

## Crystal structure of ethyl (6-hydroxy-1-benzofuran-3-yl)acetate sesquihydrate

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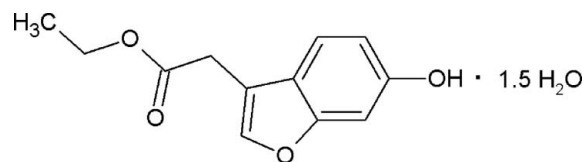
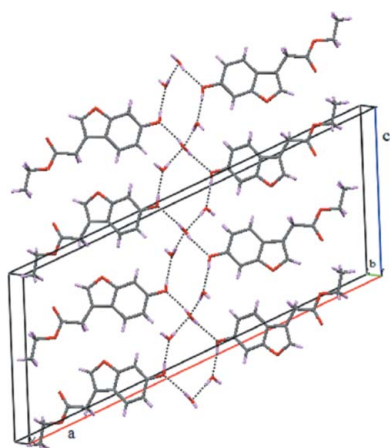
Edited by M. Gdaniec, Adam Mickiewicz University, Poland

**Keywords:** crystal structure; hydrates; O—H···O hydrogen bonds; C—H···π interactions; benzofuran**CCDC reference:** 1032887**Supporting information:** this article has supporting information at journals.iucr.org/e

In the title hydrate, C<sub>12</sub>H<sub>12</sub>O<sub>4</sub>·1.5H<sub>2</sub>O, one of the water molecules in the asymmetric unit is located on a twofold rotation axis. The molecule of the benzofuran derivative is essentially planar (r.m.s. deviation for the non-H atoms = 0.021 Å), with the ester group adopting a fully extended conformation. In the crystal, O—H···O hydrogen bonds between the water molecules and the hydroxy groups generate a centrosymmetric R<sub>6</sub><sup>6</sup>(12) ring motif. These R<sub>6</sub><sup>6</sup>(12) rings are fused, forming a one-dimensional motif extending along the *c*-axis direction.

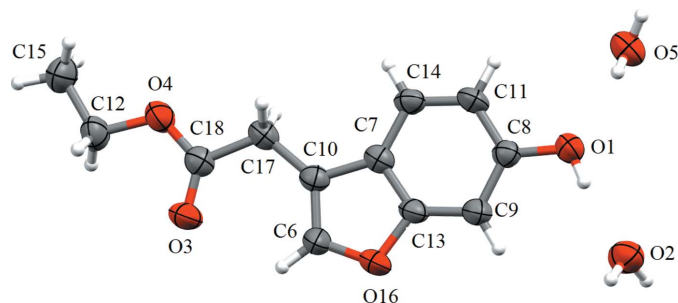
## 1. Chemical context

Furan heterocycles are of interest for synthetic chemists as they possess various pharmacological and biological activities including antituberculosis (Tawari *et al.*, 2010), anti-inflammatory (Shin *et al.*, 2011) and antibacterial (Kirilmis *et al.*, 2008) activity. Substituted benzofurans have found applications as fluorescent sensors (Oter *et al.*, 2007), anti-oxidants, brightening agents and drugs. Moreover, benzofuran carboxylic acid ethyl ester also exhibits selective cytotoxicity against a tumorigenic cell line (Hayakawa *et al.*, 2004). In view of the above facts, and as a continuation of our structural studies on benzofurans (Arunakumar, Krishnaswamy *et al.*, 2014; Arunakumar, Desai Nivedita *et al.*, 2014), the title compound has been synthesized, characterized by FT IR, <sup>1</sup>H NMR and LC-MS methods and its crystal structure determined.



## 2. Structural commentary

The title compound crystallizes as a 1.5-hydrate with one of the symmetry-independent water molecules occupying a special position of C<sub>2</sub> symmetry. The molecular structure of the title compound is shown in Fig. 1. The molecule is almost planar (r.m.s. deviation for the non-H atoms = 0.021 Å) and the ethyl acetate fragment adopts a fully extended conformation.



**Figure 1**  
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

### 3. Supramolecular features

Hydrogen bonds (Table 1) between two hydroxy groups and four water molecules generate a centrosymmetric  $R_6^6(12)$  ring motif. The rings are fused at the position of the O5 atoms, *i.e.* through water molecules located at special positions. In effect, two antiparallel chains of hydrogen bonds are formed that are fused at every fourth O atom and which propagate along the crystallographic *c*-axis (Fig. 2). In the crystal, the components are connected into a three-dimensional network through additional hydrogen bonds between the water molecule in a general position and the ester carbonyl group. In addition to strong hydrogen bonds, weaker C–H··· $\pi$  interactions are observed between the methylene group H atoms and the benzene and furan rings (Fig. 3 and Table 1).

### 4. Synthesis and crystallization

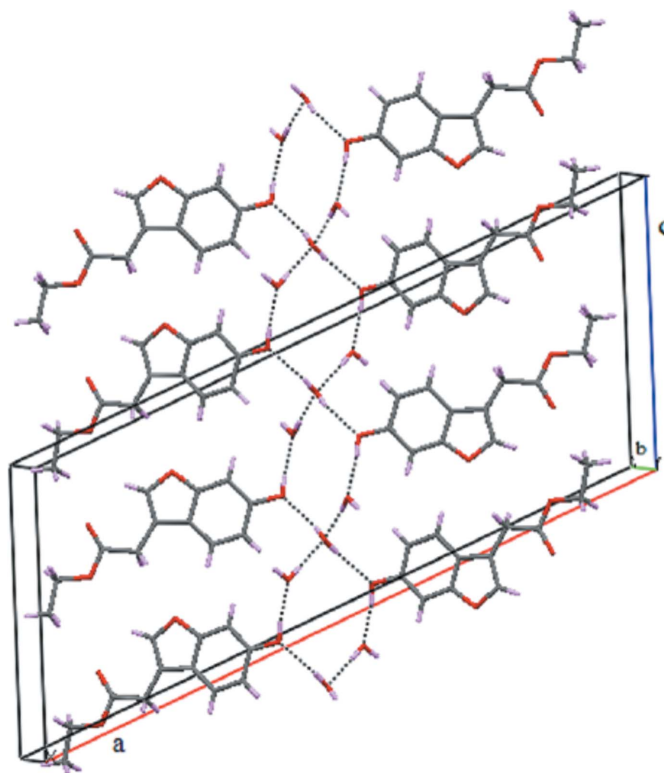
2-(6-Hydroxy-1-benzofuran-3-yl)acetic acid (2.0 g, 0.010 mmol) was taken in a round-bottomed flask containing ethanol (10 mL). Concentrated sulfuric acid (1 mL) was added and the reaction mixture was refluxed for 4 h at 353 K. After completion of the reaction, the reaction mixture was poured into ice-cold water and extracted to an ethyl acetate layer. The organic layer was washed with water followed by brine solution and dried over anhydrous sodium sulfate. The organic layer was concentrated under vacuum, giving a reddish residue. The residue was purified by column chromatography using silica gel (60–120 mesh) and ethyl acetate/petroleum ether (2:8) as eluent, affording a colourless

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

Cg1 is the centroid of the C7/C13/C9/C8/C11/C14 benzene ring and Cg2 is the centroid of the O16/C6/C10/C7/C13 furan 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>
O1–H1···O2	0.82	1.88	2.692 (4)	170
O2–H2A···O3 <sup>i</sup>	0.85	1.96	2.788 (4)	164
O2–H2B···O5 <sup>ii</sup>	0.85	2.00	2.844 (4)	174
O5–H5···O1 <sup>iii</sup>	0.85 (4)	2.09 (4)	2.870 (3)	152 (4)
C17–H17B···Cg1 <sup>iv</sup>	0.97	2.68	3.485 (3)	140
C17–H17A···Cg2 <sup>v</sup>	0.97	2.99	3.889 (3)	154

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

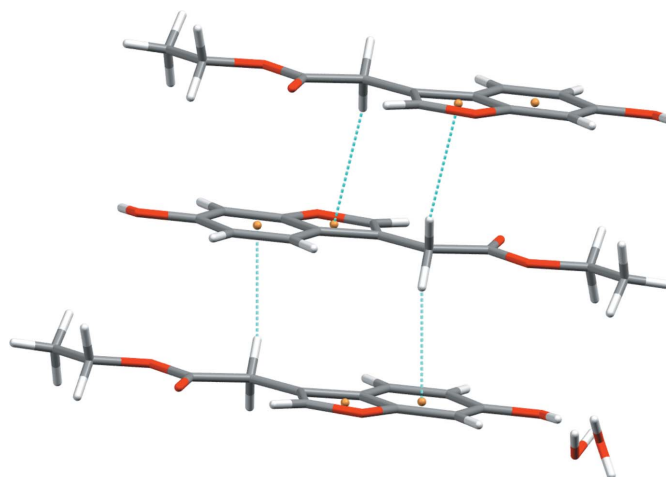


**Figure 2**  
Hydrogen-bonding interactions (dashed lines) featuring a fused  $R_6^6(12)$  ring motif.

crystalline product. Crystals suitable for X-ray analysis were formed by slow evaporation of the solution of the compound in ethyl acetate and petroleum ether (3:2) at room temperature. As the product had been water worked-up, water might have entered in the solid interstices during work-up.

### 5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H atoms of water molecules



**Figure 3**  
The C–H··· $\pi$  interactions (dashed lines) in the title compound.

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	2C <sub>12</sub> H <sub>12</sub> O <sub>4</sub> ·3H <sub>2</sub> O
<i>M</i> <sub>r</sub>	494.48
Crystal system, space group	Monoclinic, <i>C2/c</i>
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	29.191 (6), 7.3291 (17), 12.587 (3)
β (°)	113.074 (13)
<i>V</i> (Å <sup>3</sup> )	2477.4 (9)
<i>Z</i>	4
Radiation type	Cu Kα
μ (mm <sup>-1</sup> )	0.89
Crystal size (mm)	0.47 × 0.34 × 0.26
Data collection	
Diffractometer	Bruker APEXII
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2009)
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.730, 0.793
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	8441, 1968, 1132
<i>R</i> <sub>int</sub>	0.114
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.584
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.067, 0.224, 1.06
No. of reflections	1968
No. of parameters	168
No. of restraints	1
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	0.40, -0.54

Computer programs: *APEX2*, *SAINT-Plus* and *XPREP* (Bruker, 2009), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

were located from a difference Fourier map. The H atom bound to O5 was freely refined and those bound to O2 had the O—H distances restrained to 0.85 (2) Å. The remaining C/O-bound H atoms were fixed geometrically (C—H = 0.93–0.97

and O—H = 0.82 Å) and allowed to ride on their parent atoms with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C}, \text{O})$  for methyl and hydroxy H atoms, and  $1.2U_{\text{eq}}(\text{C})$  for other H atoms.

## Acknowledgements

The authors are thankful to the Department of Science and Technology, New Delhi, Government of India, for providing financial assistance under its DST FAST TRACK scheme [SR/FT/CS-81/2010 (G)]. The authors are thankful to the Institution of Excellence, Vijnana Bhavana, University of Mysore, Mysore, for providing the single-crystal X-ray diffraction facility.

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## supporting information

*Acta Cryst.* (2014). E70, 541-543 [doi:10.1107/S1600536814024349]

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### Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *APEX2* and *S SAINT-Plus* (Bruker, 2009); data reduction: *S SAINT-Plus* and *XPREP* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

### Ethyl (6-hydroxy-1-benzofuran-3-yl)acetate sesquihydrate

#### Crystal data

$2\text{C}_{12}\text{H}_{12}\text{O}_4 \cdot 3\text{H}_2\text{O}$

$M_r = 494.48$

Monoclinic, *C2/c*

Hall symbol: -C 2yc

$a = 29.191$  (6) Å

$b = 7.3291$  (17) Å

$c = 12.587$  (3) Å

$\beta = 113.074$  (13)°

$V = 2477.4$  (9) Å<sup>3</sup>

$Z = 4$

$F(000) = 1048$

prism

$D_x = 1.326$  Mg m<sup>-3</sup>

Melting point: 447 K

Cu  $K\alpha$  radiation,  $\lambda = 1.54178$  Å

Cell parameters from 125 reflections

$\theta = 6.3$ – $64.2$ °

$\mu = 0.89$  mm<sup>-1</sup>

$T = 296$  K

Prism, colourless

$0.47 \times 0.34 \times 0.26$  mm

#### Data collection

Bruker APEXII  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

phi and  $\varphi$  scans

Absorption correction: multi-scan  
(*SADABS*; Bruker, 2009)

$T_{\min} = 0.730$ ,  $T_{\max} = 0.793$

8441 measured reflections

1968 independent reflections

1132 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.114$

$\theta_{\max} = 64.2$ °,  $\theta_{\min} = 6.3$ °

$h = -31 \rightarrow 33$

$k = -8 \rightarrow 8$

$l = -13 \rightarrow 13$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.067$

$wR(F^2) = 0.224$

$S = 1.06$

1968 reflections

168 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 atoms treated by a mixture of independent  
and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.1328P)^2]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.40 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.54 \text{ e } \text{\AA}^{-3}$$

### Special details

**Experimental.** Thin-layer chromatography (TLC) was carried out on Merck pre-coated silica gel plates to monitor the progress of the reaction. The FT-IR spectra were recorded as KBr pellets using JASCO FT-IR-4100 spectrophotometer in the range 4000–400  $\text{cm}^{-1}$  at a resolution of 2  $\text{cm}^{-1}$ .  $^1\text{H}$  NMR spectra were recorded in  $\text{CDCl}_3$  and  $\text{DMSO-d}_6$  on a JEOL-400 MHz NMR instrument. Chemical shifts are reported in  $\delta$  values in parts per million relative to TMS. Mass spectral data were obtained on an Agilent LC-MS column C-18 instrument.

The IR spectrum of (I) exhibits strong bands at 1686  $\text{cm}^{-1}$  and 1193  $\text{cm}^{-1}$  due to C=O and C-O stretchings, respectively. A single band appearing at 3340  $\text{cm}^{-1}$  is due to OH group stretching. Appearance of bands in the range 3011–2907  $\text{cm}^{-1}$  is due to aromatic stretching and bands in the range 2970–2815  $\text{cm}^{-1}$  are due to C—H stretching, thus confirming the presence of the saturated hydrocarbons in (I).

The  $^1\text{H}$  NMR spectrum of (I) shows peaks at  $\delta$  9.53 (s, 1H, Ar-OH), 6.69 (s, 1H, furan-H), 7.35–7.33 (d, 1H, Ar-H), 6.88–6.87 (d, 1H, Ar-H), 6.75–6.72 (q, 1H, Ar-H), 4.12–4.07 (q, 2H,  $\text{OCH}_2$ ), 3.34 (s, 2H,  $\text{CH}_2$ ), 1.12–1.17 (t, 3H,  $\text{CH}_3$ ). The LC-MS spectrum shows the appearance of molecular ion peaks at  $m/z$  221 and 222 values, confirming the structure of the compound.

**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.** 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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O16	0.74036 (8)	0.9708 (4)	0.7193 (2)	0.0605 (10)
C7	0.71590 (10)	0.9610 (4)	0.5264 (3)	0.0378 (10)
C8	0.61898 (11)	0.8688 (4)	0.4921 (3)	0.0391 (11)
C9	0.65308 (11)	0.8957 (4)	0.6055 (3)	0.0448 (11)
H9	0.6444	0.8846	0.6689	0.054*
C10	0.76857 (11)	1.0071 (4)	0.5752 (3)	0.0389 (10)
C11	0.63322 (12)	0.8851 (4)	0.3998 (3)	0.0458 (11)
H11	0.6097	0.8646	0.3255	0.055*
C12	0.92468 (12)	1.1583 (5)	0.5340 (3)	0.0523 (12)
H12A	0.9449	1.0616	0.5824	0.063*
H12B	0.9307	1.2693	0.5793	0.063*
C13	0.70057 (11)	0.9401 (4)	0.6160 (3)	0.0405 (11)
C14	0.68085 (12)	0.9305 (4)	0.4142 (3)	0.0427 (11)
H14	0.6897	0.9409	0.3510	0.051*
C15	0.93746 (14)	1.1861 (6)	0.4312 (4)	0.0680 (15)
H15A	0.9289	1.0786	0.3839	0.102*
H15B	0.9725	1.2092	0.4564	0.102*
H15C	0.9191	1.2884	0.3873	0.102*
C17	0.79811 (11)	1.0380 (4)	0.5048 (3)	0.0420 (11)
H17A	0.7819	1.1334	0.4495	0.050*
H17B	0.7967	0.9275	0.4612	0.050*

C18	0.85173 (12)	1.0893 (4)	0.5659 (3)	0.0410 (11)
O1	0.57017 (8)	0.8246 (4)	0.4691 (2)	0.0512 (9)
H1	0.5667	0.8083	0.5301	0.077*
O2	0.54997 (10)	0.7984 (4)	0.6597 (2)	0.0639 (10)
H2A	0.5687	0.7310	0.7144	0.096*
H2B	0.5365	0.8790	0.6866	0.096*
O3	0.87331 (9)	1.1106 (3)	0.6691 (2)	0.0586 (9)
O4	0.87249 (9)	1.1095 (3)	0.4913 (2)	0.0523 (9)
O5	0.5000	0.9512 (5)	0.2500	0.0598 (13)
C6	0.77984 (12)	1.0112 (5)	0.6912 (3)	0.0526 (12)
H6	0.8114	1.0388	0.7458	0.063*
H5	0.4849 (19)	0.879 (5)	0.194 (3)	0.104 (18)*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O16	0.0473 (13)	0.0952 (19)	0.0313 (16)	-0.0166 (11)	0.0069 (14)	-0.0131 (13)
C7	0.0405 (15)	0.0324 (14)	0.036 (2)	0.0010 (10)	0.0098 (17)	0.0003 (14)
C8	0.0393 (15)	0.0418 (16)	0.035 (2)	0.0035 (10)	0.0137 (17)	0.0009 (15)
C9	0.0420 (16)	0.0557 (18)	0.034 (2)	0.0000 (12)	0.0121 (17)	-0.0065 (16)
C10	0.0428 (15)	0.0362 (15)	0.036 (2)	-0.0021 (10)	0.0130 (17)	-0.0033 (15)
C11	0.0424 (16)	0.0578 (19)	0.028 (2)	0.0010 (12)	0.0038 (18)	0.0009 (16)
C12	0.0406 (17)	0.060 (2)	0.054 (3)	-0.0104 (12)	0.0155 (19)	0.0029 (19)
C13	0.0419 (16)	0.0455 (16)	0.029 (2)	-0.0013 (12)	0.0082 (17)	-0.0069 (15)
C14	0.0474 (16)	0.0490 (17)	0.029 (2)	0.0053 (12)	0.0125 (17)	0.0032 (15)
C15	0.059 (2)	0.088 (3)	0.064 (3)	-0.0184 (18)	0.032 (2)	-0.005 (2)
C17	0.0401 (15)	0.0410 (16)	0.038 (2)	-0.0023 (11)	0.0077 (16)	-0.0006 (15)
C18	0.0442 (16)	0.0346 (15)	0.042 (2)	-0.0033 (11)	0.0148 (19)	0.0008 (15)
O1	0.0382 (11)	0.0702 (15)	0.0411 (15)	-0.0032 (9)	0.0112 (12)	0.0030 (14)
O2	0.0591 (15)	0.0818 (19)	0.0477 (17)	0.0184 (11)	0.0176 (14)	0.0097 (15)
O3	0.0555 (14)	0.0800 (17)	0.0344 (16)	-0.0188 (11)	0.0114 (14)	-0.0080 (13)
O4	0.0423 (12)	0.0624 (14)	0.0454 (16)	-0.0119 (9)	0.0100 (13)	0.0003 (12)
O5	0.0500 (18)	0.065 (2)	0.053 (3)	0.000	0.008 (2)	0.000
C6	0.0398 (17)	0.079 (2)	0.040 (2)	-0.0127 (14)	0.0166 (18)	-0.017 (2)

*Geometric parameters (Å, °)*

O16—C6	1.364 (5)	C12—H12A	0.9700
O16—C13	1.381 (3)	C12—H12B	0.9700
C7—C13	1.375 (5)	C14—H14	0.9300
C7—C14	1.399 (4)	C15—H15A	0.9600
C7—C10	1.454 (4)	C15—H15B	0.9600
C8—O1	1.377 (4)	C15—H15C	0.9600
C8—C11	1.385 (6)	C17—C18	1.496 (4)
C8—C9	1.397 (4)	C17—H17A	0.9700
C9—C13	1.379 (5)	C17—H17B	0.9700
C9—H9	0.9300	C18—O3	1.211 (4)
C10—C6	1.365 (6)	C18—O4	1.309 (5)

C10—C17	1.476 (5)	O1—H1	0.8200
C11—C14	1.371 (6)	O2—H2A	0.8499
C11—H11	0.9300	O2—H2B	0.8500
C12—O4	1.448 (4)	O5—H5	0.854 (19)
C12—C15	1.494 (6)	C6—H6	0.9300
C6—O16—C13	106.0 (3)	C11—C14—C7	118.4 (4)
C13—C7—C14	117.7 (3)	C11—C14—H14	120.8
C13—C7—C10	108.0 (3)	C7—C14—H14	120.8
C14—C7—C10	134.2 (4)	C12—C15—H15A	109.5
O1—C8—C11	118.1 (3)	C12—C15—H15B	109.5
O1—C8—C9	120.8 (4)	H15A—C15—H15B	109.5
C11—C8—C9	121.1 (3)	C12—C15—H15C	109.5
C13—C9—C8	114.7 (4)	H15A—C15—H15C	109.5
C13—C9—H9	122.6	H15B—C15—H15C	109.5
C8—C9—H9	122.6	C10—C17—C18	118.0 (3)
C6—C10—C7	103.2 (4)	C10—C17—H17A	107.8
C6—C10—C17	133.3 (3)	C18—C17—H17A	107.8
C7—C10—C17	123.5 (3)	C10—C17—H17B	107.8
C14—C11—C8	122.2 (3)	C18—C17—H17B	107.8
C14—C11—H11	118.9	H17A—C17—H17B	107.1
C8—C11—H11	118.9	O3—C18—O4	124.2 (3)
O4—C12—C15	107.3 (3)	O3—C18—C17	125.6 (4)
O4—C12—H12A	110.3	O4—C18—C17	110.2 (3)
C15—C12—H12A	110.3	C8—O1—H1	109.5
O4—C12—H12B	110.3	H2A—O2—H2B	109.5
C15—C12—H12B	110.3	C18—O4—C12	118.5 (3)
H12A—C12—H12B	108.5	O16—C6—C10	113.5 (3)
C7—C13—C9	125.9 (3)	O16—C6—H6	123.3
C7—C13—O16	109.3 (3)	C10—C6—H6	123.3
C9—C13—O16	124.9 (4)		
O1—C8—C9—C13	-179.7 (3)	C6—O16—C13—C9	-179.7 (3)
C11—C8—C9—C13	0.5 (4)	C8—C11—C14—C7	0.0 (4)
C13—C7—C10—C6	-0.6 (3)	C13—C7—C14—C11	1.2 (4)
C14—C7—C10—C6	-178.3 (3)	C10—C7—C14—C11	178.8 (3)
C13—C7—C10—C17	179.3 (3)	C6—C10—C17—C18	-1.7 (5)
C14—C7—C10—C17	1.6 (5)	C7—C10—C17—C18	178.5 (3)
O1—C8—C11—C14	179.3 (3)	C10—C17—C18—O3	-1.1 (5)
C9—C8—C11—C14	-0.9 (5)	C10—C17—C18—O4	179.3 (2)
C14—C7—C13—C9	-1.7 (5)	O3—C18—O4—C12	0.7 (5)
C10—C7—C13—C9	-179.9 (3)	C17—C18—O4—C12	-179.6 (2)
C14—C7—C13—O16	178.4 (2)	C15—C12—O4—C18	-175.7 (3)
C10—C7—C13—O16	0.2 (3)	C13—O16—C6—C10	-0.6 (4)
C8—C9—C13—C7	0.8 (4)	C7—C10—C6—O16	0.7 (4)
C8—C9—C13—O16	-179.3 (3)	C17—C10—C6—O16	-179.2 (3)
C6—O16—C13—C7	0.2 (3)		

*Hydrogen-bond geometry* ( $\text{\AA}$ ,  $^\circ$ )

Cg1 is the centroid of the C7/C13/C9/C8/C11/C14 benzene ring and Cg2 is the centroid of the O16/C6/C10/C7/C13 furan ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 $\cdots$ O2	0.82	1.88	2.692 (4)	170
O2—H2A $\cdots$ O3 <sup>i</sup>	0.85	1.96	2.788 (4)	164
O2—H2B $\cdots$ O5 <sup>ii</sup>	0.85	2.00	2.844 (4)	174
O5—H5 $\cdots$ O1 <sup>iii</sup>	0.85 (4)	2.09 (4)	2.870 (3)	152 (4)
C17—H17B $\cdots$ Cg1 <sup>iv</sup>	0.97	2.68	3.485 (3)	140
C17—H17A $\cdots$ Cg2 <sup>v</sup>	0.97	2.99	3.889 (3)	154

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