

[μ -10,21-Difluoro-3,6,14,17-tetrazatri-cyclo[17.3.1.1^{8,12}]tetracos-1(23),2,6,-8,10,12(24),13,17,19,21-decaene-23,24-diolato- κ^4 N³,N⁶,O²³,O²⁴: κ^4 N¹⁴,N¹⁷,-O²³,O²⁴]bis[methanolcopper(II)]bis(perchlorate)

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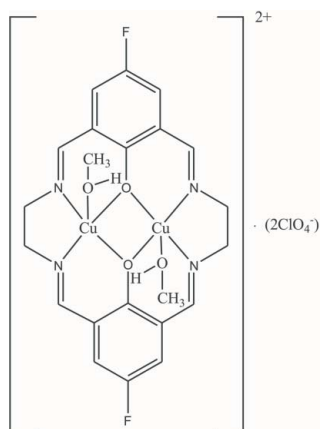
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Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.031; wR factor = 0.086; data-to-parameter ratio = 13.0.

The title complex, $[\text{Cu}_2(\text{C}_{20}\text{H}_{16}\text{F}_2\text{N}_4\text{O}_2)(\text{CH}_3\text{O})_2](\text{ClO}_4)_2$, was synthesized by cyclo-condensation between ethylenediamine and 2,6-diformyl-4-fluorophenol in the presence of Cu^{II} ions. This dinuclear copper complex is centrosymmetric. Both Cu atoms are in a distorted tetrahedral geometry, coordinated by three O atoms and two N atoms. The two Cu atoms are bridged by two endogenous phenol O atoms, with a $\text{Cu}\cdots\text{Cu}$ distance of 2.8998 (7) Å. In the crystal structure, the perchlorate ions link the macrocycles through inter- and intramolecular hydrogen bonds.

Related literature

For related literature, see: Adams *et al.* (1995); Aono *et al.* (1997); Bruker (2000); Chen *et al.* (2005, 2007); Gou & Fenton (1994); Pilkington & Robson (1970); Taniguchi (1984).



Experimental

Crystal data

$[\text{Cu}_2(\text{C}_{20}\text{H}_{16}\text{F}_2\text{N}_4\text{O}_2)-(\text{CH}_3\text{O})_2](\text{ClO}_4)_2$
 $M_r = 772.43$
 Triclinic, $P\bar{1}$
 $a = 7.8124$ (13) Å
 $b = 8.4132$ (15) Å
 $c = 10.8144$ (18) Å
 $\alpha = 103.127$ (3)°

$\beta = 96.272$ (3)°
 $\gamma = 97.569$ (3)°
 $V = 679.0$ (2) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 1.85$ mm⁻¹
 $T = 296$ (2) K
 $0.20 \times 0.20 \times 0.10$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 3953 measured reflections
 2633 independent reflections
 2268 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.011$
 SADABS; Bruker, 2000
 $T_{\text{min}} = 0.709$, $T_{\text{max}} = 0.837$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.086$
 $S = 1.07$
 2633 reflections
 203 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.31$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.24$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C10}-\text{H10}\cdots\text{O6}^{\text{i}}$	0.93	2.58	3.456 (4)	156
$\text{C7}-\text{H7}\cdots\text{O4}^{\text{ii}}$	0.93	2.53	3.364 (3)	150
$\text{C5}-\text{H5}\cdots\text{O2}^{\text{iii}}$	0.93	2.43	3.319 (3)	161
$\text{C3}-\text{H3}\cdots\text{O5}^{\text{iv}}$	0.93	2.56	3.431 (4)	156
$\text{C9}-\text{H9A}\cdots\text{O5}^{\text{v}}$	0.97	2.52	3.321 (4)	140
$\text{O2}-\text{H2}\cdots\text{O4}^{\text{v}}$	0.810 (10)	2.57 (4)	3.195 (3)	135 (4)
$\text{O2}-\text{H2}\cdots\text{O3}^{\text{v}}$	0.810 (10)	2.199 (16)	2.993 (4)	166 (5)

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

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2298).

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supplementary materials

Acta Cryst. (2007). E63, m2641 [doi:10.1107/S1600536807047009]

[μ -10,21-Difluoro-3,6,14,17-tetrazatricyclo[17.3.1.1^{8,12}]tetracos-1(23),2,6,8,10,12(24),13,17,19,21-decaene-23,24-diolato- κ^4 N³,N⁶,O²³,O²⁴: κ^4 N¹⁴,N¹⁷,O²³,O²⁴]bis[methanolcopper(II)] bis(perchlorate)

J.-L. Bai, H. Zhou, Z.-Q. Pan and X.-G. Meng

Comment

Since the Robson-style homodinuclear macrocyclic complexes were synthesized *via* template condensation, there has been an increasing interest in the research of these complexes (Pilkington & Robson, 1970; Aono *et al.*, 1997). In the past, most of these complexes were synthesized by cyclocondensation between 2,6-diformyl-4-*R*-phenol (*R* = CH₃, Cl, Br, CH₃O, *n*-butyl) and alkylenediamine by stepwise template reaction (Gou & Fenton, 1994; Adams *et al.*, 1995). But only a few crystal structures of the complexes with fluorophenyl substituents have been published (Chen *et al.*, 2005; Chen *et al.*, 2007). In this paper, we report the synthesis and crystal structure of the title complex with fluorophenyl substituents.

The crystal structure of the title complex is shown in Fig. 1. Selected bond distances and angles relevant to the coordination geometries of copper atoms are listed in Table 1. Each copper atom is coordinated by two endogenous phenolic O atoms, two azomethine nitrogen atoms and one oxygen atom from methanol molecule. The coordination polyhedron of each Cu^{II} can be described as distorted tetragonal pyramid. The deviation of Cu1 and Cu1* from the mean plane of atoms N1, N2, O1, O1* [mean deviation = 0.0182 (3) Å] and N1*, N2*, O1, O1* [mean deviation = 0.0182 (3) Å] are 0.1713 (3) Å and -0.1714 (3) Å, respectively. The two atom groups O1, O1*, Cu1, Cu1* and N1, N2, N1*, N2* are almost coplanar with the dihedral angle of the two planes 7.0 (3)°. The parallelogram formed by atoms N1, N2, N1*, N2* approximates a rectangle with the angle of N1—N2—N1* 89.7 (3)°. The Cu...Cu distance is 2.8998 (7) Å. The Cu—N bond lengths are 1.886 (2) and 1.885 (2) Å. the Cu—O bondlengths to the methanol molecule are both 2.364 (2) Å, which is much longer than those for the phenolic O atoms [1.8905 (17) Å and 1.9021 (17) Å]. The crystal structure of is stabilized by intramolecular and intermolecular hydrogen bonds of types O—H...O and C—H...O, where O atoms belong to methanol molecules or perchlorate ions.

Experimental

2, 6-Diformyl-4-fluorophenol was prepared according to the literature method of Taniguchi (1984). To a solution of 2, 6-diformyl-4-fluorophenol (0.6 mmol, 0.101 g) in absolute methanol (10 ml) was added methanol solution (10 ml) of Cu(OAc)₂H₂O (0.3 mmol, 0.06 g). The solution was stirred vigorously while a methanol solution (10 ml) containing ethylenediamine (0.6 mmol, 0.036 g) was added dropwise over a period of 2 h. The mixture was still stirred for 12 h at room temperature. Then, the Cu(ClO₄)₂·6H₂O (0.3 mmol, 0.111 g) was added to the solution and stirred for 6 h at room temperature. The dark-green block-shaped crystals suitable for X-ray diffraction were obtained by slow diffusion of ethyl acetate into the mother solution over a period of three weeks.

Refinement

All H atoms for C—H distances were placed in calculated positions in the range 0.93–0.97 Å, and included in the refinement in the riding-model approximation, with $U(\text{H})$ set to $1.2\text{--}1.5U_{\text{eq}}(\text{C})$. The methanol H atom was located in a difference Fourier map, and was refined with an O—H distance restraint of 0.808 Å; its temperature factor was set to $1.5U_{\text{eq}}(\text{O})$.

Figures

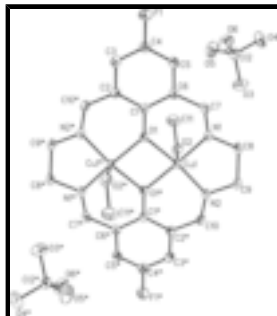


Fig. 1. A view of the title complex, showing the labeling of the non-H atoms and 30% probability ellipsoids. H atoms have been omitted. Atoms marked with an asterisk(*) are at the symmetry-generated position (Symmetry code for primed atoms: $-x, -y, 1 - z$).

[μ -10,21-Difluoro-3,6,14,17-tetrazatricyclo[17.3.1.1^{8,12}]tetracosan-1(23),2,6,8,10,12(24),13,17,19,21-decaene-23,24-diolato- $\kappa^4\text{N}^3, \text{N}^6, \text{O}^{23}, \text{O}^{24}$: $\kappa^4\text{N}^{14}, \text{N}^{17}, \text{O}^{23}, \text{O}^{24}$]bis[methanolicopper(II)] bis(perchlorate)

Crystal data

$[\text{Cu}_2(\text{C}_{20}\text{H}_{16}\text{F}_2\text{N}_4\text{O}_2)(\text{CH}_4\text{O})_2](\text{ClO}_4)_2$	$Z = 1$
$M_r = 772.43$	$F_{000} = 390$
Triclinic, $P\bar{1}$	$D_x = 1.889 \text{ Mg m}^{-3}$
Hall symbol: $-P 1$	Mo $K\alpha$ radiation
$a = 7.8124(13) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 8.4132(15) \text{ \AA}$	Cell parameters from 1982 reflections
$c = 10.8144(18) \text{ \AA}$	$\theta = 2.5\text{--}29.0^\circ$
$\alpha = 103.127(3)^\circ$	$\mu = 1.85 \text{ mm}^{-1}$
$\beta = 96.272(3)^\circ$	$T = 296(2) \text{ K}$
$\gamma = 97.569(3)^\circ$	Block, blue
$V = 679.0(2) \text{ \AA}^3$	$0.20 \times 0.20 \times 0.10 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	2633 independent reflections
Radiation source: fine-focus sealed tube	2268 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.011$
$T = 296(2) \text{ K}$	$\theta_{\text{max}} = 26.0^\circ$
φ and ω scans	$\theta_{\text{min}} = 2.5^\circ$
Absorption correction: multi-scan	$h = -9 \rightarrow 9$

(SADABS; Bruker, 2000)

$T_{\min} = 0.709$, $T_{\max} = 0.837$

3953 measured reflections

$k = -10 \rightarrow 9$

$l = -13 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.086$

$S = 1.07$

2633 reflections

203 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.1892P]$$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.31 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.24 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.01488 (4)	-0.09325 (4)	0.37234 (3)	0.04503 (13)
C1	0.2955 (3)	0.1735 (3)	0.5123 (2)	0.0370 (5)
C2	0.3570 (3)	0.3063 (3)	0.6204 (2)	0.0354 (5)
C3	0.5275 (3)	0.3910 (3)	0.6307 (2)	0.0420 (6)
H3	0.5719	0.4799	0.7003	0.050*
C4	0.6272 (3)	0.3414 (3)	0.5374 (3)	0.0442 (6)
C5	0.5696 (3)	0.2153 (3)	0.4317 (2)	0.0417 (6)
H5	0.6421	0.1883	0.3700	0.050*
C6	0.4006 (3)	0.1256 (3)	0.4157 (2)	0.0358 (5)
C7	0.3459 (3)	-0.0089 (3)	0.2995 (2)	0.0390 (5)
H7	0.4248	-0.0265	0.2412	0.047*
C8	0.1400 (4)	-0.2311 (3)	0.1512 (2)	0.0459 (6)
H8A	0.2396	-0.2760	0.1197	0.055*
H8B	0.0860	-0.1823	0.0869	0.055*

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C9	0.0077 (3)	-0.3705 (3)	0.1745 (2)	0.0432 (6)
H9A	-0.0661	-0.4279	0.0946	0.052*
H9B	0.0694	-0.4498	0.2056	0.052*
C10	-0.2534 (3)	-0.3680 (3)	0.2794 (2)	0.0386 (5)
H10	-0.3024	-0.4645	0.2179	0.046*
C11	-0.0536 (4)	0.2138 (4)	0.2389 (4)	0.0703 (9)
H11A	-0.0062	0.2864	0.3210	0.105*
H11B	-0.1355	0.2649	0.1947	0.105*
H11C	0.0391	0.1924	0.1891	0.105*
Cl2	0.37721 (9)	0.23525 (8)	0.03502 (6)	0.04801 (18)
F1	0.7932 (2)	0.4251 (2)	0.54902 (17)	0.0679 (5)
N1	0.1980 (3)	-0.1037 (2)	0.27212 (19)	0.0394 (5)
N2	-0.1008 (3)	-0.2997 (2)	0.27003 (18)	0.0368 (4)
O1	0.1343 (2)	0.0926 (2)	0.49992 (17)	0.0534 (5)
O2	-0.1394 (3)	0.0628 (2)	0.25626 (19)	0.0533 (5)
O3	0.2525 (4)	0.0916 (3)	0.0236 (3)	0.0959 (9)
O4	0.4365 (3)	0.2247 (4)	-0.0854 (2)	0.0825 (7)
O5	0.2965 (4)	0.3775 (3)	0.0673 (3)	0.0877 (8)
O6	0.5174 (3)	0.2428 (3)	0.1313 (2)	0.0847 (8)
H2	-0.178 (6)	0.007 (5)	0.185 (2)	0.127*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0476 (2)	0.0403 (2)	0.03627 (19)	-0.00728 (14)	0.01882 (14)	-0.01080 (13)
C1	0.0417 (13)	0.0348 (12)	0.0315 (12)	0.0000 (10)	0.0084 (10)	0.0038 (10)
C2	0.0400 (12)	0.0314 (12)	0.0326 (12)	0.0025 (10)	0.0041 (10)	0.0056 (9)
C3	0.0412 (13)	0.0396 (13)	0.0391 (13)	0.0004 (11)	0.0001 (11)	0.0036 (11)
C4	0.0329 (12)	0.0492 (15)	0.0474 (15)	-0.0003 (11)	0.0016 (11)	0.0111 (12)
C5	0.0363 (12)	0.0491 (15)	0.0408 (14)	0.0062 (11)	0.0098 (10)	0.0119 (11)
C6	0.0395 (12)	0.0365 (12)	0.0322 (12)	0.0049 (10)	0.0085 (10)	0.0089 (10)
C7	0.0430 (13)	0.0401 (13)	0.0355 (13)	0.0083 (11)	0.0170 (10)	0.0065 (10)
C8	0.0538 (15)	0.0460 (14)	0.0324 (13)	0.0045 (12)	0.0163 (11)	-0.0045 (11)
C9	0.0511 (14)	0.0359 (13)	0.0363 (13)	0.0047 (11)	0.0125 (11)	-0.0056 (10)
C10	0.0480 (14)	0.0310 (12)	0.0316 (12)	0.0035 (10)	0.0026 (10)	0.0001 (9)
C11	0.0641 (19)	0.063 (2)	0.089 (3)	0.0053 (16)	0.0208 (18)	0.0283 (19)
Cl2	0.0509 (4)	0.0473 (4)	0.0397 (4)	0.0023 (3)	0.0051 (3)	0.0021 (3)
F1	0.0386 (8)	0.0844 (13)	0.0654 (11)	-0.0136 (8)	0.0076 (8)	0.0003 (9)
N1	0.0470 (11)	0.0349 (11)	0.0326 (10)	0.0030 (9)	0.0131 (9)	-0.0008 (8)
N2	0.0432 (11)	0.0340 (10)	0.0295 (10)	0.0037 (9)	0.0090 (8)	-0.0002 (8)
O1	0.0478 (10)	0.0536 (11)	0.0412 (10)	-0.0181 (9)	0.0211 (8)	-0.0163 (8)
O2	0.0550 (11)	0.0431 (11)	0.0543 (12)	0.0014 (9)	0.0079 (9)	0.0001 (9)
O3	0.0901 (18)	0.0763 (18)	0.103 (2)	-0.0284 (14)	0.0149 (16)	0.0088 (15)
O4	0.0919 (18)	0.113 (2)	0.0528 (13)	0.0309 (16)	0.0281 (13)	0.0240 (14)
O5	0.0994 (18)	0.0747 (17)	0.0813 (17)	0.0365 (15)	0.0077 (15)	-0.0065 (13)
O6	0.0933 (18)	0.0789 (17)	0.0677 (16)	0.0063 (14)	-0.0271 (14)	0.0115 (13)

Geometric parameters (Å, °)

Cu1—N2	1.885 (2)	C8—N1	1.473 (3)
Cu1—N1	1.886 (2)	C8—C9	1.543 (4)
Cu1—O1	1.8905 (17)	C8—H8A	0.9700
Cu1—O1 ⁱ	1.9021 (17)	C8—H8B	0.9700
Cu1—O2	2.364 (2)	C9—N2	1.479 (3)
Cu1—Cu1 ⁱ	2.8998 (7)	C9—H9A	0.9700
C1—O1	1.327 (3)	C9—H9B	0.9700
C1—C2	1.409 (3)	C10—N2	1.278 (3)
C1—C6	1.418 (3)	C10—C2 ⁱ	1.465 (3)
C2—C3	1.406 (3)	C10—H10	0.9300
C2—C10 ⁱ	1.465 (3)	C11—O2	1.418 (4)
C3—C4	1.366 (4)	C11—H11A	0.9600
C3—H3	0.9300	C11—H11B	0.9600
C4—C5	1.359 (4)	C11—H11C	0.9600
C4—F1	1.370 (3)	Cl2—O6	1.411 (2)
C5—C6	1.404 (3)	Cl2—O4	1.417 (2)
C5—H5	0.9300	Cl2—O5	1.417 (2)
C6—C7	1.467 (3)	Cl2—O3	1.421 (3)
C7—N1	1.279 (3)	O1—Cu1 ⁱ	1.9022 (17)
C7—H7	0.9300	O2—H2	0.810 (10)
N2—Cu1—N1	90.13 (8)	C9—C8—H8A	109.8
N2—Cu1—O1	169.19 (9)	N1—C8—H8B	109.8
N1—Cu1—O1	94.42 (8)	C9—C8—H8B	109.8
N2—Cu1—O1 ⁱ	93.32 (8)	H8A—C8—H8B	108.2
N1—Cu1—O1 ⁱ	167.69 (9)	N2—C9—C8	109.70 (19)
O1—Cu1—O1 ⁱ	80.26 (8)	N2—C9—H9A	109.7
N2—Cu1—O2	94.58 (8)	C8—C9—H9A	109.7
N1—Cu1—O2	95.01 (8)	N2—C9—H9B	109.7
O1—Cu1—O2	94.78 (8)	C8—C9—H9B	109.7
O1 ⁱ —Cu1—O2	96.48 (8)	H9A—C9—H9B	108.2
N2—Cu1—Cu1 ⁱ	132.72 (6)	N2—C10—C2 ⁱ	125.1 (2)
N1—Cu1—Cu1 ⁱ	133.72 (6)	N2—C10—H10	117.5
O1—Cu1—Cu1 ⁱ	40.28 (5)	C2 ⁱ —C10—H10	117.5
O1 ⁱ —Cu1—Cu1 ⁱ	39.98 (5)	O2—C11—H11A	109.5
O2—Cu1—Cu1 ⁱ	97.38 (5)	O2—C11—H11B	109.5
O1—C1—C2	119.1 (2)	H11A—C11—H11B	109.5
O1—C1—C6	119.2 (2)	O2—C11—H11C	109.5
C2—C1—C6	121.7 (2)	H11A—C11—H11C	109.5
C3—C2—C1	118.1 (2)	H11B—C11—H11C	109.5
C3—C2—C10 ⁱ	117.1 (2)	O6—Cl2—O4	110.58 (16)
C1—C2—C10 ⁱ	124.8 (2)	O6—Cl2—O5	109.79 (16)
C4—C3—C2	119.3 (2)	O4—Cl2—O5	109.75 (16)
C4—C3—H3	120.4	O6—Cl2—O3	109.72 (18)

supplementary materials

C2—C3—H3	120.4	O4—Cl2—O3	107.74 (18)
C5—C4—C3	123.6 (2)	O5—Cl2—O3	109.22 (18)
C5—C4—F1	117.9 (2)	C7—N1—C8	124.5 (2)
C3—C4—F1	118.5 (2)	C7—N1—Cu1	126.02 (17)
C4—C5—C6	120.0 (2)	C8—N1—Cu1	109.37 (15)
C4—C5—H5	120.0	C10—N2—C9	124.4 (2)
C6—C5—H5	120.0	C10—N2—Cu1	125.07 (17)
C5—C6—C1	117.4 (2)	C9—N2—Cu1	110.53 (15)
C5—C6—C7	117.4 (2)	C1—O1—Cu1	130.12 (15)
C1—C6—C7	125.2 (2)	C1—O1—Cu1 ⁱ	128.21 (16)
N1—C7—C6	125.0 (2)	Cu1—O1—Cu1 ⁱ	99.74 (8)
N1—C7—H7	117.5	C11—O2—Cu1	119.82 (19)
C6—C7—H7	117.5	C11—O2—H2	105 (4)
N1—C8—C9	109.45 (19)	Cu1—O2—H2	110 (4)
N1—C8—H8A	109.8		
O1—C1—C2—C3	-179.4 (2)	C2 ⁱ —C10—N2—C9	174.9 (2)
C6—C1—C2—C3	-0.2 (4)	C2 ⁱ —C10—N2—Cu1	-6.7 (3)
O1—C1—C2—C10 ⁱ	-2.3 (4)	C8—C9—N2—C10	155.9 (2)
C6—C1—C2—C10 ⁱ	176.8 (2)	C8—C9—N2—Cu1	-22.7 (2)
C1—C2—C3—C4	-0.6 (4)	N1—Cu1—N2—C10	-174.2 (2)
C10 ⁱ —C2—C3—C4	-177.9 (2)	O1—Cu1—N2—C10	70.8 (5)
C2—C3—C4—C5	1.6 (4)	O1 ⁱ —Cu1—N2—C10	17.6 (2)
C2—C3—C4—F1	-179.9 (2)	O2—Cu1—N2—C10	-79.2 (2)
C3—C4—C5—C6	-1.6 (4)	Cu1 ⁱ —Cu1—N2—C10	25.3 (2)
F1—C4—C5—C6	179.9 (2)	N1—Cu1—N2—C9	4.38 (17)
C4—C5—C6—C1	0.7 (4)	O1—Cu1—N2—C9	-110.6 (4)
C4—C5—C6—C7	179.9 (2)	O1 ⁱ —Cu1—N2—C9	-163.80 (16)
O1—C1—C6—C5	179.4 (2)	O2—Cu1—N2—C9	99.42 (16)
C2—C1—C6—C5	0.2 (3)	Cu1 ⁱ —Cu1—N2—C9	-156.14 (13)
O1—C1—C6—C7	0.2 (4)	C2—C1—O1—Cu1	-177.49 (18)
C2—C1—C6—C7	-178.9 (2)	C6—C1—O1—Cu1	3.3 (4)
C5—C6—C7—N1	178.6 (2)	C2—C1—O1—Cu1 ⁱ	-16.6 (3)
C1—C6—C7—N1	-2.3 (4)	C6—C1—O1—Cu1 ⁱ	164.21 (18)
N1—C8—C9—N2	35.4 (3)	N2—Cu1—O1—C1	110.7 (4)
C6—C7—N1—C8	175.7 (2)	N1—Cu1—O1—C1	-4.0 (2)
C6—C7—N1—Cu1	0.6 (4)	O1 ⁱ —Cu1—O1—C1	164.9 (3)
C9—C8—N1—C7	152.6 (2)	O2—Cu1—O1—C1	-99.4 (2)
C9—C8—N1—Cu1	-31.5 (2)	Cu1 ⁱ —Cu1—O1—C1	164.9 (3)
N2—Cu1—N1—C7	-168.4 (2)	N2—Cu1—O1—Cu1 ⁱ	-54.2 (4)
O1—Cu1—N1—C7	1.8 (2)	N1—Cu1—O1—Cu1 ⁱ	-168.81 (10)
O1 ⁱ —Cu1—N1—C7	-62.0 (5)	O1 ⁱ —Cu1—O1—Cu1 ⁱ	0.0
O2—Cu1—N1—C7	97.0 (2)	O2—Cu1—O1—Cu1 ⁱ	95.78 (9)
Cu1 ⁱ —Cu1—N1—C7	-8.2 (3)	N2—Cu1—O2—C11	-144.7 (2)
N2—Cu1—N1—C8	15.90 (17)	N1—Cu1—O2—C11	-54.2 (2)
O1—Cu1—N1—C8	-173.91 (17)	O1—Cu1—O2—C11	40.7 (2)

O1 ⁱ —Cu1—N1—C8	122.3 (4)	O1 ⁱ —Cu1—O2—C11	121.4 (2)
O2—Cu1—N1—C8	-78.71 (17)	Cu1 ⁱ —Cu1—O2—C11	81.1 (2)
Cu1 ⁱ —Cu1—N1—C8	176.09 (13)		

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C10—H10 \cdots O6 ⁱⁱ	0.93	2.58	3.456 (4)	156
C7—H7 \cdots O4 ⁱⁱⁱ	0.93	2.53	3.364 (3)	150
C5—H5 \cdots O2 ^{iv}	0.93	2.43	3.319 (3)	161
C3—H3 \cdots O5 ^v	0.93	2.56	3.431 (4)	156
C9—H9A \cdots O5 ^{vi}	0.97	2.52	3.321 (4)	140
O2—H2 \cdots O4 ^{vi}	0.810 (10)	2.57 (4)	3.195 (3)	135 (4)
O2—H2 \cdots O3 ^{vi}	0.810 (10)	2.199 (16)	2.993 (4)	166 (5)

Symmetry codes: (ii) $x-1, y-1, z$; (iii) $-x+1, -y, -z$; (iv) $x+1, y, z$; (v) $-x+1, -y+1, -z+1$; (vi) $-x, -y, -z$.

Fig. 1

