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8-Hydroxy-3,4-bis(4-methoxyphenyl)-1*H*-isochromen-1-one

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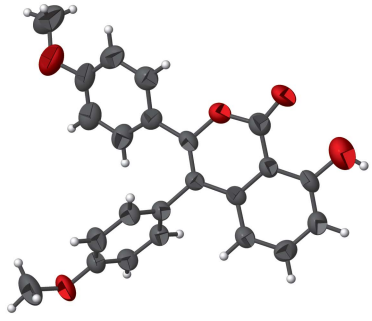
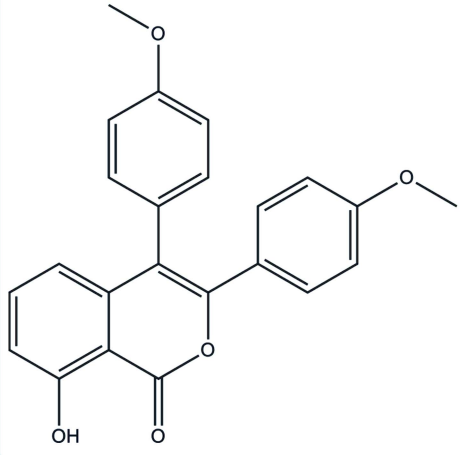
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{23}H_{18}O_5$, the two methoxy-substituted benzene rings are inclined to one another by 67.0 (2)° and to the mean plane of the 1*H*-isochromene ring system by 67.21 (16) and 27.61 (17)°. There is an intramolecular C—H···π interaction present involving the two 4-methoxyphenyl rings. In the crystal, molecules are linked by O—H···O hydrogen bonds, forming chains propagating along the [301] direction. The chains are linked by a number of C—H···π interactions, forming a three-dimensional structure.

3D view



Chemical scheme



Structure description

Chromene derivatives are important heterocyclic compounds that have a variety of industrial, biological and chemical synthesis applications (Geen *et al.*, 1996; Ercole *et al.*, 2009). They exhibit a number of pharmacological activities, such as anti-HIV, anti-inflammatory, antibacterial, anti-allergic and anticancer (Khan *et al.*, 2010; Raj *et al.*, 2010).

The title compound, Fig. 1, consists of a chromene moiety substituted by two methoxyphenyl groups and an hydroxy group. The two benzene rings (C10–C15 and C17–C22) are inclined to one another by 67.0 (2)° and to the mean plane of the 1*H*-isochromene ring system (O1/C1–C9) by 67.21 (16) and 27.61 (17)°, respectively. The 1*H*-isochromene moiety is planar (r.m.s. deviation = 0.043 Å) and atoms O2 and O3 deviate from this mean plane by −0.121 (3) and 0.058 (5) Å, respectively. There is an intramolecular C—H···π interaction present involving the two 4-methoxyphenyl rings (Table 1 and Fig. 1).

In the crystal, molecules are linked by O—H···O hydrogen bonds, forming chains propagating along [301]; Table 1 and Fig. 2. The chains are linked by a number of C—H···π interactions, forming a three-dimensional structure

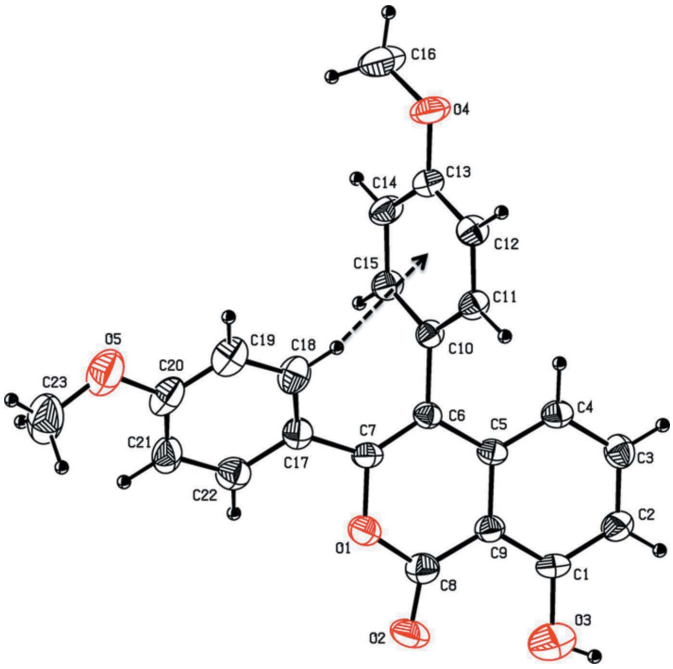


Figure 1
The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level. The intramolecular C—H···π interaction (Table 1) is shown as a dashed arrow.

Synthesis and crystallization

To a dried 50 ml round-bottom flask, fitted with a reflux condenser, were added 2-hydroxybenzoic acid (0.3 mmol), 1,2-bis(4-methoxyphenyl)ethyne (0.3 mmol), [$RuCl_2$(*p*-cymene)] (5.0 mol %), AgOAc (1.0 equiv) and $AgSbF_6$ (20 mol %) in 1,2-dichloroethane. The reaction mixture was refluxed for 12 h. After cooling to ambient temperature, the reaction mixture was diluted with CH_2Cl_2, filtered through Celite and the filtrate was concentrated under reduced pressure. The crude product was purified through a silica gel column using hexane and ethyl acetate as eluent. The title compound was obtained in 65% yield. It was recrystallized by slow evaporation of a solution in chloroform, yielding colourless block-like crystals.

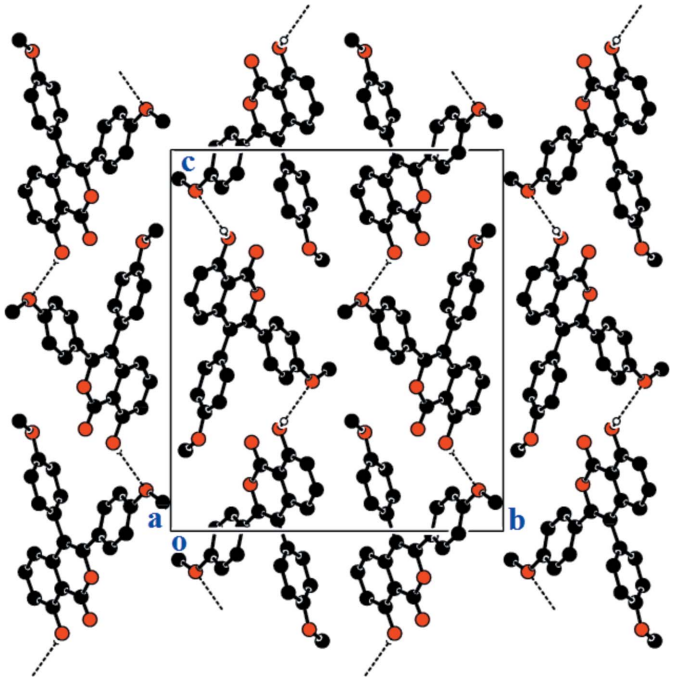


Figure 2
A view along the *a* axis of the crystal packing of the title compound. The dashed lines represent the hydrogen bonds (see Table 1). For clarity, H atoms not involved in hydrogen bonding have been omitted.

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

*Cg*3 and *Cg*4 are the centroids of benzene rings C10–C15 and C17–C22, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O5^{i}	0.82	2.56	3.236 (5)	140
C18—H18···*Cg*3	0.93	2.77	3.494 (5)	135
C3—H3···*Cg*3^{ii}	0.93	2.79	3.611 (5)	148
C11—H11···*Cg*4^{iii}	0.93	2.73	3.593 (4)	155
C23—H23*C*···*Cg*4^{iv}	0.96	3.00	3.872 (7)	152

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{18}O_5$
M_r	374.37
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, *b*, *c* (Å)	5.8882 (7), 16.418 (3), 18.894 (3)
β (°)	95.016 (5)
V (Å^3)	1819.5 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.25 × 0.22 × 0.16
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.976, 0.985
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9449, 2910, 1375
R_{int}	0.068
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.576
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.061, 0.197, 1.01
No. of reflections	2910
No. of parameters	257
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.23

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97 SHELXL97* and *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170535 [https://doi.org/10.1107/S2414314617005351]

8-Hydroxy-3,4-bis(4-methoxyphenyl)-1*H*-isochromen-1-one

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8-Hydroxy-3,4-bis(4-methoxyphenyl)-1*H*-isochromen-1-one

Crystal data

$C_{23}H_{18}O_5$
M_r = 374.37
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 5.8882 (7) Å
b = 16.418 (3) Å
c = 18.894 (3) Å
β = 95.016 (5)°
V = 1819.5 (5) Å^3
Z = 4
$F(000)$ = 784
D_x = 1.367 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1375 reflections
θ = 2.2–24.2°
μ = 0.10 mm^{-1}
T = 296 K
Block, colourless
0.25 × 0.22 × 0.16 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
T_{min} = 0.976, T_{max} = 0.985
9449 measured reflections
2910 independent reflections
1375 reflections with $I > 2\sigma(I)$
R_{int} = 0.068
θ_{max} = 24.2°, θ_{min} = 2.2°
h = −6→4
k = −15→18
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.197
S = 1.01
2910 reflections
257 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
$w = 1/[\sigma^2(F_o^2) + (0.0901P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.006 (2)

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. 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.4796 (7)	0.1453 (3)	0.6993 (2)	0.0573 (12)
C2	1.6348 (7)	0.0900 (3)	0.6765 (2)	0.0606 (12)
H2	1.7539	0.0716	0.7081	0.073*
C3	1.6147 (6)	0.0621 (3)	0.6080 (2)	0.0583 (12)
H3	1.7190	0.0243	0.5936	0.070*
C4	1.4399 (6)	0.0896 (2)	0.55963 (19)	0.0490 (11)
H4	1.4289	0.0704	0.5132	0.059*
C5	1.2825 (6)	0.1453 (2)	0.58020 (18)	0.0423 (10)
C6	1.1052 (6)	0.1788 (2)	0.52959 (18)	0.0420 (10)
C7	0.9648 (6)	0.2358 (3)	0.55146 (18)	0.0470 (10)
C8	1.1367 (7)	0.2303 (3)	0.6731 (2)	0.0594 (12)
C9	1.3006 (6)	0.1729 (2)	0.65103 (19)	0.0469 (10)
C10	1.0851 (5)	0.1492 (2)	0.45471 (18)	0.0433 (10)
C11	1.2498 (6)	0.1688 (2)	0.40897 (19)	0.0483 (11)
H11	1.3791	0.1975	0.4263	0.058*
C12	1.2242 (6)	0.1464 (3)	0.33848 (19)	0.0514 (11)
H12	1.3341	0.1612	0.3084	0.062*
C13	1.0352 (6)	0.1020 (3)	0.3123 (2)	0.0522 (11)
C14	0.8745 (6)	0.0802 (3)	0.3572 (2)	0.0586 (12)
H14	0.7480	0.0499	0.3401	0.070*
C15	0.9007 (6)	0.1033 (2)	0.4279 (2)	0.0527 (11)
H15	0.7918	0.0876	0.4580	0.063*
C16	0.8276 (8)	0.0444 (4)	0.2115 (2)	0.1003 (19)
H16A	0.8093	−0.0066	0.2352	0.150*
H16B	0.8410	0.0347	0.1619	0.150*
H16C	0.6973	0.0783	0.2168	0.150*
C17	0.7859 (6)	0.2841 (2)	0.5105 (2)	0.0508 (11)
C18	0.7925 (7)	0.3006 (3)	0.4386 (2)	0.0651 (13)
H18	0.9111	0.2796	0.4147	0.078*
C19	0.6284 (8)	0.3471 (3)	0.4019 (3)	0.0772 (14)
H19	0.6361	0.3570	0.3537	0.093*
C20	0.4544 (8)	0.3789 (3)	0.4359 (3)	0.0720 (14)
C21	0.4392 (6)	0.3655 (3)	0.5068 (3)	0.0709 (14)
H21	0.3202	0.3878	0.5297	0.085*
C22	0.6072 (7)	0.3173 (3)	0.5446 (2)	0.0628 (12)

H22	0.5985	0.3076	0.5927	0.075*
C23	0.1536 (9)	0.4761 (4)	0.4247 (4)	0.126 (2)
H23A	0.0418	0.4439	0.4461	0.189*
H23B	0.0787	0.5117	0.3898	0.189*
H23C	0.2381	0.5079	0.4607	0.189*
O1	0.9793 (4)	0.26094 (17)	0.62196 (13)	0.0592 (8)
O2	1.1211 (5)	0.2567 (2)	0.73262 (15)	0.0907 (12)
O3	1.5022 (7)	0.1731 (3)	0.76879 (19)	0.1251 (15)
H3A	1.6270	0.1594	0.7878	0.188*
O4	1.0245 (5)	0.08343 (19)	0.24135 (14)	0.0747 (10)
O5	0.2996 (6)	0.4257 (2)	0.3928 (2)	0.1062 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.067 (3)	0.066 (3)	0.038 (2)	−0.002 (2)	−0.003 (2)	−0.014 (2)
C2	0.063 (2)	0.066 (3)	0.050 (3)	0.007 (2)	−0.007 (2)	−0.001 (2)
C3	0.059 (2)	0.054 (3)	0.062 (3)	0.009 (2)	0.007 (2)	0.005 (2)
C4	0.055 (2)	0.052 (3)	0.040 (2)	−0.005 (2)	0.0045 (19)	0.000 (2)
C5	0.050 (2)	0.035 (3)	0.042 (2)	−0.006 (2)	0.0065 (18)	−0.0031 (19)
C6	0.044 (2)	0.044 (3)	0.039 (2)	−0.0020 (19)	0.0070 (17)	−0.0011 (19)
C7	0.051 (2)	0.052 (3)	0.038 (2)	−0.007 (2)	0.0047 (18)	−0.007 (2)
C8	0.066 (3)	0.061 (3)	0.051 (3)	0.000 (2)	0.004 (2)	−0.001 (2)
C9	0.052 (2)	0.049 (3)	0.040 (2)	0.001 (2)	0.0012 (18)	−0.0017 (19)
C10	0.042 (2)	0.046 (3)	0.042 (2)	−0.0021 (19)	0.0036 (17)	0.0012 (19)
C11	0.046 (2)	0.049 (3)	0.049 (2)	−0.0093 (19)	0.0027 (18)	0.001 (2)
C12	0.054 (2)	0.058 (3)	0.043 (2)	−0.007 (2)	0.0113 (18)	0.007 (2)
C13	0.054 (2)	0.059 (3)	0.043 (2)	0.000 (2)	−0.001 (2)	−0.004 (2)
C14	0.052 (2)	0.068 (3)	0.054 (3)	−0.017 (2)	−0.004 (2)	−0.008 (2)
C15	0.048 (2)	0.063 (3)	0.048 (3)	−0.011 (2)	0.0079 (18)	−0.001 (2)
C16	0.112 (4)	0.120 (5)	0.065 (3)	−0.021 (4)	−0.013 (3)	−0.026 (3)
C17	0.049 (2)	0.039 (3)	0.064 (3)	−0.005 (2)	0.002 (2)	−0.002 (2)
C18	0.060 (3)	0.067 (4)	0.067 (3)	0.000 (2)	−0.001 (2)	0.017 (3)
C19	0.071 (3)	0.076 (4)	0.082 (3)	−0.006 (3)	−0.007 (3)	0.011 (3)
C20	0.067 (3)	0.054 (3)	0.090 (4)	−0.005 (3)	−0.025 (3)	0.009 (3)
C21	0.046 (2)	0.058 (4)	0.107 (4)	−0.005 (2)	−0.006 (3)	−0.020 (3)
C22	0.066 (3)	0.054 (3)	0.068 (3)	−0.008 (2)	0.004 (2)	−0.005 (2)
C23	0.084 (4)	0.080 (5)	0.207 (7)	0.014 (4)	−0.026 (4)	−0.037 (5)
O1	0.0656 (17)	0.061 (2)	0.0511 (18)	0.0081 (15)	0.0062 (14)	−0.0058 (15)
O2	0.109 (2)	0.113 (3)	0.0491 (19)	0.037 (2)	0.0023 (17)	−0.0251 (19)
O3	0.136 (3)	0.156 (4)	0.079 (3)	0.016 (3)	−0.015 (2)	−0.019 (3)
O4	0.083 (2)	0.095 (3)	0.0435 (18)	−0.0101 (18)	−0.0063 (14)	−0.0165 (16)
O5	0.085 (2)	0.096 (3)	0.131 (3)	0.010 (2)	−0.028 (2)	0.003 (2)

Geometric parameters (Å, º)

C1—C2	1.383 (5)	C13—C14	1.372 (5)
C1—O3	1.386 (5)	C14—C15	1.384 (5)

C1—C9	1.407 (5)	C14—H14	0.9300
C2—C3	1.369 (5)	C15—H15	0.9300
C2—H2	0.9300	C16—O4	1.400 (5)
C3—C4	1.391 (5)	C16—H16A	0.9600
C3—H3	0.9300	C16—H16B	0.9600
C4—C5	1.382 (5)	C16—H16C	0.9600
C4—H4	0.9300	C17—C18	1.389 (5)
C5—C9	1.408 (5)	C17—C22	1.392 (5)
C5—C6	1.460 (5)	C18—C19	1.371 (6)
C6—C7	1.338 (5)	C18—H18	0.9300
C6—C10	1.491 (5)	C19—C20	1.359 (6)
C7—O1	1.390 (4)	C19—H19	0.9300
C7—C17	1.482 (5)	C20—C21	1.369 (6)
C8—O2	1.216 (4)	C20—O5	1.398 (5)
C8—O1	1.374 (4)	C21—C22	1.411 (6)
C8—C9	1.436 (6)	C21—H21	0.9300
C10—C15	1.381 (5)	C22—H22	0.9300
C10—C11	1.392 (5)	C23—O5	1.370 (6)
C11—C12	1.377 (5)	C23—H23A	0.9600
C11—H11	0.9300	C23—H23B	0.9600
C12—C13	1.385 (5)	C23—H23C	0.9600
C12—H12	0.9300	O3—H3A	0.8200
C13—O4	1.371 (4)		

C2—C1—O3	119.9 (4)	C13—C14—H14	120.0
C2—C1—C9	119.2 (4)	C15—C14—H14	120.0
O3—C1—C9	120.8 (4)	C10—C15—C14	121.4 (4)
C3—C2—C1	120.6 (4)	C10—C15—H15	119.3
C3—C2—H2	119.7	C14—C15—H15	119.3
C1—C2—H2	119.7	O4—C16—H16A	109.5
C2—C3—C4	120.7 (4)	O4—C16—H16B	109.5
C2—C3—H3	119.6	H16A—C16—H16B	109.5
C4—C3—H3	119.6	O4—C16—H16C	109.5
C5—C4—C3	120.4 (4)	H16A—C16—H16C	109.5
C5—C4—H4	119.8	H16B—C16—H16C	109.5
C3—C4—H4	119.8	C18—C17—C22	117.6 (4)
C4—C5—C9	118.9 (3)	C18—C17—C7	122.4 (4)
C4—C5—C6	121.6 (3)	C22—C17—C7	119.9 (4)
C9—C5—C6	119.5 (3)	C19—C18—C17	121.5 (4)
C7—C6—C5	119.1 (3)	C19—C18—H18	119.2
C7—C6—C10	121.4 (3)	C17—C18—H18	119.2
C5—C6—C10	119.5 (3)	C20—C19—C18	120.2 (5)
C6—C7—O1	121.1 (3)	C20—C19—H19	119.9
C6—C7—C17	130.0 (3)	C18—C19—H19	119.9
O1—C7—C17	108.9 (3)	C19—C20—C21	121.2 (4)
O2—C8—O1	114.8 (4)	C19—C20—O5	114.6 (5)
O2—C8—C9	127.5 (4)	C21—C20—O5	124.2 (5)
O1—C8—C9	117.7 (4)	C20—C21—C22	118.8 (4)

C1—C9—C5	120.1 (4)	C20—C21—H21	120.6
C1—C9—C8	120.5 (4)	C22—C21—H21	120.6
C5—C9—C8	119.3 (3)	C17—C22—C21	120.7 (4)
C15—C10—C11	117.8 (3)	C17—C22—H22	119.6
C15—C10—C6	121.4 (3)	C21—C22—H22	119.6
C11—C10—C6	120.8 (3)	O5—C23—H23A	109.5
C12—C11—C10	121.1 (3)	O5—C23—H23B	109.5
C12—C11—H11	119.5	H23A—C23—H23B	109.5
C10—C11—H11	119.5	O5—C23—H23C	109.5
C11—C12—C13	120.1 (3)	H23A—C23—H23C	109.5
C11—C12—H12	119.9	H23B—C23—H23C	109.5
C13—C12—H12	119.9	C8—O1—C7	123.1 (3)
O4—C13—C14	124.8 (3)	C1—O3—H3A	109.5
O4—C13—C12	115.6 (3)	C13—O4—C16	117.5 (3)
C14—C13—C12	119.5 (3)	C23—O5—C20	118.6 (5)
C13—C14—C15	120.0 (3)		

O3—C1—C2—C3	−179.9 (4)	C6—C10—C11—C12	−175.5 (4)
C9—C1—C2—C3	−0.2 (6)	C10—C11—C12—C13	−1.6 (6)
C1—C2—C3—C4	0.9 (6)	C11—C12—C13—O4	179.4 (4)
C2—C3—C4—C5	−0.4 (6)	C11—C12—C13—C14	−0.3 (6)
C3—C4—C5—C9	−0.8 (6)	O4—C13—C14—C15	−179.0 (4)
C3—C4—C5—C6	176.4 (3)	C12—C13—C14—C15	0.7 (6)
C4—C5—C6—C7	−176.4 (4)	C11—C10—C15—C14	−2.6 (6)
C9—C5—C6—C7	0.8 (5)	C6—C10—C15—C14	175.8 (4)
C4—C5—C6—C10	3.2 (5)	C13—C14—C15—C10	0.8 (6)
C9—C5—C6—C10	−179.6 (3)	C6—C7—C17—C18	−26.0 (6)
C5—C6—C7—O1	−2.8 (5)	O1—C7—C17—C18	151.4 (4)
C10—C6—C7—O1	177.6 (3)	C6—C7—C17—C22	156.4 (4)
C5—C6—C7—C17	174.4 (3)	O1—C7—C17—C22	−26.2 (5)
C10—C6—C7—C17	−5.3 (6)	C22—C17—C18—C19	−0.6 (6)
C2—C1—C9—C5	−1.0 (6)	C7—C17—C18—C19	−178.3 (4)
O3—C1—C9—C5	178.8 (4)	C17—C18—C19—C20	0.4 (7)
C2—C1—C9—C8	−180.0 (4)	C18—C19—C20—C21	0.2 (7)
O3—C1—C9—C8	−0.3 (6)	C18—C19—C20—O5	179.5 (4)
C4—C5—C9—C1	1.4 (6)	C19—C20—C21—C22	−0.5 (7)
C6—C5—C9—C1	−175.8 (3)	O5—C20—C21—C22	−179.7 (4)
C4—C5—C9—C8	−179.5 (4)	C18—C17—C22—C21	0.3 (6)
C6—C5—C9—C8	3.2 (5)	C7—C17—C22—C21	178.0 (4)
O2—C8—C9—C1	−5.2 (7)	C20—C21—C22—C17	0.2 (6)
O1—C8—C9—C1	173.9 (3)	O2—C8—O1—C7	−177.5 (4)
O2—C8—C9—C5	175.8 (4)	C9—C8—O1—C7	3.4 (5)
O1—C8—C9—C5	−5.2 (6)	C6—C7—O1—C8	0.7 (5)
C7—C6—C10—C15	−68.8 (5)	C17—C7—O1—C8	−177.0 (3)
C5—C6—C10—C15	111.6 (4)	C14—C13—O4—C16	4.8 (6)
C7—C6—C10—C11	109.6 (4)	C12—C13—O4—C16	−174.9 (4)
C5—C6—C10—C11	−70.0 (5)	C19—C20—O5—C23	−164.1 (5)
C15—C10—C11—C12	3.0 (6)	C21—C20—O5—C23	15.2 (7)

Hydrogen-bond geometry (Å, º)

Cg3 and Cg4 are the centroids of benzene rings C10–C15 and C17–C22, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*A*···O5^{i}	0.82	2.56	3.236 (5)	140
C18—H18···*Cg*3	0.93	2.77	3.494 (5)	135
C3—H3···*Cg*3^{ii}	0.93	2.79	3.611 (5)	148
C11—H11···*Cg*4^{iii}	0.93	2.73	3.593 (4)	155
C23—H23*C*···*Cg*4^{iv}	0.96	3.00	3.872 (7)	152

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