

Table 1. Crystal data and structure refinement for structure15.

Identification code	structure15
Empirical formula	C ₂₄ H ₃₄ Cu N ₄ Na ₂ O ₁₉
Formula weight	792.07
Temperature	153(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2(1)/c
Unit cell dimensions	a = 14.507(3) Å α = 90°. b = 7.007(2) Å β = 90.015(3)°. c = 31.118(5) Å γ = 90°.
Volume	3163.2(12) Å ³
Z	4
Calculated density	1.663 Mg/m ³
Absorption coefficient	0.810 mm ⁻¹
F(000)	1636
Crystal size	0.35 x 0.08 x 0.05 mm ³
Theta range for data collection	1.40 to 25.00°.
Limiting indices	-17<=h<=16, -8<=k<=8, -37<=l<=36
Reflections collected	29738
Independent reflections	5548 [R(int) = 0.0787]
Completeness to theta = 25.00°	99.4%
Absorption correction	Empirical
Max. and min. transmission	1.000 and 0.898
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5548 / 433 / 333
Goodness-of-fit on F ²	1.228
Final R indices [I>2sigma(I)]	R1 = 0.0814, wR2 = 0.1851
R indices (all data)	R1 = 0.0947, wR2 = 0.1906
Largest diff. peak and hole	1.297 and -0.728 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct15. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cu(1)	2497(1)	1210(1)	-36(1)	15(1)
N(1)	1381(5)	2437(10)	239(2)	13(2)
C(1)	1341(6)	3274(11)	620(2)	13(2)
C(2)	542(5)	4019(12)	798(3)	17(2)
C(3)	-269(5)	3804(12)	572(2)	14(2)
C(11)	-1183(5)	4406(12)	766(2)	13(2)
O(1)	-1887(4)	4370(9)	538(2)	23(2)
O(2)	-1173(4)	5006(8)	1145(2)	16(1)
C(4)	-234(5)	2925(12)	168(2)	16(2)
C(5)	599(5)	2276(11)	9(2)	12(2)
C(6)	733(5)	1414(12)	-425(2)	14(2)
C(7)	51(5)	1115(11)	-723(2)	10(2)
O(4)	-181(4)	-812(8)	-1798(2)	18(1)
O(3)	-1285(4)	-12(7)	-1330(2)	9(1)
C(12)	-476(5)	-179(11)	-1444(2)	9(2)
C(8)	277(5)	289(12)	-1120(2)	13(2)
C(9)	1184(5)	-186(13)	-1204(3)	17(2)
C(10)	1823(6)	153(11)	-887(2)	11(2)
N(2)	1616(4)	913(10)	-510(2)	12(2)
N(3)	3374(4)	1163(10)	442(2)	14(2)
C(13)	3177(6)	439(12)	827(2)	16(2)
C(14)	3838(5)	243(11)	1142(2)	7(2)
C(15)	4735(5)	851(12)	1054(2)	12(2)
C(23)	5462(5)	755(11)	1402(2)	11(2)
O(5)	6263(4)	1286(9)	1297(2)	28(2)
O(6)	5212(4)	166(8)	1760(2)	17(1)
C(16)	4936(5)	1548(11)	647(2)	11(2)
C(17)	4254(5)	1649(11)	345(2)	7(2)
C(18)	4378(5)	2383(11)	-101(2)	10(2)
C(19)	5194(5)	3058(11)	-260(2)	12(2)
O(8)	6137(4)	5026(8)	-1251(2)	19(1)
O(7)	6861(4)	4192(9)	-649(2)	23(2)
C(24)	6155(5)	4373(12)	-873(2)	14(2)
C(20)	5241(5)	3719(12)	-680(2)	16(2)
C(21)	4430(5)	3858(12)	-906(2)	14(2)
C(22)	3623(6)	3167(12)	-730(2)	16(2)
N(4)	3599(4)	2382(10)	-337(2)	11(1)
Na(1)	2504(3)	3342(4)	2470(1)	16(1)
Na(2)	2493(3)	-1649(4)	2553(1)	18(1)
O(9)	2520(5)	-1758(7)	17(2)	23(1)
O(10)	1415(5)	848(10)	2480(2)	17(1)
O(11)	3702(4)	736(10)	2434(2)	19(2)
O(12)	3573(4)	5859(10)	2567(2)	15(1)
O(13)	1287(5)	5822(10)	2554(2)	22(2)
O(14)	2735(5)	3018(10)	3209(2)	29(2)
O(15)	2387(5)	3377(9)	1703(2)	29(2)
O(16)	2464(5)	-2230(8)	1805(2)	27(1)
O(17)	2625(4)	-992(9)	3316(2)	21(1)
O(18)	-87(4)	4969(10)	1878(2)	22(1)
O(19)	4878(4)	6410(9)	1928(2)	21(1)

Table 3. Bond lengths [Å] and angles [°] for struct15.

Cu(1)-N(3)	1.955(7)
Cu(1)-N(2)	1.962(6)
Cu(1)-N(1)	2.022(7)
Cu(1)-N(4)	2.028(6)
Cu(1)-O(9)	2.086(5)
N(1)-C(1)	1.323(9)
N(1)-C(5)	1.345(9)
C(1)-C(2)	1.388(10)
C(2)-C(3)	1.378(10)
C(3)-C(4)	1.402(9)
C(3)-C(11)	1.518(9)
C(11)-O(1)	1.244(9)
C(11)-O(2)	1.251(8)
C(4)-C(5)	1.381(9)
C(5)-C(6)	1.493(10)
C(6)-N(2)	1.354(9)
C(6)-C(7)	1.372(9)
C(7)-C(8)	1.403(9)
O(4)-C(12)	1.262(8)
O(3)-C(12)	1.232(8)
C(12)-C(8)	1.524(9)
C(8)-C(9)	1.383(10)
C(9)-C(10)	1.373(10)
C(10)-N(2)	1.325(9)
N(3)-C(13)	1.334(9)
N(3)-C(17)	1.356(9)
C(13)-C(14)	1.379(9)
C(14)-C(15)	1.396(9)
C(15)-C(16)	1.388(9)
C(15)-C(23)	1.514(9)
C(23)-O(6)	1.242(8)
C(23)-O(5)	1.262(9)
C(16)-C(17)	1.367(9)
C(17)-C(18)	1.491(9)
C(18)-N(4)	1.346(9)
C(18)-C(19)	1.367(9)
C(19)-C(20)	1.389(9)
O(8)-C(24)	1.262(8)
O(7)-C(24)	1.244(9)
C(24)-C(20)	1.527(9)
C(20)-C(21)	1.374(9)
C(21)-C(22)	1.381(10)
C(22)-N(4)	1.343(9)
Na(1)-O(14)	2.335(6)
Na(1)-O(10)	2.356(8)
Na(1)-O(12)	2.368(7)
Na(1)-O(15)	2.394(6)
Na(1)-O(13)	2.491(8)
Na(1)-O(11)	2.523(8)
Na(1)-Na(2)	3.507(4)
Na(1)-Na(2)#1	3.519(4)
Na(2)-O(12)#2	2.346(7)
Na(2)-O(10)	2.358(8)
Na(2)-O(16)	2.365(6)
Na(2)-O(17)	2.427(6)
Na(2)-O(11)	2.451(8)
Na(2)-O(13)#2	2.490(8)

Na (2) -Na (1) #2	3.519 (4)
O (12) -Na (2) #1	2.346 (7)
O (13) -Na (2) #1	2.490 (8)

N (3) -Cu (1) -N (2)	173.0 (3)
N (3) -Cu (1) -N (1)	102.0 (3)
N (2) -Cu (1) -N (1)	80.9 (3)
N (3) -Cu (1) -N (4)	81.1 (3)
N (2) -Cu (1) -N (4)	102.0 (3)
N (1) -Cu (1) -N (4)	130.9 (3)
N (3) -Cu (1) -O (9)	85.0 (3)
N (2) -Cu (1) -O (9)	88.0 (3)
N (1) -Cu (1) -O (9)	113.8 (3)
N (4) -Cu (1) -O (9)	115.3 (3)
C (1) -N (1) -C (5)	118.4 (7)
C (1) -N (1) -Cu (1)	127.0 (6)
C (5) -N (1) -Cu (1)	114.5 (5)
N (1) -C (1) -C (2)	124.1 (8)
C (3) -C (2) -C (1)	117.9 (7)
C (2) -C (3) -C (4)	118.3 (7)
C (2) -C (3) -C (11)	120.8 (6)
C (4) -C (3) -C (11)	120.8 (7)
O (1) -C (11) -O (2)	123.7 (7)
O (1) -C (11) -C (3)	118.9 (6)
O (2) -C (11) -C (3)	117.3 (6)
C (5) -C (4) -C (3)	119.8 (7)
N (1) -C (5) -C (4)	121.3 (7)
N (1) -C (5) -C (6)	113.8 (6)
C (4) -C (5) -C (6)	124.8 (6)
N (2) -C (6) -C (7)	120.7 (7)
N (2) -C (6) -C (5)	113.9 (6)
C (7) -C (6) -C (5)	125.4 (6)
C (6) -C (7) -C (8)	119.3 (7)
O (3) -C (12) -O (4)	127.5 (7)
O (3) -C (12) -C (8)	118.1 (6)
O (4) -C (12) -C (8)	114.3 (6)
C (9) -C (8) -C (7)	119.3 (7)
C (9) -C (8) -C (12)	120.3 (6)
C (7) -C (8) -C (12)	120.3 (6)
C (10) -C (9) -C (8)	117.7 (7)
N (2) -C (10) -C (9)	123.6 (8)
C (10) -N (2) -C (6)	119.4 (7)
C (10) -N (2) -Cu (1)	124.2 (5)
C (6) -N (2) -Cu (1)	116.2 (5)
C (13) -N (3) -C (17)	119.9 (7)
C (13) -N (3) -Cu (1)	123.3 (5)
C (17) -N (3) -Cu (1)	116.1 (5)
N (3) -C (13) -C (14)	121.9 (8)
C (13) -C (14) -C (15)	118.5 (7)
C (16) -C (15) -C (14)	118.9 (7)
C (16) -C (15) -C (23)	121.4 (7)
C (14) -C (15) -C (23)	119.7 (6)
O (6) -C (23) -O (5)	126.7 (7)
O (6) -C (23) -C (15)	116.9 (6)
O (5) -C (23) -C (15)	116.4 (6)
C (17) -C (16) -C (15)	119.6 (7)
N (3) -C (17) -C (16)	121.0 (6)
N (3) -C (17) -C (18)	114.0 (6)
C (16) -C (17) -C (18)	124.9 (6)
N (4) -C (18) -C (19)	122.1 (7)
N (4) -C (18) -C (17)	113.9 (6)

C (19) -C (18) -C (17)	124.0 (6)
C (18) -C (19) -C (20)	119.8 (7)
O (7) -C (24) -O (8)	125.1 (7)
O (7) -C (24) -C (20)	117.6 (7)
O (8) -C (24) -C (20)	117.2 (6)
C (21) -C (20) -C (19)	117.6 (7)
C (21) -C (20) -C (24)	121.4 (6)
C (19) -C (20) -C (24)	120.9 (6)
C (20) -C (21) -C (22)	119.9 (7)
N (4) -C (22) -C (21)	121.8 (8)
C (22) -N (4) -C (18)	118.3 (7)
C (22) -N (4) -Cu (1)	127.4 (5)
C (18) -N (4) -Cu (1)	114.3 (5)
O (14) -Na (1) -O (10)	90.6 (2)
O (14) -Na (1) -O (12)	81.5 (2)
O (10) -Na (1) -O (12)	171.9 (2)
O (14) -Na (1) -O (15)	173.5 (3)
O (10) -Na (1) -O (15)	88.5 (2)
O (12) -Na (1) -O (15)	99.6 (2)
O (14) -Na (1) -O (13)	93.8 (2)
O (10) -Na (1) -O (13)	92.3 (3)
O (12) -Na (1) -O (13)	86.1 (2)
O (15) -Na (1) -O (13)	92.7 (3)
O (14) -Na (1) -O (11)	82.8 (2)
O (10) -Na (1) -O (11)	85.7 (2)
O (12) -Na (1) -O (11)	95.4 (3)
O (15) -Na (1) -O (11)	90.7 (2)
O (13) -Na (1) -O (11)	176.0 (2)
O (14) -Na (1) -Na (2)	80.28 (19)
O (10) -Na (1) -Na (2)	41.95 (18)
O (12) -Na (1) -Na (2)	137.4 (2)
O (15) -Na (1) -Na (2)	94.78 (19)
O (13) -Na (1) -Na (2)	133.2 (2)
O (11) -Na (1) -Na (2)	44.35 (18)
O (14) -Na (1) -Na (2) #1	91.44 (19)
O (10) -Na (1) -Na (2) #1	137.4 (3)
O (12) -Na (1) -Na (2) #1	41.47 (18)
O (15) -Na (1) -Na (2) #1	93.61 (19)
O (13) -Na (1) -Na (2) #1	45.04 (18)
O (11) -Na (1) -Na (2) #1	136.7 (2)
Na (2) -Na (1) -Na (2) #1	171.54 (12)
O (12) #2 -Na (2) -O (10)	175.5 (2)
O (12) #2 -Na (2) -O (16)	84.4 (2)
O (10) -Na (2) -O (16)	91.2 (2)
O (12) #2 -Na (2) -O (17)	94.1 (2)
O (10) -Na (2) -O (17)	90.3 (2)
O (16) -Na (2) -O (17)	176.3 (3)
O (12) #2 -Na (2) -O (11)	91.8 (3)
O (10) -Na (2) -O (11)	87.4 (2)
O (16) -Na (2) -O (11)	88.9 (3)
O (17) -Na (2) -O (11)	87.8 (2)
O (12) #2 -Na (2) -O (13) #2	86.5 (2)
O (10) -Na (2) -O (13) #2	93.6 (3)
O (16) -Na (2) -O (13) #2	82.3 (3)
O (17) -Na (2) -O (13) #2	100.9 (2)
O (11) -Na (2) -O (13) #2	171.2 (2)
O (12) #2 -Na (2) -Na (1)	137.8 (2)
O (10) -Na (2) -Na (1)	41.92 (18)
O (16) -Na (2) -Na (1)	95.69 (17)
O (17) -Na (2) -Na (1)	83.25 (17)
O (11) -Na (2) -Na (1)	46.01 (17)

O(13) #2-Na(2)-Na(1)	135.5(2)
O(12) #2-Na(2)-Na(1) #2	41.95(18)
O(10)-Na(2)-Na(1) #2	137.4(2)
O(16)-Na(2)-Na(1) #2	75.88(17)
O(17)-Na(2)-Na(1) #2	105.13(18)
O(11)-Na(2)-Na(1) #2	131.7(2)
O(13) #2-Na(2)-Na(1) #2	45.07(18)
Na(1)-Na(2)-Na(1) #2	171.54(12)
Na(1)-O(10)-Na(2)	96.1(3)
Na(2)-O(11)-Na(1)	89.6(2)
Na(2) #1-O(12)-Na(1)	96.6(3)
Na(2) #1-O(13)-Na(1)	89.9(2)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct15.
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)	11 (1)	24 (1)	9 (1)	-1 (1)	-2 (1)	0 (1)
Na (1)	19 (2)	17 (2)	13 (1)	0 (1)	0 (2)	-4 (2)
Na (2)	20 (2)	14 (1)	19 (1)	2 (1)	2 (2)	0 (2)
O (10)	19 (3)	16 (3)	15 (3)	-6 (3)	-5 (3)	1 (3)
O (11)	13 (3)	29 (4)	15 (3)	-1 (3)	4 (3)	4 (3)
O (12)	11 (3)	22 (4)	11 (3)	-3 (3)	1 (2)	-1 (3)
O (13)	26 (4)	19 (4)	21 (3)	5 (3)	3 (3)	0 (3)
O (14)	44 (5)	30 (4)	12 (3)	1 (3)	-1 (3)	-10 (3)
O (15)	28 (4)	45 (4)	15 (3)	-4 (3)	7 (3)	-9 (4)
O (16)	35 (4)	23 (3)	22 (3)	1 (2)	-5 (4)	12 (4)
O (17)	16 (4)	31 (3)	17 (3)	5 (3)	6 (3)	4 (3)
O (18)	5 (3)	49 (4)	11 (3)	-2 (3)	-3 (3)	3 (3)
O (19)	22 (4)	25 (4)	15 (3)	-4 (3)	0 (3)	7 (3)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for struct15.

	x	y	z	U(eq)
H(1)	1895	3371	781	16
H(2)	553	4656	1068	20
H(4)	-780	2775	3	19
H(7)	-568	1464	-661	12
H(9)	1360	-727	-1472	20
H(10)	2448	-176	-942	13
H(13)	2563	46	886	19
H(14)	3687	-293	1414	8
H(16)	5544	1953	579	13
H(19)	5728	3074	-83	14
H(21)	4425	4428	-1183	17
H(22)	3069	3249	-892	19
H(9A)	2130 (20)	-2430 (30)	-143 (10)	34
H(9B)	2740 (8)	-2460 (30)	237 (5)	34
H(10A)	1065 (16)	866 (15)	2244 (5)	25
H(10B)	1154 (17)	200 (60)	2694 (8)	25
H(11A)	4069 (16)	544 (13)	2212 (6)	29
H(11B)	4000 (16)	870 (110)	2685 (6)	29
H(12A)	3890 (17)	5614 (12)	2809 (5)	22
H(12B)	3946 (16)	6270 (80)	2356 (8)	22
H(13A)	907 (15)	5857 (13)	2783 (5)	33
H(13B)	947 (18)	5640 (110)	2311 (6)	33
H(14A)	2814 (15)	1840 (16)	3311 (9)	43
H(14B)	3070 (30)	3840 (40)	3375 (14)	43
H(15A)	2129 (16)	2409 (13)	1557 (10)	44
H(15B)	2880 (30)	3820 (80)	1558 (15)	44
H(16A)	2080 (13)	-1500 (40)	1650 (6)	40
H(16B)	2390 (50)	-3470 (20)	1730 (20)	40
H(17A)	2157 (8)	-670 (30)	3490 (8)	31
H(17B)	3040 (30)	-1700 (80)	3459 (12)	31
H(18A)	-448 (6)	5150 (40)	1645 (3)	33
H(18B)	90 (50)	3730 (30)	1892 (18)	33
H(19A)	4547 (6)	5880 (40)	1714 (6)	31
H(19B)	4860 (30)	7691 (17)	1906 (12)	31

