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catena-Poly[[aquadioxidouranium(VI)]-μ_3-4,4′-oxydibenzoato]

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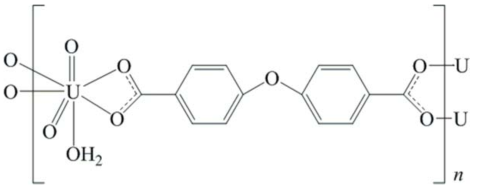
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.019; wR factor = 0.064; data-to-parameter ratio = 17.3.

The title compound, $[UO_2(C_{14}H_8O_5)(H_2O)]_n$, is a polymeric UO_2 complex bridged by 4,4′-oxydibenzoate ligands. One carboxylate group of the bridging ligand chelates a uranyl cation while the other carboxylate group of the ligand bridges two other two uranyl cations, forming a double-chain polymeric structure. The central U^{VI} atom is seven-coordinated in a distorted UO_7 pentagonal-bipyramidal geometry. In the crystal structure, O—H···O hydrogen bonding links the polymeric chains into a three-dimensional supramolecular framework. Within the bridging ligand, the two benzene rings are oriented at a dihedral angle of 59.0 (2)°.

Related literature

For the potential applications of porous uranyl-organic frameworks, see: Thuéry & Masci (2008); Cahill *et al.* (2007); Masci & Thuéry (2008). For a related structure, see: Yu *et al.* (2004).



Experimental

Crystal data

$[U(C_{14}H_8O_5)O_2(H_2O)]$
M_r = 544.25
Monoclinic, $P2_1/c$
a = 16.0160 (6) Å
b = 8.8832 (3) Å
c = 10.1952 (4) Å
β = 95.736 (1)°
V = 1443.24 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 11.29 mm^{-1}
T = 296 K
0.19 × 0.18 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.135, T_{max} = 0.147
10376 measured reflections
3606 independent reflections
3188 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.064
S = 1.17
3606 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.88 e Å^{-3}

Table 1
Selected bond lengths (Å).

U1—O1^{i}	2.337 (3)	U1—O6	1.759 (3)
U1—O2	2.315 (3)	U1—O7	1.765 (3)
U1—O4^{ii}	2.407 (3)	U1—O8	2.461 (3)
U1—O5^{ii}	2.437 (3)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O8—H8···O7^{iii}	0.85	2.05	2.812 (4)	150
O8—H11···O2^{iv}	0.85	2.37	3.083 (4)	142

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2712).

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supporting information

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S1. Comment

Recently the design and synthesis of porous uranyl-organic frameworks (UOFs) have received rather considerable attention due to their potential applications (Thuéry & Masci, 2008; Cahill *et al.*, 2007; Masci & Thuéry, 2008; Yu *et al.*, 2004; Chen *et al.*, 2003). However the coordination polymers of uranyl with 4,4′-oxydibenzoate ligand (oba) have not been reported to our knowledge. We are currently interested in using oba as a bridging ligand to build novel UOFs. Herein we report a novel UOF of $[UO_2(oba)(H_2O)]_n$.

The compound possesses a 1-D double chain architecture, in which the asymmetric unit consists of one UO_2^{2+} cation, one oxy-bis(benzoate) anion and one coordinated water molecule. The central U atom is seven-coordinated in a UO_7 pentagonal-bipyramidal geometry by four O atoms from three different oba^{2-} ligands and one water O atom, and other two O atoms are oxo groups in axial positions (Fig. 1). The coordinate bond distances are listed in Table 1, which are comparable to the related uranyl carboxylate compound (Yu *et al.*, 2004). The terminal groups of the oba ligand coordinate to three U centers to form the 1D double chain framework (Fig. 2). The O—H···O hydrogen bonding links the polymeric chains into 3D supramolecular structure (Table 2 and Fig. 3).

S2. Experimental

For the preparation of the title compound, a mixture of uranium oxynitrate hexahydrate (0.1025 g, 0.21 mmol), 4,4′-oxybis(benzoic acid) (0.1092 g, 0.42 mmol), potassium hydroxide (0.0470 g, 0.84 mmol) and 6 mL water was sealed in a 23 mLstainless steel reactor with a Teflon liner. The reaction system was heated at 423 K for 48 h, and then cooled slowly to room temperature. A large number of pale-yellow crystals of the title compound were obtained and collected by filtration, washed with water and dried in air.

S3. Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic) and with $U_{iso}(H) = 1.2U_{eq}(C)$. Water H atoms were initially located in a difference Fourier map, but they were treated as riding on their parent atoms with O—H = 0.85 Å and with $U_{iso}(H) = 1.5U_{eq}(O)$.

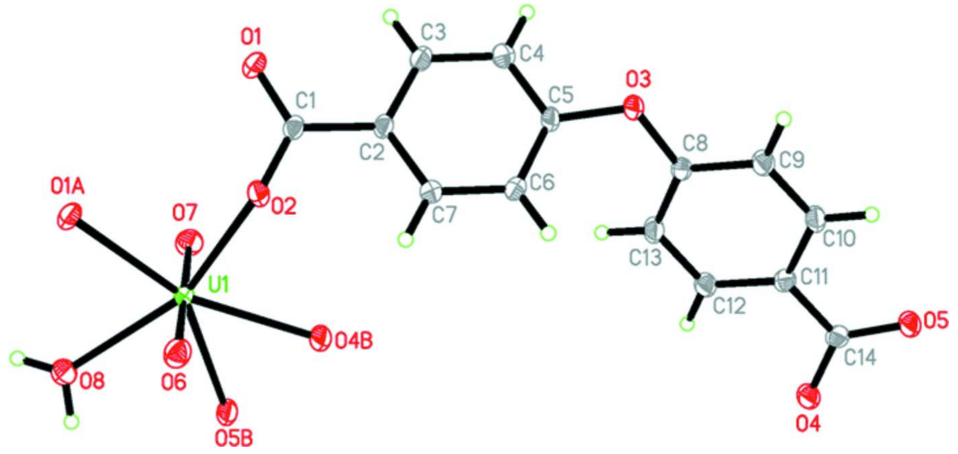

Figure 1

Thermal ellipsoid plot of a portion of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry codes (A): -x + 1, -y + 1, -z + 1; (B): -x + 2, -y + 1, -z + 1].

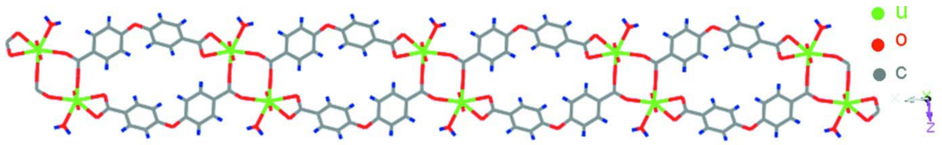

Figure 2

View of one-dimensional double chain structure of the title compound.

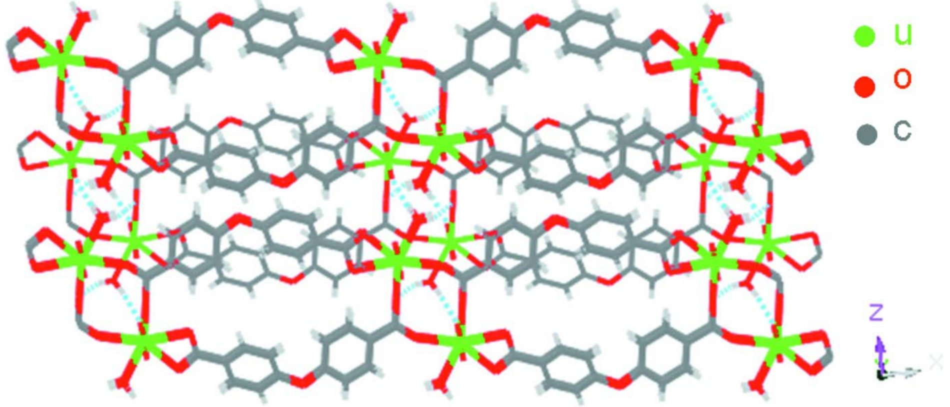

Figure 3

View of three-dimensional supramolecular structure with hydrogen bond interactions shown as dashed lines.

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Crystal data

$[U(C_{14}H_8O_5)O_2(H_2O)]$
M_r = 544.25
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 16.0160 (6) Å
b = 8.8832 (3) Å
c = 10.1952 (4) Å
β = 95.736 (1)°
V = 1443.24 (9) Å^3
Z = 4
F(000) = 1000
D_x = 2.505 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4425 reflections

θ = 2.5–25.0°	Block, yellow
μ = 11.29 mm^{-1}	0.19 × 0.18 × 0.17 mm
T = 296 K	

Data collection

Rigaku R-AXIS RAPID diffractometer	10376 measured reflections
Radiation source: fine-focus sealed tube	3606 independent reflections
Graphite monochromator	3188 reflections with $I > 2\sigma(I)$
ω scan	$R_{\rm int}$ = 0.020
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$\theta_{\rm max}$ = 28.4°, $\theta_{\rm min}$ = 1.3°
$T_{\rm min}$ = 0.135, $T_{\rm max}$ = 0.147	$h = -21 \rightarrow 20$
	$k = -11 \rightarrow 11$
	$l = -13 \rightarrow 11$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.019	H-atom parameters constrained
$wR(F^2)$ = 0.064	$w = 1/[\sigma^2(F_o^2) + (0.0365P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.17	$(\Delta/\sigma)_{\rm max}$ = 0.002
3606 reflections	$\Delta\rho_{\rm max}$ = 0.74 e Å^{-3}
208 parameters	$\Delta\rho_{\rm min}$ = −0.88 e Å^{-3}
0 restraints	
Primary atom site location: structure-invariant direct methods	

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	$U_{\rm iso}$*/$U_{\rm eq}$
U1	0.586399 (8)	0.547362 (15)	0.296990 (13)	0.02255 (6)
O1	0.55538 (19)	0.4926 (4)	0.6780 (3)	0.0334 (6)
O4	1.2633 (2)	0.4586 (4)	0.6570 (3)	0.0393 (8)
O5	1.31269 (18)	0.3423 (4)	0.8388 (3)	0.0366 (7)
C14	1.2507 (3)	0.3891 (5)	0.7634 (4)	0.0287 (8)
C11	1.1633 (2)	0.3682 (4)	0.7976 (4)	0.0259 (8)
C12	1.0998 (3)	0.4558 (4)	0.7347 (4)	0.0293 (9)
H12	1.1117	0.5218	0.6683	0.035*
C10	1.1455 (3)	0.2688 (5)	0.8968 (4)	0.0303 (8)
H10	1.1882	0.2115	0.9408	0.036*
C13	1.0187 (3)	0.4458 (4)	0.7699 (4)	0.0316 (9)
H13	0.9765	0.5067	0.7294	0.038*
C9	1.0644 (2)	0.2558 (5)	0.9295 (4)	0.0308 (8)

H9	1.0521	0.1877	0.9941	0.037*
C8	1.0012 (2)	0.3435 (5)	0.8665 (4)	0.0269 (8)
C1	0.6145 (3)	0.4466 (4)	0.6168 (4)	0.0251 (8)
C2	0.6980 (2)	0.4239 (4)	0.6891 (4)	0.0243 (8)
C7	0.7623 (2)	0.3572 (5)	0.6279 (4)	0.0279 (8)
H7	0.7535	0.3328	0.5389	0.033*
C6	0.8389 (3)	0.3266 (5)	0.6969 (4)	0.0304 (9)
H6	0.8814	0.2807	0.6555	0.037*
C5	0.8514 (2)	0.3659 (5)	0.8298 (4)	0.0273 (8)
C4	0.7882 (3)	0.4337 (5)	0.8920 (4)	0.0321 (9)
H4	0.7974	0.4596	0.9806	0.038*
C3	0.7115 (3)	0.4629 (4)	0.8222 (4)	0.0307 (9)
H3	0.6690	0.5084	0.8638	0.037*
O3	0.92367 (17)	0.3279 (4)	0.9105 (3)	0.0370 (7)
O2	0.60500 (19)	0.4162 (4)	0.4939 (3)	0.0345 (7)
O7	0.5825 (2)	0.7188 (3)	0.3837 (3)	0.0359 (7)
O6	0.58900 (19)	0.3749 (3)	0.2127 (3)	0.0350 (7)
O8	0.50947 (19)	0.6486 (3)	0.0952 (3)	0.0369 (7)
H11	0.4613	0.6883	0.0787	0.055*
H8	0.5375	0.6547	0.0288	0.055*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
U1	0.01670 (9)	0.02981 (9)	0.02128 (9)	0.00041 (5)	0.00266 (6)	−0.00035 (5)
O1	0.0196 (15)	0.0439 (16)	0.0374 (17)	0.0045 (13)	0.0064 (12)	0.0048 (14)
O4	0.0205 (16)	0.066 (2)	0.0309 (16)	−0.0022 (14)	0.0011 (12)	0.0114 (14)
O5	0.0197 (14)	0.0566 (19)	0.0330 (15)	−0.0005 (14)	0.0010 (12)	0.0132 (14)
C14	0.022 (2)	0.037 (2)	0.0282 (19)	−0.0036 (17)	0.0037 (15)	−0.0004 (17)
C11	0.0195 (18)	0.032 (2)	0.0260 (18)	−0.0040 (16)	0.0004 (14)	−0.0040 (16)
C12	0.023 (2)	0.036 (2)	0.029 (2)	−0.0037 (16)	0.0002 (16)	0.0052 (16)
C10	0.023 (2)	0.035 (2)	0.031 (2)	0.0035 (17)	−0.0028 (15)	0.0052 (17)
C13	0.022 (2)	0.038 (2)	0.035 (2)	0.0007 (16)	−0.0016 (17)	0.0073 (17)
C9	0.022 (2)	0.038 (2)	0.032 (2)	−0.0036 (17)	0.0006 (15)	0.0086 (17)
C8	0.0161 (18)	0.040 (2)	0.0235 (18)	−0.0034 (16)	−0.0017 (14)	−0.0002 (16)
C1	0.0184 (19)	0.0268 (19)	0.030 (2)	−0.0022 (14)	0.0024 (15)	0.0066 (15)
C2	0.0156 (18)	0.0284 (19)	0.029 (2)	−0.0013 (14)	0.0012 (15)	0.0050 (15)
C7	0.024 (2)	0.036 (2)	0.0233 (18)	0.0026 (17)	0.0018 (15)	−0.0009 (16)
C6	0.0204 (19)	0.044 (2)	0.027 (2)	0.0069 (17)	0.0026 (15)	−0.0029 (17)
C5	0.0165 (18)	0.038 (2)	0.0270 (18)	−0.0005 (16)	−0.0020 (14)	0.0056 (16)
C4	0.025 (2)	0.044 (2)	0.026 (2)	−0.0015 (18)	−0.0005 (16)	−0.0021 (17)
C3	0.023 (2)	0.040 (2)	0.030 (2)	0.0051 (16)	0.0025 (17)	−0.0051 (16)
O3	0.0169 (14)	0.066 (2)	0.0278 (14)	0.0009 (14)	−0.0014 (11)	0.0103 (14)
O2	0.0238 (16)	0.0517 (17)	0.0270 (15)	0.0005 (13)	−0.0015 (12)	0.0113 (13)
O7	0.0363 (17)	0.0354 (16)	0.0362 (16)	0.0002 (13)	0.0045 (13)	−0.0099 (13)
O6	0.0298 (16)	0.0351 (16)	0.0399 (17)	0.0026 (13)	0.0024 (12)	−0.0072 (13)
O8	0.0334 (17)	0.0473 (17)	0.0298 (15)	0.0056 (14)	0.0027 (12)	0.0101 (13)

Geometric parameters (Å, º)

U1—O1$^{\rm i}$	2.337 (3)	C10—H10	0.9300
U1—O2	2.315 (3)	C13—C8	1.389 (6)
U1—O4$^{\rm ii}$	2.407 (3)	C13—H13	0.9300
U1—O5$^{\rm ii}$	2.437 (3)	C9—C8	1.384 (5)
U1—O6	1.759 (3)	C9—H9	0.9300
U1—O7	1.765 (3)	C8—O3	1.369 (5)
U1—O8	2.461 (3)	C1—O2	1.275 (5)
U1—C14$^{\rm ii}$	2.798 (4)	C1—C2	1.475 (5)
O1—C1	1.254 (5)	C2—C7	1.389 (5)
O1—U1$^{\rm i}$	2.337 (3)	C2—C3	1.396 (6)
O4—C14	1.282 (5)	C7—C6	1.379 (5)
O4—U1$^{\rm ii}$	2.407 (3)	C7—H7	0.9300
O5—C14	1.263 (5)	C6—C5	1.395 (5)
O5—U1$^{\rm ii}$	2.437 (3)	C6—H6	0.9300
C14—C11	1.488 (5)	C5—C4	1.385 (6)
C14—U1$^{\rm ii}$	2.798 (4)	C5—O3	1.393 (4)
C11—C12	1.386 (6)	C4—C3	1.381 (6)
C11—C10	1.393 (5)	C4—H4	0.9300
C12—C13	1.384 (6)	C3—H3	0.9300
C12—H12	0.9300	O8—H11	0.8499
C10—C9	1.377 (6)	O8—H8	0.8500
O6—U1—O7	178.90 (14)	C13—C12—H12	119.7
O6—U1—O2	88.75 (12)	C11—C12—H12	119.7
O7—U1—O2	90.45 (12)	C9—C10—C11	119.6 (4)
O6—U1—O1$^{\rm i}$	89.53 (13)	C9—C10—H10	120.2
O7—U1—O1$^{\rm i}$	89.62 (13)	C11—C10—H10	120.2
O2—U1—O1$^{\rm i}$	82.59 (10)	C12—C13—C8	119.2 (4)
O6—U1—O4$^{\rm ii}$	90.22 (13)	C12—C13—H13	120.4
O7—U1—O4$^{\rm ii}$	90.34 (13)	C8—C13—H13	120.4
O2—U1—O4$^{\rm ii}$	77.30 (10)	C10—C9—C8	120.3 (4)
O1$^{\rm i}$—U1—O4$^{\rm ii}$	159.90 (11)	C10—C9—H9	119.8
O6—U1—O5$^{\rm ii}$	91.33 (12)	C8—C9—H9	119.8
O7—U1—O5$^{\rm ii}$	89.77 (13)	O3—C8—C9	115.9 (3)
O2—U1—O5$^{\rm ii}$	131.32 (10)	O3—C8—C13	123.5 (4)
O1$^{\rm i}$—U1—O5$^{\rm ii}$	146.09 (10)	C9—C8—C13	120.5 (4)
O4$^{\rm ii}$—U1—O5$^{\rm ii}$	54.01 (10)	O1—C1—O2	122.4 (4)
O6—U1—O8	86.79 (12)	O1—C1—C2	119.2 (4)
O7—U1—O8	93.66 (12)	O2—C1—C2	118.4 (4)
O2—U1—O8	156.87 (10)	C7—C2—C3	119.5 (4)
O1$^{\rm i}$—U1—O8	74.70 (10)	C7—C2—C1	120.6 (4)
O4$^{\rm ii}$—U1—O8	125.36 (10)	C3—C2—C1	119.8 (4)
O5$^{\rm ii}$—U1—O8	71.51 (10)	C6—C7—C2	121.1 (4)
O6—U1—C14$^{\rm ii}$	90.00 (13)	C6—C7—H7	119.4
O7—U1—C14$^{\rm ii}$	90.93 (13)	C2—C7—H7	119.4
O2—U1—C14$^{\rm ii}$	104.52 (11)	C7—C6—C5	118.7 (4)

O1^{i}—U1—C14^{ii}	172.86 (11)	C7—C6—H6	120.6
O4^{ii}—U1—C14^{ii}	27.22 (11)	C5—C6—H6	120.6
O5^{ii}—U1—C14^{ii}	26.82 (10)	C4—C5—O3	116.0 (3)
O8—U1—C14^{ii}	98.17 (11)	C4—C5—C6	120.9 (4)
C1—O1—U1^{i}	142.7 (3)	O3—C5—C6	122.9 (4)
C14—O4—U1^{ii}	93.6 (2)	C3—C4—C5	119.9 (4)
C14—O5—U1^{ii}	92.7 (2)	C3—C4—H4	120.0
O5—C14—O4	119.6 (4)	C5—C4—H4	120.0
O5—C14—C11	121.1 (3)	C4—C3—C2	119.9 (4)
O4—C14—C11	119.3 (4)	C4—C3—H3	120.1
O5—C14—U1^{ii}	60.5 (2)	C2—C3—H3	120.1
O4—C14—U1^{ii}	59.2 (2)	C8—O3—C5	120.7 (3)
C11—C14—U1^{ii}	175.5 (3)	C1—O2—U1	137.5 (3)
C12—C11—C10	119.9 (4)	U1—O8—H11	133.3
C12—C11—C14	119.1 (4)	U1—O8—H8	115.4
C10—C11—C14	121.0 (4)	H11—O8—H8	110.9
C13—C12—C11	120.5 (4)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8—H8···O7^{iii}	0.85	2.05	2.812 (4)	150
O8—H11···O2^{iv}	0.85	2.37	3.083 (4)	142

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