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## Structure Reports

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Tetraaquabis(4-formylbenzoato- $\kappa$ O)-cobalt(II) tetrahydrateZhao-Peng Deng,<sup>a</sup> Shan Gao,<sup>a</sup> Li-Hua Huo<sup>a</sup> and Seik Weng Ng<sup>b\*</sup><sup>a</sup>School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and <sup>b</sup>Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

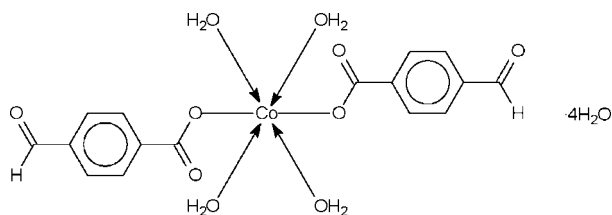
Received 11 January 2008; accepted 28 January 2008

Key indicators: single-crystal X-ray study;  $T = 295$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.027;  $wR$  factor = 0.080; data-to-parameter ratio = 13.9.

The  $\text{Co}^{\text{II}}$  atom in the title compound,  $[\text{Co}(\text{C}_8\text{H}_5\text{O}_3)_2(\text{H}_2\text{O})_4] \cdot 4\text{H}_2\text{O}$ , which exists in an all-*trans* octahedral coordination geometry, lies on a center of inversion. The coordinated and uncoordinated water molecules engage in extensive hydrogen-bonding interactions, forming a three-dimensional hydrogen-bonded network.

## Related literature

Hexaaquacobalt(II) bis(4-formylbenzoate) dihydrate was isolated from the reaction of cobalt(II) acetate and 4-formylbenzoic acid in the presence of sodium hydroxide; see Deng *et al.* (2006*b*). The reaction with pyridine in place of sodium hydroxide yielded the formylbenzoate-coordinated title compound. This is isostructural with the nickel analog; see Deng *et al.* (2006*a*).



## Experimental

## Crystal data

 $[\text{Co}(\text{C}_8\text{H}_5\text{O}_3)_2(\text{H}_2\text{O})_4] \cdot 4\text{H}_2\text{O}$  $M_r = 501.30$ Triclinic,  $P\bar{1}$  $a = 7.1472$  (3) Å $b = 7.4759$  (4) Å $c = 11.5720$  (6) Å $\alpha = 77.114$  (2)° $\beta = 77.905$  (2)° $\gamma = 63.839$  (1)° $V = 536.61$  (5) Å<sup>3</sup> $Z = 1$ Mo  $K\alpha$  radiation $\mu = 0.87$  mm<sup>-1</sup> $T = 295$  (2) K

0.30 × 0.26 × 0.22 mm

## Data collection

Rigaku R-Axis RAPID

diffractometer

Absorption correction: multi-scan

(ABSCOR; Higashi, 1995)

 $T_{\text{min}} = 0.666$ ,  $T_{\text{max}} = 0.832$ 

5294 measured reflections

2426 independent reflections

2270 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.015$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.027$  $wR(F^2) = 0.080$  $S = 1.03$ 

2426 reflections

174 parameters

12 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.35$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.27$  e Å<sup>-3</sup>

Table 1

Selected bond lengths (Å).

Co1—O1	2.098 (1)	Co1—O2W	2.116 (1)
Co1—O1W	2.113 (1)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1W—H1W1 $\cdots$ O3 <sup>i</sup>	0.86 (1)	1.77 (1)	2.611 (2)	166 (2)
O1W—H1W2 $\cdots$ O3W <sup>ii</sup>	0.84 (1)	2.11 (1)	2.925 (2)	161 (2)
O2W—H2W1 $\cdots$ O3W	0.85 (1)	1.97 (1)	2.808 (2)	168 (2)
O2W—H2W2 $\cdots$ O4W <sup>iii</sup>	0.85 (1)	1.97 (1)	2.808 (2)	169 (2)
O3W—H3W1 $\cdots$ O4W	0.85 (1)	2.00 (1)	2.810 (2)	159 (2)
O3W—H3W2 $\cdots$ O1 <sup>iii</sup>	0.84 (1)	2.19 (1)	2.992 (2)	159 (2)
O4W—H4W1 $\cdots$ O2 <sup>iv</sup>	0.85 (1)	1.93 (1)	2.771 (2)	169 (3)
O4W—H4W2 $\cdots$ O3 <sup>i</sup>	0.85 (1)	2.00 (1)	2.841 (2)	172 (3)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); method used to solve structure: atomic coordinates taken from the isostructural nickel analog; program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2668).

## References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.  
 Deng, Z.-P., Gao, S. & Ng, S. W. (2006*a*). *Acta Cryst.* **E62**, m2904–m2905.  
 Deng, Z.-P., Gao, S. & Ng, S. W. (2006*b*). *Acta Cryst.* **E62**, m3423–m3424.  
 Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.  
 Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.  
 Rigaku/MS (2002). *CrystalStructure*. Rigaku/MS, The Woodlands, Texas, USA.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Westrip, S. P. (2008). *pubCIF*. In preparation.

## supporting information

*Acta Cryst.* (2008). E64, m446 [doi:10.1107/S1600536808003140]

**Tetraaquabis(4-formylbenzoato- $\kappa$ O)cobalt(II) tetrahydrate**

**Zhao-Peng Deng, Shan Gao, Li-Hua Huo and Seik Weng Ng**

**S1. Comment**

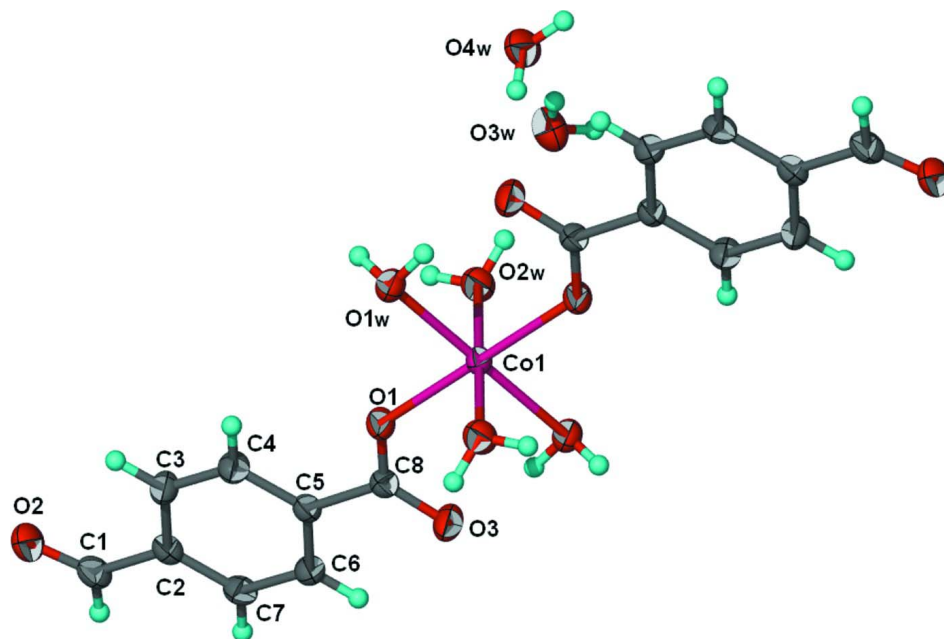
Hexaaquacobalt(II) bis(4-formylbenzoate) dihydrate was isolated from the reaction of cobalt(II) acetate and 4-formylbenzoic acid in the presence of sodium hydroxide (Deng *et al.*, 2006b). The reaction with pyridine in place of sodium hydroxide yielded the formylbenzoate-coordinated title compound.

**S2. Experimental**

Cobalt diacetate dihydrate (2.32 g, 10 mmol) was added to an aqueous solution of 4-formylbenzoic acid (3.0 g, 20 mmol) that was earlier been treated with 1 ml pyridine to give a pH of 6. The solution was allowed to evaporate at room temperature; pink prismatic crystals separated from the filtered solution after several days. C&H elemental analysis. Calc. for  $C_{16}H_{26}O_{14}Co$ : C 38.33, H 5.23%. Found: C 38.36, H 5.24%.

**S3. Refinement**

The carbon-bound H atoms were placed in calculated positions [C–H 0.93 Å and  $U_{iso}(H)$  1.2 $U_{eq}(C)$ ], and were included in the refinement in the riding-model approximation. The water H-atoms were located in a difference Fourier map, and were refined with distance restraints of O–H 0.85±0.01 Å and H··H 1.39±0.01 Å; their displacement parameters were freely refined.

**Figure 1**

Anisotropic displacement parameter plot of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms as spheres of arbitrary radius.

### Tetraaquabis(4-formylbenzoato- $\kappa$ O)cobalt(II) tetrahydrate

#### Crystal data

$[\text{Co}(\text{C}_8\text{H}_5\text{O}_3)_2(\text{H}_2\text{O})_4] \cdot 4\text{H}_2\text{O}$

$M_r = 501.30$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 7.1472$  (3) Å

$b = 7.4759$  (4) Å

$c = 11.5720$  (6) Å

$\alpha = 77.114$  (2)°

$\beta = 77.905$  (2)°

$\gamma = 63.839$  (1)°

$V = 536.61$  (5) Å<sup>3</sup>

$Z = 1$

$F(000) = 261$

$D_x = 1.551$  Mg m<sup>-3</sup>

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

Cell parameters from 4983 reflections

$\theta = 3.1\text{--}27.5^\circ$

$\mu = 0.87$  mm<sup>-1</sup>

$T = 295$  K

Prism, pink

$0.30 \times 0.26 \times 0.22$  mm

#### Data collection

Rigaku R-Axis RAPID  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 10.000 pixels mm<sup>-1</sup>

$\omega$  scans

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

$T_{\min} = 0.666$ ,  $T_{\max} = 0.832$

5294 measured reflections

2426 independent reflections

2270 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.016$

$\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 3.1^\circ$

$h = -9 \rightarrow 9$

$k = -9 \rightarrow 9$

$l = -15 \rightarrow 14$

Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.080$

$S = 1.03$

2426 reflections

174 parameters

12 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

$w = 1/[\sigma^2(F_o^2) + (0.0481P)^2 + 0.1724P]$

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

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

$\Delta\rho_{\max} = 0.36 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Co1	0.5000	0.5000	0.5000	0.02806 (11)
O1	0.45499 (18)	0.39037 (19)	0.36093 (10)	0.0359 (3)
O2	0.0927 (2)	0.2392 (2)	-0.11561 (12)	0.0492 (3)
O3	0.76754 (19)	0.3176 (2)	0.25021 (12)	0.0460 (3)
O1W	0.19780 (18)	0.52308 (19)	0.58061 (11)	0.0381 (3)
H1W1	0.192 (3)	0.570 (3)	0.6429 (14)	0.057 (7)*
H1W2	0.091 (3)	0.602 (3)	0.5461 (19)	0.071 (8)*
O2W	0.3680 (2)	0.79054 (18)	0.40003 (12)	0.0408 (3)
H2W1	0.329 (4)	0.893 (3)	0.434 (2)	0.067 (8)*
H2W2	0.271 (3)	0.807 (4)	0.362 (2)	0.069 (8)*
O3W	0.2016 (3)	1.1588 (2)	0.48800 (14)	0.0544 (4)
H3W1	0.152 (3)	1.158 (3)	0.5610 (10)	0.051 (6)*
H3W2	0.282 (4)	1.218 (4)	0.470 (2)	0.096 (11)*
O4W	-0.0173 (2)	1.1045 (2)	0.71542 (13)	0.0534 (4)
H4W1	0.001 (4)	1.159 (3)	0.767 (2)	0.076 (8)*
H4W2	0.048 (5)	0.9775 (14)	0.731 (3)	0.096 (11)*
C1	0.2664 (3)	0.2311 (2)	-0.11986 (15)	0.0384 (4)
H1	0.3563	0.2070	-0.1910	0.046*
C2	0.3455 (2)	0.2570 (2)	-0.01950 (13)	0.0311 (3)
C3	0.2157 (2)	0.3005 (3)	0.08787 (15)	0.0351 (3)
H3	0.0779	0.3139	0.0967	0.042*
C4	0.2921 (2)	0.3237 (3)	0.18106 (14)	0.0344 (3)
H4	0.2052	0.3537	0.2525	0.041*
C5	0.4989 (2)	0.3026 (2)	0.16869 (13)	0.0279 (3)
C6	0.6284 (2)	0.2574 (2)	0.06149 (14)	0.0321 (3)
H6	0.7668	0.2420	0.0528	0.039*
C7	0.5514 (3)	0.2353 (2)	-0.03205 (14)	0.0334 (3)
H7	0.6380	0.2059	-0.1037	0.040*
C8	0.5803 (2)	0.3383 (2)	0.26758 (13)	0.0297 (3)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Co1	0.02531 (16)	0.03279 (16)	0.02910 (16)	-0.01180 (12)	-0.00411 (10)	-0.01027 (11)

O1	0.0324 (5)	0.0492 (6)	0.0324 (6)	-0.0187 (5)	-0.0014 (4)	-0.0167 (5)
O2	0.0491 (8)	0.0561 (8)	0.0500 (8)	-0.0196 (6)	-0.0160 (6)	-0.0179 (6)
O3	0.0315 (6)	0.0714 (9)	0.0433 (7)	-0.0231 (6)	-0.0004 (5)	-0.0248 (6)
O1W	0.0298 (6)	0.0469 (7)	0.0409 (7)	-0.0161 (5)	-0.0034 (5)	-0.0134 (5)
O2W	0.0431 (7)	0.0362 (6)	0.0432 (7)	-0.0124 (5)	-0.0143 (5)	-0.0063 (5)
O3W	0.0666 (9)	0.0547 (8)	0.0556 (9)	-0.0350 (8)	-0.0125 (7)	-0.0084 (7)
O4W	0.0528 (8)	0.0562 (9)	0.0547 (9)	-0.0140 (7)	-0.0207 (6)	-0.0204 (7)
C1	0.0468 (9)	0.0372 (8)	0.0326 (8)	-0.0149 (7)	-0.0078 (7)	-0.0104 (6)
C2	0.0378 (8)	0.0278 (7)	0.0290 (7)	-0.0132 (6)	-0.0063 (6)	-0.0055 (5)
C3	0.0300 (7)	0.0459 (9)	0.0341 (8)	-0.0184 (7)	-0.0029 (6)	-0.0102 (6)
C4	0.0325 (8)	0.0448 (8)	0.0276 (7)	-0.0171 (7)	0.0008 (6)	-0.0106 (6)
C5	0.0300 (7)	0.0268 (6)	0.0278 (7)	-0.0114 (6)	-0.0048 (5)	-0.0056 (5)
C6	0.0292 (7)	0.0348 (7)	0.0331 (8)	-0.0137 (6)	-0.0007 (6)	-0.0084 (6)
C7	0.0379 (8)	0.0340 (7)	0.0273 (7)	-0.0143 (6)	0.0017 (6)	-0.0093 (6)
C8	0.0295 (7)	0.0297 (7)	0.0305 (7)	-0.0110 (6)	-0.0050 (6)	-0.0071 (5)

*Geometric parameters (Å, °)*

Co1—O1	2.098 (1)	O4W—H4W1	0.847 (10)
Co1—O1 <sup>i</sup>	2.098 (1)	O4W—H4W2	0.849 (10)
Co1—O1W <sup>i</sup>	2.113 (1)	C1—C2	1.475 (2)
Co1—O1w	2.113 (1)	C1—H1	0.9300
Co1—O2w	2.116 (1)	C2—C7	1.388 (2)
Co1—O2W <sup>i</sup>	2.116 (1)	C2—C3	1.393 (2)
O1—C8	1.2630 (18)	C3—C4	1.381 (2)
O2—C1	1.207 (2)	C3—H3	0.9300
O3—C8	1.2543 (19)	C4—C5	1.395 (2)
O1W—H1W1	0.858 (9)	C4—H4	0.9300
O1W—H1W2	0.844 (9)	C5—C6	1.393 (2)
O2W—H2W1	0.849 (9)	C5—C8	1.507 (2)
O2W—H2W2	0.848 (9)	C6—C7	1.382 (2)
O3W—H3W1	0.845 (9)	C6—H6	0.9300
O3W—H3W2	0.838 (10)	C7—H7	0.9300
O1—Co1—O1 <sup>i</sup>	180.0	O2—C1—C2	124.23 (16)
O1—Co1—O1W <sup>i</sup>	93.12 (5)	O2—C1—H1	117.9
O1 <sup>i</sup> —Co1—O1W <sup>i</sup>	86.88 (5)	C2—C1—H1	117.9
O1—Co1—O1W	86.88 (5)	C7—C2—C3	119.95 (14)
O1 <sup>i</sup> —Co1—O1W	93.12 (5)	C7—C2—C1	119.56 (14)
O1W <sup>i</sup> —Co1—O1W	180.0	C3—C2—C1	120.49 (14)
O1—Co1—O2W	86.82 (5)	C4—C3—C2	119.79 (14)
O1 <sup>i</sup> —Co1—O2W	93.18 (5)	C4—C3—H3	120.1
O1W <sup>i</sup> —Co1—O2W	89.23 (5)	C2—C3—H3	120.1
O1W—Co1—O2W	90.77 (5)	C3—C4—C5	120.42 (14)
O1—Co1—O2W <sup>i</sup>	93.18 (5)	C3—C4—H4	119.8
O1 <sup>i</sup> —Co1—O2W <sup>i</sup>	86.82 (5)	C5—C4—H4	119.8
O1W <sup>i</sup> —Co1—O2W <sup>i</sup>	90.77 (5)	C6—C5—C4	119.52 (14)
O1W—Co1—O2W <sup>i</sup>	89.23 (5)	C6—C5—C8	119.64 (13)

O2W—Co1—O2W <sup>i</sup>	180.0	C4—C5—C8	120.77 (13)
C8—O1—Co1	127.37 (10)	C7—C6—C5	120.04 (14)
Co1—O1W—H1W1	97.7 (16)	C7—C6—H6	120.0
Co1—O1W—H1W2	120.0 (19)	C5—C6—H6	120.0
H1W1—O1W—H1W2	108.3 (14)	C6—C7—C2	120.27 (14)
Co1—O2W—H2W1	118.7 (17)	C6—C7—H7	119.9
Co1—O2W—H2W2	113.8 (17)	C2—C7—H7	119.9
H2W1—O2W—H2W2	108.9 (15)	O3—C8—O1	124.60 (14)
H3W1—O3W—H3W2	110.9 (15)	O3—C8—C5	117.39 (13)
H4W1—O4W—H4W2	109.2 (15)	O1—C8—C5	118.00 (13)
O1 <sup>i</sup> —Co1—O1—C8	0 (100)	C4—C5—C6—C7	0.5 (2)
O1W <sup>i</sup> —Co1—O1—C8	-0.75 (13)	C8—C5—C6—C7	-176.45 (13)
O1W—Co1—O1—C8	179.25 (13)	C5—C6—C7—C2	-0.4 (2)
O2W—Co1—O1—C8	88.31 (13)	C3—C2—C7—C6	-0.2 (2)
O2W <sup>i</sup> —Co1—O1—C8	-91.69 (13)	C1—C2—C7—C6	-179.45 (14)
O2—C1—C2—C7	176.99 (16)	Co1—O1—C8—O3	10.4 (2)
O2—C1—C2—C3	-2.3 (3)	Co1—O1—C8—C5	-168.27 (9)
C7—C2—C3—C4	0.6 (2)	C6—C5—C8—O3	-2.7 (2)
C1—C2—C3—C4	179.83 (15)	C4—C5—C8—O3	-179.67 (15)
C2—C3—C4—C5	-0.4 (2)	C6—C5—C8—O1	176.00 (14)
C3—C4—C5—C6	-0.1 (2)	C4—C5—C8—O1	-0.9 (2)
C3—C4—C5—C8	176.80 (15)		

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

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

<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>
O1W—H1W1 $\cdots$ O3 <sup>i</sup>	0.86 (1)	1.77 (1)	2.611 (2)	166 (2)
O1W—H1W2 $\cdots$ O3W <sup>ii</sup>	0.84 (1)	2.11 (1)	2.925 (2)	161 (2)
O2W—H2W1 $\cdots$ O3W	0.85 (1)	1.97 (1)	2.808 (2)	168 (2)
O2W—H2W2 $\cdots$ O4W <sup>ii</sup>	0.85 (1)	1.97 (1)	2.808 (2)	169 (2)
O3W—H3W1 $\cdots$ O4W	0.85 (1)	2.00 (1)	2.810 (2)	159 (2)
O3W—H3W2 $\cdots$ O1 <sup>iii</sup>	0.84 (1)	2.19 (1)	2.992 (2)	159 (2)
O4W—H4W1 $\cdots$ O2 <sup>iv</sup>	0.85 (1)	1.93 (1)	2.771 (2)	169 (3)
O4W—H4W2 $\cdots$ O3 <sup>i</sup>	0.85 (1)	2.00 (1)	2.841 (2)	172 (3)

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