

(8-Hydroxy-6-methoxy-1-oxo-1*H*-isochromen-3-yl)methyl formate: a supramolecular framework

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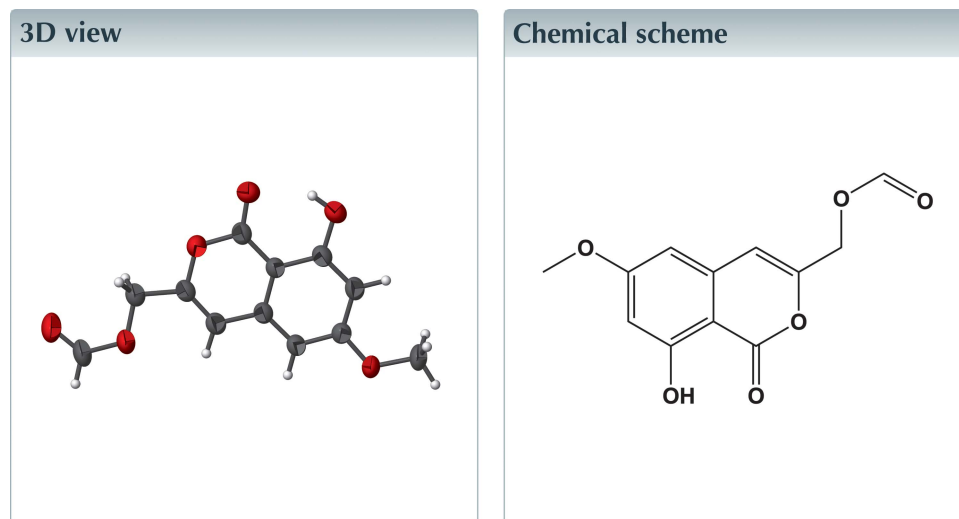
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Keywords: crystal structure; isocoumarin; cyto-genin; hydrogen bonding; C—H··· π interaction; supramolecular framework.

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Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, C₁₂H₁₀O₆, an intramolecular O—H···O hydrogen bond forms an *S*(6) ring motif. The molecule is essentially planar with an r.m.s. deviation of 0.051 Å for all non-H atoms. In the crystal molecules are linked by C—H···O hydrogen bonds and a C—H··· π interaction, forming a supra-molecular framework.



Structure description

The title compound, **I**, is an intermediate in the synthesis of cyto-genin, a naturally occurring isocoumarin that was first isolated from a cultured broth of *Streptovercillium eurociticum* (Kumagai *et al.*, 1990, 1995). It was shown by these authors to have both antibiotic properties and antitumor activity. The first synthesis of cyto-genin was reported in 2004 (Saeed, 2004). More recently, a new synthetic route to cyto-genin and similar isocoumarins has been reported (Gadakh & Sudalai, 2014).

As shown in Fig. 1, compound **I** was prepared *via* two pathways (see *Synthesis and crystallization*). The details of the syntheses of the precursors **A** and **B** and cyto-genin have been described elsewhere (Tiouabi, 2005).

The molecule of **I** (Fig. 2), is essentially planar with an r.m.s. deviation of 0.051 Å for all non-H atoms (O1–O6/C1/C3–C13); the maximum deviations from this mean plane are 0.080 (6) Å for atom C12 and –0.091 (8) Å for atom C13. There is an intramolecular O—H···O hydrogen bond present, forming an *S*(6) ring motif (Fig. 2 and Table 1).

In the crystal, molecules are linked by a series of C—H···O hydrogen bonds (Table 1), forming interconnected ribbons running normal to each other in planes (012) and (01 $\bar{2}$): see Fig. 3. These interactions lead to the formation of a supramolecular framework, which is reinforced by a C—H··· π interaction (Fig. 4 and Table 1).

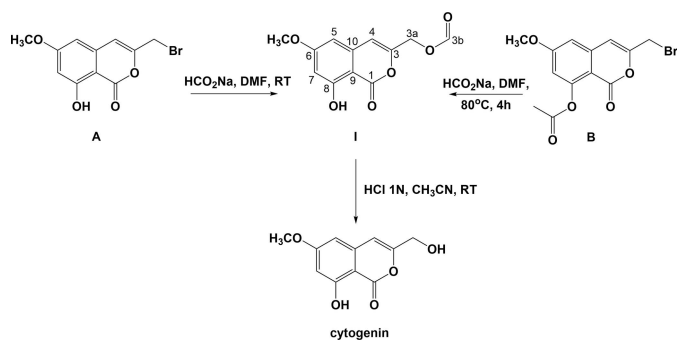


Figure 1
The reaction pathways for the synthesis of compound **I** and cytogenin (Tiouabi, 2005).

Synthesis and crystallization

The syntheses of the title compound, **I**, and cytogenin, are illustrated in Fig. 1. The syntheses of the precursors, 3-(bromomethyl)-8-hydroxy-6-methoxy-1*H*-isochromen-1-one (**A**), 3-(bromomethyl)-6-methoxy-1-oxo-1*H*-isochromen-8-yl acetate (**B**), and cytogenin, are described in the PhD thesis of Tiouabi (2005), which can be downloaded from the website <https://doc.rero.ch/record>, a digital library where many theses of Swiss universities are deposited. The numbering scheme of **I** in Fig. 1 is with reference to the NMR spectra.

Method 1: The hydroxybromoisocoumarin **A** (0.14 g, 0.49 mmol) was dissolved with stirring in 5 ml of anhydrous DMF in a 50 ml flask equipped with a magnetic stirrer and under an atmosphere of argon. HCO₂Na (0.167 g, 2.46 mmol) was added and the mixture was stirred overnight at room temperature. The evolution of the reaction was monitored by thin-layer chromatography, using dimethylchloride as eluent. On completion of the reaction, the mixture was diluted with ethyl acetate and then washed with an aqueous saturated solution of NaCl. The organic phase was dried using anhydrous Na₂SO₄, then filtered and concentrated using a rotary evaporator, yielding compound **I** in the form of a white solid (yield 0.118 g, 96%).

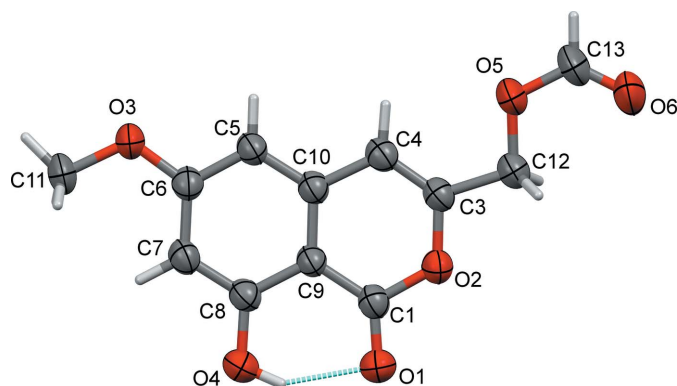


Figure 2
A view of the molecular structure of compound **I**, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level. The intramolecular O—H···O hydrogen bond (see Table 1) is shown as a dashed line.

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

C_g is the centroid of the C5–C10 ring.

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O4—H40···O1	0.84	1.88	2.616 (5)	146
C4—H4···O1 ⁱ	0.95	2.38	3.326 (6)	173
C5—H5···O2 ⁱ	0.95	2.59	3.541 (6)	176
C7—H7···O6 ⁱⁱ	0.95	2.55	3.499 (5)	175
C11—H11C···O6 ⁱ	0.98	2.57	3.388 (8)	141
C12—H12B···C _g ⁱⁱⁱ	0.99	2.88	3.788 (6)	153

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

Method 2: The acetoxybromoisocoumarin **B** (34.2 mg, 0.104 mmol) was dissolved with stirring in 3 ml of anhydrous DMF in a 50 ml flask equipped with a magnetic stirrer and under an atmosphere of argon. HCO₂Na (47 mg, 0.69 mmol) was added, the temperature was raised to 80°C and the

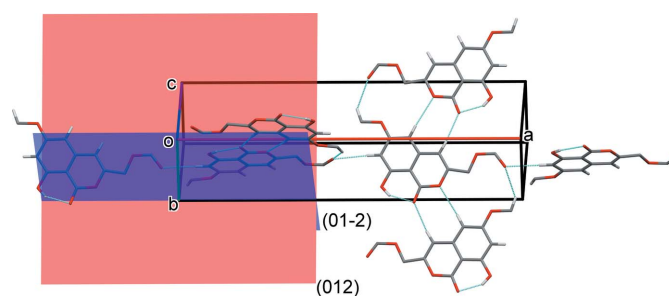


Figure 3
A partial view of the crystal packing of compound **I**, viewed normal to plane (011). Hydrogen bonds (see Table 1) are shown as dashed lines.

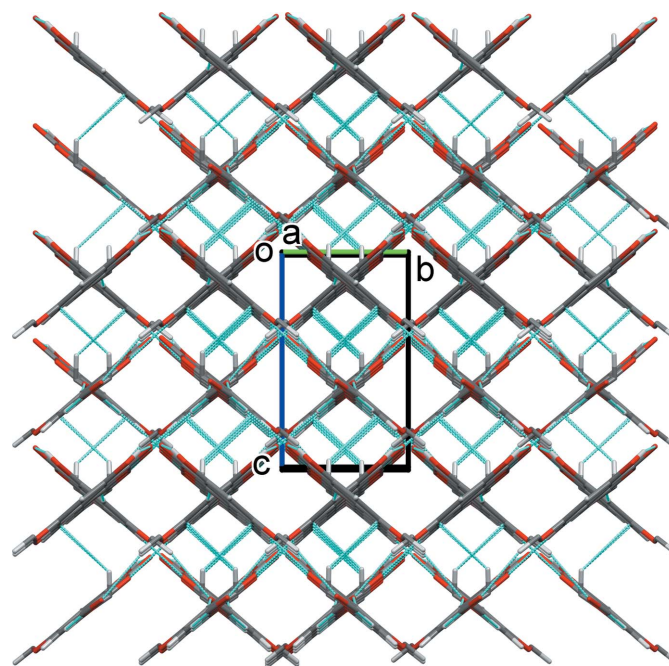


Figure 4
A view along the *a* axis of the crystal packing of compound **I**. Hydrogen bonds and C—H···π interactions (see Table 1) are shown as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₂ H ₁₀ O ₆
<i>M_r</i>	250.20
Crystal system, space group	Orthorhombic, <i>Pca</i> 2 ₁
Temperature (K)	173
<i>a</i> , <i>b</i> , <i>c</i> (Å)	25.006 (2), 5.0337 (6), 8.5646 (6)
<i>V</i> (Å ³)	1078.05 (17)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.13
Crystal size (mm)	0.50 × 0.50 × 0.50
Data collection	
Diffractometer	STOE IPDS 1
Absorption correction	Multi-scan (<i>MULABS</i> ; Spek, 2020)
<i>T_{min}</i> , <i>T_{max}</i>	0.763, 1.000
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	7630, 2012, 1249
<i>R_{int}</i>	0.070
(sin θ/λ) _{max} (Å ⁻¹)	0.619
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.050, 0.135, 0.91
No. of reflections	2012
No. of parameters	166
No. of restraints	1
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.32, -0.27

Computer programs: *EXPOSE*, *CELL* and *INTEGRATE* in *IPDS-I* (Stoe & Cie, 2004), *SHELXS97* (Sheldrick, 2008), *Mercury* (Macrae et al., 2020), *SHELXL2018/3* (Sheldrick, 2015), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

mixture stirred for 4 h. The evolution of the reaction was monitored by thin-layer chromatography, using dimethylchloride as eluent. On completion of the reaction, the mixture was diluted with ethyl acetate and then washed with an aqueous saturated solution of NaCl. The organic phase was dried using anhydrous Na₂SO₄, then purified by column chromatography (silica, eluent CH₂Cl₂/hexane 10/1). Compound **I** was obtained in the form of a white solid (yield 18.7 mg, 72%).

Analytical data for I: *R_f* (CH₂Cl₂, UV) 0.44. ¹H NMR (400 MHz, CDCl₃, 298 K): 3.90 (*s*, 3H, OCH₃), 4.99 (*s*, 2H, CH₂-3a), 6.42 (*d*, *J_m* = 2.3 Hz, 1H, ArH-7), 6.53 (*s*, 1H, H-4), 6.55 (*d*, *J_m* = 2.3 Hz, 1H, ArH-5), 8.17 (*s*, 1H, CHO-3 b), 11.0 (*s*, 1H, OH-8). ¹³C NMR (100 Hz, CDCl₃, 298 K, HETCOR-

SR/LR): 56.19 C(OCH₃), 61.61 C(3a), 100.67 C(9), 101.80 C(5), 103.13 C(7), 107.82 C(4), 138.21 C(10), 150.27 C(3), 160.37 C(3 b), 164.23 C(1), 165.75 C(8), 167.35 C(6). HR-MS [ESI(+)]: *m/z* 273.03634 [*M* + Na]⁺. IR (KBr disk, cm⁻¹): 3129 *br*, 1728 *s*, 1690 *vs*, 1622 *m*, 1400 *vs*, 1164 *vs*, 1064 *w*.

Colourless block-like crystals of **I** were obtained by slow evaporation of a solution in chloroform.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Intensity data were measured using a Stoe IPDS I, a one-circle diffractometer. The alert *diffrn_reflns_laue_measured_fraction_full_value* (0.947) below minimum (0.95) is given. This involves 29 random reflections out of the expected 1034 for the IUCr cut-off limit of (sin θ)/λ = 0.6 Å⁻¹; viz. 2.8%.

Acknowledgements

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full crystallographic data

IUCrData (2020). 5, x201391 [https://doi.org/10.1107/S2414314620013917]

(8-Hydroxy-6-methoxy-1-oxo-1*H*-isochromen-3-yl)methyl formate: a supramolecular framework

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(8-Hydroxy-6-methoxy-1-oxo-1*H*-isochromen-3-yl)methyl formate

Crystal data

C₁₂H₁₀O₆

$M_r = 250.20$

Orthorhombic, *Pca*2₁

$a = 25.006$ (2) Å

$b = 5.0337$ (6) Å

$c = 8.5646$ (6) Å

$V = 1078.05$ (17) Å³

$Z = 4$

$F(000) = 520$

$D_x = 1.542$ Mg m⁻³

Mo *K*α radiation, $\lambda = 0.71073$ Å

Cell parameters from 3909 reflections

$\theta = 2.2$ – 25.8°

$\mu = 0.13$ mm⁻¹

$T = 173$ K

Block, colorless

0.50 × 0.50 × 0.50 mm

Data collection

STOE IPDS 1

diffractometer

Radiation source: fine-focus sealed tube

Plane graphite monochromator

φ rotation scans

Absorption correction: multi-scan

(MULABS; Spek, 2020)

$T_{\min} = 0.763$, $T_{\max} = 1.000$

7630 measured reflections

2012 independent reflections

1249 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.070$

$\theta_{\max} = 26.1^\circ$, $\theta_{\min} = 2.9^\circ$

$h = -30 \rightarrow 30$

$k = -6 \rightarrow 6$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.135$

$S = 0.91$

2012 reflections

166 parameters

1 restraint

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier

map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0852P)^2]$

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

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

$\Delta\rho_{\max} = 0.32$ e Å⁻³

$\Delta\rho_{\min} = -0.27$ e Å⁻³

Extinction correction: (SHELXL-2018/3;

Sheldrick, 2015),

$F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.061 (11)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Flack $x = 0.223$ (999) by classical fit to all intensities 1.664 (999) from 481 selected quotients (Parsons' method)

** Absolute structure cannot be determined reliably **

The hydroxyl H atom and the C-bound H atoms were included in calculated positions and treated as riding on their parent O or C atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.68528 (13)	0.9547 (7)	-0.0918 (5)	0.0500 (9)
O2	0.75876 (11)	0.7819 (6)	0.0089 (4)	0.0461 (9)
O3	0.58898 (11)	0.0468 (7)	0.3437 (5)	0.0511 (10)
O4	0.59095 (13)	0.7730 (7)	-0.0142 (5)	0.0531 (10)
H40	0.613134	0.862673	-0.065697	0.080*
O5	0.86682 (12)	0.4224 (8)	0.1774 (5)	0.0657 (12)
O6	0.94909 (14)	0.5664 (9)	0.1136 (6)	0.0732 (13)
C1	0.70366 (17)	0.7848 (9)	-0.0037 (6)	0.0433 (11)
C3	0.78373 (18)	0.5948 (9)	0.1006 (7)	0.0428 (12)
C4	0.75774 (17)	0.4136 (9)	0.1838 (6)	0.0443 (12)
H4	0.776871	0.288244	0.245052	0.053*
C5	0.67032 (17)	0.2286 (9)	0.2657 (6)	0.0438 (11)
H5	0.687823	0.104223	0.331620	0.053*
C6	0.61467 (17)	0.2302 (9)	0.2549 (7)	0.0434 (12)
C7	0.58804 (17)	0.4147 (10)	0.1602 (7)	0.0455 (12)
H7	0.550100	0.414965	0.154550	0.055*
C8	0.61731 (18)	0.5950 (9)	0.0759 (6)	0.0437 (13)
C9	0.67425 (17)	0.5970 (9)	0.0848 (7)	0.0399 (11)
C10	0.69987 (16)	0.4093 (9)	0.1799 (7)	0.0411 (11)
C11	0.53177 (17)	0.0277 (11)	0.3310 (8)	0.0614 (15)
H11C	0.518847	-0.116607	0.397911	0.092*
H11B	0.521957	-0.008880	0.222346	0.092*
H11A	0.515514	0.195648	0.364158	0.092*
C12	0.84306 (18)	0.6344 (10)	0.0911 (7)	0.0493 (13)
H12B	0.855082	0.629778	-0.019002	0.059*
H12A	0.853189	0.807981	0.136752	0.059*
C13	0.92037 (19)	0.4136 (14)	0.1770 (10)	0.0726 (19)
H13	0.936777	0.272176	0.232693	0.087*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0486 (18)	0.0487 (18)	0.053 (2)	0.0019 (15)	-0.0012 (16)	0.0089 (19)
O2	0.0381 (16)	0.0448 (17)	0.055 (2)	-0.0039 (13)	-0.0010 (15)	0.0043 (17)
O3	0.0330 (15)	0.0564 (19)	0.064 (3)	-0.0051 (14)	0.0021 (16)	0.0138 (19)

O4	0.0425 (17)	0.055 (2)	0.062 (3)	0.0046 (16)	-0.0054 (17)	0.0109 (19)
O5	0.0318 (16)	0.076 (2)	0.089 (3)	-0.0021 (17)	-0.002 (2)	0.026 (2)
O6	0.040 (2)	0.099 (3)	0.080 (3)	-0.012 (2)	0.0013 (19)	0.016 (3)
C1	0.036 (2)	0.046 (3)	0.048 (3)	0.0014 (19)	0.001 (2)	-0.001 (2)
C3	0.035 (2)	0.045 (2)	0.048 (3)	0.003 (2)	-0.002 (2)	-0.002 (2)
C4	0.038 (2)	0.044 (2)	0.051 (3)	0.0004 (19)	-0.004 (2)	-0.002 (2)
C5	0.034 (2)	0.044 (2)	0.053 (3)	-0.001 (2)	-0.004 (2)	0.002 (2)
C6	0.038 (2)	0.039 (2)	0.053 (3)	-0.0005 (19)	0.002 (2)	0.001 (2)
C7	0.035 (2)	0.048 (2)	0.053 (4)	-0.003 (2)	-0.003 (2)	-0.002 (2)
C8	0.036 (2)	0.044 (3)	0.052 (4)	0.003 (2)	-0.002 (2)	0.001 (2)
C9	0.033 (2)	0.038 (2)	0.049 (3)	0.0002 (19)	-0.001 (2)	0.001 (2)
C10	0.035 (2)	0.041 (2)	0.048 (3)	0.0008 (18)	0.000 (2)	-0.001 (2)
C11	0.031 (2)	0.073 (3)	0.080 (4)	-0.011 (2)	-0.001 (3)	0.013 (3)
C12	0.036 (2)	0.055 (3)	0.057 (4)	0.000 (2)	-0.002 (2)	0.005 (3)
C13	0.031 (3)	0.088 (4)	0.098 (6)	0.000 (3)	-0.003 (3)	0.021 (4)

Geometric parameters (Å, °)

O1—C1	1.230 (6)	C5—C10	1.383 (7)
O2—C3	1.376 (6)	C5—C6	1.395 (6)
O2—C1	1.382 (5)	C5—H5	0.9500
O3—C6	1.358 (6)	C6—C7	1.401 (7)
O3—C11	1.438 (5)	C7—C8	1.371 (7)
O4—C8	1.354 (6)	C7—H7	0.9500
O4—H40	0.8400	C8—C9	1.426 (6)
O5—C13	1.340 (6)	C9—C10	1.402 (7)
O5—C12	1.428 (6)	C11—H11C	0.9800
O6—C13	1.184 (7)	C11—H11B	0.9800
C1—C9	1.417 (7)	C11—H11A	0.9800
C3—C4	1.327 (7)	C12—H12B	0.9900
C3—C12	1.499 (6)	C12—H12A	0.9900
C4—C10	1.447 (6)	C13—H13	0.9500
C4—H4	0.9500		
C3—O2—C1	120.3 (4)	O4—C8—C9	120.8 (4)
C6—O3—C11	118.3 (4)	C7—C8—C9	120.6 (4)
C8—O4—H40	109.5	C10—C9—C1	121.5 (4)
C13—O5—C12	116.1 (4)	C10—C9—C8	118.8 (4)
O1—C1—O2	115.3 (4)	C1—C9—C8	119.6 (4)
O1—C1—C9	126.7 (4)	C5—C10—C9	120.5 (4)
O2—C1—C9	117.9 (4)	C5—C10—C4	122.1 (4)
C4—C3—O2	123.7 (4)	C9—C10—C4	117.4 (4)
C4—C3—C12	127.2 (5)	O3—C11—H11C	109.5
O2—C3—C12	109.1 (4)	O3—C11—H11B	109.5
C3—C4—C10	119.2 (5)	H11C—C11—H11B	109.5
C3—C4—H4	120.4	O3—C11—H11A	109.5
C10—C4—H4	120.4	H11C—C11—H11A	109.5
C10—C5—C6	119.6 (5)	H11B—C11—H11A	109.5

C10—C5—H5	120.2	O5—C12—C3	106.5 (4)
C6—C5—H5	120.2	O5—C12—H12B	110.4
O3—C6—C5	115.5 (4)	C3—C12—H12B	110.4
O3—C6—C7	123.4 (4)	O5—C12—H12A	110.4
C5—C6—C7	121.1 (4)	C3—C12—H12A	110.4
C8—C7—C6	119.3 (4)	H12B—C12—H12A	108.6
C8—C7—H7	120.3	O6—C13—O5	125.8 (6)
C6—C7—H7	120.3	O6—C13—H13	117.1
O4—C8—C7	118.6 (4)	O5—C13—H13	117.1
C3—O2—C1—O1	-178.0 (4)	O2—C1—C9—C8	179.5 (4)
C3—O2—C1—C9	2.3 (6)	O4—C8—C9—C10	179.9 (5)
C1—O2—C3—C4	-1.6 (7)	C7—C8—C9—C10	0.8 (8)
C1—O2—C3—C12	179.1 (4)	O4—C8—C9—C1	-1.0 (8)
O2—C3—C4—C10	-0.2 (8)	C7—C8—C9—C1	179.9 (5)
C12—C3—C4—C10	179.0 (5)	C6—C5—C10—C9	1.3 (8)
C11—O3—C6—C5	-176.5 (5)	C6—C5—C10—C4	-178.7 (5)
C11—O3—C6—C7	4.8 (8)	C1—C9—C10—C5	179.7 (5)
C10—C5—C6—O3	-179.7 (5)	C8—C9—C10—C5	-1.2 (8)
C10—C5—C6—C7	-1.0 (8)	C1—C9—C10—C4	-0.3 (8)
O3—C6—C7—C8	179.2 (5)	C8—C9—C10—C4	178.8 (5)
C5—C6—C7—C8	0.6 (8)	C3—C4—C10—C5	-178.9 (5)
C6—C7—C8—O4	-179.6 (5)	C3—C4—C10—C9	1.1 (8)
C6—C7—C8—C9	-0.5 (8)	C13—O5—C12—C3	176.8 (5)
O1—C1—C9—C10	179.0 (5)	C4—C3—C12—O5	5.5 (8)
O2—C1—C9—C10	-1.4 (7)	O2—C3—C12—O5	-175.2 (4)
O1—C1—C9—C8	-0.1 (8)	C12—O5—C13—O6	0.9 (12)

*Hydrogen-bond geometry (Å, °)*C_g is the centroid of the C5–C10 ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O4—H40...O1	0.84	1.88	2.616 (5)	146
C4—H4...O1 ⁱ	0.95	2.38	3.326 (6)	173
C5—H5...O2 ⁱ	0.95	2.59	3.541 (6)	176
C7—H7...O6 ⁱⁱ	0.95	2.55	3.499 (5)	175
C11—H11C...O6 ⁱ	0.98	2.57	3.388 (8)	141
C12—H12B...C _g ⁱⁱⁱ	0.99	2.88	3.788 (6)	153

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