

## catena-Poly[[triaquacopper(II)]- $\mu_2$ -furan-2,5-dicarboxylato- $\kappa^4 O^1, O^2: O^2, O^{2'}$ ]

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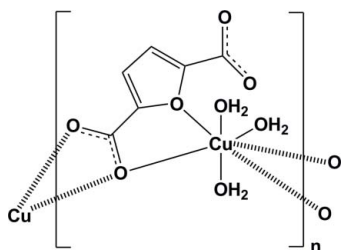
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(C-C) = 0.003$  Å;  $R$  factor = 0.031;  $wR$  factor = 0.070; data-to-parameter ratio = 12.9.

In the title compound,  $[Cu(C_6H_2O_5)(H_2O)_3]_n$ , an infinite chain is formed along [001] by linking of the  $Cu(OH_2)_3O_4$  cluster with one carboxylate group of the furan-2,5-dicarboxylate ligand. Adjacent chains are linked by  $O_{\text{water}}-H \cdots O$  hydrogen-bonding interactions. The  $Cu(OH_2)_3O_4$  cluster displays a pentagonal bipyramidal geometry with two weak coordinations [ $Cu-O_{\text{furan}} = 2.790$  (2) Å] and  $Cu-O_{\text{carboxylate}} = 2.684$  (2) Å] and two water molecules located in axial positions.

### Related literature

For background to metalorganic framework materials, see: Chui *et al.* (1999); Corma *et al.* (2010); Ferey (2008); Li *et al.* (1999); Murray *et al.* (2009); Tranchemontagne *et al.* (2009).



### Experimental

#### Crystal data

$[Cu(C_6H_2O_5)(H_2O)_3]$   
 $M_r = 271.66$   
 Monoclinic,  $P2_1/c$   
 $a = 7.0559$  (14) Å  
 $b = 15.040$  (3) Å  
 $c = 8.1578$  (16) Å  
 $\beta = 93.92$  (3)°

$V = 863.7$  (3) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 2.55$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.15 \times 0.14 \times 0.12$  mm

#### Data collection

Rigaku R-Axis RAPID  
 diffractometer  
 Absorption correction: multi-scan  
 (ABSCOR; Higashi, 1995)  
 $T_{\min} = 0.701$ ,  $T_{\max} = 0.749$

8400 measured reflections  
 1985 independent reflections  
 1656 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.039$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$   
 $wR(F^2) = 0.070$   
 $S = 1.09$   
 1985 reflections  
 154 parameters  
 10 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.43$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.44$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O1W-H1A \cdots O5^i$	0.81 (2)	2.04 (2)	2.843 (3)	173 (3)
$O1W-H1B \cdots O4^{ii}$	0.79 (2)	1.95 (2)	2.729 (3)	170 (3)
$O2W-H2A \cdots O5^{iii}$	0.82 (2)	1.91 (2)	2.690 (3)	161 (3)
$O2W-H2B \cdots O4^{iv}$	0.80 (2)	2.55 (3)	3.118 (3)	129 (3)
$O3W-H3A \cdots O4$	0.81 (2)	1.90 (2)	2.704 (3)	171 (3)
$O3W-H3B \cdots O1^v$	0.80 (2)	1.92 (2)	2.715 (2)	172 (3)

Symmetry codes: (i)  $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$ ; (ii)  $-x + 1, -y + 1, -z + 1$ ; (iii)  $-x, y + \frac{1}{2}, -z + \frac{3}{2}$ ; (iv)  $-x, -y + 1, -z + 1$ ; (v)  $x, y, z - 1$ .

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2000); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZJ2064).

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## supplementary materials

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**catena-Poly[[triaquacopper(II)]- $\mu_2$ -furan-2,5-dicarboxylato- $\kappa^4 O^1, O^2: O^2, O^2'$ ]**

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**Comment**

During past decades, the MOF materials have being attracted huge attentions due to the applications including gas absorption and catalyst reactions (Murray, *et al.*, 2009; Corma, *et al.*, 2010). The more efforts have been focused on the MOF based on the phenyl ring with carboxyl groups (Chui, *et al.*, 1999; Li, *et al.*, 1999; Ferey, 2008; Tranchemontagne, *et al.*, 2009). Compared with phenyl ring with carboxyl groups, the 5-membered rings with carboxyl groups as the ligand are rarely studied. Recently, we utilize furan-2,5-dicarboxyl acid as the ligand to constructed the MOFs. In this work, chainlike compound,  $[Cu(C_6O_5H_2)3H_2O]_n$  (I), is synthesized.

The asymmetric unit of (I) comprises of one Cu(II) cation, one furan-2,5-dicarboxylate anion and three  $H_2O$  (Fig.1). Cu cation is coordinated by three carboxyl O atoms, one oxygen of furan ring, and three water molecules of which two locate at the poles, exhibiting pentagonal bipyrimad geometry. It is necessarily noted that oxygen of furan ring ( $d_{O-Cu}=2.790$  (2) Å) and  $\eta^2$ -oxygen of carboxyl ( $d_{O-Cu}=2.684$  (2) Å) are very weakly ligated to Cu cation. If excluding this two O atoms, Cu displays trigonal bipyramid geometry and the chain property may not be changed. Only one carboxyl of furan-2,5-dicarboxylate involves in the formation of Cu polyhedron. The carboxyl shows  $\mu_2:\eta^1,\eta^2$  mode.

Cu cations are linked by one carboxyl of furan-2,5-dicarboxylate to give rise to the infinite chain (Fig.2). The H-bond of  $OW-H\cdots O$  holds together adjacent chains (Fig.3).

**Experimental**

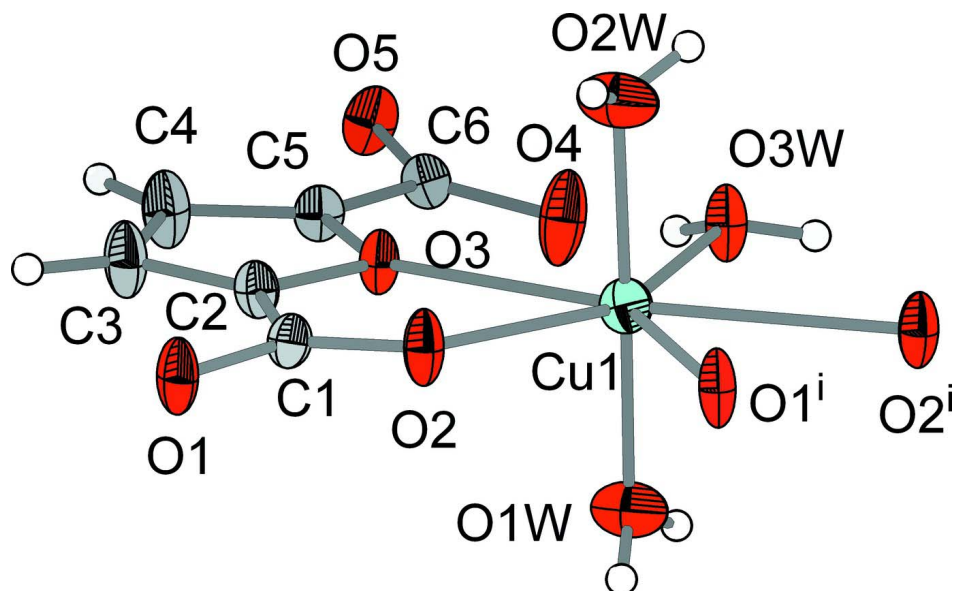
(I) was synthesized under solvothermal condition. In a typically route, furan-2,5-dicarboxyl acid (0.312 g, 2.0 mmol) and  $Cu(NO_3)_2\cdot 3H_2O$  (0.48 g, 2.0 mmol) were dissolved in the mixture of EtOH (2.9 ml, 50 mmol) and DMF (3.9 ml, 50 mmol) under stirring. Then, the clear solution with molar ratio of 1 (furan-2,5-dicarboxyl acid): 1 ( $Cu(NO_3)_2\cdot 3H_2O$ ): 25 (EtOH): 25 (DMF) was transferred into 23 ml autoclave and heated at 393 K for 24hrs. After naturally cooling to room temperature, blue block product was collected by filtration as a single phase.

**Refinement**

Water H atoms were located in a difference Fourier map and were refined with  $O-H = 0.82$  (2) Å,  $H\cdots H = 1.37$  (2) Å and  $U_{iso}(H) = 1.2U_{eq}(O)$ . The carbon H-atoms were placed in calculated positions ( $C-H = 0.93$  Å) and were included in the refinement in the riding-model approximation, with  $U_{iso}(H) = 1.2U_{eq}(C)$ .

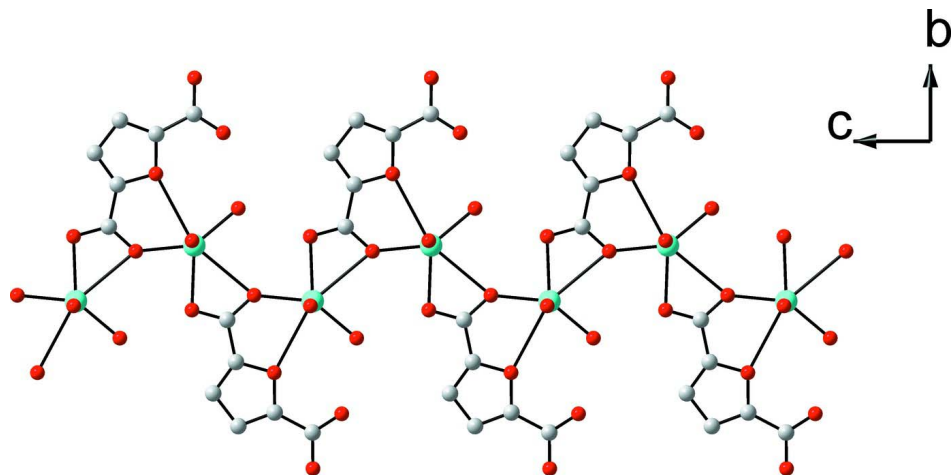
**Computing details**

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2000); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).



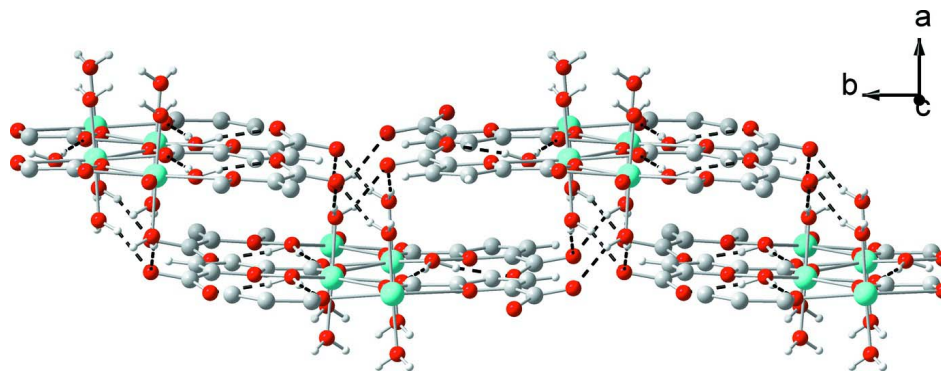
**Figure 1**

The unit cell of (I), showing the atomic labelling scheme and displacement ellipsoids at the 50% probability level. [Symmetry codes: (i)  $x, 1.5 - y, -0.5 + z$ .]



**Figure 2**

The stick plot of (I), displaying the infinite chain along (001) direction formed by linking the Cu with carboxyl of furan-2,5-dicarboxylate.


**Figure 3**

The ball-stick packing diagram of (I). The H-bond of OW—H...O holds together adjacent chains.

**catena-Poly[[triaquacopper(II)]- $\mu_2$ -furan-2,5-dicarboxylato-  $\kappa^4 O^1, O^2: O^2, O^2$ ]**

*Crystal data*

[Cu(C<sub>6</sub>H<sub>2</sub>O<sub>5</sub>)(H<sub>2</sub>O)<sub>3</sub>]

$M_r = 271.66$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 7.0559$  (14) Å

$b = 15.040$  (3) Å

$c = 8.1578$  (16) Å

$\beta = 93.92$  (3)°

$V = 863.7$  (3) Å<sup>3</sup>

$Z = 4$

$F(000) = 548$

$D_x = 2.089$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2000 reflections

$\theta = 3.2$ – $27.5$ °

$\mu = 2.55$  mm<sup>-1</sup>

$T = 296$  K

Block, light blue

$0.15 \times 0.14 \times 0.12$  mm

*Data collection*

Rigaku R-AXIS RAPID  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 10.00 pixels mm<sup>-1</sup>

$\omega$  scans

Absorption correction: multi-scan  
(*ABSCOR*; Higashi, 1995)

$T_{\min} = 0.701$ ,  $T_{\max} = 0.749$

8400 measured reflections

1985 independent reflections

1656 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 27.5$ °,  $\theta_{\min} = 3.2$ °

$h = -9 \rightarrow 9$

$k = -18 \rightarrow 19$

$l = -10 \rightarrow 10$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

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

$wR(F^2) = 0.070$

$S = 1.09$

1985 reflections

154 parameters

10 restraints

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

$w = 1/[\sigma^2(F_o^2) + (0.0277P)^2 + 0.660P]$

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

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

$\Delta\rho_{\max} = 0.43$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.44$  e Å<sup>-3</sup>

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.25359 (5)	0.68635 (2)	0.66688 (4)	0.02149 (11)
O1	0.2757 (3)	0.66588 (12)	1.1767 (2)	0.0271 (5)
O2	0.2608 (3)	0.69971 (11)	0.9141 (2)	0.0260 (4)
O3	0.2629 (3)	0.52292 (11)	0.82901 (19)	0.0198 (4)
O4	0.3038 (3)	0.42902 (12)	0.5442 (2)	0.0370 (5)
O5	0.2282 (3)	0.30371 (11)	0.6657 (2)	0.0263 (4)
C1	0.2663 (4)	0.64357 (16)	1.0277 (3)	0.0183 (5)
C2	0.2593 (4)	0.54734 (15)	0.9908 (3)	0.0188 (5)
C3	0.2454 (5)	0.47559 (17)	1.0867 (3)	0.0288 (6)
H3	0.2409	0.4750	1.2003	0.035*
C4	0.2389 (5)	0.40085 (17)	0.9808 (3)	0.0285 (6)
H4	0.2283	0.3416	1.0116	0.034*
C5	0.2511 (4)	0.43186 (15)	0.8272 (3)	0.0192 (5)
C6	0.2608 (4)	0.38628 (16)	0.6674 (3)	0.0198 (5)
O1W	0.5258 (3)	0.67555 (14)	0.6763 (2)	0.0320 (5)
H1A	0.588 (4)	0.7150 (17)	0.721 (4)	0.038*
H1B	0.573 (4)	0.6500 (19)	0.605 (3)	0.038*
O2W	-0.0197 (3)	0.69352 (15)	0.6594 (3)	0.0356 (5)
H2A	-0.060 (5)	0.7333 (18)	0.716 (3)	0.043*
H2B	-0.074 (5)	0.690 (2)	0.570 (2)	0.043*
O3W	0.2223 (3)	0.60185 (12)	0.4812 (2)	0.0261 (4)
H3A	0.258 (4)	0.5519 (10)	0.503 (3)	0.031*
H3B	0.245 (4)	0.6171 (18)	0.391 (2)	0.031*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Cu1	0.02457 (18)	0.02215 (17)	0.01807 (16)	0.00066 (14)	0.00374 (11)	-0.00597 (13)
O1	0.0528 (14)	0.0170 (9)	0.0118 (8)	-0.0027 (8)	0.0048 (8)	-0.0024 (7)
O2	0.0502 (13)	0.0154 (8)	0.0128 (8)	0.0014 (8)	0.0053 (8)	0.0000 (7)
O3	0.0368 (11)	0.0108 (8)	0.0120 (7)	-0.0012 (7)	0.0037 (7)	-0.0012 (7)
O4	0.0747 (17)	0.0181 (9)	0.0202 (9)	0.0038 (10)	0.0169 (10)	0.0004 (8)
O5	0.0432 (13)	0.0127 (9)	0.0237 (9)	-0.0066 (8)	0.0073 (8)	-0.0050 (7)
C1	0.0236 (14)	0.0162 (11)	0.0156 (11)	0.0012 (10)	0.0041 (9)	-0.0006 (10)
C2	0.0276 (14)	0.0152 (11)	0.0138 (10)	0.0013 (10)	0.0019 (9)	-0.0023 (10)
C3	0.053 (2)	0.0201 (12)	0.0129 (12)	-0.0026 (13)	0.0030 (11)	-0.0011 (11)
C4	0.0534 (19)	0.0132 (11)	0.0187 (12)	-0.0006 (12)	0.0014 (12)	0.0001 (11)

C5	0.0272 (13)	0.0109 (10)	0.0196 (11)	-0.0008 (10)	0.0018 (9)	-0.0026 (10)
C6	0.0236 (13)	0.0173 (12)	0.0184 (11)	0.0023 (10)	0.0014 (9)	-0.0021 (10)
O1W	0.0244 (11)	0.0360 (12)	0.0357 (11)	0.0011 (9)	0.0028 (9)	-0.0173 (9)
O2W	0.0238 (11)	0.0479 (13)	0.0353 (11)	0.0004 (10)	0.0025 (8)	-0.0235 (11)
O3W	0.0484 (13)	0.0161 (8)	0.0144 (8)	0.0038 (9)	0.0057 (8)	0.0012 (7)

*Geometric parameters (Å, °)*

Cu1—O1W	1.924 (2)	C2—C3	1.340 (4)
Cu1—O2W	1.928 (2)	C3—C4	1.416 (4)
Cu1—O3W	1.9782 (18)	C3—H3	0.9300
Cu1—O2	2.0243 (17)	C4—C5	1.345 (3)
Cu1—O1 <sup>i</sup>	2.2289 (18)	C4—H4	0.9300
O1—C1	1.258 (3)	C5—C6	1.479 (3)
O1—Cu1 <sup>ii</sup>	2.2289 (18)	C6—O4	1.248 (3)
O2—C1	1.252 (3)	O1W—H1A	0.809 (17)
O3—C2	1.372 (3)	O1W—H1B	0.791 (17)
O3—C5	1.372 (3)	O2W—H2A	0.816 (17)
O4—C6	1.248 (3)	O2W—H2B	0.802 (17)
O5—C6	1.263 (3)	O3W—H3A	0.807 (15)
C1—C2	1.478 (3)	O3W—H3B	0.799 (16)
O1W—Cu1—O2W	178.29 (10)	C4—C3—H3	126.8
O1W—Cu1—O3W	92.01 (9)	C5—C4—C3	106.9 (2)
O2W—Cu1—O3W	87.28 (9)	C5—C4—H4	126.5
O1W—Cu1—O2	90.67 (9)	C3—C4—H4	126.5
O2W—Cu1—O2	89.03 (9)	C4—C5—O3	110.1 (2)
O3W—Cu1—O2	145.16 (7)	C4—C5—C6	132.1 (2)
O1W—Cu1—O1 <sup>i</sup>	90.89 (8)	O3—C5—C6	117.8 (2)
O2W—Cu1—O1 <sup>i</sup>	90.73 (9)	O4—C6—O5	123.5 (2)
O3W—Cu1—O1 <sup>i</sup>	132.21 (7)	O4—C6—O5	123.5 (2)
O2—Cu1—O1 <sup>i</sup>	82.44 (6)	O4—C6—C5	120.0 (2)
C1—O1—Cu1 <sup>ii</sup>	103.45 (15)	O4—C6—C5	120.0 (2)
C1—O2—Cu1	131.89 (15)	O5—C6—C5	116.5 (2)
C2—O3—C5	105.81 (17)	Cu1—O1W—H1A	118 (2)
O2—C1—O1	122.1 (2)	Cu1—O1W—H1B	119 (2)
O2—C1—C2	120.7 (2)	H1A—O1W—H1B	116 (3)
O1—C1—C2	117.2 (2)	Cu1—O2W—H2A	114 (2)
C3—C2—O3	110.7 (2)	Cu1—O2W—H2B	116 (3)
C3—C2—C1	132.2 (2)	H2A—O2W—H2B	113 (3)
O3—C2—C1	117.1 (2)	Cu1—O3W—H3A	114.5 (15)
C2—C3—C4	106.5 (2)	Cu1—O3W—H3B	120 (2)
C2—C3—H3	126.8	H3A—O3W—H3B	113 (2)
O1W—Cu1—O2—C1	-84.2 (2)	C1—C2—C3—C4	178.1 (3)
O2W—Cu1—O2—C1	94.1 (2)	C2—C3—C4—C5	0.6 (4)
O3W—Cu1—O2—C1	10.3 (3)	C3—C4—C5—O3	-0.7 (3)
O1 <sup>i</sup> —Cu1—O2—C1	-175.0 (3)	C3—C4—C5—C6	176.7 (3)
Cu1—O2—C1—O1	177.90 (19)	C2—O3—C5—C4	0.5 (3)
Cu1—O2—C1—C2	-3.0 (4)	C2—O3—C5—C6	-177.2 (2)

Cu1 <sup>ii</sup> —O1—C1—O2	4.6 (3)	O4—O4—C6—O5	0.0 (3)
Cu1 <sup>ii</sup> —O1—C1—C2	-174.55 (19)	O4—O4—C6—C5	0.0 (3)
C5—O3—C2—C3	-0.2 (3)	C4—C5—C6—O4	-167.8 (3)
C5—O3—C2—C1	-178.8 (2)	O3—C5—C6—O4	9.3 (4)
O2—C1—C2—C3	-172.9 (3)	C4—C5—C6—O4	-167.8 (3)
O1—C1—C2—C3	6.3 (5)	O3—C5—C6—O4	9.3 (4)
O2—C1—C2—O3	5.4 (4)	C4—C5—C6—O5	10.6 (5)
O1—C1—C2—O3	-175.4 (2)	O3—C5—C6—O5	-172.3 (2)
O3—C2—C3—C4	-0.2 (3)		

Symmetry codes: (i)  $x, -y+3/2, z-1/2$ ; (ii)  $x, -y+3/2, z+1/2$ .

*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>
O1 <i>W</i> —H1 <i>A</i> $\cdots$ O5 <sup>iii</sup>	0.81 (2)	2.04 (2)	2.843 (3)	173 (3)
O1 <i>W</i> —H1 <i>B</i> $\cdots$ O4 <sup>iv</sup>	0.79 (2)	1.95 (2)	2.729 (3)	170 (3)
O2 <i>W</i> —H2 <i>A</i> $\cdots$ O5 <sup>v</sup>	0.82 (2)	1.91 (2)	2.690 (3)	161 (3)
O2 <i>W</i> —H2 <i>B</i> $\cdots$ O4 <sup>vi</sup>	0.80 (2)	2.55 (3)	3.118 (3)	129 (3)
O3 <i>W</i> —H3 <i>A</i> $\cdots$ O4	0.81 (2)	1.90 (2)	2.704 (3)	171 (3)
O3 <i>W</i> —H3 <i>B</i> $\cdots$ O1 <sup>vii</sup>	0.80 (2)	1.92 (2)	2.715 (2)	172 (3)

Symmetry codes: (iii)  $-x+1, y+1/2, -z+3/2$ ; (iv)  $-x+1, -y+1, -z+1$ ; (v)  $-x, y+1/2, -z+3/2$ ; (vi)  $-x, -y+1, -z+1$ ; (vii)  $x, y, z-1$ .