(5)
O(1)	41(3)	52(3)	22(2)	-8(2)	10(2)	14(2)
O(2)	36(3)	55(3)	33(2)	8(2)	21(2)	17(2)
O(3)	38(3)	79(4)	17(2)	-5(2)	10(2)	-6(2)
O(4)	29(3)	177(7)	28(3)	3(3)	5(2)	17(3)
O(5)	38(4)	33(4)	33(4)	0	-6(3)	0
O(6)	47(3)	104(5)	54(3)	18(3)	27(3)	19(3)
O(7)	67(4)	204(8)	61(4)	-10(5)	21(3)	2(5)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Struct14.

	x	y	z	U(eq)
H(1)	912	1935	2540	29
H(2)	1212	717	1399	30
H(4)	48	2012	-715	23
H(7)	-644	3114	-1017	24
H(9)	-1528	5411	179	31
H(10)	-977	5226	1694	31
H(13A)	2859	-2434	1954	170
H(13B)	3165	-1650	1337	170
H(13C)	2674	-2491	787	170
H(14A)	1985	-652	843	171
H(14B)	2077	1287	1420	171
H(14C)	2189	-638	2008	171
H(3A)	2651	649	775	107
H(3B)	2839	736	1856	107
H(5)	250 (2)	7550 (30)	2720 (30)	58
H(6A)	1525 (18)	190 (80)	-1250 (40)	99
H(6B)	1570 (20)	1570 (70)	-1980 (50)	99
H(7A)	2770 (30)	920 (70)	-980 (60)	166
H(7B)	2313 (9)	430 (70)	-930 (60)	166

