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catena-Poly[[methanolcopper(II)-potassium(I)]-μ_3-1-(3-methoxy-2-oxidobenzylideneamino)-2-(2-oxidobenzamido)ethane]

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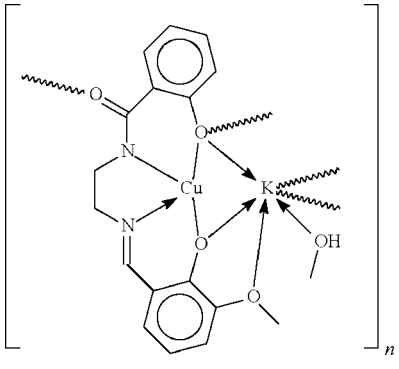
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.042; wR factor = 0.091; data-to-parameter ratio = 17.1.

In the title compound, $[CuK(C_{17}H_{15}N_2O_4)(CH_3OH)]_n$, the Cu^{II} ion has a square-planar coordination geometry and is coordinated by two N and two O atoms. One phenoxo and the amide O atom also interact with the methanol-coordinated K^+ ion along with the methoxy O atom of the trianion. Two bridging interactions to K^+ give rise to a linear chain structure. The chains are further linked by hydrogen bonds involving the amido methanol O atoms into a two-dimensional network structure.

Related literature

For other polynuclear complexes, see Kido *et al.* (2000, 2003); Osa *et al.* (2003). For related literature, see: Hamamatsu *et al.* (2007).



Experimental

Crystal data

$[CuK(C_{17}H_{15}N_2O_4)(CH_4O)]$
M_r = 445.99
Triclinic, $P\overline{1}$
a = 8.851 (6) Å
b = 9.139 (6) Å
c = 12.458 (6) Å
α = 72.19 (2)°
β = 77.68 (3)°
γ = 78.69 (2)°
V = 928.0 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.43 mm^{-1}
T = 293 (2) K
0.2 × 0.2 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.732, T_{max} = 0.759
9074 measured reflections
4201 independent reflections
3241 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.091
S = 1.02
4201 reflections
246 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.893 (2)	K1—O1	2.714 (2)
Cu1—N1	1.922 (3)	K1—O3^{i}	2.726 (3)
Cu1—O2	1.937 (2)	K1—O4	2.736 (3)
Cu1—N2	1.940 (3)	K1—O5	2.740 (3)
K1—O2	2.701 (3)	K1—O1^{ii}	2.886 (3)
O1—Cu1—N1	95.19 (10)	O2—K1—O5	162.88 (7)
O1—Cu1—O2	88.75 (9)	O1—K1—O5	130.64 (8)
N1—Cu1—O2	169.99 (10)	O3^{i}—K1—O5	90.63 (9)
O1—Cu1—N2	173.78 (10)	O4—K1—O5	110.44 (8)
N1—Cu1—N2	85.22 (11)	O2—K1—O1^{ii}	90.43 (7)
O2—Cu1—N2	91.86 (10)	O1—K1—O1^{ii}	97.52 (7)
O2—K1—O1	59.32 (7)	O3^{i}—K1—O1^{ii}	165.31 (7)
O2—K1—O3^{i}	104.21 (8)	O4—K1—O1^{ii}	81.53 (8)
O1—K1—O3^{i}	89.14 (8)	O5—K1—O1^{ii}	75.08 (8)
O2—K1—O4	57.36 (7)	Cu1—O1—K1^{ii}	100.64 (9)
O1—K1—O4	116.65 (7)	K1—O1—K1^{ii}	82.48 (7)
O3^{i}—K1—O4	107.21 (8)	Cu1—O2—K1	103.83 (9)

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x, -y+1, -z$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5···O3^{iii}	0.85	1.90	2.703 (4)	156

Symmetry code: (iii) $x-1, y+1, z$.

Data collection: *CrystalStructure* (Rigaku/MSC, 2004); cell refinement: *CrystalStructure*; data reduction: *CrystalStructure*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1998); software used to prepare material for publication: *XP*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2273).

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supplementary materials

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catena-Poly[[methanolcopper(II)potassium(I)]-μ_3-1-(3-methoxy-2-oxidobenzylideneamino)-2-(2-oxidobenzamido)ethane]

W.-X. Luo, M.-M. Yu, L. Zheng, A.-L. Cui and H.-Z. Kou

Comment

1-(2-hydroxybenzamido)-2-(2-hydroxy-3-methoxybenzylideneamino)ethane, abbreviated as H_3L, is an excellent bridging ligand that can link two metal atoms *via* the phenolato and the amido oxgen atoms to form polynuclear complexes (Kido *et al.*, 2000). A few cyclic heterometallic tetranuclear complexes have been synthesize and their structures have been characterized by diffraction analysis and magnetic studies (Hamamatsu *et al.*, 2007; Kido *et al.*, 2003; Osa *et al.*, 2003). The syntheses requires K[CuL] as the starting reactant. This compound crystallizes from methanol as the title compound.

The structure consists of $[CuL]^-$ and $[K(MeOH)]^+$ moieties connected by the phenolato and amido oxygen atoms (Fig. 1). The coordination geometry of potassium is an octahedron, and that of copper is a square plane. Two N atoms and two O atoms are linked to the copper atom. The coordination environment is similar to those found in other cyclic heterometallic tetranuclear complexes.

The phenolato oxygen and amido oxgen atoms are involving in bridging to form a ladder structure (Fig. 2). Adjacent ladders are further linked by hydrogen bonds (involving the amido group and the methanol molecule) (O···O 2.702 (4) Å) to form a two-dimensional, hydrogen-bonded network.

Experimental

The compound was prepared according to the literature method (Kido *et al.*, 2003), and recrystallization from methanol afforded violet, block-shaped crystals.

Refinement

The H atoms bound to C atoms were placed in caculated positions with C—H = 0.93–0.77 Å and included in the refinement with $U_{iso}(H) = 1.2U_{eq}(C)$. The H atom attached to the methanol O atom were found from E-map, and was fixed with O—H = 0.85 Å and refined isotropically.

Figures

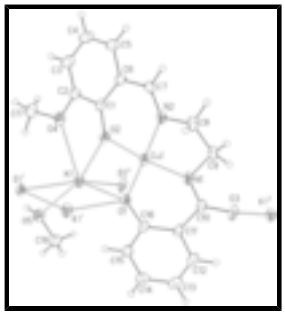

Fig. 1. A view of complex (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Symmetry code: i −*x*, 1 − *y*, −*z*; ii 1 − *x*, 1 − *y*, −*z*.

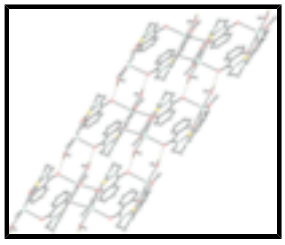

Fig. 2. The hydrogen-bonded layer structure.

catena-Poly[[methanolcopper(II)potassium(I)]-μ$_3$– 1-(3-methoxy-2-oxidobenzylideneamino)-2-(2-oxidobenzamido)ethane]

Crystal data

[CuK($C_{17}H_{15}N_2O_4$)(CH_4O)]	Z = 2
M_r = 445.99	F_{000} = 458
Triclinic, $P\overline{1}$	D_x = 1.596 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 8.851 (6) Å	Cell parameters from 4201 reflections
b = 9.139 (6) Å	θ = 3.0–27.5º
c = 12.458 (6) Å	μ = 1.43 mm^{-1}
α = 72.19 (2)º	T = 293 (2) K
β = 78.68 (3)º	Block, violet
γ = 78.69 (2)º	0.2 × 0.2 × 0.18 mm
V = 928.0 (10) Å^3	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	4201 independent reflections
Radiation source: fine-focus sealed tube	3241 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.045
Detector resolution: 0.1 pixels mm^{-1}	θ_{max} = 27.5º
T = 293(2) K	θ_{min} = 3.0º
ω scans	h = −11→11
Absorption correction: multi-scan	k = −11→11

(ABSCOR; Higashi, 1995)
T_{min} = 0.732, T_{max} = 0.759
9074 measured reflections

l = −16→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.091
S = 1.02
4201 reflections
246 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.01P)^2 + P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.27702 (4)	0.27166 (4)	0.12226 (3)	0.03185 (11)
K1	0.03569 (8)	0.65451 (7)	0.05460 (6)	0.03864 (17)
O1	0.2426 (2)	0.4267 (2)	−0.01471 (17)	0.0358 (5)
O2	0.0917 (2)	0.3708 (2)	0.20129 (17)	0.0358 (5)
N2	0.3005 (3)	0.0990 (3)	0.2574 (2)	0.0325 (5)
N1	0.4802 (3)	0.1843 (3)	0.0599 (2)	0.0344 (6)
C16	0.3546 (3)	0.4689 (3)	−0.1033 (2)	0.0311 (6)
C11	0.5110 (3)	0.3922 (3)	−0.1150 (3)	0.0324 (6)
O3	0.7203 (2)	0.2010 (3)	−0.0501 (2)	0.0442 (5)
C1	0.0455 (3)	0.3377 (3)	0.3110 (3)	0.0314 (6)
C2	−0.0732 (4)	0.4438 (3)	0.3569 (3)	0.0350 (7)
C7	0.2269 (4)	0.0894 (3)	0.3583 (3)	0.0359 (7)
H7A	0.2556	0.0012	0.4153	0.043*
C12	0.6138 (4)	0.4529 (4)	−0.2151 (3)	0.0414 (7)
H12A	0.7163	0.4038	−0.2241	0.050*

C8	0.4203 (4)	−0.0246 (3)	0.2303 (3)	0.0413 (7)
H8A	0.3758	−0.0905	0.2010	0.050*
H8B	0.4613	−0.0879	0.2987	0.050*
C10	0.5754 (3)	0.2510 (3)	−0.0307 (3)	0.0328 (6)
C6	0.1032 (3)	0.2026 (3)	0.3925 (3)	0.0336 (6)
C4	−0.0790 (5)	0.2770 (4)	0.5471 (3)	0.0513 (9)
H4A	−0.1221	0.2557	0.6243	0.062*
C15	0.3135 (4)	0.6004 (4)	−0.1913 (3)	0.0394 (7)
H15A	0.2120	0.6524	−0.1840	0.047*
C13	0.5699 (4)	0.5814 (4)	−0.3001 (3)	0.0477 (8)
H13A	0.6415	0.6179	−0.3650	0.057*
C9	0.5501 (4)	0.0481 (4)	0.1414 (3)	0.0411 (7)
H9A	0.6202	0.0791	0.1780	0.049*
H9B	0.6098	−0.0264	0.1017	0.049*
C5	0.0393 (4)	0.1755 (4)	0.5088 (3)	0.0438 (8)
H5A	0.0784	0.0865	0.5608	0.053*
C3	−0.1347 (4)	0.4125 (4)	0.4699 (3)	0.0489 (8)
H3A	−0.2148	0.4823	0.4958	0.059*
C14	0.4183 (4)	0.6552 (4)	−0.2879 (3)	0.0445 (8)
H14A	0.3868	0.7421	−0.3449	0.053*
C17	−0.2533 (4)	0.6761 (4)	0.3077 (3)	0.0544 (9)
H17A	−0.3396	0.6178	0.3350	0.082*
H17B	−0.2751	0.7612	0.2427	0.082*
H17C	−0.2377	0.7154	0.3672	0.082*
O4	−0.1159 (3)	0.5782 (2)	0.27564 (19)	0.0434 (5)
O5	−0.1113 (3)	0.9268 (3)	−0.06939 (19)	0.0465 (6)
C18	0.0008 (4)	0.9855 (4)	−0.1635 (3)	0.0485 (8)
H18C	−0.0447	1.0816	−0.2103	0.073*
H18D	0.0358	0.9119	−0.2076	0.073*
H18A	0.0880	1.0031	−0.1369	0.073*
H5	−0.1666	0.9996	−0.0431	0.051 (10)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.02267 (18)	0.0323 (2)	0.0352 (2)	0.00534 (14)	−0.00369 (14)	−0.00796 (15)
K1	0.0325 (4)	0.0315 (3)	0.0475 (4)	0.0003 (3)	−0.0073 (3)	−0.0071 (3)
O1	0.0230 (10)	0.0383 (11)	0.0373 (11)	0.0031 (9)	−0.0011 (8)	−0.0051 (9)
O2	0.0295 (11)	0.0350 (11)	0.0335 (11)	0.0051 (9)	0.0009 (9)	−0.0060 (9)
N2	0.0260 (13)	0.0281 (12)	0.0404 (14)	0.0042 (10)	−0.0064 (11)	−0.0094 (10)
N1	0.0241 (12)	0.0313 (13)	0.0436 (15)	0.0057 (10)	−0.0048 (11)	−0.0109 (11)
C16	0.0279 (15)	0.0329 (15)	0.0333 (15)	−0.0044 (12)	0.0013 (12)	−0.0145 (12)
C11	0.0268 (15)	0.0351 (15)	0.0390 (16)	−0.0021 (12)	−0.0017 (12)	−0.0196 (13)
O3	0.0213 (11)	0.0412 (13)	0.0683 (15)	0.0018 (9)	0.0018 (10)	−0.0223 (11)
C1	0.0239 (14)	0.0300 (14)	0.0384 (16)	−0.0044 (11)	−0.0005 (12)	−0.0094 (12)
C2	0.0331 (16)	0.0312 (15)	0.0394 (17)	−0.0031 (13)	−0.0032 (13)	−0.0105 (13)
C7	0.0370 (17)	0.0283 (15)	0.0382 (17)	−0.0015 (13)	−0.0096 (13)	−0.0029 (12)
C12	0.0313 (17)	0.0494 (19)	0.0463 (19)	−0.0108 (14)	0.0043 (14)	−0.0213 (15)

C8	0.0355 (17)	0.0314 (16)	0.053 (2)	0.0070 (13)	−0.0089 (15)	−0.0121 (14)
C10	0.0244 (14)	0.0320 (15)	0.0464 (18)	0.0024 (12)	−0.0046 (13)	−0.0218 (13)
C6	0.0314 (16)	0.0311 (15)	0.0365 (16)	−0.0056 (12)	−0.0026 (12)	−0.0082 (12)
C4	0.060 (2)	0.053 (2)	0.0355 (18)	−0.0069 (18)	0.0074 (16)	−0.0154 (16)
C15	0.0357 (17)	0.0386 (17)	0.0408 (17)	0.0005 (14)	−0.0030 (14)	−0.0121 (14)
C13	0.048 (2)	0.053 (2)	0.0407 (19)	−0.0169 (17)	0.0088 (15)	−0.0162 (16)
C9	0.0300 (16)	0.0368 (17)	0.052 (2)	0.0101 (13)	−0.0085 (14)	−0.0142 (15)
C5	0.050 (2)	0.0398 (18)	0.0374 (17)	−0.0071 (15)	−0.0047 (15)	−0.0060 (14)
C3	0.050 (2)	0.047 (2)	0.047 (2)	−0.0006 (16)	0.0064 (16)	−0.0215 (16)
C14	0.054 (2)	0.0429 (18)	0.0345 (17)	−0.0118 (16)	−0.0017 (15)	−0.0080 (14)
C17	0.041 (2)	0.047 (2)	0.069 (2)	0.0122 (16)	−0.0041 (18)	−0.0220 (18)
O4	0.0370 (13)	0.0357 (12)	0.0485 (13)	0.0106 (10)	−0.0024 (10)	−0.0113 (10)
O5	0.0439 (14)	0.0376 (13)	0.0495 (14)	0.0036 (11)	−0.0018 (11)	−0.0096 (11)
C18	0.0379 (19)	0.048 (2)	0.053 (2)	−0.0013 (16)	−0.0014 (16)	−0.0107 (16)

Geometric parameters (Å, °)

Cu1—O1	1.893 (2)	C7—H7A	0.9300
Cu1—N1	1.922 (3)	C12—C13	1.374 (5)
Cu1—O2	1.937 (2)	C12—H12A	0.9300
Cu1—N2	1.940 (3)	C8—C9	1.515 (5)
K1—O2	2.701 (3)	C8—H8A	0.9700
K1—O1	2.714 (2)	C8—H8B	0.9700
K1—O3^{i}	2.726 (3)	C6—C5	1.402 (4)
K1—O4	2.736 (3)	C4—C5	1.364 (5)
K1—O5	2.740 (3)	C4—C3	1.392 (5)
K1—O1^{ii}	2.886 (3)	C4—H4A	0.9300
O1—C16	1.331 (3)	C15—C14	1.377 (5)
O1—K1^{ii}	2.886 (3)	C15—H15A	0.9300
O2—C1	1.298 (4)	C13—C14	1.378 (5)
N2—C7	1.272 (4)	C13—H13A	0.9300
N2—C8	1.457 (4)	C9—H9A	0.9700
N1—C10	1.315 (4)	C9—H9B	0.9700
N1—C9	1.469 (4)	C5—H5A	0.9300
C16—C15	1.403 (4)	C3—H3A	0.9300
C16—C11	1.423 (4)	C14—H14A	0.9300
C11—C12	1.407 (4)	C17—O4	1.422 (4)
C11—C10	1.494 (4)	C17—H17A	0.9600
O3—C10	1.272 (3)	C17—H17B	0.9600
O3—K1^{i}	2.726 (3)	C17—H17C	0.9600
C1—C6	1.422 (4)	O5—C18	1.406 (4)
C1—C2	1.433 (4)	O5—H5	0.8521
C2—C3	1.358 (5)	C18—H18C	0.9600
C2—O4	1.377 (4)	C18—H18D	0.9600
C7—C6	1.441 (4)	C18—H18A	0.9600
O1—Cu1—N1	95.19 (10)	N2—C8—C9	108.7 (3)
O1—Cu1—O2	88.75 (9)	N2—C8—H8A	110.0
N1—Cu1—O2	169.99 (10)	C9—C8—H8A	110.0

O1—Cu1—N2	173.78 (10)	N2—C8—H8B	110.0
N1—Cu1—N2	85.22 (11)	C9—C8—H8B	110.0
O2—Cu1—N2	91.86 (10)	H8A—C8—H8B	108.3
O2—K1—O1	59.32 (7)	O3—C10—N1	123.1 (3)
O2—K1—O3^{i}	104.21 (8)	O3—C10—C11	118.2 (3)
O1—K1—O3^{i}	89.14 (8)	N1—C10—C11	118.7 (2)
O2—K1—O4	57.36 (7)	C5—C6—C1	120.4 (3)
O1—K1—O4	116.65 (7)	C5—C6—C7	118.2 (3)
O3^{i}—K1—O4	107.21 (8)	C1—C6—C7	121.4 (3)
O2—K1—O5	162.88 (7)	C5—C4—C3	119.4 (3)
O1—K1—O5	130.64 (8)	C5—C4—H4A	120.3
O3^{i}—K1—O5	90.63 (9)	C3—C4—H4A	120.3
O4—K1—O5	110.44 (8)	C14—C15—C16	122.3 (3)
O2—K1—O1^{ii}	90.43 (7)	C14—C15—H15A	118.8
O1—K1—O1^{ii}	97.52 (7)	C16—C15—H15A	118.8
O3^{i}—K1—O1^{ii}	165.31 (7)	C12—C13—C14	119.0 (3)
O4—K1—O1^{ii}	81.53 (8)	C12—C13—H13A	120.5
O5—K1—O1^{ii}	75.08 (8)	C14—C13—H13A	120.5
C16—O1—Cu1	124.07 (18)	N1—C9—C8	108.6 (2)
C16—O1—K1	117.80 (17)	N1—C9—H9A	110.0
Cu1—O1—K1	104.65 (9)	C8—C9—H9A	110.0
C16—O1—K1^{ii}	118.66 (17)	N1—C9—H9B	110.0
Cu1—O1—K1^{ii}	100.64 (9)	C8—C9—H9B	110.0
K1—O1—K1^{ii}	82.48 (7)	H9A—C9—H9B	108.4
C1—O2—Cu1	126.37 (18)	C4—C5—C6	121.4 (3)
C1—O2—K1	124.59 (17)	C4—C5—H5A	119.3
Cu1—O2—K1	103.83 (9)	C6—C5—H5A	119.3
C7—N2—C8	122.0 (3)	C2—C3—C4	120.7 (3)
C7—N2—Cu1	127.1 (2)	C2—C3—H3A	119.7
C8—N2—Cu1	110.9 (2)	C4—C3—H3A	119.7
C10—N1—C9	116.5 (2)	C15—C14—C13	120.0 (3)
C10—N1—Cu1	127.7 (2)	C15—C14—H14A	120.0
C9—N1—Cu1	113.3 (2)	C13—C14—H14A	120.0
O1—C16—C15	116.7 (3)	O4—C17—H17A	109.5
O1—C16—C11	125.2 (3)	O4—C17—H17B	109.5
C15—C16—C11	118.1 (3)	H17A—C17—H17B	109.5
C12—C11—C16	117.5 (3)	O4—C17—H17C	109.5
C12—C11—C10	117.0 (3)	H17A—C17—H17C	109.5
C16—C11—C10	125.6 (3)	H17B—C17—H17C	109.5
C10—O3—K1^{i}	127.29 (18)	C2—O4—C17	117.3 (3)
O2—C1—C6	125.4 (3)	C2—O4—K1	123.72 (17)
O2—C1—C2	118.9 (3)	C17—O4—K1	118.8 (2)
C6—C1—C2	115.7 (3)	C18—O5—K1	105.91 (19)
C3—C2—O4	124.5 (3)	C18—O5—H5	110.9
C3—C2—C1	122.2 (3)	K1—O5—H5	126.3
O4—C2—C1	113.2 (3)	O5—C18—H18C	109.5

N2—C7—C6	126.0 (3)	O5—C18—H18D	109.5
N2—C7—H7A	117.0	H18C—C18—H18D	109.5
C6—C7—H7A	117.0	O5—C18—H18A	109.5
C13—C12—C11	123.1 (3)	H18C—C18—H18A	109.5
C13—C12—H12A	118.4	H18D—C18—H18A	109.5
C11—C12—H12A	118.4		
N1—Cu1—O1—C16	−15.7 (2)	K1—O2—C1—C6	−164.0 (2)
O2—Cu1—O1—C16	155.1 (2)	Cu1—O2—C1—C2	166.0 (2)
K1^{ii}—Cu1—O1—C16	−135.7 (2)	K1—O2—C1—C2	15.8 (4)
N1—Cu1—O1—K1	−155.04 (10)	O2—C1—C2—C3	175.7 (3)
O2—Cu1—O1—K1	15.73 (9)	C6—C1—C2—C3	−4.5 (4)
N1—Cu1—O1—K1^{ii}	120.04 (10)	O2—C1—C2—O4	−4.8 (4)
O2—Cu1—O1—K1^{ii}	−69.19 (9)	C6—C1—C2—O4	175.1 (3)
O2—K1—O1—C16	−155.5 (2)	C8—N2—C7—C6	−177.6 (3)
O3^{i}—K1—O1—C16	−48.4 (2)	Cu1—N2—C7—C6	3.8 (5)
O4—K1—O1—C16	−157.23 (18)	C16—C11—C12—C13	0.2 (5)
O5—K1—O1—C16	41.7 (2)	C10—C11—C12—C13	179.5 (3)
O1^{ii}—K1—O1—C16	118.5 (2)	C7—N2—C8—C9	−142.6 (3)
O3^{i}—K1—O1—Cu1	94.05 (10)	Cu1—N2—C8—C9	36.3 (3)
O4—K1—O1—Cu1	−14.83 (12)	K1^{i}—O3—C10—N1	−114.3 (3)
O5—K1—O1—Cu1	−175.86 (8)	K1^{i}—O3—C10—C11	65.8 (3)
O1^{ii}—K1—O1—Cu1	−99.09 (10)	C9—N1—C10—O3	1.4 (4)
O2—K1—O1—K1^{ii}	86.02 (8)	Cu1—N1—C10—O3	162.2 (2)
O3^{i}—K1—O1—K1^{ii}	−166.86 (7)	C9—N1—C10—C11	−178.6 (2)
O4—K1—O1—K1^{ii}	84.26 (8)	Cu1—N1—C10—C11	−17.8 (4)
O5—K1—O1—K1^{ii}	−76.77 (10)	C12—C11—C10—O3	4.8 (4)
O1^{ii}—K1—O1—K1^{ii}	0.0	C16—C11—C10—O3	−176.0 (3)
Cu1^{ii}—K1—O1—K1^{ii}	−29.86 (5)	C12—C11—C10—N1	−175.2 (3)
O1—Cu1—O2—C1	−170.9 (2)	C16—C11—C10—N1	4.1 (4)
N1—Cu1—O2—C1	−57.5 (7)	O2—C1—C6—C5	−177.1 (3)
N2—Cu1—O2—C1	15.3 (2)	C2—C1—C6—C5	3.1 (4)
K1^{ii}—Cu1—O2—C1	141.3 (2)	O2—C1—C6—C7	2.2 (5)
O1—Cu1—O2—K1	−15.75 (9)	C2—C1—C6—C7	−177.6 (3)
N1—Cu1—O2—K1	97.6 (6)	N2—C7—C6—C5	−177.6 (3)
N2—Cu1—O2—K1	170.44 (9)	N2—C7—C6—C1	3.1 (5)
O1—K1—O2—C1	168.4 (2)	O1—C16—C15—C14	−179.5 (3)
O3^{i}—K1—O2—C1	88.1 (2)	C11—C16—C15—C14	0.9 (5)
O4—K1—O2—C1	−13.4 (2)	C11—C12—C13—C14	0.0 (5)
O5—K1—O2—C1	−61.3 (3)	C10—N1—C9—C8	−172.4 (3)
O1^{ii}—K1—O2—C1	−93.1 (2)	Cu1—N1—C9—C8	24.0 (3)
K1^{ii}—K1—O2—C1	−135.3 (2)	N2—C8—C9—N1	−38.5 (3)
Cu1^{ii}—K1—O2—C1	−102.8 (2)	C3—C4—C5—C6	−1.8 (6)
O1—K1—O2—Cu1	12.72 (7)	C1—C6—C5—C4	−0.1 (5)
O3^{i}—K1—O2—Cu1	−67.59 (10)	C7—C6—C5—C4	−179.4 (3)

O4—K1—O2—Cu1	−169.14 (12)	O4—C2—C3—C4	−176.7 (3)
O5—K1—O2—Cu1	143.0 (2)	C1—C2—C3—C4	2.8 (5)
O1^{ii}—K1—O2—Cu1	111.21 (10)	C5—C4—C3—C2	0.5 (6)
N1—Cu1—N2—C7	159.9 (3)	C16—C15—C14—C13	−0.7 (5)
O2—Cu1—N2—C7	−10.5 (3)	C12—C13—C14—C15	0.3 (5)
O2—Cu1—N2—C8	170.7 (2)	C3—C2—O4—C17	−12.8 (5)
K1^{ii}—Cu1—N2—C8	99.6 (2)	C1—C2—O4—C17	167.7 (3)
O1—Cu1—N1—C10	21.4 (3)	C3—C2—O4—K1	171.7 (3)
O2—Cu1—N1—C10	−91.5 (6)	C1—C2—O4—K1	−7.8 (3)
N2—Cu1—N1—C10	−164.9 (3)	O2—K1—O4—C2	10.4 (2)
O1—Cu1—N1—C9	−177.3 (2)	O1—K1—O4—C2	12.2 (2)
O2—Cu1—N1—C9	69.8 (6)	O3^{i}—K1—O4—C2	−85.7 (2)
N2—Cu1—N1—C9	−3.5 (2)	O5—K1—O4—C2	177.0 (2)
Cu1—O1—C16—C15	−171.1 (2)	O1^{ii}—K1—O4—C2	106.4 (2)
K1—O1—C16—C15	−36.5 (3)	O2—K1—O4—C17	−165.0 (3)
K1^{ii}—O1—C16—C15	60.3 (3)	O1—K1—O4—C17	−163.2 (2)
Cu1—O1—C16—C11	8.5 (4)	O3^{i}—K1—O4—C17	98.9 (2)
K1—O1—C16—C11	143.1 (2)	O5—K1—O4—C17	1.6 (2)
K1^{ii}—O1—C16—C11	−120.0 (3)	O1^{ii}—K1—O4—C17	−69.0 (2)
O1—C16—C11—C12	179.8 (3)	O2—K1—O5—C18	−159.7 (2)
C15—C16—C11—C12	−0.6 (4)	O1—K1—O5—C18	−39.6 (2)
O1—C16—C11—C10	0.6 (4)	O3^{i}—K1—O5—C18	49.8 (2)
C15—C16—C11—C10	−179.8 (3)	O4—K1—O5—C18	158.47 (19)
Cu1—O2—C1—C6	−13.8 (4)	O1^{ii}—K1—O5—C18	−126.7 (2)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5···O3^{iii}	0.85	1.90	2.703 (4)	156

Symmetry codes: (iii) *x*−1, *y*+1, *z*.

Fig. 1

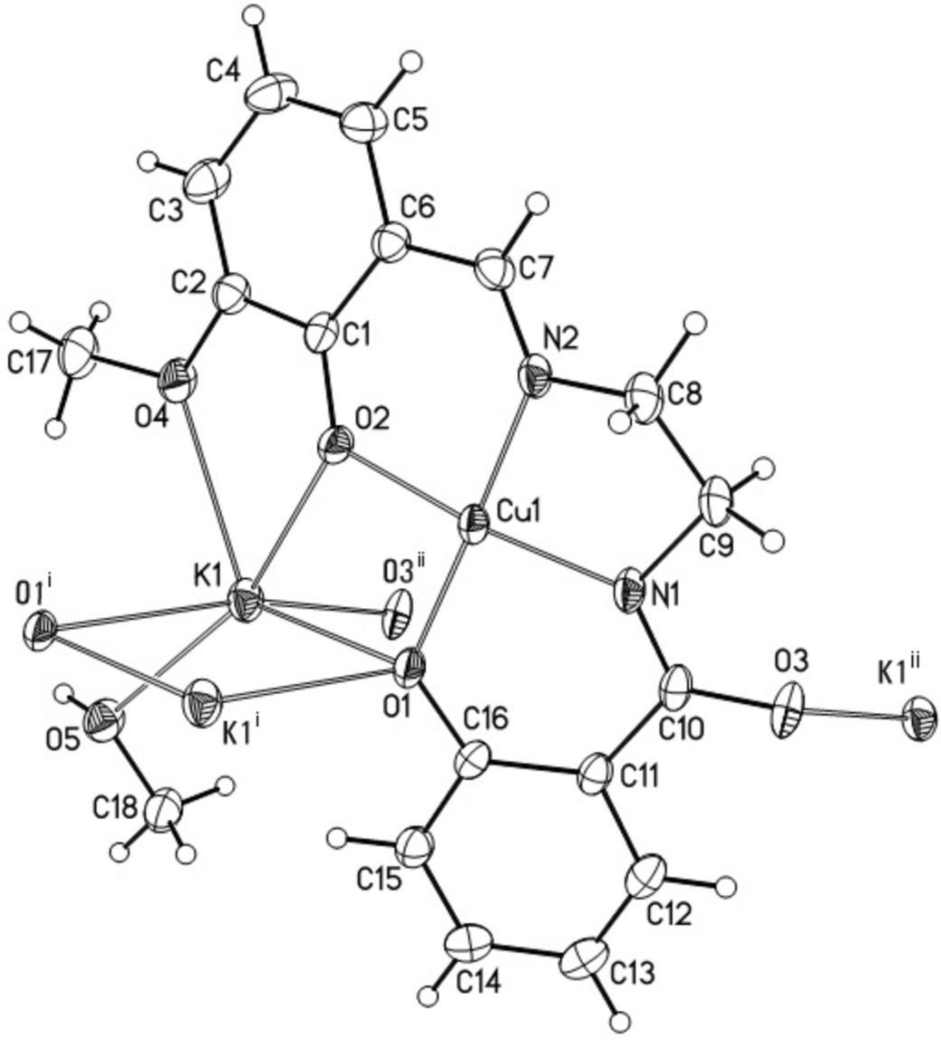
C4
C5
C3
C6
C7
C2
C1
N2
C17
O4
O2
C8
Cu1
C9
K1
O3ii
O1i
N1
O3
K1ii
O1
O5
K1i
C16
C10
C11
C18
C15
C12
C14
C13

Fig. 2