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1,7-Dihydroxy-2,3,4-trimethoxy-9*H*-xanthen-9-one monohydrate from *Halenia elliptica*

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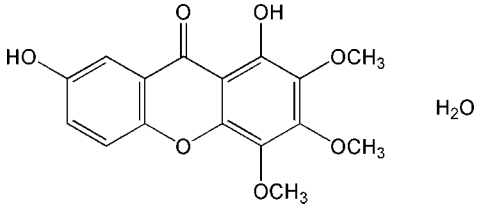
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.142; data-to-parameter ratio = 15.3.

The title compound, $C_{16}H_{14}O_7\cdot H_2O$, possesses a planar three-ring skeleton; its carbonyl, one of the two hydroxy and two of the three methoxy O atoms and the water molecule form hydrogen bonds, giving rise to a layer structure.

Related literature

For the antidepressant, antitumor, antimicrobial, antifungal, anti-inflammatory, antiviral, cardiotonic, hypoglycemic, anti-hepatotoxic and immunomodulatory activities of simple xanthones, see: Basnet *et al.* (1994); Fernandes *et al.* (1995); Karan *et al.* (1999); Liou *et al.* (1993); Miura *et al.* (2001); Parmar *et al.* (1996); Pedro *et al.* (2002); Sousa *et al.* (2002). For the crystal structures of oxygenated xanthones, see: Evans *et al.* (2004); Gales *et al.* (2001); Jiang *et al.* (2004); Kabaleeswaran *et al.* (2003); Kato *et al.* (2005); Kijjoa *et al.* (1998); Shi *et al.* (2004, 2005); Stout *et al.* (1969); Vijayalakshmi *et al.* (1987).



Experimental

Crystal data

$C_{16}H_{14}O_7\cdot H_2O$
M_r = 336.29
Monoclinic, $P2_1/c$
a = 10.9272 (9) Å
b = 10.4511 (8) Å
c = 14.0201 (11) Å
β = 111.6830 (10)°
V = 1487.8 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 298 K
0.2 × 0.1 × 0.05 mm

Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: none
8808 measured reflections
3563 independent reflections
2848 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.141
S = 1.06
3563 reflections
233 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O8^{i}—H16^{i}···O2	0.73 (3)	2.58 (3)	3.091 (2)	129.4
O8^{i}—H16^{i}···O3	0.73 (3)	2.46 (3)	3.177 (2)	167.3
O8^{ii}—H15^{ii}···O6	0.84 (5)	2.08 (5)	2.923 (2)	172.3
O7—H7···O8^{iii}	0.83	1.88	2.706 (2)	169

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

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: NG2424).

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Acta Cryst. (2008). E**64**, o651–o652 [doi:10.1107/S1600536808004832]

1,7-Dihydroxy-2,3,4-trimethoxy-9*H*-xanthen-9-one monohydrate from *Halenia elliptica*

Peizhong Yu, Xiaojuan Shen, Changqi Hu, Edward J. Meehan and Liqing Chen

S1. Comment

Xanthone compounds commonly occur in several higher plant families, such as *Gentianaceae,Guttiferae, Moraceae* and *Polygalaceae.* Simple oxygenated xanthones possess different biological activities such as antidepressant, antitumor, antimicrobial, antifungal, anti-inflammatory, antiviral, cardiotonic, hypoglycemic, antihepatotoxic and immunomodulatory (Liou *et al.*, 1993; Basnet *et al.,* 1994; Fernandes *et al.*, 1995; Parmar *et al.*, 1996; Karan *et al.*, 1999; Miura *et al.*, 2001; Pedro *et al.,* 2002; Sousa *et al.,* 2002). The majority of the xanthones isolated so far are hydroxyl or methoxy substituted in the xanthone skeleton. Up to present, only ten simple oxygenated xanthones were characterized by X-ray diffraction (Stout *et al.,* 1969; Vijayalakshmi *et al.,* 1987; Kijjoa *et al.*, 1998; Gales *et al.,* 2001; Kabaleeswaran *et al.,* 2003; Jiang *et al.,* 2004; Shi *et al.,* 2004; Evans *et al.*, 2004; Kato *et al.*, 2005; Shi *et al.*, 2005). 1,7-dihydroxy-2,3,4-trimethoxyxanthone (I) was first isolated from *Halenia elliptica* D. Don (Gentianaceae) and has antioxidant activity. Its crystal structure is reported for the first time in this paper. The structure of I (Figure 1) is similar to other xanthones reported with a planar three-ring skeleton. The asymmetric unit of crystal I contains one molecule I plus one water molecule. I forms hydrogen bonds with the water molecule through its carbonyl, one of the two hydroxyl and two of the three methoxyl O atoms (Table 1, Figure 2). The crystal structure is stabilized by the extensive hydrogen bond network.

S2. Experimental

Halenia elliptica D. Don was collected in *DALI*, Yunnan Province, in April 2005 and was identified by Professor Xiaokuang Ma, Department of Pharmacognosy, School of Pharmacy, *DALI* University, People's Republic of China.

Extraction and isolation: 1,7-dihydroxy-2,3,4-trimethoxyxanthone (I) was isolated from ethyl acetate fraction of the ethanol extract of the aerial parts of *Halenia elliptica* with other four 1,7-dihydroxy substituted xanthones by silica gel column chromatography with gradient mixtures of petroleum ether and ethyl acetate. Yellow crystals of I were obtained by slow evaporation of a solution in EtOH. *M*.p.164–165°C. ESI-MS *m/z* (*rel*. %): 319[*M*+H]$^{+.1}$H-NMR (400 MHz, $CDCl_3$), *d*12.60 (1*H*, *s*, OH-1), 7.60 (1*H*, *d*, *J*=3.0 Hz, H-8), 7.49 (1*H*, *d*, *J*=9.3 Hz, H-5), 7.34 (1*H*, *dd*, *J*=3.0, 9.0 Hz, H-6), 5.32 (1*H*, *br. s*, OH-7), 4.15 (3*H*, *s*, OCH_3), 3.96 (3*H*, *s*, OCH_3), 3.95 (3*H*, *s*, OCH_3).

S3. Refinement

H atoms attached to O atoms were located in a difference map and refined with bond restraints O—H = 0.82 (2) Å. C-bound H atoms were positioned geometrically (C—H 0.93 - 0.96 Å). All H atoms were refined as riding, with U_{iso}(H) = 1.2 - 1.5 U_{eq} of the parent atom.

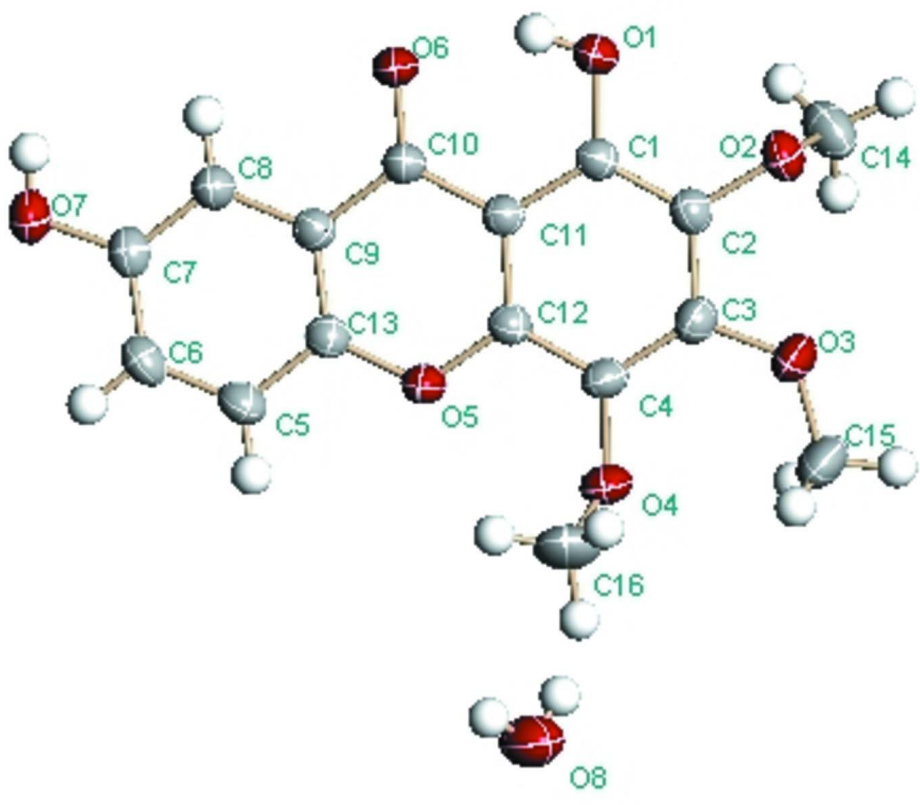

Figure 1

The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. Arbitrary atom numbering.

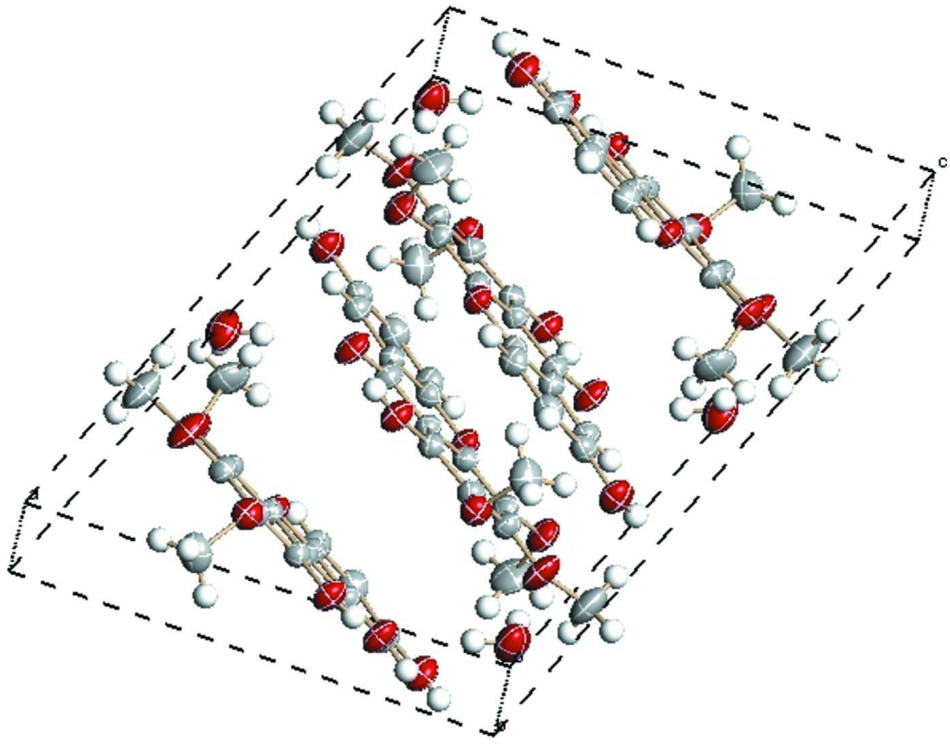

Figure 2

The packing of (I), viewed down the *b* axis.

1,7-dihydroxy-2,3,4-trimethoxy-9*H*-xanthen-9-one monohydrate

Crystal data

$C_{16}H_{14}O_7 \cdot H_2O$
$M_r = 336.29$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.9272\ (9)$ Å
$b = 10.4511\ (8)$ Å
$c = 14.0201\ (11)$ Å
$\beta = 111.683\ (1)°$
$V = 1487.8\ (2)$ Å^3
$Z = 4$

$F(000) = 704$
$D_x = 1.501$ Mg m^{-3}
Melting point: 437 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3563 reflections
$\theta = 2.5–28.3°$
$\mu = 0.12$ mm^{-1}
$T = 298$ K
Block, yellow
0.2 × 0.1 × 0.05 mm

Data collection

Bruker SMART 1K CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Thin–slice ω scans
8808 measured reflections
3563 independent reflections

2848 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 28.3°$, $\theta_{min} = 2.5°$
$h = -14 \rightarrow 14$
$k = -8 \rightarrow 13$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.142$
$S = 1.06$
3563 reflections
233 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0743P)^2 + 0.2855P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0085 (18)

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_{iso}*/U_{eq}
O5	0.62447 (9)	0.47253 (9)	0.17678 (8)	0.0374 (2)
O1	0.44791 (10)	0.90069 (10)	0.12081 (9)	0.0441 (3)
H1	0.3758	0.8590	0.0943	0.066*
C11	0.52749 (12)	0.68367 (13)	0.14635 (9)	0.0315 (3)
O6	0.29738 (10)	0.70239 (10)	0.06007 (9)	0.0492 (3)
O2	0.69716 (11)	0.99477 (10)	0.21570 (8)	0.0437 (3)
C2	0.67515 (14)	0.86433 (13)	0.20640 (10)	0.0361 (3)
C12	0.63679 (13)	0.60211 (13)	0.18592 (10)	0.0325 (3)
C10	0.39784 (13)	0.63185 (13)	0.09340 (10)	0.0343 (3)
C13	0.50227 (13)	0.41989 (13)	0.12579 (10)	0.0336 (3)
C4	0.76454 (13)	0.64776 (14)	0.23766 (11)	0.0370 (3)
C8	0.26918 (14)	0.43164 (14)	0.02687 (11)	0.0371 (3)
H8	0.1934	0.4798	−0.0049	0.045*
O3	0.89800 (11)	0.84290 (12)	0.29620 (11)	0.0599 (4)
C3	0.78279 (13)	0.78037 (15)	0.24786 (11)	0.0385 (3)
C9	0.38925 (13)	0.49338 (13)	0.08075 (10)	0.0331 (3)
C1	0.54949 (13)	0.81769 (13)	0.15801 (10)	0.0331 (3)
O7	0.14973 (11)	0.23466 (11)	−0.03034 (10)	0.0517 (3)
H7	0.0882	0.2864	−0.0560	0.078*
C7	0.26315 (14)	0.30003 (14)	0.02086 (11)	0.0386 (3)
O4	0.86845 (10)	0.56302 (11)	0.26990 (9)	0.0500 (3)
C5	0.49582 (15)	0.28688 (14)	0.12202 (11)	0.0398 (3)
H5	0.5711	0.2383	0.1543	0.048*

C6	0.37723 (16)	0.22793 (14)	0.07010 (11)	0.0421 (3)
H6	0.3727	0.1391	0.0677	0.051*
C15	1.02209 (16)	0.7842 (2)	0.32996 (18)	0.0673 (5)
H15A	1.0321	0.7309	0.3881	0.101*
H15B	1.0895	0.8486	0.3492	0.101*
H15C	1.0297	0.7329	0.2756	0.101*
C14	0.7299 (2)	1.04398 (18)	0.13328 (16)	0.0595 (5)
H14A	0.8034	0.9974	0.1290	0.089*
H14B	0.7526	1.1328	0.1453	0.089*
H14C	0.6557	1.0349	0.0700	0.089*
C16	0.8790 (2)	0.4892 (2)	0.35909 (16)	0.0701 (6)
H16A	0.8795	0.5457	0.4132	0.105*
H16B	0.9592	0.4406	0.3811	0.105*
H16C	0.8052	0.4321	0.3425	0.105*
O8	0.92795 (15)	0.37653 (18)	0.88918 (14)	0.0695 (4)
H15	0.862 (4)	0.361 (4)	0.905 (3)	0.123 (12)*
H16	0.912 (3)	0.436 (3)	0.860 (2)	0.104 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O5	0.0319 (5)	0.0313 (5)	0.0448 (5)	0.0041 (4)	0.0093 (4)	0.0004 (4)
O1	0.0363 (5)	0.0311 (5)	0.0567 (6)	0.0041 (4)	0.0076 (5)	0.0031 (4)
C11	0.0310 (6)	0.0309 (6)	0.0311 (6)	0.0016 (5)	0.0098 (5)	0.0008 (5)
O6	0.0318 (5)	0.0347 (5)	0.0694 (7)	0.0041 (4)	0.0048 (5)	0.0046 (5)
O2	0.0460 (6)	0.0323 (5)	0.0512 (6)	−0.0056 (4)	0.0160 (5)	−0.0051 (4)
C2	0.0382 (7)	0.0318 (6)	0.0374 (7)	−0.0016 (5)	0.0128 (6)	−0.0024 (5)
C12	0.0329 (6)	0.0314 (6)	0.0328 (6)	0.0024 (5)	0.0116 (5)	−0.0001 (5)
C10	0.0322 (6)	0.0318 (6)	0.0359 (6)	0.0017 (5)	0.0089 (5)	0.0031 (5)
C13	0.0348 (7)	0.0328 (7)	0.0336 (6)	0.0019 (5)	0.0132 (5)	−0.0006 (5)
C4	0.0297 (6)	0.0379 (7)	0.0396 (7)	0.0051 (5)	0.0086 (5)	0.0001 (5)
C8	0.0352 (7)	0.0341 (7)	0.0393 (7)	−0.0005 (5)	0.0107 (6)	0.0001 (5)
O3	0.0317 (5)	0.0457 (7)	0.0854 (9)	−0.0031 (5)	0.0018 (5)	−0.0102 (6)
C3	0.0318 (6)	0.0401 (7)	0.0401 (7)	−0.0028 (5)	0.0091 (5)	−0.0042 (6)
C9	0.0345 (7)	0.0314 (6)	0.0328 (6)	0.0006 (5)	0.0119 (5)	0.0011 (5)
C1	0.0342 (6)	0.0310 (6)	0.0333 (6)	0.0024 (5)	0.0113 (5)	0.0014 (5)
O7	0.0443 (6)	0.0396 (6)	0.0659 (7)	−0.0102 (5)	0.0139 (5)	−0.0092 (5)
C7	0.0422 (7)	0.0356 (7)	0.0398 (7)	−0.0061 (6)	0.0175 (6)	−0.0047 (6)
O4	0.0329 (5)	0.0435 (6)	0.0661 (7)	0.0095 (4)	0.0095 (5)	0.0028 (5)
C5	0.0433 (7)	0.0315 (7)	0.0449 (7)	0.0061 (6)	0.0166 (6)	0.0003 (6)
C6	0.0519 (8)	0.0294 (6)	0.0483 (8)	−0.0010 (6)	0.0222 (7)	−0.0033 (6)
C15	0.0329 (8)	0.0638 (12)	0.0911 (14)	−0.0019 (8)	0.0063 (8)	−0.0113 (10)
C14	0.0677 (11)	0.0416 (9)	0.0790 (12)	−0.0009 (8)	0.0387 (10)	0.0066 (8)
C16	0.0575 (11)	0.0644 (12)	0.0714 (12)	0.0185 (9)	0.0038 (9)	0.0198 (10)
O8	0.0527 (8)	0.0662 (10)	0.0874 (11)	0.0122 (7)	0.0232 (7)	0.0162 (8)

Geometric parameters (Å, º)

O5—C12	1.3623 (16)	O3—C3	1.3567 (17)
O5—C13	1.3753 (17)	O3—C15	1.402 (2)
O1—C1	1.3523 (16)	O7—C7	1.3640 (17)
O1—H1	0.8561	O7—H7	0.8336
C11—C12	1.4040 (18)	C7—C6	1.401 (2)
C11—C1	1.4204 (19)	O4—C16	1.437 (2)
C11—C10	1.4402 (18)	C5—C6	1.375 (2)
O6—C10	1.2601 (16)	C5—H5	0.9300
O2—C2	1.3820 (17)	C6—H6	0.9300
O2—C14	1.426 (2)	C15—H15A	0.9600
C2—C1	1.3765 (19)	C15—H15B	0.9600
C2—C3	1.409 (2)	C15—H15C	0.9600
C12—C4	1.3979 (19)	C14—H14A	0.9600
C10—C9	1.4568 (19)	C14—H14B	0.9600
C13—C5	1.3919 (19)	C14—H14C	0.9600
C13—C9	1.3920 (19)	C16—H16A	0.9600
C4—O4	1.3779 (16)	C16—H16B	0.9600
C4—C3	1.400 (2)	C16—H16C	0.9600
C8—C7	1.3781 (19)	O8—H15	0.85 (4)
C8—C9	1.4057 (19)	O8—H16	0.73 (4)
C8—H8	0.9300		
C12—O5—C13	119.33 (10)	O1—C1—C11	120.54 (12)
C1—O1—H1	109.5	C2—C1—C11	120.10 (12)
C12—C11—C1	118.04 (12)	C7—O7—H7	109.5
C12—C11—C10	120.44 (12)	O7—C7—C8	123.07 (14)
C1—C11—C10	121.51 (12)	O7—C7—C6	117.39 (13)
C2—O2—C14	111.49 (12)	C8—C7—C6	119.54 (13)
C1—C2—O2	120.20 (12)	C4—O4—C16	114.94 (13)
C1—C2—C3	120.75 (13)	C6—C5—C13	119.48 (14)
O2—C2—C3	119.05 (12)	C6—C5—H5	120.3
O5—C12—C4	115.67 (12)	C13—C5—H5	120.3
O5—C12—C11	121.75 (12)	C5—C6—C7	120.84 (13)
C4—C12—C11	122.58 (13)	C5—C6—H6	119.6
O6—C10—C11	121.83 (12)	C7—C6—H6	119.6
O6—C10—C9	121.87 (12)	O3—C15—H15A	109.5
C11—C10—C9	116.31 (12)	O3—C15—H15B	109.5
O5—C13—C5	116.43 (12)	H15A—C15—H15B	109.5
O5—C13—C9	122.92 (12)	O3—C15—H15C	109.5
C5—C13—C9	120.65 (13)	H15A—C15—H15C	109.5
O4—C4—C12	119.65 (13)	H15B—C15—H15C	109.5
O4—C4—C3	122.26 (12)	O2—C14—H14A	109.5
C12—C4—C3	117.91 (12)	O2—C14—H14B	109.5
C7—C8—C9	120.33 (13)	H14A—C14—H14B	109.5
C7—C8—H8	119.8	O2—C14—H14C	109.5
C9—C8—H8	119.8	H14A—C14—H14C	109.5

C3—O3—C15	124.13 (14)	H14B—C14—H14C	109.5
O3—C3—C4	126.78 (13)	O4—C16—H16A	109.5
O3—C3—C2	112.65 (13)	O4—C16—H16B	109.5
C4—C3—C2	120.57 (12)	H16A—C16—H16B	109.5
C13—C9—C8	119.08 (12)	O4—C16—H16C	109.5
C13—C9—C10	119.11 (12)	H16A—C16—H16C	109.5
C8—C9—C10	121.79 (12)	H16B—C16—H16C	109.5
O1—C1—C2	119.35 (12)	H15—O8—H16	106 (3)
C14—O2—C2—C1	−93.37 (16)	O5—C13—C9—C8	177.67 (12)
C14—O2—C2—C3	87.18 (17)	C5—C13—C9—C8	−3.1 (2)
C13—O5—C12—C4	−179.21 (11)	O5—C13—C9—C10	−4.2 (2)
C13—O5—C12—C11	1.25 (19)	C5—C13—C9—C10	175.03 (12)
C1—C11—C12—O5	−179.12 (11)	C7—C8—C9—C13	1.5 (2)
C10—C11—C12—O5	−0.6 (2)	C7—C8—C9—C10	−176.60 (13)
C1—C11—C12—C4	1.4 (2)	O6—C10—C9—C13	−175.33 (13)
C10—C11—C12—C4	179.86 (12)	C11—C10—C9—C13	4.52 (19)
C12—C11—C10—O6	177.61 (13)	O6—C10—C9—C8	2.7 (2)
C1—C11—C10—O6	−4.0 (2)	C11—C10—C9—C8	−177.40 (12)
C12—C11—C10—C9	−2.24 (18)	O2—C2—C1—O1	−0.8 (2)
C1—C11—C10—C9	176.19 (12)	C3—C2—C1—O1	178.70 (12)
C12—O5—C13—C5	−178.02 (12)	O2—C2—C1—C11	178.48 (12)
C12—O5—C13—C9	1.24 (19)	C3—C2—C1—C11	−2.1 (2)
O5—C12—C4—O4	3.85 (19)	C12—C11—C1—O1	179.59 (11)
C11—C12—C4—O4	−176.61 (12)	C10—C11—C1—O1	1.1 (2)
O5—C12—C4—C3	179.11 (12)	C12—C11—C1—C2	0.37 (19)
C11—C12—C4—C3	−1.4 (2)	C10—C11—C1—C2	−178.10 (12)
C15—O3—C3—C4	10.8 (3)	C9—C8—C7—O7	−179.92 (13)
C15—O3—C3—C2	−169.68 (17)	C9—C8—C7—C6	0.9 (2)
O4—C4—C3—O3	−5.7 (2)	C12—C4—O4—C16	−75.54 (18)
C12—C4—C3—O3	179.12 (14)	C3—C4—O4—C16	109.41 (18)
O4—C4—C3—C2	174.75 (13)	O5—C13—C5—C6	−178.43 (12)
C12—C4—C3—C2	−0.4 (2)	C9—C13—C5—C6	2.3 (2)
C1—C2—C3—O3	−177.47 (13)	C13—C5—C6—C7	0.2 (2)
O2—C2—C3—O3	1.98 (19)	O7—C7—C6—C5	179.03 (13)
C1—C2—C3—C4	2.1 (2)	C8—C7—C6—C5	−1.8 (2)
O2—C2—C3—C4	−178.45 (12)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O8^{i}—H16^{i}···O2	0.73 (3)	2.58 (3)	3.091 (2)	129.4
O8^{i}—H16^{i}···O3	0.73 (3)	2.46 (3)	3.177 (2)	167.3
O8^{ii}—H15^{ii}···O6	0.84 (5)	2.08 (5)	2.923 (2)	172.3
O7—H7···O8^{iii}	0.83	1.88	2.706 (2)	169

Symmetry codes: (i) *x*, −*y*+3/2, *z*−1/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*−1, *y*, *z*−1.