IUCrData

ISSN 2414-3146

9-Fluoro-2,4,4a,6-tetrahydrospiro[benzo[*c*]-chromene-3,2′-[1,3]dioxolane]

I. Ayswariya,[a] P. Rajalakshmi,[b] R.V. Krishnakumar[a] and N. Srinivasan[a]*

[a]Department of Physics, Thiagarajar College, Madurai 625 009, India, and [b]Department of Physics, M.G.R. College, Hosur 635 109, India. *Correspondence e-mail: vasan692000@yahoo.co.in

Received 3 January 2017
Accepted 10 January 2017

Edited by P. C. Healy, Griffith University, Australia

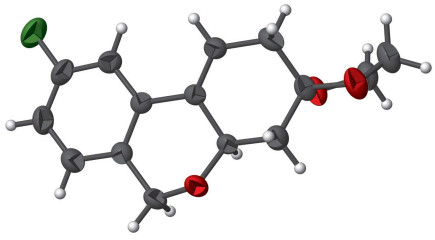
Keywords: crystal structure; 1,3-dioxolane derivative; spiro; isochromane; C—H···O hydrogen bonding; C—H···π interactions.

CCDC reference: 1444815

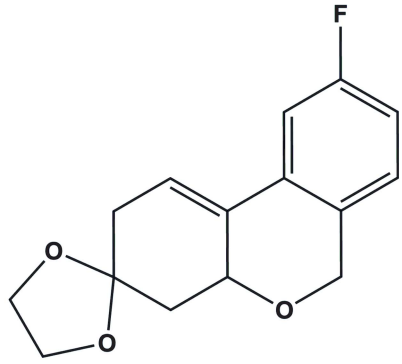
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{15}H_{15}FO_3$, the dihedral angle between the mean plane through all the non-H atoms of the dioxolane ring with those of the rest of the atoms of the chromene ring system, including the substituent F atom, is 81.1 (1)°. The pyran ring has an envelope conformation with the O atom as the flap. The cyclohexene ring has a half-chair conformation, while the dioxolane ring has a twisted conformation on an –O—CH_2– bond. In the crystal, molecules are linked *via* C—H···O hydrogen bonds, forming chains along [100]. The chains are linked by C—H···π interactions, involving the fluorobenzene ring, forming layers parallel to the *ac* plane.

3D view



Chemical scheme



Structure description

The title compound belongs to a novel class of spiro heterocycles consisting of a chromene ring system with a fused 4-fluorobenzene on one side and a spiro-fused 1,3-dioxolane ring on the other. Several dioxolane–indoline derivatives are known to be anticonvulsants (Rajopadhye & Popp, 1988) and the crystal structures of a few of them, closely related to the title compound, have been elucidated (De, 2008; Bjerrum *et al.*, 2009; Meng & Miao, 2010; Wang *et al.*, 2010). Chromene scaffolds are basic components of innumerable natural products which exhibit a variety of biological activities, in particular as anti-JH activity in the context of safe inspect-specific pesticides (Bowers *et al.*, 1976) and antiprotozoal agents (Harel *et al.*, 2013). In a recent study, several chromene derivatives were evaluated and shown to possess antiproliferative activity against cancer cells (Parthiban *et al.*, 2016). The importance of chromene as a promising pharmacophore with numerous activities such as anticancer, antimicrobial, antiviral, anti-inflammatory, antioxidant and antithrombotic was emphasized in a recent review on structurally diversified chromenes (Costa *et al.*, 2016). 1,3-Dioxolane is regarded as a green solvent as it produces stable carbon nanotube dispersions, which leave no residue

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

Cg is the centroid of the C7–C12 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15*B*···O3^{i}	0.97	2.52	3.448 (2)	161
C4—H4*A*···*Cg*^{ii}	0.97	2.99	3.933 (3)	164

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

on electrodes when it evaporates (Moscoso *et al.*, 2014). A survey of the Cambridge Structural Database (Groom *et al.*, 2016) shows that crystal structures incorporating spiro-fused dioxolane-chromene ring systems are scarce and, to the best of our knowledge, the title structure is the first of its kind. Details of its molecular and crystal structure are presented herein.

The molecular structure of the title compound is shown in Fig. 1. The dihedral angle between the mean plane through all non-H atoms of the dioxolane ring with those of the rest of the fused benzo[*c*]chromene unit, including atom F1, is 81.1 (1)°. The puckering parameters of the pyran ring (O3/C5–C7/C12/C13), *viz.* Q = 0.5012 (2) Å, θ = 129.8 (2)° and φ = 196.7 (3)°, describe a distorted envelope conformation. Those for the cyclohexene ring (C3/C4/C5/C13/C14/C15), *viz.* Q =

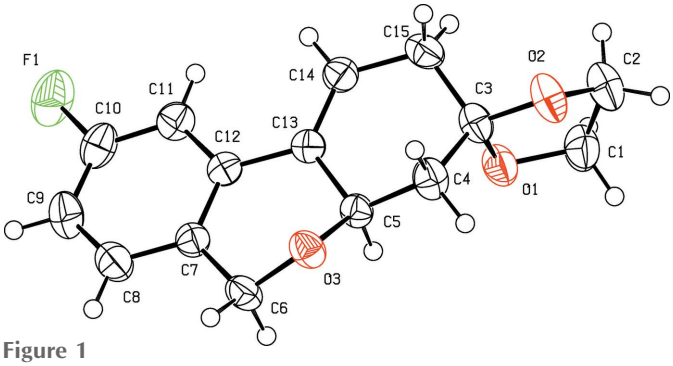


Figure 1
The molecular structure of the title compound, showing the atom-labelling scheme and 50% probability displacement ellipsoids.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{15}FO_3$
M_r	262.28
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	295
a, b, c (Å)	7.0373 (4), 20.7068 (14), 8.4725 (6)
β (°)	92.088 (3)
V (Å^3)	1233.79 (14)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.30 × 0.23 × 0.18
Data collection	
Diffractometer	Bruker SMART APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.978, 0.986
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23436, 2802, 1702
R_{int}	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.045, 0.121, 1.01
No. of reflections	2802
No. of parameters	173
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.20

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS2013/1* (Sheldrick, 2008), *SHELXL2013/1* (Sheldrick, 2015), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

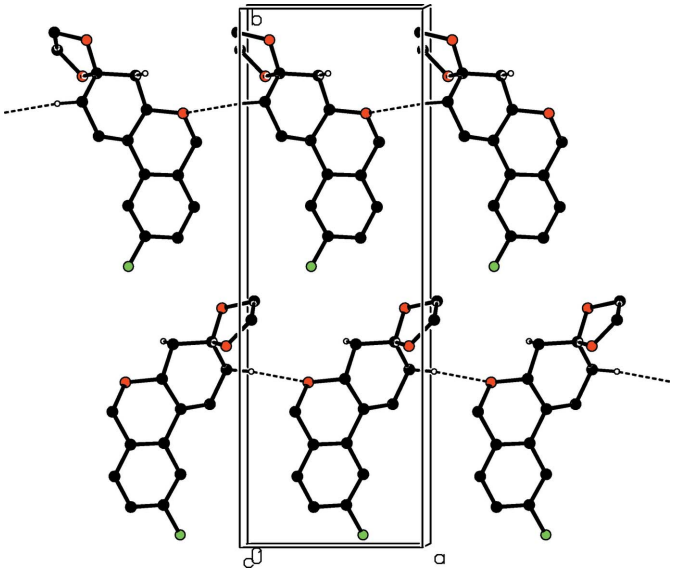


Figure 2
A partial view along the *c* axis of the crystal packing of the title compound, showing the hydrogen-bonded chains propagating along the *a* axis. Hydrogen bonds (see Table 1) are shown as dashed lines, and only H atoms H15*B* and H4*A* have been included.

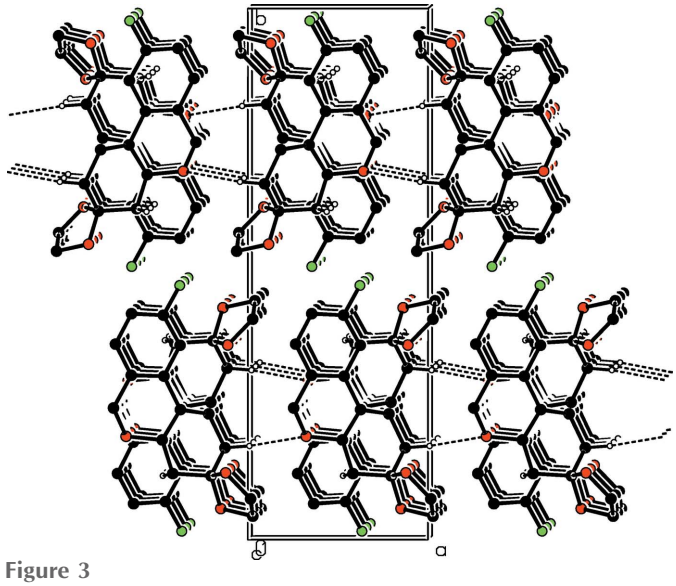


Figure 3
A view along the *c* axis of the crystal packing of the title compound. Hydrogen bonds (see Table 1) are shown as dashed lines, and only H atoms H15*B* and H4*A* have been included. The C—H···π interactions involve the fluorobenzene rings (see Table 1).

0.480 (2) Å, θ = 130.4 (2)° and φ = 212.8 (3)°, described a half-chair conformation. The dioxolane ring (C3/C2/C1/O1/O2) has a slightly twisted conformation about the C2—O2 bond, and is close to $^3T_4$ with puckering parameters of Q = 0.295 (2) Å and φ = 98.2 (2)°.

In the crystal, molecules are linked by C—H···O hydrogen bonds, involving the pyran O atom, O3, forming chains propagating along the *a*-axis direction (Table 1 and Fig. 2). The chains are linked by C—H···π interactions, forming layers parallel to the *ac* plane (Table 1 and Fig. 3).

Synthesis and crystallization

To a solution of 8-[5-fluoro-2-(hydroxymethyl)phenyl]-1,4-dioxaspiro[4,5]dec-8-en-7-ol (100 mmol) in dry THF (10 vol), cooled to 273 K, was added triphenylphosphane (15 mmol) and diisopropyl azodicarboxylate (120 mmol) under N_2. The reaction mixture was heated to 353 K for 6 h. The reaction mixture was quenched with ice and extracted with ethyl acetate, washed with saturated brine solution, dried over sodium sulfate and concentrated under vacuum. The crude product was purified by flash chromatography (silica gel, 50% EtOAc in hexanes), to give the title compound as colourless needle-like crystals on evaporation of the solvent.

Refinement

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

Acknowledgements

The authors thank the Sophisticated Analytical Instrumentation Centre (SAIF), Indian Institute of Technology (IIT), Chennai, for the X-ray intensity data collection and the School of Physics, Madurai Kamaraj University, Madurai, for access to the Cambridge Structural Database.

References

Bjerrum, J. V., Ulven, T. & Bond, A. D. (2009). *Acta Cryst.* E**65**, o579.
Bowers, W. S., Ohta, T., Cleere, J. S. & Marsella, P. A. (1976). *Science*, **193**, 542–547.
Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Costa, M., Dias, T., Brito, A. & Proença, F. (2016). *Eur. J. Med. Chem.* **123**, 487–507.
De, A. (2008). *Acta Cryst.* E**64**, o562.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Harel, D., Schepmann, D., Prinz, H., Brun, R., Schmidt, T. J. & Wünsch, B. (2013). *J. Med. Chem.* **56**, 7442–7448.
Meng, Y. & Miao, Y. (2010). *Acta Cryst.* E**66**, o1305.
Moscoso, R., Carbajo, J. & Squella, J. A. (2014). *Electrochem. Commun.* **48**, 69–72.
Parthiban, A., Kumaravel, M., Muthukumaran, J., Rukkumani, R., Krishna, R. & Rao, H. S. P. (2016). *Med. Chem. Res.* **25**, 1308–1315.
Rajopadhye, M. & Popp, F. D. (1988). *J. Med. Chem.* **31**, 1001–1005.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Wang, K., Yang, W., Wang, L.-L., Zhu, J. & Hu, Y. (2010). *Acta Cryst.* E**66**, o2431.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2017). **2**, x170045 [https://doi.org/10.1107/S2414314617000451]

9-Fluoro-2,4,4a,6-tetrahydrospiro[benzo[*c*]chromene-3,2′-[1,3]dioxolane]

I. Ayswariya, P. Rajalakshmi, R.V. Krishnakumar and N. Srinivasan

9-Fluoro-2,4,4a,6-tetrahydrospiro[benzo[*c*]chromene-3,2′-[1,3]dioxolane]

Crystal data

$C_{15}H_{15}FO_3$
M_r = 262.28
Monoclinic, $P2_1/c$
a = 7.0373 (4) Å
b = 20.7068 (14) Å
c = 8.4725 (6) Å
β = 92.088 (3)°
V = 1233.79 (14) Å^3
Z = 4
$F(000)$ = 552
D_x = 1.412 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2803 reflections
θ = 1.0–27.8°
μ = 0.11 mm^{-1}
T = 295 K
Needle, colourless
0.30 × 0.23 × 0.18 mm

Data collection

Bruker Smart APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.978, T_{max} = 0.986
23436 measured reflections
2802 independent reflections
1702 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 27.5°, θ_{min} = 2.6°
h = −9→8
k = −26→26
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.121
S = 1.01
2802 reflections
173 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
$w = 1/[\sigma^2(F_o^2) + (0.0413P)^2 + 0.5912P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: SHELXL-2013/1 (Sheldrick, 2015), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0044 (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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.63642 (19)	0.01685 (6)	0.13314 (18)	0.0690 (4)
O1	0.89547 (19)	0.36864 (7)	0.30809 (15)	0.0458 (4)
O2	0.86401 (19)	0.43734 (7)	0.10063 (17)	0.0507 (4)
O3	0.34019 (17)	0.30048 (6)	0.20342 (15)	0.0381 (3)
C1	1.0345 (3)	0.41731 (11)	0.3309 (3)	0.0524 (6)
H1A	1.1568	0.3985	0.3609	0.063*
H1B	0.9982	0.4472	0.4128	0.063*
C2	1.0432 (3)	0.45101 (12)	0.1753 (3)	0.0562 (6)
H2A	1.0608	0.4971	0.1895	0.067*
H2B	1.1461	0.4342	0.1141	0.067*
C3	0.8108 (3)	0.37529 (9)	0.1533 (2)	0.0376 (5)
C4	0.5986 (3)	0.37102 (9)	0.1610 (3)	0.0418 (5)
H4A	0.5413	0.3758	0.0558	0.050*
H4B	0.5525	0.4058	0.2262	0.050*
C5	0.5414 (2)	0.30716 (9)	0.2291 (2)	0.0314 (4)
H5	0.5707	0.3075	0.3430	0.038*
C6	0.2724 (3)	0.24662 (9)	0.2886 (2)	0.0388 (5)
H6A	0.1367	0.2421	0.2675	0.047*
H6B	0.2930	0.2543	0.4009	0.047*
C7	0.3699 (3)	0.18527 (9)	0.2448 (2)	0.0338 (4)
C8	0.2831 (3)	0.12635 (10)	0.2685 (3)	0.0472 (5)
H8	0.1625	0.1253	0.3098	0.057*
C9	0.3712 (3)	0.06928 (11)	0.2324 (3)	0.0523 (6)
H9	0.3129	0.0297	0.2496	0.063*
C10	0.5467 (3)	0.07270 (10)	0.1707 (3)	0.0463 (5)
C11	0.6385 (3)	0.12945 (10)	0.1444 (2)	0.0400 (5)
H11	0.7585	0.1295	0.1019	0.048*
C12	0.5501 (2)	0.18748 (9)	0.1821 (2)	0.0318 (4)
C13	0.6407 (2)	0.25062 (9)	0.1568 (2)	0.0307 (4)
C14	0.7963 (3)	0.25918 (10)	0.0756 (2)	0.0376 (5)
H14	0.8534	0.2229	0.0334	0.045*
C15	0.8856 (3)	0.32319 (10)	0.0475 (2)	0.0406 (5)
H15A	0.8617	0.3355	−0.0619	0.049*
H15B	1.0221	0.3196	0.0654	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0713 (9)	0.0369 (8)	0.0983 (11)	0.0132 (7)	−0.0042 (8)	−0.0096 (7)
O1	0.0481 (8)	0.0513 (9)	0.0376 (8)	−0.0185 (7)	−0.0033 (6)	0.0042 (6)
O2	0.0455 (8)	0.0425 (9)	0.0635 (10)	−0.0123 (7)	−0.0051 (7)	0.0165 (7)
O3	0.0275 (7)	0.0374 (8)	0.0496 (8)	0.0016 (6)	0.0034 (6)	0.0049 (6)
C1	0.0508 (13)	0.0471 (14)	0.0588 (14)	−0.0138 (11)	−0.0034 (11)	−0.0039 (11)
C2	0.0477 (13)	0.0528 (15)	0.0681 (15)	−0.0177 (11)	−0.0005 (11)	0.0059 (12)
C3	0.0361 (10)	0.0362 (11)	0.0402 (10)	−0.0058 (9)	−0.0024 (8)	0.0085 (8)

C4	0.0351 (11)	0.0343 (11)	0.0557 (12)	0.0009 (9)	−0.0008 (9)	0.0034 (9)
C5	0.0245 (9)	0.0331 (11)	0.0366 (9)	0.0003 (8)	0.0000 (7)	−0.0007 (8)
C6	0.0304 (10)	0.0408 (12)	0.0458 (11)	−0.0021 (9)	0.0083 (8)	0.0034 (9)
C7	0.0343 (10)	0.0346 (11)	0.0324 (9)	−0.0012 (8)	0.0006 (8)	0.0007 (8)
C8	0.0425 (12)	0.0452 (13)	0.0543 (13)	−0.0058 (10)	0.0085 (10)	0.0022 (10)
C9	0.0568 (14)	0.0353 (13)	0.0647 (15)	−0.0093 (11)	0.0015 (11)	0.0033 (11)
C10	0.0524 (13)	0.0312 (12)	0.0546 (13)	0.0082 (10)	−0.0070 (10)	−0.0052 (10)
C11	0.0369 (11)	0.0401 (12)	0.0430 (11)	0.0041 (9)	−0.0007 (9)	−0.0016 (9)
C12	0.0322 (10)	0.0341 (11)	0.0289 (9)	0.0023 (8)	−0.0020 (7)	0.0003 (8)
C13	0.0271 (9)	0.0350 (10)	0.0298 (9)	0.0012 (8)	−0.0022 (7)	0.0005 (7)
C14	0.0323 (10)	0.0401 (12)	0.0405 (11)	−0.0009 (8)	0.0028 (8)	−0.0050 (9)
C15	0.0325 (10)	0.0526 (13)	0.0370 (10)	−0.0059 (9)	0.0039 (8)	0.0031 (9)

Geometric parameters (Å, º)

F1—C10	1.361 (2)	C6—C7	1.497 (3)
O1—C1	1.413 (2)	C6—H6A	0.9700
O1—C3	1.427 (2)	C6—H6B	0.9700
O2—C3	1.415 (2)	C7—C8	1.382 (3)
O2—C2	1.419 (2)	C7—C12	1.393 (2)
O3—C6	1.420 (2)	C8—C9	1.374 (3)
O3—C5	1.431 (2)	C8—H8	0.9300
C1—C2	1.495 (3)	C9—C10	1.361 (3)
C1—H1A	0.9700	C9—H9	0.9300
C1—H1B	0.9700	C10—C11	1.363 (3)
C2—H2A	0.9700	C11—C12	1.395 (3)
C2—H2B	0.9700	C11—H11	0.9300
C3—C4	1.500 (3)	C12—C13	1.474 (3)
C3—C15	1.510 (3)	C13—C14	1.326 (2)
C4—C5	1.503 (3)	C14—C15	1.490 (3)
C4—H4A	0.9700	C14—H14	0.9300
C4—H4B	0.9700	C15—H15A	0.9700
C5—C13	1.505 (2)	C15—H15B	0.9700
C5—H5	0.9800		
C1—O1—C3	108.71 (15)	C7—C6—H6A	109.2
C3—O2—C2	106.36 (15)	O3—C6—H6B	109.2
C6—O3—C5	110.31 (14)	C7—C6—H6B	109.2
O1—C1—C2	105.23 (17)	H6A—C6—H6B	107.9
O1—C1—H1A	110.7	C8—C7—C12	119.84 (18)
C2—C1—H1A	110.7	C8—C7—C6	120.27 (17)
O1—C1—H1B	110.7	C12—C7—C6	119.88 (17)
C2—C1—H1B	110.7	C9—C8—C7	121.4 (2)
H1A—C1—H1B	108.8	C9—C8—H8	119.3
O2—C2—C1	103.62 (17)	C7—C8—H8	119.3
O2—C2—H2A	111.0	C10—C9—C8	117.7 (2)
C1—C2—H2A	111.0	C10—C9—H9	121.2
O2—C2—H2B	111.0	C8—C9—H9	121.2

C1—C2—H2B	111.0	C9—C10—F1	118.76 (19)
H2A—C2—H2B	109.0	C9—C10—C11	123.34 (19)
O2—C3—O1	105.74 (15)	F1—C10—C11	117.90 (19)
O2—C3—C4	110.03 (16)	C10—C11—C12	119.15 (19)
O1—C3—C4	109.72 (16)	C10—C11—H11	120.4
O2—C3—C15	111.08 (16)	C12—C11—H11	120.4
O1—C3—C15	109.50 (16)	C7—C12—C11	118.59 (17)
C4—C3—C15	110.65 (16)	C7—C12—C13	119.29 (16)
C3—C4—C5	110.45 (15)	C11—C12—C13	122.12 (16)
C3—C4—H4A	109.6	C14—C13—C12	124.32 (17)
C5—C4—H4A	109.6	C14—C13—C5	120.78 (17)
C3—C4—H4B	109.6	C12—C13—C5	114.90 (15)
C5—C4—H4B	109.6	C13—C14—C15	124.24 (18)
H4A—C4—H4B	108.1	C13—C14—H14	117.9
O3—C5—C4	107.68 (14)	C15—C14—H14	117.9
O3—C5—C13	109.54 (14)	C14—C15—C3	112.52 (16)
C4—C5—C13	113.16 (15)	C14—C15—H15A	109.1
O3—C5—H5	108.8	C3—C15—H15A	109.1
C4—C5—H5	108.8	C14—C15—H15B	109.1
C13—C5—H5	108.8	C3—C15—H15B	109.1
O3—C6—C7	112.04 (15)	H15A—C15—H15B	107.8
O3—C6—H6A	109.2		

C3—O1—C1—C2	−4.9 (2)	C8—C9—C10—C11	0.5 (3)
C3—O2—C2—C1	−32.3 (2)	C9—C10—C11—C12	0.0 (3)
O1—C1—C2—O2	22.7 (2)	F1—C10—C11—C12	−179.87 (17)
C2—O2—C3—O1	29.8 (2)	C8—C7—C12—C11	0.1 (3)
C2—O2—C3—C4	148.23 (18)	C6—C7—C12—C11	179.13 (16)
C2—O2—C3—C15	−88.89 (19)	C8—C7—C12—C13	179.76 (17)
C1—O1—C3—O2	−14.9 (2)	C6—C7—C12—C13	−1.2 (3)
C1—O1—C3—C4	−133.47 (17)	C10—C11—C12—C7	−0.3 (3)
C1—O1—C3—C15	104.90 (18)	C10—C11—C12—C13	−179.96 (18)
O2—C3—C4—C5	−175.51 (16)	C7—C12—C13—C14	−168.76 (18)
O1—C3—C4—C5	−59.6 (2)	C11—C12—C13—C14	10.9 (3)
C15—C3—C4—C5	61.4 (2)	C7—C12—C13—C5	10.4 (2)
C6—O3—C5—C4	−169.93 (15)	C11—C12—C13—C5	−169.99 (16)
C6—O3—C5—C13	66.62 (18)	O3—C5—C13—C14	137.18 (17)
C3—C4—C5—O3	−168.26 (15)	C4—C5—C13—C14	17.0 (2)
C3—C4—C5—C13	−47.0 (2)	O3—C5—C13—C12	−42.0 (2)
C5—O3—C6—C7	−57.3 (2)	C4—C5—C13—C12	−162.16 (15)
O3—C6—C7—C8	−156.86 (17)	C12—C13—C14—C15	178.77 (17)
O3—C6—C7—C12	24.1 (2)	C5—C13—C14—C15	−0.3 (3)
C12—C7—C8—C9	0.4 (3)	C13—C14—C15—C3	14.2 (3)
C6—C7—C8—C9	−178.6 (2)	O2—C3—C15—C14	−166.59 (15)
C7—C8—C9—C10	−0.7 (3)	O1—C3—C15—C14	76.99 (19)
C8—C9—C10—F1	−179.63 (19)	C4—C3—C15—C14	−44.1 (2)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C7–C12 benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15*B*···O3^{i}	0.97	2.52	3.448 (2)	161
C4—H4*A*···*Cg*^{ii}	0.97	2.99	3.933 (3)	164

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