



Crystal structure of bergapten: a photomutagenic and photobiologically active furanocoumarin

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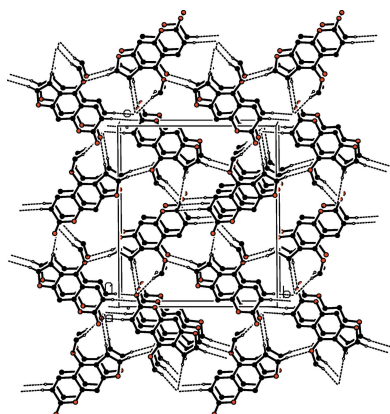
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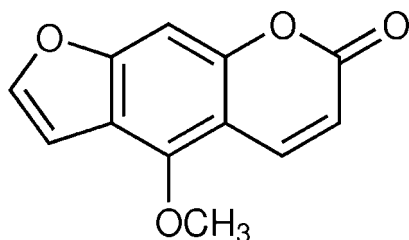
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The title compound, C₁₂H₈O₄, is a furanocoumarin [systematic name: 4-methoxy-7*H*-furo[3,2-*g*]chromen-7-one], which was isolated from the Indian herb *T. stictocarpum*. The molecule is almost planar with an r.m.s. deviation of 0.024 Å for the hetero atoms of the fused-ring system. In the crystal, molecules are linked by C—H...O hydrogen bonds, forming a three-dimensional framework. There are offset π – π interactions present involving the coumarin moieties stacking along the *a*-axis direction [shortest inter-centroid distance = 3.717 (3) Å].

1. Chemical context

The title molecule, bergapten, is a linear furanocoumarin having a methoxy group in the benzene ring at position C5. This class of furano coumarins have absorption bands in the near UV region due to the presence of conjugated double bonds, and exhibit photomutagenic (Appendino, *et al.*, 2004) and photocarcinogenic properties, binding with purine bases of DNA in living cells to yield photoadducts (Filomena *et al.*, 2009). Based on this property, they are employed to treat numerous inflammatory skin diseases, such as atopic dermatitis, and pigment disorders like vitiligo and psoriasis by UV photodynamic therapy. In addition, due to their strong ability to absorb UV radiation, this class of molecules are utilized as photoprotective agents, to prevent the absorption of harmful UV radiation by the skin. A variety of sun-screen lotions are widely used in dermatological applications in the cosmetic and pharmaceutical industries (Chen *et al.*, 2007, 2009). In addition, the *in vitro* antiproliferation activity and *in vivo* phototoxicity of the title molecule has been reported against epithelial cancer cell lines, including HL60, A431 (Conconi *et al.*, 1998). Bergapten (5-methoxy psoralen/methoxsalen) has been used successfully in combination with UV photodynamic therapy to manage psoriasis and vitiligo; it inhibits proliferation in human hepatocellular carcinoma cell line (March *et al.*, 1993). Experimental results revealed that its phototoxicity and photomutagenicity is exerted *via* a Diels–Alder reaction binding the double bond of a purine base of DNA in a living cell with the double bonds of bergapten to yield mono- and di-adducts (Conforti *et al.*, 2009).





While this is the first report of the crystal structure of the title compound, its chemical structure was determined by spectrometric and spectroscopic analysis many years ago (Howell & Robertson, 1937; Ray *et al.*, 1937; Lin *et al.*, 1979; Confalone & Confalone, 1983).

2. Structural commentary

The title compound (Fig. 1), belongs to the psoralen class of compounds and is composed of three fused rings *viz.* furan, benzene and pyrone. It is an almost planar molecule with an r.m.s. deviation of 0.024 Å for the atoms of the fused ring system, O1–O2/C1–C11. The methoxy C atom, C12, is displaced from this mean plane by 0.925 (5) Å, while atoms O3 and O4 are displaced from the mean plane by 0.069 (3) and 0.035 (3) Å, respectively.

3. Supramolecular features

In the crystal, molecules are linked by a series of C–H···O hydrogen bonds, which are illustrated in Fig. 2 (see also Table 1). They form a three-dimensional network (Table 1 and Fig. 3). There are offset π – π interactions present involving the coumarin moieties stacking along the *a*-axis direction [shortest inter-centroid distance $Cg2 \cdots Cg3^i = 3.717$ (3) Å, interplanar distance = 3.425 (2) Å, slippage = 1.356 Å, $Cg2$ and $Cg3$ are

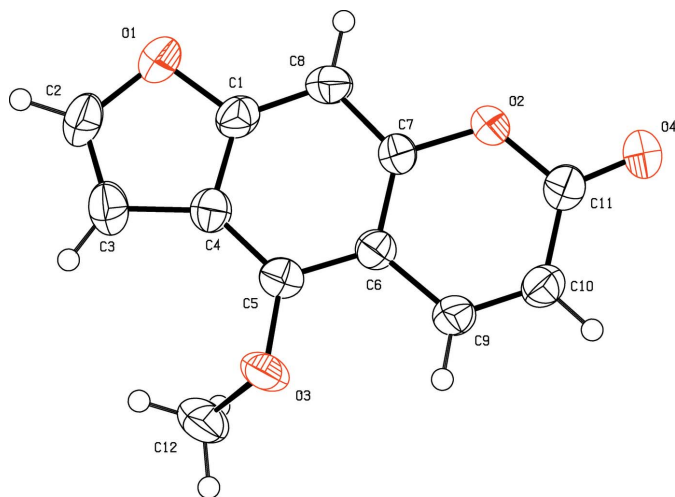


Figure 1
A view of the molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

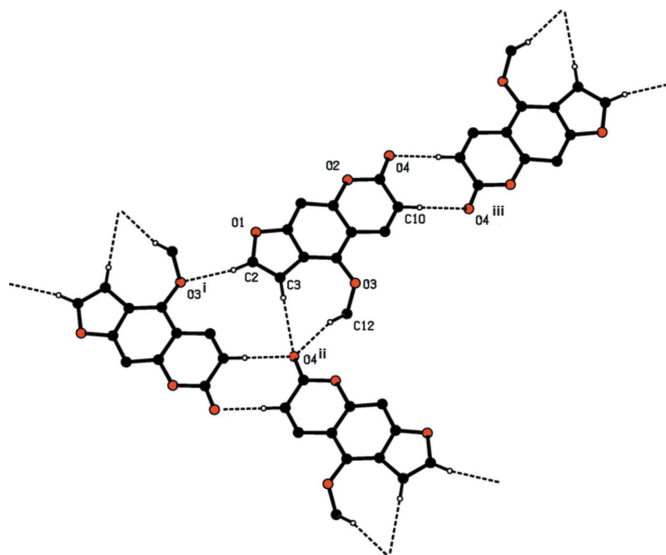


Figure 2
A view of the various C–H···O hydrogen bonds (dashed lines; see Table 1 for details) in the crystal of the title compound.

the centroids of rings O2/C6/C7/C9–C11 and C1/C4–C8, respectively, symmetry code: (i) $x - 1, y, z$].

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 5.37, last update May 2016; Groom *et al.*, 2016) gave 16 hits for the furanocoumarin skeleton with an O atom

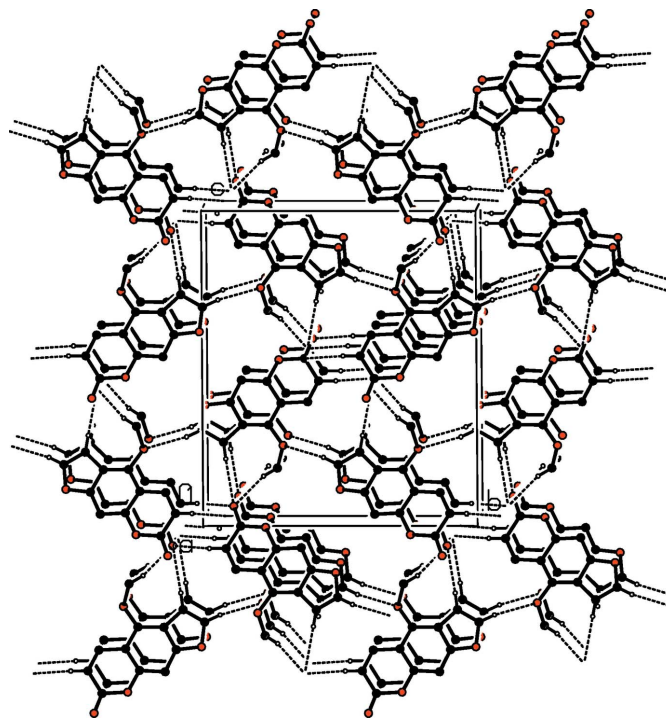


Figure 3
A view along the *a* axis of the crystal packing of the title compound. Hydrogen bonds are drawn as dashed lines (see Table 1) and H atoms not involved in these interactions have been omitted for clarity.

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

<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>
C2—H2...O3 ⁱ	0.93	2.49	3.406 (5)	170
C3—H3...O4 ⁱⁱ	0.93	2.57	3.484 (6)	170
C10—H10...O4 ⁱⁱⁱ	0.93	2.51	3.387 (5)	158
C12—H12A...O4 ⁱⁱ	0.96	2.44	3.376 (5)	165

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

substituent in position 5, similar to the title compound. Two compounds closely resemble the title compound, *viz.* 5-hydroxypsoralen [JIXBOH; Ginderow, 1991] isolated from the bark of *Citrus bergamia*, and 5,8-dimethoxypsoralen [ISIMP (293 K); Gopalakrishna *et al.*, 1977] and [ISIMP01 (120 K); Napolitano *et al.*, 2003]. The latter was isolated from the roots and leaves of *Adiscanthus fusciflorus* (*Rutaceae*).

5. Synthesis and crystallization

The title compound was isolated as a colourless solid from the methanol extract of *T. stictocarpum* by means of column chromatography over silica gel by gradient elution with a mixture of binary solvents system hexane and ethyl acetate. It was purified by reverse phase high-pressure liquid chromatography. Colourless rod-like crystals, suitable crystals for X ray diffraction analysis, were obtained after the title compound

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₂ H ₈ O ₄
<i>M_r</i>	216.18
Crystal system, space group	Monoclinic, <i>P</i> ₂ ₁ / <i>c</i>
Temperature (K)	299
<i>a</i> , <i>b</i> , <i>c</i> (Å)	3.8486 (8), 14.676 (2), 16.866 (3)
β (°)	92.12 (2)
<i>V</i> (Å ³)	952.0 (3)
<i>Z</i>	4
Radiation type	Mo Kα
μ (mm ⁻¹)	0.12
Crystal size (mm)	0.44 × 0.08 × 0.02
Data collection	
Diffractometer	Oxford Diffraction Xcalibur with a Sapphire CCD detector
Absorption correction	Multi-scan (<i>CrysAlis RED</i> ; Oxford Diffraction, 2009) [*]
<i>T_{min}</i> , <i>T_{max}</i>	0.951, 0.998
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	7096, 7096, 3811
<i>R_{int}</i>	0.08
(sin θ/λ) _{max} (Å ⁻¹)	0.602
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.055, 0.138, 0.86
No. of reflections	7096
No. of parameters	147
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.19, -0.22

Computer programs: *CrysAlis CCD* and *CrysAlis RED* (Oxford Diffraction, 2009), *SHELXS2014* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

was recrystallized three times from ethyl acetate:hexane (1:4) mixed solvents at room temperature by slow evaporation of the solvents (m.p. 469 K).

¹H NMR data (CHCl₃, 200 MHz) 8.13 (*d*, 1H, *J* = 9.8 Hz, H-9), 7.57 (*d*, 1H, *J* = 2.2 Hz, H-2), 7.11 (*s*, 1H, H-8), 7.05 (*d*, 1H, *J* = 2.2 Hz, H-3), 6.25 (*d*, 1H, *J* = 9.8 Hz, H-10), 4.26 (*s*, 3H, OCH₃). EIMS (70 ev) data: *m/z* (%) 216 (100; base peak/molecular ion peak) [*M*⁺], 201 (25.2%) [*M*⁺—CH₃], 188 (25.7) [*M*⁺—OCH₃], 173 (25.6) [*M*⁺—(CH₃—CO)], 145 (33.8) [*M*⁺—(OCH₃—CO₂)], 89(17.0).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C-bound H atoms were included in calculated positions and treated as riding atoms: C—H = 0.93–0.96 Å with *U*_{iso}(H) = 1.5*U*_{eq}(C-methyl) and 1.2*U*_{eq}(C) for other H atoms. The structure was refined as a two-component twin [180° rotation about the *a** axis; BASF = 0.3955 (2)].

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Computing details

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis CCD* (Oxford Diffraction, 2009); data reduction: *CrysAlis RED* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS2014* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015).

4-Methoxy-7H-furo[3,2-g]chromen-7-one

Crystal data

$C_{12}H_8O_4$

$M_r = 216.18$

Monoclinic, $P2_1/c$

$a = 3.8486$ (8) Å

$b = 14.676$ (2) Å

$c = 16.866$ (3) Å

$\beta = 92.12$ (2)°

$V = 952.0$ (3) Å³

$Z = 4$

$F(000) = 448$

$D_x = 1.508$ Mg m⁻³

Melting point: 469 K

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

Cell parameters from 870 reflections

$\theta = 2.8$ – 27.9 °

$\mu = 0.12$ mm⁻¹

$T = 299$ K

Needle, colourless

$0.44 \times 0.08 \times 0.02$ mm

Data collection

Oxford Diffraction Xcalibur with a Sapphire
CCD detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Rotation method data acquisition using ω and
phi scans.

Absorption correction: multi-scan

(*CrysAlis RED*; Oxford Diffraction, 2009)

$T_{\min} = 0.951$, $T_{\max} = 0.998$

7096 measured reflections

7096 independent reflections

3811 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.08$

$\theta_{\max} = 25.4$ °, $\theta_{\min} = 2.8$ °

$h = -4 \rightarrow 4$

$k = -17 \rightarrow 17$

$l = -20 \rightarrow 20$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.055$

$wR(F^2) = 0.138$

$S = 0.86$

7096 reflections

147 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-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0738P)^2]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$

$$\Delta\rho_{\max} = 0.19 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.22 \text{ e } \text{\AA}^{-3}$$

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. Refined as a 2-component twin.

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	0.7447 (9)	0.00489 (18)	0.37565 (18)	0.0525 (10)
O2	0.3156 (8)	0.26727 (18)	0.50579 (14)	0.0399 (9)
O3	0.7860 (9)	0.28906 (17)	0.24893 (16)	0.0510 (10)
O4	0.1046 (9)	0.3863 (2)	0.56614 (18)	0.0617 (11)
C1	0.6682 (13)	0.0956 (3)	0.3822 (3)	0.0392 (13)
C2	0.8854 (13)	-0.0043 (3)	0.3016 (3)	0.0534 (15)
H2	0.9619	-0.0595	0.2814	0.064*
C3	0.8989 (13)	0.0740 (3)	0.2626 (3)	0.0477 (14)
H3	0.9832	0.0833	0.2123	0.057*
C4	0.7573 (13)	0.1417 (3)	0.3137 (2)	0.0369 (12)
C5	0.6975 (12)	0.2354 (3)	0.3111 (2)	0.0344 (12)
C6	0.5523 (11)	0.2781 (3)	0.3757 (2)	0.0304 (11)
C7	0.4677 (11)	0.2262 (3)	0.4418 (2)	0.0348 (12)
C8	0.5234 (12)	0.1339 (3)	0.4477 (3)	0.0397 (13)
H8	0.4679	0.1003	0.4922	0.048*
C9	0.4692 (12)	0.3738 (3)	0.3771 (3)	0.0373 (13)
H9	0.5221	0.4101	0.3339	0.045*
C10	0.3191 (12)	0.4114 (3)	0.4385 (2)	0.0431 (13)
H10	0.2654	0.4732	0.4371	0.052*
C11	0.2370 (13)	0.3592 (3)	0.5074 (3)	0.0433 (13)
C12	0.6549 (14)	0.2653 (3)	0.1726 (2)	0.0652 (17)
H12A	0.7936	0.2173	0.1516	0.098*
H12B	0.6630	0.3175	0.1384	0.098*
H12C	0.4187	0.2450	0.1758	0.098*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.075 (3)	0.0265 (17)	0.056 (2)	0.0074 (19)	0.006 (2)	-0.0024 (16)
O2	0.054 (2)	0.0343 (18)	0.0321 (16)	0.0034 (18)	0.0073 (19)	0.0003 (14)
O3	0.081 (3)	0.0419 (18)	0.0300 (17)	-0.0206 (19)	0.005 (2)	0.0006 (15)
O4	0.089 (3)	0.052 (2)	0.045 (2)	0.018 (2)	0.025 (2)	-0.0027 (18)
C1	0.045 (4)	0.029 (3)	0.043 (3)	0.000 (3)	-0.007 (3)	0.000 (2)
C2	0.063 (4)	0.040 (3)	0.058 (3)	0.009 (3)	0.010 (3)	-0.013 (3)
C3	0.054 (4)	0.041 (3)	0.048 (3)	-0.001 (3)	0.007 (3)	-0.006 (2)

C4	0.040 (3)	0.032 (3)	0.039 (3)	-0.002 (3)	-0.001 (3)	-0.0073 (19)
C5	0.036 (3)	0.037 (3)	0.030 (2)	-0.006 (3)	0.001 (3)	0.001 (2)
C6	0.029 (3)	0.029 (2)	0.033 (2)	-0.002 (2)	-0.002 (2)	-0.001 (2)
C7	0.041 (3)	0.033 (3)	0.031 (2)	-0.002 (3)	0.005 (2)	-0.002 (2)
C8	0.049 (4)	0.033 (3)	0.038 (3)	-0.002 (3)	0.004 (3)	0.008 (2)
C9	0.047 (3)	0.030 (3)	0.035 (3)	-0.004 (2)	0.002 (3)	0.005 (2)
C10	0.056 (4)	0.029 (2)	0.044 (3)	0.004 (3)	0.001 (3)	0.003 (2)
C11	0.046 (4)	0.036 (3)	0.048 (3)	0.007 (3)	0.006 (3)	-0.001 (2)
C12	0.099 (5)	0.060 (3)	0.037 (3)	-0.013 (4)	0.001 (3)	-0.003 (2)

Geometric parameters (Å, °)

O1—C1	1.369 (5)	C4—C5	1.394 (6)
O1—C2	1.386 (5)	C5—C6	1.391 (5)
O2—C7	1.385 (4)	C6—C7	1.398 (5)
O2—C11	1.383 (5)	C6—C9	1.442 (5)
O3—C5	1.365 (4)	C7—C8	1.374 (5)
O3—C12	1.409 (4)	C8—H8	0.9300
O4—C11	1.200 (5)	C9—C10	1.325 (5)
C1—C8	1.376 (5)	C9—H9	0.9300
C1—C4	1.393 (6)	C10—C11	1.435 (5)
C2—C3	1.327 (6)	C10—H10	0.9300
C2—H2	0.9300	C12—H12A	0.9600
C3—C4	1.435 (6)	C12—H12B	0.9600
C3—H3	0.9300	C12—H12C	0.9600
C1—O1—C2	105.1 (3)	C8—C7—O2	116.2 (4)
C7—O2—C11	122.6 (3)	C8—C7—C6	123.7 (4)
C5—O3—C12	117.9 (3)	O2—C7—C6	120.1 (4)
O1—C1—C8	123.8 (4)	C1—C8—C7	114.2 (4)
O1—C1—C4	110.2 (4)	C1—C8—H8	122.9
C8—C1—C4	126.0 (4)	C7—C8—H8	122.9
C3—C2—O1	112.7 (4)	C10—C9—C6	121.4 (4)
C3—C2—H2	123.7	C10—C9—H9	119.3
O1—C2—H2	123.7	C6—C9—H9	119.3
C2—C3—C4	106.2 (4)	C9—C10—C11	121.7 (4)
C2—C3—H3	126.9	C9—C10—H10	119.1
C4—C3—H3	126.9	C11—C10—H10	119.1
C5—C4—C1	117.3 (4)	O4—C11—O2	116.1 (4)
C5—C4—C3	136.9 (4)	O4—C11—C10	127.2 (4)
C1—C4—C3	105.8 (4)	O2—C11—C10	116.8 (4)
O3—C5—C6	117.4 (4)	O3—C12—H12A	109.5
O3—C5—C4	123.2 (4)	O3—C12—H12B	109.5
C6—C5—C4	119.4 (4)	H12A—C12—H12B	109.5
C5—C6—C7	119.4 (4)	O3—C12—H12C	109.5
C5—C6—C9	123.2 (4)	H12A—C12—H12C	109.5
C7—C6—C9	117.4 (4)	H12B—C12—H12C	109.5

C2—O1—C1—C8	-179.8 (5)	C4—C5—C6—C9	-177.6 (4)
C2—O1—C1—C4	0.3 (5)	C11—O2—C7—C8	-178.5 (4)
C1—O1—C2—C3	-0.2 (6)	C11—O2—C7—C6	0.9 (6)
O1—C2—C3—C4	0.0 (6)	C5—C6—C7—C8	0.8 (6)
O1—C1—C4—C5	-179.6 (4)	C9—C6—C7—C8	178.3 (4)
C8—C1—C4—C5	0.5 (7)	C5—C6—C7—O2	-178.5 (4)
O1—C1—C4—C3	-0.3 (5)	C9—C6—C7—O2	-1.1 (6)
C8—C1—C4—C3	179.8 (5)	O1—C1—C8—C7	-179.9 (5)
C2—C3—C4—C5	179.2 (6)	C4—C1—C8—C7	-0.1 (7)
C2—C3—C4—C1	0.2 (6)	O2—C7—C8—C1	178.7 (4)
C12—O3—C5—C6	-126.8 (4)	C6—C7—C8—C1	-0.6 (7)
C12—O3—C5—C4	55.5 (6)	C5—C6—C9—C10	177.4 (5)
C1—C4—C5—O3	177.3 (4)	C7—C6—C9—C10	0.1 (7)
C3—C4—C5—O3	-1.7 (9)	C6—C9—C10—C11	1.1 (7)
C1—C4—C5—C6	-0.3 (7)	C7—O2—C11—O4	179.7 (4)
C3—C4—C5—C6	-179.3 (5)	C7—O2—C11—C10	0.3 (6)
O3—C5—C6—C7	-178.0 (4)	C9—C10—C11—O4	179.3 (5)
C4—C5—C6—C7	-0.3 (6)	C9—C10—C11—O2	-1.3 (7)
O3—C5—C6—C9	4.7 (6)		

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>
C2—H2 \cdots O3 ⁱ	0.93	2.49	3.406 (5)	170
C3—H3 \cdots O4 ⁱⁱ	0.93	2.57	3.484 (6)	170
C10—H10 \cdots O4 ⁱⁱⁱ	0.93	2.51	3.387 (5)	158
C12—H12 <i>A</i> \cdots O4 ⁱⁱ	0.96	2.44	3.376 (5)	165

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