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4-[(Hydroxy)(4-methylphenyl)methylidene]isochroman-1,3-dione

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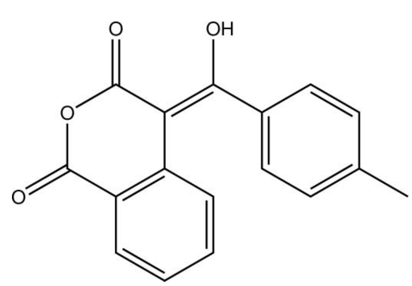
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.057; wR factor = 0.150; data-to-parameter ratio = 17.1.

In the title compound, $C_{17}H_{12}O_4$, the six-membered heterocyclic ring adopts a distorted screw-boat conformation. The molecular structure exhibits an $S(6)$ ring motif, owing to an intramolecular O—H···O hydrogen bond. In the crystal, weak C—H···O contacts generate an infinite chain along the c axis. There are also π–π stacking interactions between neighbouring isochromanedione benzene rings, with a centroid–centroid distance of 3.755 (1) Å, and C—O···π interactions with an O···centroid distance of 3.964 (2) Å.

Related literature

For the biological activity of isochromanones, see: Bianchi *et al.*, (2004); Buntin *et al.* (2008). For π–π stacking interactions, see: Janiak (2000). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For ring puckering parameters, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{17}H_{12}O_4$
M_r = 280.27
Monoclinic, $P2_1/c$
a = 15.6767 (6) Å
b = 5.9655 (2) Å
c = 14.4589 (4) Å
β = 102.961 (1)°
V = 1317.74 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 K
0.40 × 0.34 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
12419 measured reflections
3304 independent reflections
2684 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.150
S = 1.08
3304 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O3	0.82	1.75	2.485 (2)	148
C7—H7···O2^{i}	0.93	2.57	3.299 (2)	136

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

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO*/*SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO*/*SCALEPACK*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*, *publCIF* (Westrip, 2010) and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2488).

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4-[(Hydroxy)(4-methylphenyl)methylidene]isochroman-1,3-dione

Akoun Abou, Abdoulaye Djandé, Adama Saba, Thierry Chiavassa and Rita Kakou-Yao

S1. Comment

The title molecule is related to the isochromanone derivatives that are generally known as regulators of plant growth (Bianchi *et al.*, 2004). Depending on their chemical structure and concentration they can act either as inhibitors or stimulators in these processes. Some substituted isochromanones isolated from myxobacteria strains were introduced as anti-fungal agents (Buntin *et al.*, 2008).

The structure of the title compound (I) (Fig. 1) consists of two essentially planar benzene rings with the maximum deviations from the best planes of 0.035 (1) Å for atom C6 (benzene ring C4—C9) and 0.008 (2) Å for atoms C12 and C15 (benzene ring C11—C16). An S(6) ring motifs (Bernstein *et al.*, 1995), arising from the intramolecular hydrogen bond O—H···O, generates a planar pseudo six-membered ring (maximum deviation from planarity being ∓0.055 (2) Å for atoms C1 and C10) to result in a tricyclic ring (Fig. 1). The dihedral angles between two benzene rings is 58.99 (8)° and that between the pseudo six-membered ring and benzene rings are 13.75 (8) ° (ring C4—C9) and 53.96 (8)° (ring C11—C16). The heterocyclic ring O1/C1—C5 adopts a distorted screw-boat conformation as judged from the puckering parameters (Cremer & Pople, 1975): Q = 0.0974 (17) Å, θ = 69.6 (1)° and φ = 132.6 (1)°. Furthermore, intermolecular C—H···O hydrogen bonds (Table 1) link molecules into infinite chains along the [001] (Fig. 2).

The supramolecular aggregation is completed by the presence of C—O···π interactions (O3···*Cg3*[*x*,1/2 - *y*,-3/2 + *z*] = 3.964 (2) Å, C2—O3···*Cg3* = 83.89 (12)°, where *Cg3* is the centroid of the benzene ring C11—C16 and π–π stacking between two parallel isochromandione-benzene C4—C9 rings; in the latter, the centroid···centroid distance, (*Cg2*···*Cg2*(-*x*,2 - *y*,-*z*) of 3.755 (1) Å), is less than 3.8 Å, the maximum regarded as relevant for π–π interactions (Janiak, 2000) (Fig.3).

S2. Experimental

To a solution of *p*-Toluoyl chloride (4.10^{-2} mole) in dried tetrahydrofuran (150 ml), was added dried triethylamine (0.12 mole) and homophtalic anhydride (4.10^{-2} mole) by small portions over 30 min. The mixture was then refluxed for 3 h and poured in 300 ml of chloroform. The solution was acidified with dilute hydrochloric acid until the pH was 2 - 3. The organic layer was extracted, washed with water, dried over MgSO4 and the solvent removed. The crude product was recrystallized from chloroform-hexane (1/1, *v*/*v*) mixture. Yellow crystals of the title compound were obtained in a good yield: 85%; *M*.pt. 387–388 K.

S3. Refinement

H atoms were placed in calculated positions [O—H = 0.82 Å and C—H = 0.93 (aromatic) or 0.96 Å (methyl group)] and refined using a riding model approximation with U_{iso}(H) constrained to 1.2 (aromatic) or 1.5 (methyle, O—H) times U_{eq} of the respective parent atom.

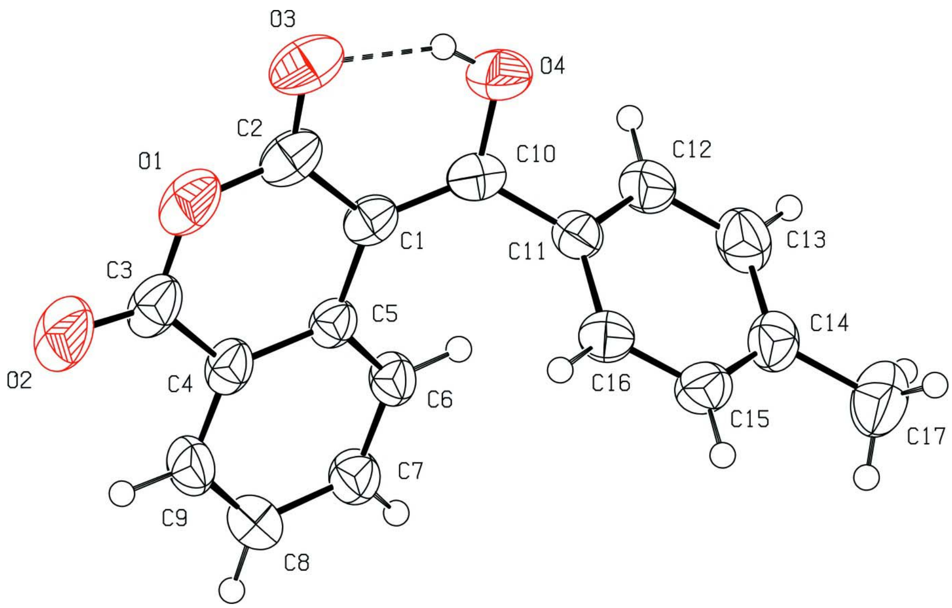

Figure 1

The molecular structure of (I) showing the atomic labeling scheme with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitary radius. Dashed lines indicate an hydrogen bond.

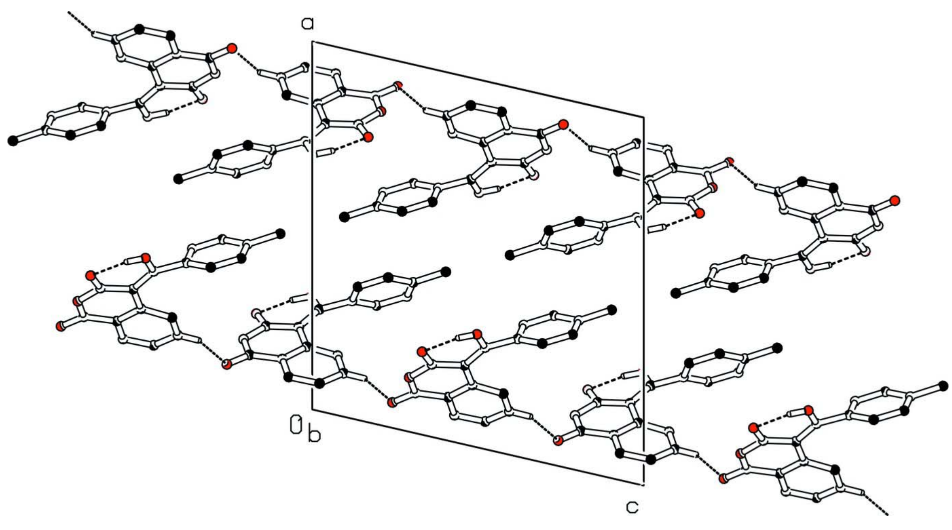

Figure 2

Crystal packing, viewed down the *b* axis, showing parallel chains along the *c* direction. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonds have been omitted for clarity.

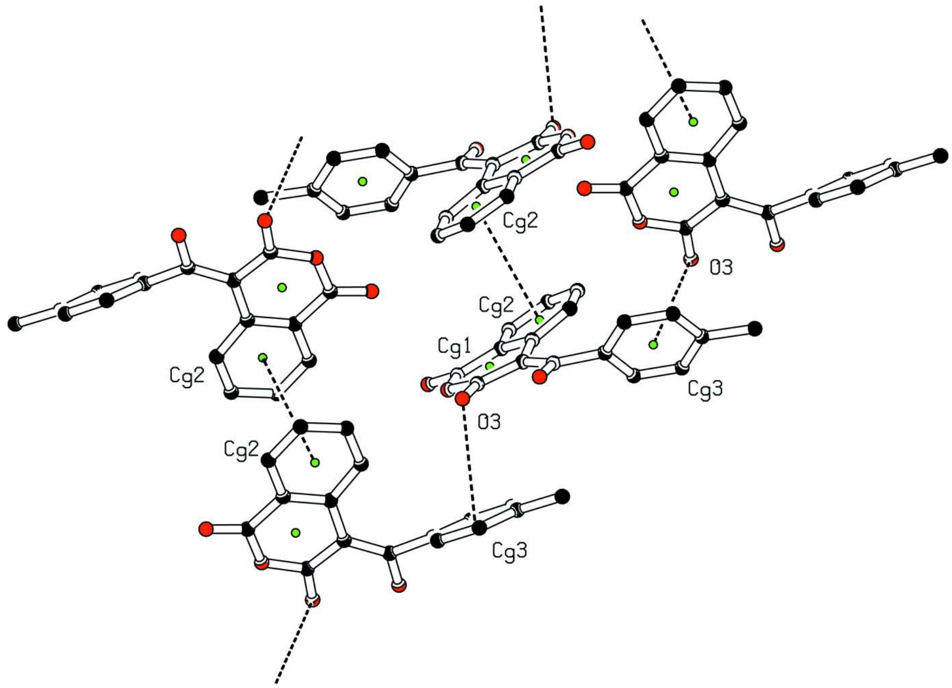

Figure 3

A view of the crystal packing, showing C—O···π and π–π stacking interactions (dashed lines). The green dots are centroids of rings. H atoms have been omitted for clarity.

4-[(Hydroxy)(4-methylphenyl)methylidene]isochroman-1,3-dione

Crystal data

$C_{17}H_{12}O_4$	$F(000) = 584$
$M_r = 280.27$	$D_x = 1.413$ Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point = 387–388 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 15.6767$ (6) Å	Cell parameters from 12419 reflections
$b = 5.9655$ (2) Å	$\theta = 2.9$–$29.0°$
$c = 14.4589$ (4) Å	$\mu = 0.10$ mm^{-1}
$\beta = 102.961$ (1)°	$T = 298$ K
$V = 1317.74$ (8) Å^3	Prism, yellow
$Z = 4$	0.40 × 0.34 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer	2684 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.053$
Graphite monochromator	$\theta_{max} = 29.0°$, $\theta_{min} = 2.9°$
φ and ω scans	$h = -21 \rightarrow 20$
12419 measured reflections	$k = -7 \rightarrow 7$
3304 independent reflections	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.150$
$S = 1.08$
3304 reflections
193 parameters
0 restraints
48 constraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0625P)^2 + 0.424P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.20$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.11 (2)

Special details

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

Refinement. The 2 reflections [(-5 2 1), (2 0 0)] whith (Iobs-Icalc)/Sigma(I) superior to 10, are not used in the refinement. 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 $F^2 > 2\sigma(F^2)$ 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}
O1	0.85227 (9)	0.2252 (2)	0.70711 (8)	0.0608 (4)
C5	0.83327 (9)	0.3569 (2)	0.51682 (9)	0.0361 (3)
C4	0.88171 (10)	0.4900 (3)	0.59015 (10)	0.0420 (4)
O3	0.77485 (10)	−0.0788 (3)	0.66859 (10)	0.0690 (4)
O4	0.69333 (9)	−0.1556 (2)	0.50349 (10)	0.0632 (4)
H4	0.7147	−0.1802	0.5597	0.095*
C15	0.59439 (11)	0.3609 (3)	0.27099 (12)	0.0484 (4)
H15	0.5656	0.4979	0.2599	0.058*
C1	0.78494 (10)	0.1628 (3)	0.54105 (10)	0.0405 (4)
C6	0.83808 (10)	0.4128 (3)	0.42383 (10)	0.0401 (4)
H6	0.8110	0.3211	0.3738	0.048*
C9	0.92667 (11)	0.6800 (3)	0.57079 (12)	0.0514 (4)
H9	0.9579	0.7670	0.6204	0.062*
C16	0.63851 (10)	0.3071 (3)	0.36170 (12)	0.0454 (4)
H16	0.6403	0.4089	0.4108	0.054*
C11	0.68042 (10)	0.1011 (3)	0.38016 (11)	0.0412 (4)
C10	0.72372 (10)	0.0383 (3)	0.47841 (12)	0.0441 (4)
C12	0.67731 (11)	−0.0477 (3)	0.30589 (13)	0.0515 (4)
H12	0.7043	−0.1870	0.3173	0.062*
C8	0.92474 (12)	0.7385 (3)	0.47832 (13)	0.0530 (4)
H8	0.9519	0.8693	0.4648	0.064*
C3	0.89085 (12)	0.4261 (3)	0.68931 (11)	0.0532 (5)

O2	0.93083 (11)	0.5246 (3)	0.75773 (9)	0.0782 (5)
C14	0.59194 (10)	0.2147 (3)	0.19552 (12)	0.0487 (4)
C13	0.63411 (12)	0.0107 (3)	0.21485 (13)	0.0567 (5)
H13	0.6334	−0.0896	0.1654	0.068*
C7	0.88200 (11)	0.6007 (3)	0.40553 (11)	0.0461 (4)
H7	0.8831	0.6360	0.3432	0.055*
C2	0.80260 (12)	0.0934 (3)	0.63907 (12)	0.0504 (4)
C17	0.54283 (14)	0.2771 (4)	0.09711 (14)	0.0719 (6)
H17A	0.4814	0.2511	0.0913	0.108*
H17B	0.5634	0.1874	0.0514	0.108*
H17C	0.5524	0.4327	0.0859	0.108*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0781 (9)	0.0731 (9)	0.0303 (6)	0.0141 (7)	0.0104 (5)	0.0079 (5)
C5	0.0390 (7)	0.0374 (8)	0.0311 (7)	0.0060 (5)	0.0063 (5)	−0.0008 (5)
C4	0.0461 (8)	0.0458 (9)	0.0313 (7)	0.0105 (6)	0.0029 (6)	−0.0061 (6)
O3	0.0837 (10)	0.0700 (9)	0.0572 (8)	0.0078 (7)	0.0242 (7)	0.0287 (7)
O4	0.0656 (8)	0.0478 (7)	0.0736 (9)	−0.0084 (6)	0.0102 (7)	0.0191 (6)
C15	0.0448 (8)	0.0428 (9)	0.0566 (10)	0.0044 (7)	0.0092 (7)	0.0052 (7)
C1	0.0452 (8)	0.0419 (8)	0.0357 (7)	0.0064 (6)	0.0116 (6)	0.0047 (6)
C6	0.0435 (8)	0.0450 (8)	0.0306 (7)	−0.0051 (6)	0.0056 (6)	−0.0029 (6)
C9	0.0527 (9)	0.0473 (9)	0.0474 (9)	−0.0001 (7)	−0.0031 (7)	−0.0147 (7)
C16	0.0481 (8)	0.0383 (8)	0.0491 (9)	0.0034 (6)	0.0094 (7)	−0.0026 (6)
C11	0.0382 (7)	0.0355 (8)	0.0482 (8)	−0.0021 (6)	0.0064 (6)	0.0002 (6)
C10	0.0463 (8)	0.0371 (8)	0.0509 (9)	0.0039 (6)	0.0149 (7)	0.0069 (6)
C12	0.0520 (9)	0.0383 (9)	0.0606 (10)	0.0032 (7)	0.0048 (8)	−0.0059 (7)
C8	0.0551 (10)	0.0438 (9)	0.0567 (10)	−0.0094 (7)	0.0053 (8)	−0.0031 (7)
C3	0.0648 (11)	0.0583 (11)	0.0328 (8)	0.0203 (8)	0.0030 (7)	−0.0057 (7)
O2	0.1091 (12)	0.0797 (10)	0.0345 (6)	0.0199 (9)	−0.0081 (7)	−0.0154 (6)
C14	0.0380 (8)	0.0586 (10)	0.0478 (9)	−0.0055 (7)	0.0060 (6)	0.0021 (7)
C13	0.0563 (10)	0.0564 (11)	0.0544 (10)	−0.0008 (8)	0.0059 (8)	−0.0161 (8)
C7	0.0487 (9)	0.0504 (9)	0.0380 (8)	−0.0070 (7)	0.0069 (6)	0.0024 (6)
C2	0.0563 (10)	0.0564 (10)	0.0414 (8)	0.0153 (8)	0.0169 (7)	0.0108 (7)
C17	0.0641 (12)	0.0963 (17)	0.0503 (11)	−0.0034 (11)	0.0024 (9)	0.0090 (10)

Geometric parameters (Å, º)

O1—C2	1.360 (2)	C9—H9	0.9300
O1—C3	1.392 (2)	C16—C11	1.391 (2)
C5—C4	1.404 (2)	C16—H16	0.9300
C5—C6	1.404 (2)	C11—C12	1.386 (2)
C5—C1	1.469 (2)	C11—C10	1.479 (2)
C4—C9	1.396 (2)	C12—C13	1.383 (3)
C4—C3	1.459 (2)	C12—H12	0.9300
O3—C2	1.229 (2)	C8—C7	1.384 (2)
O4—C10	1.3316 (19)	C8—H8	0.9300

O4—H4	0.8200	C3—O2	1.199 (2)
C15—C16	1.376 (2)	C14—C13	1.383 (3)
C15—C14	1.391 (2)	C14—C17	1.505 (2)
C15—H15	0.9300	C13—H13	0.9300
C1—C10	1.380 (2)	C7—H7	0.9300
C1—C2	1.443 (2)	C17—H17A	0.9600
C6—C7	1.372 (2)	C17—H17B	0.9600
C6—H6	0.9300	C17—H17C	0.9600
C9—C8	1.376 (3)		

C2—O1—C3	124.49 (13)	C1—C10—C11	126.59 (14)
C4—C5—C6	116.93 (14)	C13—C12—C11	120.05 (16)
C4—C5—C1	119.11 (13)	C13—C12—H12	120.0
C6—C5—C1	123.87 (13)	C11—C12—H12	120.0
C9—C4—C5	121.33 (14)	C9—C8—C7	119.32 (16)
C9—C4—C3	117.80 (15)	C9—C8—H8	120.3
C5—C4—C3	120.78 (16)	C7—C8—H8	120.3
C10—O4—H4	109.5	O2—C3—O1	115.94 (16)
C16—C15—C14	121.40 (16)	O2—C3—C4	126.9 (2)
C16—C15—H15	119.3	O1—C3—C4	117.10 (15)
C14—C15—H15	119.3	C13—C14—C15	117.73 (15)
C10—C1—C2	116.26 (15)	C13—C14—C17	121.93 (18)
C10—C1—C5	126.02 (13)	C15—C14—C17	120.32 (17)
C2—C1—C5	117.72 (14)	C12—C13—C14	121.58 (16)
C7—C6—C5	121.07 (14)	C12—C13—H13	119.2
C7—C6—H6	119.5	C14—C13—H13	119.2
C5—C6—H6	119.5	C6—C7—C8	121.13 (15)
C8—C9—C4	119.92 (15)	C6—C7—H7	119.4
C8—C9—H9	120.0	C8—C7—H7	119.4
C4—C9—H9	120.0	O3—C2—O1	114.97 (15)
C15—C16—C11	120.24 (16)	O3—C2—C1	125.20 (18)
C15—C16—H16	119.9	O1—C2—C1	119.82 (16)
C11—C16—H16	119.9	C14—C17—H17A	109.5
C12—C11—C16	118.97 (15)	C14—C17—H17B	109.5
C12—C11—C10	120.72 (14)	H17A—C17—H17B	109.5
C16—C11—C10	120.24 (15)	C14—C17—H17C	109.5
O4—C10—C1	121.84 (15)	H17A—C17—H17C	109.5
O4—C10—C11	111.50 (14)	H17B—C17—H17C	109.5

C6—C5—C4—C9	5.1 (2)	C16—C11—C12—C13	0.9 (3)
C1—C5—C4—C9	−178.11 (14)	C10—C11—C12—C13	177.89 (16)
C6—C5—C4—C3	−171.19 (14)	C4—C9—C8—C7	−3.5 (3)
C1—C5—C4—C3	5.6 (2)	C2—O1—C3—O2	178.20 (16)
C4—C5—C1—C10	168.82 (15)	C2—O1—C3—C4	−4.3 (2)
C6—C5—C1—C10	−14.7 (2)	C9—C4—C3—O2	3.0 (3)
C4—C5—C1—C2	−11.4 (2)	C5—C4—C3—O2	179.43 (17)
C6—C5—C1—C2	165.14 (14)	C9—C4—C3—O1	−174.25 (14)
C4—C5—C6—C7	−5.5 (2)	C5—C4—C3—O1	2.2 (2)

C1—C5—C6—C7	177.88 (14)	C16—C15—C14—C13	1.2 (2)
C5—C4—C9—C8	−0.7 (2)	C16—C15—C14—C17	179.69 (16)
C3—C4—C9—C8	175.73 (16)	C11—C12—C13—C14	−1.1 (3)
C14—C15—C16—C11	−1.4 (3)	C15—C14—C13—C12	0.1 (3)
C15—C16—C11—C12	0.3 (2)	C17—C14—C13—C12	−178.41 (18)
C15—C16—C11—C10	−176.67 (15)	C5—C6—C7—C8	1.5 (3)
C2—C1—C10—O4	−10.7 (2)	C9—C8—C7—C6	3.2 (3)
C5—C1—C10—O4	169.10 (15)	C3—O1—C2—O3	179.33 (15)
C2—C1—C10—C11	165.94 (15)	C3—O1—C2—C1	−1.8 (2)
C5—C1—C10—C11	−14.3 (3)	C10—C1—C2—O3	8.2 (2)
C12—C11—C10—O4	−52.7 (2)	C5—C1—C2—O3	−171.65 (16)
C16—C11—C10—O4	124.25 (16)	C10—C1—C2—O1	−170.55 (14)
C12—C11—C10—C1	130.41 (18)	C5—C1—C2—O1	9.6 (2)
C16—C11—C10—C1	−52.7 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O3	0.82	1.75	2.485 (2)	148
C7—H7···O2^{i}	0.93	2.57	3.299 (2)	136

Symmetry code: (i) *x*, −*y*+3/2, *z*−1/2.