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Tetra-μ-acetato-bis[(benzofuro[3,2-*c*]pyridine)copper(II)]

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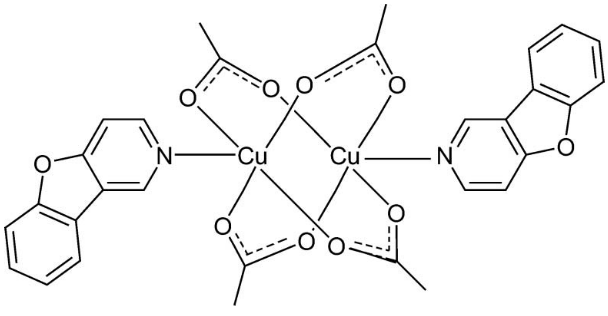
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.034; wR factor = 0.103; data-to-parameter ratio = 15.8.

The title compound, $[Cu_2(C_2H_3O_2)_4(C_{11}H_7NO)_2]$, has a centrosymmetric dinuclear structure in which two symmetry-related Cu^{II} centres are bridged by four acetate groups, with a Cu$\cdots$Cu separation of 2.6330 (6) Å. Each Cu^{II} centre is five-coordinated in a distorted square-pyramidal coordination geometry by four O atoms from four bridging acetate groups in the basal plane and the N atom of a benzofuropyridine ligand in the apical position. Each Cu^{II} atom is displaced from the basal plane by 0.2064 (3) Å towards the apical N atom. In the crystal structure, the complexes are linked by C—H$\cdots$O interactions to form zigzag layers.

Related literature

For related literature, see: Baran *et al.* (2005); Bencková & Krutošíková (1995, 1999); Berners-Price *et al.* (1987); Bobošík *et al.* (1995); Comba *et al.* (1999); Cox *et al.* (2000); Francesca *et al.* (2005); Miklovič *et al.* (2004); Moncol *et al.* (2007); Musie *et al.* (2006); Nikhil *et al.* (2001); Su *et al.* (2006).



Experimental

Crystal data

$[Cu_2(C_2H_3O_2)_4(C_{11}H_7NO)_2]$
M_r = 701.60
Orthorhombic, *Pbca*
a = 13.6706 (2) Å
b = 8.2336 (1) Å
c = 27.7541 (4) Å
V = 3123.95 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.42 mm^{-1}
T = 298 (2) K
0.42 × 0.29 × 0.17 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: analytical (Clark & Reid, 1995)
T_{min} = 0.542, T_{max} = 0.785
65563 measured reflections
3185 independent reflections
2574 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.103
S = 1.09
3185 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2001); software used to prepare material for publication: *enCIFer* (Allen *et al.*, 2004).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2409).

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supplementary materials

Acta Cryst. (2007). E**63**, m2112-m2113 [**doi:10.1107/S1600536807032242**]

Tetra-μ-acetato-bis[(benzofuro[3,2-*c*]pyridine)copper(II)]

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Comment

Copper(II) complexes have attracted much attention over the past decade due to their role in biological systems. A great number of copper(II) complexes with various organic ligands have been a subject of intense study because of their interesting properties from many different (chemical, structural and biological) points of view. Copper(II) complexes with bridging acetate ligands have received much attention for their various coordination geometries (Comba *et al.*, 1999; Cox *et al.*, 2000) and potential biological significance (Berners-Price *et al.*, 1987). In addition, some copper(II) complexes also have shown antitumor and antiproliferative effects (Francesca *et al.*, 2005; Nikhil *et al.*, 2001). The furo[3,2-*c*]pyridine and its derivatives represent quinoline isosters, in which the benzene ring is replaced by the furan and pyridine ring can be readily coordinated to metal centers through N-donor atom (Miklovič *et al.*, 2004; Baran *et al.*, 2005). We report here the synthesis and crystal structure of the title compound.

Molecules of the title compound lie on centers of inversion. As illustrated in Fig.1, the two Cu^{II} atoms are bridged by four acetate groups in the *syn*-*syn* mode, forming a dinuclear structure. The $Cu1\cdots Cu1^{i}$ [symmetry code: (i) $1 - x, -y, 1 - z$] distance is 2.6330 (6) Å, very similar to the values found in other dimeric copper(II) carboxylate complexes (Musie *et al.*, 2006; Su *et al.*, 2006; Moncol *et al.*, 2007). Each Cu^{II} atom displays an approximate square-pyramidal geometry with four acetate O atoms in the basal plane [Cu—O = 1.9562 (19)–1.9731 (19) Å] and the N atom of the benzofuro[3,2-*c*]pyridine ligand (BFP) in the apical position [Cu—N = 2.180 (2) Å]. Atom Cu1 is displaced from the least-squares plane defined by the basal atoms by 0.2064 (3) Å towards the apical N atom. The BFP ligand is almost planar (mean deviation is 0.01 (3) Å), the dihedral angle between the O16/O14/Cu1/O16'/O14'/Cu1' plane and the BFP ring is 24.51 (4)°.

In the crystal structure, the complexes are linked by C—H···O interactions (H···O = 2.41–2.42 Å and C···O = 3.210 (3)–3.364 (3) Å] to form zigzag layers parallel to the *ab* plane.

Experimental

The organic ligand, [1]benzofuro[3,2-*c*]pyridine, was prepared according literature procedures of Bobošík *et al.* (1995) and Bencková & Krutošíková (1995, 1999). To a $Cu(CH_3CO_2)_2{\cdot}H_2O$ (1.5 mmol) solution in ethanol (5 ml) was added the solution of [1]benzofuro[3,2-*c*]pyridine (3.2 mmol) in ethanol (2 ml). Small blue-green crystals were collected after 2 d. These were filtered off, washed with ethanol and recrystallized from THF.

Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å and U_{iso} set at $1.2U_{eq}$ ($1.5U_{eq}$ for methyl) of the parent atom.

Figures

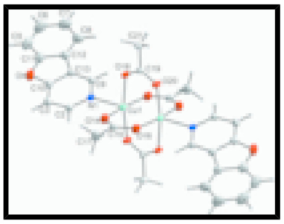


Fig. 1. The molecular structure of the title compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operation ($1 - x$, $-y$, $1 - z$).

Tetra-μ-acetato-bis[(benzofuro[3,2-*c*]pyridine)copper(II)]

Crystal data

$[Cu_2(C_2H_3O_2)_4(C_{11}H_7NO)_2]$

$M_r = 701.60$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 13.6706$ (2) Å

$b = 8.2336$ (1) Å

$c = 27.7541$ (4) Å

$V = 3123.95$ (7) Å^3

$Z = 4$

$F_{000} = 1432$

$D_x = 1.492$ Mg m^{-3}

Mo *Kα* radiation
λ = 0.71073 Å

Cell parameters from 22540 reflections

θ = 2.9–27.0°

μ = 1.42 mm^{-1}

$T = 298$ (2) K

Block, blue-green

0.42 × 0.29 × 0.17 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298(2)$ K

Rotation method data acquisition using ω and φ scans

Absorption correction: analytical (Clark & Reid, 1995)

$T_{min} = 0.542$, $T_{max} = 0.785$

65563 measured reflections

3185 independent reflections

2574 reflections with $I > 2\sigma(I)$

$R_{int} = 0.029$

$\theta_{max} = 26.4°$

$\theta_{min} = 4.1°$

$h = -17 \rightarrow 17$

$k = -10 \rightarrow 10$

$l = -34 \rightarrow 34$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.103$

$S = 1.09$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2 + 2.9514P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.002$

3185 reflections	$\Delta\rho_{max}$ = 0.48 e Å^{-3}
201 parameters	$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. face-indexed (*CrysAlis RED*; Oxford Diffraction, 2006)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C2	0.70235 (19)	0.2627 (3)	0.40930 (10)	0.0478 (6)
H2A	0.7306	0.2572	0.4397	0.057*
C3	0.7556 (2)	0.3325 (4)	0.37304 (10)	0.0565 (7)
H3A	0.8180	0.3743	0.3781	0.068*
C5	0.6905 (4)	0.4181 (6)	0.20420 (14)	0.1018 (15)
H5A	0.7467	0.4678	0.1925	0.122*
C6	0.6130 (4)	0.3843 (7)	0.17489 (14)	0.1127 (18)
H6A	0.6168	0.4113	0.1424	0.135*
C7	0.5302 (4)	0.3122 (7)	0.19172 (14)	0.1055 (16)
H7A	0.4791	0.2917	0.1705	0.127*
C8	0.5200 (3)	0.2682 (6)	0.23994 (12)	0.0854 (12)
H8A	0.4631	0.2194	0.2512	0.103*
C9	0.5702 (2)	0.2094 (3)	0.36038 (9)	0.0459 (6)
H9A	0.5070	0.1697	0.3564	0.055*
C10	0.7114 (2)	0.3368 (4)	0.32895 (10)	0.0537 (7)
C11	0.6812 (3)	0.3746 (5)	0.25224 (12)	0.0747 (10)
C12	0.5977 (2)	0.2997 (4)	0.27031 (10)	0.0628 (8)
C13	0.6181 (2)	0.2743 (4)	0.32132 (9)	0.0487 (6)
C15	0.6669 (2)	−0.0453 (4)	0.53715 (10)	0.0517 (7)
C17	0.7680 (2)	−0.0657 (5)	0.55807 (13)	0.0756 (10)
H17A	0.7629	−0.0931	0.5916	0.113*
H17B	0.8037	0.0341	0.5547	0.113*
H17C	0.8017	−0.1508	0.5413	0.113*
C19	0.51878 (19)	−0.2616 (3)	0.45388 (9)	0.0432 (6)
C21	0.5319 (3)	−0.4195 (3)	0.42755 (13)	0.0645 (9)
H21A	0.4842	−0.4275	0.4023	0.097*
H21B	0.5235	−0.5082	0.4496	0.097*
H21C	0.5964	−0.4239	0.4139	0.097*
N1	0.61150 (15)	0.2016 (2)	0.40376 (7)	0.0403 (5)
O4	0.75112 (18)	0.3981 (3)	0.28729 (8)	0.0785 (7)
O14	0.66150 (14)	0.0289 (3)	0.49771 (7)	0.0605 (5)
O16	0.59648 (15)	−0.1010 (3)	0.56013 (7)	0.0599 (5)

O18	0.54378 (14)	−0.1354 (2)	0.43235 (7)	0.0528 (5)
O20	0.48062 (16)	−0.2675 (2)	0.49478 (7)	0.0548 (5)
Cu1	0.53871 (2)	0.07893 (4)	0.463419 (10)	0.03838 (14)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0516 (14)	0.0546 (15)	0.0371 (13)	0.0007 (12)	−0.0041 (11)	−0.0014 (11)
C3	0.0459 (14)	0.073 (2)	0.0507 (16)	−0.0091 (14)	−0.0022 (13)	0.0041 (14)
C5	0.112 (3)	0.143 (4)	0.051 (2)	0.019 (3)	0.017 (2)	0.037 (2)
C6	0.130 (4)	0.169 (5)	0.040 (2)	0.041 (4)	0.001 (2)	0.027 (3)
C7	0.125 (4)	0.148 (5)	0.043 (2)	0.022 (3)	−0.025 (2)	0.007 (3)
C8	0.096 (3)	0.114 (3)	0.046 (2)	0.002 (2)	−0.0189 (18)	0.005 (2)
C9	0.0458 (13)	0.0538 (15)	0.0381 (14)	−0.0032 (12)	−0.0015 (11)	0.0009 (11)
C10	0.0533 (15)	0.0664 (18)	0.0415 (15)	−0.0018 (13)	0.0043 (12)	0.0073 (13)
C11	0.081 (2)	0.099 (3)	0.0434 (17)	0.005 (2)	0.0041 (16)	0.0211 (17)
C12	0.072 (2)	0.078 (2)	0.0377 (15)	0.0072 (17)	−0.0059 (14)	0.0064 (14)
C13	0.0539 (15)	0.0585 (16)	0.0338 (13)	0.0033 (13)	−0.0016 (11)	0.0030 (11)
C15	0.0570 (17)	0.0584 (16)	0.0396 (15)	0.0185 (14)	−0.0043 (12)	−0.0090 (12)
C17	0.0528 (18)	0.106 (3)	0.068 (2)	0.0206 (18)	−0.0119 (16)	−0.004 (2)
C19	0.0480 (13)	0.0389 (13)	0.0428 (15)	0.0084 (11)	0.0091 (11)	−0.0001 (11)
C21	0.092 (2)	0.0427 (16)	0.0593 (19)	0.0002 (14)	0.0242 (17)	−0.0096 (13)
N1	0.0463 (11)	0.0432 (11)	0.0315 (10)	0.0019 (9)	0.0000 (9)	−0.0002 (8)
O4	0.0671 (14)	0.115 (2)	0.0535 (13)	−0.0139 (13)	0.0089 (12)	0.0285 (13)
O14	0.0484 (11)	0.0798 (14)	0.0534 (12)	0.0052 (10)	−0.0035 (9)	0.0102 (11)
O16	0.0558 (12)	0.0810 (15)	0.0428 (11)	0.0132 (10)	−0.0063 (9)	0.0065 (10)
O18	0.0747 (13)	0.0408 (10)	0.0427 (11)	−0.0008 (9)	0.0190 (9)	−0.0060 (8)
O20	0.0849 (14)	0.0396 (10)	0.0399 (10)	−0.0005 (9)	0.0170 (10)	−0.0027 (8)
Cu1	0.0451 (2)	0.0407 (2)	0.02941 (19)	0.00430 (12)	0.00409 (12)	0.00026 (12)

Geometric parameters (Å, °)

C2—N1	1.349 (3)	C12—C13	1.458 (4)
C2—C3	1.369 (4)	C15—O16	1.242 (4)
C2—H2A	0.93	C15—O14	1.256 (3)
C3—C10	1.365 (4)	C15—C17	1.509 (4)
C3—H3A	0.93	C17—H17A	0.96
C5—C6	1.364 (7)	C17—H17B	0.96
C5—C11	1.386 (5)	C17—H17C	0.96
C5—H5A	0.93	C19—O18	1.246 (3)
C6—C7	1.360 (7)	C19—O20	1.250 (3)
C6—H6A	0.93	C19—C21	1.503 (4)
C7—C8	1.393 (6)	C21—H21A	0.96
C7—H7A	0.93	C21—H21B	0.96
C8—C12	1.381 (5)	C21—H21C	0.96
C8—H8A	0.93	N1—Cu1	2.180 (2)
C9—N1	1.331 (3)	O14—Cu1	1.9731 (19)
C9—C13	1.375 (4)	O16—Cu1^{i}	1.969 (2)

C9—H9A	0.93	O18—Cu1	1.9650 (19)
C10—O4	1.373 (3)	O20—Cu1^{i}	1.9562 (19)
C10—C13	1.392 (4)	Cu1—O20^{i}	1.9562 (19)
C11—O4	1.377 (4)	Cu1—O16^{i}	1.969 (2)
C11—C12	1.391 (5)	Cu1—Cu1^{i}	2.6330 (6)

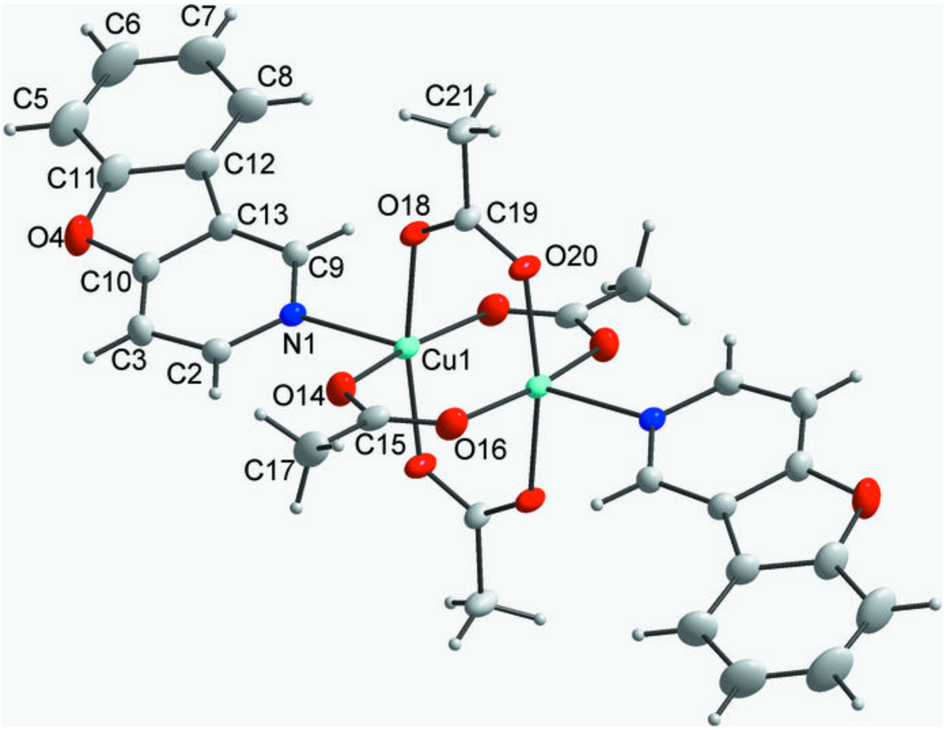
N1—C2—C3	124.3 (2)	C15—C17—H17B	109.5
N1—C2—H2A	117.9	H17A—C17—H17B	109.5
C3—C2—H2A	117.9	C15—C17—H17C	109.5
C10—C3—C2	115.7 (3)	H17A—C17—H17C	109.5
C10—C3—H3A	122.1	H17B—C17—H17C	109.5
C2—C3—H3A	122.1	O18—C19—O20	125.6 (2)
C6—C5—C11	116.8 (4)	O18—C19—C21	117.1 (2)
C6—C5—H5A	121.6	O20—C19—C21	117.2 (2)
C11—C5—H5A	121.6	C19—C21—H21A	109.5
C7—C6—C5	122.0 (4)	C19—C21—H21B	109.5
C7—C6—H6A	119.0	H21A—C21—H21B	109.5
C5—C6—H6A	119.0	C19—C21—H21C	109.5
C6—C7—C8	121.8 (4)	H21A—C21—H21C	109.5
C6—C7—H7A	119.1	H21B—C21—H21C	109.5
C8—C7—H7A	119.1	C9—N1—C2	118.4 (2)
C12—C8—C7	117.4 (4)	C9—N1—Cu1	121.04 (17)
C12—C8—H8A	121.3	C2—N1—Cu1	120.44 (17)
C7—C8—H8A	121.3	C10—O4—C11	105.6 (2)
N1—C9—C13	122.0 (2)	C15—O14—Cu1	124.9 (2)
N1—C9—H9A	119.0	C15—O16—Cu1^{i}	121.51 (18)
C13—C9—H9A	119.0	C19—O18—Cu1	121.90 (16)
C3—C10—O4	126.1 (3)	C19—O20—Cu1^{i}	124.31 (18)
C3—C10—C13	122.2 (3)	O20^{i}—Cu1—O18	167.88 (8)
O4—C10—C13	111.7 (2)	O20^{i}—Cu1—O16^{i}	89.82 (9)
O4—C11—C5	125.4 (4)	O18—Cu1—O16^{i}	88.29 (9)
O4—C11—C12	112.2 (3)	O20^{i}—Cu1—O14	89.69 (10)
C5—C11—C12	122.4 (4)	O18—Cu1—O14	89.67 (9)
C8—C12—C11	119.7 (3)	O16^{i}—Cu1—O14	167.97 (9)
C8—C12—C13	135.5 (3)	O20^{i}—Cu1—N1	98.31 (8)
C11—C12—C13	104.9 (3)	O18—Cu1—N1	93.81 (8)
C9—C13—C10	117.4 (2)	O16^{i}—Cu1—N1	97.68 (8)
C9—C13—C12	136.9 (3)	O14—Cu1—N1	94.29 (8)
C10—C13—C12	105.7 (3)	O20^{i}—Cu1—Cu1^{i}	83.12 (6)
O16—C15—O14	125.6 (3)	O18—Cu1—Cu1^{i}	84.80 (6)
O16—C15—C17	118.1 (3)	O16^{i}—Cu1—Cu1^{i}	85.65 (6)
O14—C15—C17	116.3 (3)	O14—Cu1—Cu1^{i}	82.35 (6)
C15—C17—H17A	109.5	N1—Cu1—Cu1^{i}	176.36 (6)

N1—C2—C3—C10	−0.5 (5)	C5—C11—O4—C10	−179.8 (4)
C11—C5—C6—C7	0.3 (8)	C12—C11—O4—C10	0.0 (4)
C5—C6—C7—C8	−0.2 (9)	O16—C15—O14—Cu1	1.4 (4)

C6—C7—C8—C12	−0.4 (8)	C17—C15—O14—Cu1	−177.9 (2)
C2—C3—C10—O4	−178.9 (3)	O14—C15—O16—Cu1$^{\mathrm{i}}$	0.0 (4)
C2—C3—C10—C13	0.0 (5)	C17—C15—O16—Cu1$^{\mathrm{i}}$	179.2 (2)
C6—C5—C11—O4	179.9 (4)	O20—C19—O18—Cu1	6.5 (4)
C6—C5—C11—C12	0.1 (7)	C21—C19—O18—Cu1	−176.2 (2)
C7—C8—C12—C11	0.8 (6)	O18—C19—O20—Cu1$^{\mathrm{i}}$	−5.3 (4)
C7—C8—C12—C13	−179.7 (4)	C21—C19—O20—Cu1$^{\mathrm{i}}$	177.4 (2)
O4—C11—C12—C8	179.5 (3)	C19—O18—Cu1—O20$^{\mathrm{i}}$	−8.4 (6)
C5—C11—C12—C8	−0.7 (6)	C19—O18—Cu1—O16$^{\mathrm{i}}$	−89.6 (2)
O4—C11—C12—C13	−0.1 (4)	C19—O18—Cu1—O14	78.5 (2)
C5—C11—C12—C13	179.6 (4)	C19—O18—Cu1—N1	172.8 (2)
N1—C9—C13—C10	−1.8 (4)	C19—O18—Cu1—Cu1$^{\mathrm{i}}$	−3.8 (2)
N1—C9—C13—C12	178.7 (3)	C15—O14—Cu1—O20$^{\mathrm{i}}$	81.6 (2)
C3—C10—C13—C9	1.1 (5)	C15—O14—Cu1—O18	−86.3 (2)
O4—C10—C13—C9	−179.9 (3)	C15—O14—Cu1—O16$^{\mathrm{i}}$	−6.1 (6)
C3—C10—C13—C12	−179.3 (3)	C15—O14—Cu1—N1	179.9 (2)
O4—C10—C13—C12	−0.2 (4)	C15—O14—Cu1—Cu1$^{\mathrm{i}}$	−1.5 (2)
C8—C12—C13—C9	0.1 (7)	C9—N1—Cu1—O20$^{\mathrm{i}}$	−115.6 (2)
C11—C12—C13—C9	179.7 (4)	C2—N1—Cu1—O20$^{\mathrm{i}}$	68.5 (2)
C8—C12—C13—C10	−179.4 (4)	C9—N1—Cu1—O18	64.1 (2)
C11—C12—C13—C10	0.2 (4)	C2—N1—Cu1—O18	−111.78 (19)
C13—C9—N1—C2	1.4 (4)	C9—N1—Cu1—O16$^{\mathrm{i}}$	−24.6 (2)
C13—C9—N1—Cu1	−174.6 (2)	C2—N1—Cu1—O16$^{\mathrm{i}}$	159.43 (19)
C3—C2—N1—C9	−0.2 (4)	C9—N1—Cu1—O14	154.1 (2)
C3—C2—N1—Cu1	175.8 (2)	C2—N1—Cu1—O14	−21.8 (2)
C3—C10—O4—C11	179.2 (3)	C9—N1—Cu1—Cu1$^{\mathrm{i}}$	131.5 (8)
C13—C10—O4—C11	0.2 (4)	C2—N1—Cu1—Cu1$^{\mathrm{i}}$	−44.4 (10)

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

Fig. 1


C6
C7
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O4
O20
C10
C9
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C3
C2
Cu1
O14
C15
O16
C17