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Crystal structure of benzyl 2-naphthyl ether, a sensitiser for thermal paper

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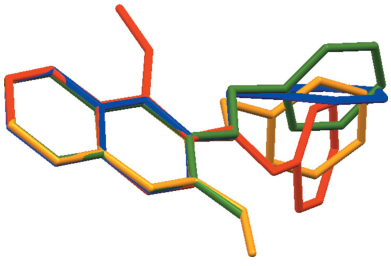
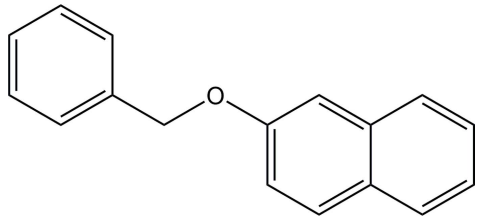
The title compound [systematic name: 2-(benzyloxy)naphthalene], $C_{17}H_{14}O$, which is used as a sensitiser for thermal paper, has a twisted conformation with a dihedral angle of 48.71 (12)° between the phenyl ring and the naphthyl ring system. In the crystal, one molecule interacts with six neighbouring molecules *via* intermolecular C—H···π interactions to form a herringbone molecular arrangement.

1. Chemical context

Thermal printing is a rapid and inexpensive printing technology widely used in commercial applications such as receipts, faxes and tickets (Gregory, 1991; Mendum *et al.*, 2011). Many structural reports are available for thermosensitive dyes and developers (Matsumoto *et al.*, 2010; Kodama *et al.*, 2013; Gontani *et al.*, 2017; Ohashi *et al.*, 2017). On the other hand, we found only one report on the crystal structure of a compound commonly used as a sensitiser for the thermosensitive layer (Rudolph *et al.*, 2010), which can facilitate the dye coloration process by lowering the melting point of the dye/developer composite on thermal paper (US EPA, 2014). The title compound, benzyl 2-naphthyl ether, **1**, is known as another commonly used sensitiser. Herein, we report the crystal structure of **1** as fundamental data for the investigation of its influence on the solid-state physicochemical properties of the thermosensitive layer of the thermal paper.





2. Structural commentary

The title compound (Fig. 1) is a simple ether compound in which a benzyl group is connected to a naphthyl group *via* an ether bond. The two aromatic rings are twisted, which is

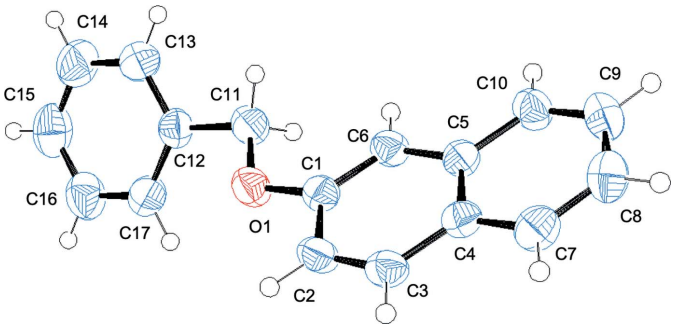


Figure 1
The molecular structure of the title compound, **1**, with displacement ellipsoids drawn at the 50% probability level.

mainly attributable to the rotation about the C11—C12 bond. The dihedral angle between the mean planes of the naphthyl ring system (C1–C10) and the phenyl ring (C12–C17) is 48.71 (12)°. The related torsion angles for this dihedral angle are −44.9 (3)° (O1—C11—C12—C17), 178.7 (2)° (C1—O1—C11—C12) and −5.6 (3)° (C6—C1—O1—C11).

3. Supramolecular features

In the crystal, one molecule interacts with six neighbouring molecules *via* intermolecular C—H···π interactions (Table 1; Fig. 2). The molecules are linked by a C—H···π interaction between the benzene C1–C6 rings (C3—H3···*Cg*1^{i}; symmetry code as in Table 1), forming a zigzag chain along the *a*-axis direction. The chains are connected into a layer structure parallel to the *ab* plane *via* a C—H···π interaction between the benzene C4/C5/C7–C10 ring and the methylene hydrogen atom (C11—H11*A*···*Cg*2^{ii}; Table 1). A weak C—H···π interaction between the C12–C17 phenyl rings (C16—H16···*Cg*3^{iii}; Table 1) links the layers and thus the molecules form a herringbone arrangement when viewed along the *a* axis, as shown in Fig. 3.

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C1–C6, C4/C5/C7–C10 and C12–C17 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···*Cg*1^{i}	0.93	2.71	3.439 (2)	135
C11—H11*A*···*Cg*2^{ii}	0.97	2.63	3.512 (3)	150
C16—H16···*Cg*3^{iii}	0.93	2.87	3.586 (3)	135

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

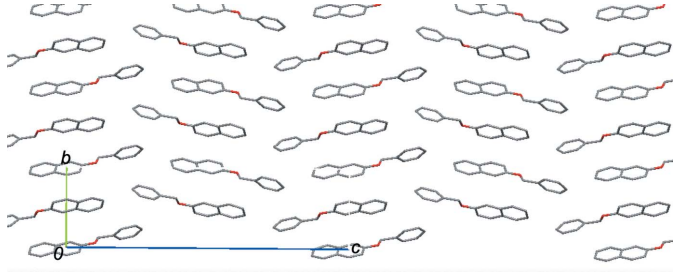


Figure 3
A packing diagram of the title compound, **1**, viewed along the *a* axis, showing a herringbone arrangement. H atoms have been omitted for clarity.

4. Database survey

Three analogous compounds of **1**, namely, 2-benzyloxy-1-naphthaldehyde, **2** [CSD (Groom *et al.*, 2016) refcode SOLVUL; Gao *et al.*, 2009], 2-benzyloxy-3-methoxynaphthalene, **3** (MEBYIC; Huang *et al.*, 2004) and 2-benzyloxy-3-hydroxynaphthalene, **4** (SICGEQ; Peters *et al.*, 1998), have been reported. Compounds, **2**, **3** and **4**, crystallize in the centrosymmetric space groups $P2_1/c$, $P2_1/c$ and $P\overline{1}$, respectively. Fig. 4 shows an overlay of the molecular geometries of compounds **1**–**4**, which indicates significant geometrical differences in the conformation of the benzyl unit caused by the rotations around the C1—O1 and C11—C12 bonds. Fig. 5

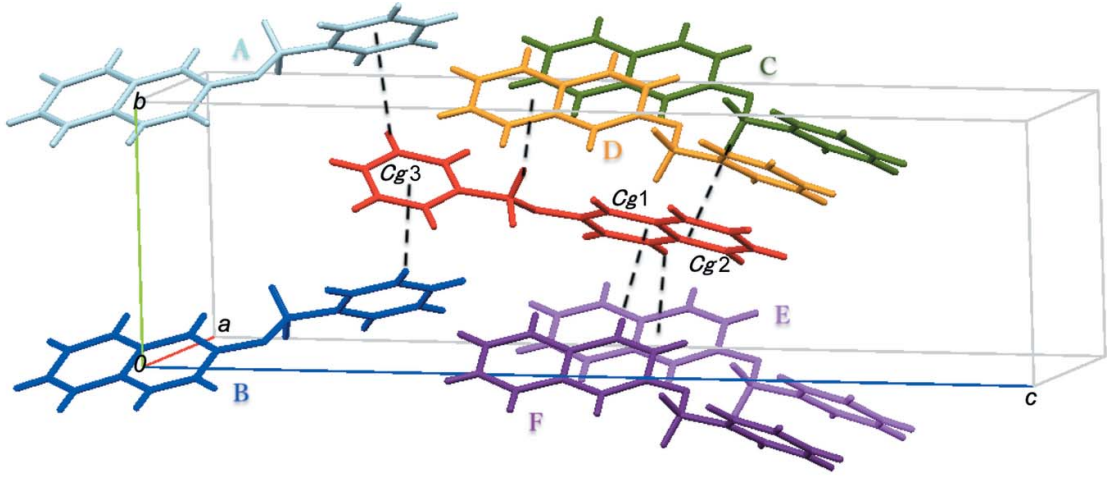


Figure 2
A packing diagram of the title compound, **1**, showing intermolecular C—H···π interactions (dashed lines). [Symmetry codes: (A) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (B) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (C) $x+\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (D) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (E) $x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (F) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$.]

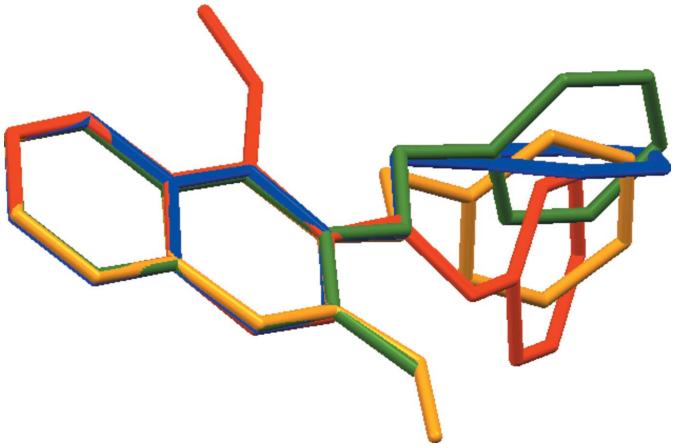


Figure 4
An overlay of the molecular conformation of four analogous benzyl-2-naphthyl ether derivatives, **1** (blue), **2** (red), **3** (yellow) and **4** (green). All H atoms have been omitted for clarity.

shows packing diagrams for compounds **2**–**4**. In the crystals of **2**–**4**, the molecules form zigzag chains *via* C—H···O interactions. In **2**, the chains are linked by π–π interactions into a three-dimensional network, whereas C—H···π interactions contribute to the arrangement of the chains in **3** and **4**.

5. Synthesis and crystallization

The title compound was purchased from Tokyo Kasei Kogyo Co., Ltd., and used without further purification. X-ray diffraction quality colourless platelets were obtained using a liquid–liquid diffusion method, with combination of chloroform and ethanol at 278 K.

6. Refinement

The crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were positioned geometrically (C—H = 0.93 Å) and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C).

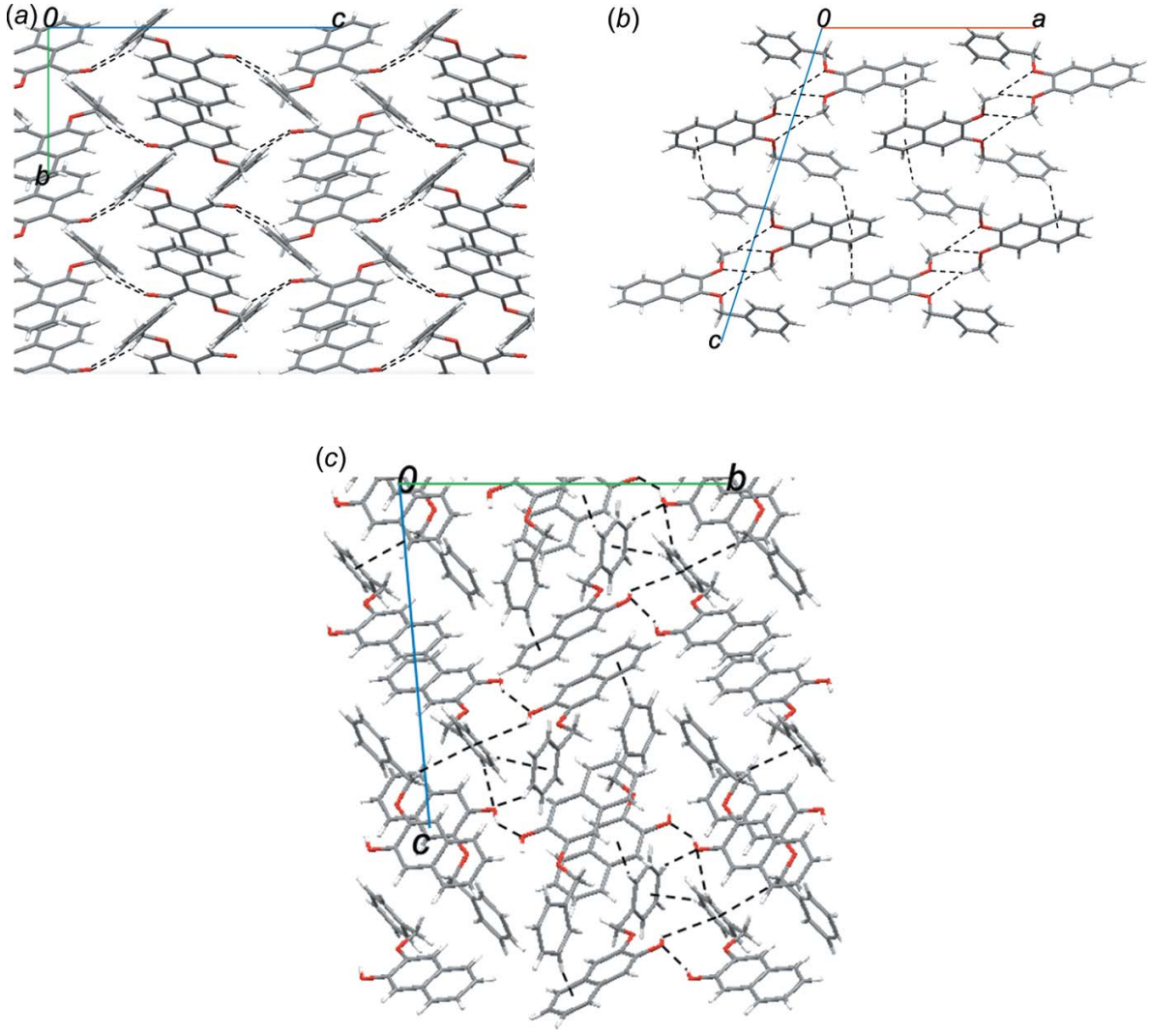


Figure 5
Packing diagrams of compounds **2** (*a*), **3** (*b*) and **4** (*c*). The dotted lines indicate intermolecular C—H···O and C—H···π interactions.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{14}O$
M_r	234.30
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	298
a, b, c (Å)	6.10537 (10), 7.58687 (13), 26.8196 (5)
V (Å^3)	1242.30 (4)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.59
Crystal size (mm)	0.61 × 0.42 × 0.04
Data collection	
Diffractometer	Rigaku XtaLAB PRO
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.396, 0.976
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	3724, 2017, 1841
R_{int}	0.033
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.107, 1.01
No. of reflections	2017
No. of parameters	163
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.12, −0.20
Absolute structure	Flack x determined using 601 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.3 (3)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *CrystalStructure* (Rigaku, 2018).

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supporting information

Acta Cryst. (2019). E**75**, 242-245 [https://doi.org/10.1107/S2056989019000690]

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2015); cell refinement: *CrysAlis PRO* (Rigaku OD, 2015); data reduction: *CrysAlis PRO* (Rigaku OD, 2015); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015*b*); molecular graphics: *CrystalStructure* (Rigaku, 2018); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2018).

2-(Benzyloxy)naphthalene

Crystal data

$C_{17}H_{14}O$
$M_r = 234.30$
Orthorhombic, $P2_12_12_1$
$a = 6.10537$ (10) Å
$b = 7.58687$ (13) Å
$c = 26.8196$ (5) Å
$V = 1242.30$ (4) Å^3
$Z = 4$
$F(000) = 496.00$
$D_x = 1.253$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 2523 reflections
$\theta = 6.1$–$71.1°$
$\mu = 0.59$ mm^{-1}
$T = 298$ K
Plate, colourless
0.61 × 0.42 × 0.04 mm

Data collection

Rigaku XtaLAB PRO diffractometer
Detector resolution: 5.811 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2015)
$T_{min} = 0.396$, $T_{max} = 0.976$
3724 measured reflections
2017 independent reflections
1841 reflections with $F^2 > 2.0\sigma(F^2)$
$R_{int} = 0.033$
$\theta_{max} = 66.4°$, $\theta_{min} = 3.3°$
$h = -3\rightarrow7$
$k = -9\rightarrow8$
$l = -31\rightarrow31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.107$
$S = 1.01$
2017 reflections
163 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
$w = 1/[\sigma^2(F_o^2) + (0.0559P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.12$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

Absolute structure: Flack *x* determined using 601 quotients [(I^+)-(I^-)]/[(I^+)+(I^-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.3 (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. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.5853 (3)	0.5557 (2)	0.39703 (5)	0.0492 (4)
C1	0.6358 (4)	0.5250 (3)	0.44606 (8)	0.0394 (5)
C5	0.5738 (4)	0.5198 (3)	0.53498 (7)	0.0380 (5)
C3	0.9115 (3)	0.4027 (3)	0.50010 (8)	0.0432 (5)
H3	1.0488	0.3518	0.5045	0.052*
C4	0.7789 (4)	0.4363 (3)	0.54226 (8)	0.0393 (5)
C12	0.3435 (4)	0.6519 (3)	0.33234 (8)	0.0446 (5)
C6	0.5058 (3)	0.5652 (3)	0.48601 (8)	0.0405 (5)
H6	0.3728	0.6223	0.4811	0.049*
C7	0.8415 (4)	0.3848 (3)	0.59097 (9)	0.0494 (6)
H7	0.9760	0.3300	0.5960	0.059*
C2	0.8426 (4)	0.4432 (3)	0.45349 (9)	0.0447 (5)
H2	0.9310	0.4173	0.4262	0.054*
C10	0.4399 (4)	0.5505 (3)	0.57705 (8)	0.0466 (5)
H10	0.3060	0.6072	0.5731	0.056*
C11	0.3713 (4)	0.6215 (4)	0.38720 (8)	0.0491 (6)
H11A	0.3492	0.7313	0.4051	0.059*
H11B	0.2628	0.5374	0.3987	0.059*
C8	0.7069 (5)	0.4148 (4)	0.63052 (9)	0.0561 (6)
H8	0.7496	0.3798	0.6623	0.067*
C9	0.5047 (5)	0.4980 (3)	0.62363 (9)	0.0547 (6)
H9	0.4136	0.5177	0.6509	0.066*
C13	0.1486 (4)	0.6077 (4)	0.30972 (9)	0.0572 (6)
H13	0.0402	0.5509	0.3280	0.069*
C17	0.5030 (5)	0.7337 (4)	0.30452 (9)	0.0557 (6)
H17	0.6365	0.7617	0.3192	0.067*
C16	0.4669 (6)	0.7750 (4)	0.25472 (10)	0.0650 (8)
H16	0.5752	0.8315	0.2363	0.078*
C14	0.1122 (5)	0.6472 (5)	0.25993 (10)	0.0721 (9)
H14	−0.0195	0.6162	0.2449	0.086*
C15	0.2717 (5)	0.7322 (4)	0.23289 (10)	0.0706 (9)
H15	0.2467	0.7607	0.1996	0.085*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0436 (8)	0.0647 (10)	0.0394 (8)	0.0042 (7)	0.0028 (7)	0.0050 (7)
C1	0.0388 (11)	0.0405 (11)	0.0387 (11)	−0.0026 (9)	0.0009 (9)	0.0015 (8)
C5	0.0394 (11)	0.0352 (10)	0.0393 (11)	−0.0026 (8)	0.0009 (9)	−0.0017 (9)
C3	0.0325 (9)	0.0461 (11)	0.0510 (13)	0.0024 (9)	0.0007 (11)	−0.0012 (10)
C4	0.0366 (10)	0.0367 (10)	0.0448 (11)	−0.0015 (9)	−0.0019 (10)	−0.0017 (9)
C12	0.0473 (12)	0.0465 (11)	0.0401 (11)	0.0038 (10)	−0.0003 (10)	−0.0054 (9)
C6	0.0342 (10)	0.0439 (11)	0.0435 (11)	0.0035 (8)	0.0025 (10)	0.0006 (9)
C7	0.0474 (12)	0.0489 (12)	0.0517 (13)	0.0047 (11)	−0.0082 (12)	0.0020 (10)
C2	0.0342 (10)	0.0509 (12)	0.0490 (12)	−0.0003 (9)	0.0086 (10)	−0.0012 (10)
C10	0.0438 (12)	0.0505 (12)	0.0454 (12)	0.0058 (10)	0.0058 (11)	−0.0035 (10)
C11	0.0433 (12)	0.0619 (14)	0.0423 (12)	0.0026 (11)	0.0017 (10)	0.0014 (10)
C8	0.0682 (16)	0.0590 (14)	0.0411 (12)	0.0024 (13)	−0.0041 (13)	0.0023 (11)
C9	0.0633 (15)	0.0595 (14)	0.0414 (12)	0.0015 (13)	0.0100 (12)	−0.0025 (11)
C13	0.0472 (12)	0.0702 (16)	0.0542 (14)	−0.0016 (12)	−0.0033 (12)	−0.0035 (12)
C17	0.0600 (14)	0.0602 (15)	0.0470 (13)	−0.0119 (12)	−0.0011 (13)	−0.0033 (11)
C16	0.085 (2)	0.0626 (16)	0.0473 (14)	−0.0058 (16)	0.0077 (15)	0.0040 (12)
C14	0.0624 (17)	0.099 (2)	0.0545 (16)	0.0074 (17)	−0.0178 (15)	−0.0066 (16)
C15	0.092 (2)	0.0753 (19)	0.0444 (13)	0.0178 (18)	−0.0101 (16)	0.0030 (13)

Geometric parameters (Å, º)

O1—C1	1.370 (2)	C2—H2	0.9300
O1—C11	1.423 (3)	C10—C9	1.370 (3)
C1—C6	1.368 (3)	C10—H10	0.9300
C1—C2	1.421 (3)	C11—H11A	0.9700
C5—C10	1.413 (3)	C11—H11B	0.9700
C5—C4	1.417 (3)	C8—C9	1.399 (4)
C5—C6	1.420 (3)	C8—H8	0.9300
C3—C2	1.354 (3)	C9—H9	0.9300
C3—C4	1.414 (3)	C13—C14	1.387 (4)
C3—H3	0.9300	C13—H13	0.9300
C4—C7	1.416 (3)	C17—C16	1.390 (4)
C12—C17	1.374 (3)	C17—H17	0.9300
C12—C13	1.377 (3)	C16—C15	1.367 (4)
C12—C11	1.499 (3)	C16—H16	0.9300
C6—H6	0.9300	C14—C15	1.375 (4)
C7—C8	1.361 (4)	C14—H14	0.9300
C7—H7	0.9300	C15—H15	0.9300
C1—O1—C11	116.36 (18)	O1—C11—C12	109.85 (19)
C6—C1—O1	125.7 (2)	O1—C11—H11A	109.7
C6—C1—C2	120.2 (2)	C12—C11—H11A	109.7
O1—C1—C2	114.1 (2)	O1—C11—H11B	109.7
C10—C5—C4	118.4 (2)	C12—C11—H11B	109.7
C10—C5—C6	122.0 (2)	H11A—C11—H11B	108.2

C4—C5—C6	119.61 (19)	C7—C8—C9	120.4 (2)
C2—C3—C4	121.3 (2)	C7—C8—H8	119.8
C2—C3—H3	119.4	C9—C8—H8	119.8
C4—C3—H3	119.4	C10—C9—C8	120.4 (2)
C3—C4—C7	122.2 (2)	C10—C9—H9	119.8
C3—C4—C5	118.47 (19)	C8—C9—H9	119.8
C7—C4—C5	119.3 (2)	C12—C13—C14	120.7 (3)
C17—C12—C13	118.9 (2)	C12—C13—H13	119.7
C17—C12—C11	121.5 (2)	C14—C13—H13	119.7
C13—C12—C11	119.5 (2)	C12—C17—C16	120.8 (3)
C1—C6—C5	120.1 (2)	C12—C17—H17	119.6
C1—C6—H6	120.0	C16—C17—H17	119.6
C5—C6—H6	120.0	C15—C16—C17	119.8 (3)
C8—C7—C4	120.6 (2)	C15—C16—H16	120.1
C8—C7—H7	119.7	C17—C16—H16	120.1
C4—C7—H7	119.7	C15—C14—C13	119.7 (3)
C3—C2—C1	120.3 (2)	C15—C14—H14	120.1
C3—C2—H2	119.8	C13—C14—H14	120.1
C1—C2—H2	119.8	C16—C15—C14	120.2 (3)
C9—C10—C5	120.9 (2)	C16—C15—H15	119.9
C9—C10—H10	119.5	C14—C15—H15	119.9
C5—C10—H10	119.5		

C11—O1—C1—C6	−5.6 (3)	C4—C5—C10—C9	−1.2 (3)
C11—O1—C1—C2	174.04 (19)	C6—C5—C10—C9	176.9 (2)
C2—C3—C4—C7	175.9 (2)	C1—O1—C11—C12	178.72 (19)
C2—C3—C4—C5	−2.3 (3)	C17—C12—C11—O1	−44.9 (3)
C10—C5—C4—C3	178.9 (2)	C13—C12—C11—O1	139.5 (2)
C6—C5—C4—C3	0.8 (3)	C4—C7—C8—C9	−0.3 (4)
C10—C5—C4—C7	0.8 (3)	C5—C10—C9—C8	0.9 (4)
C6—C5—C4—C7	−177.4 (2)	C7—C8—C9—C10	−0.1 (4)
O1—C1—C6—C5	177.4 (2)	C17—C12—C13—C14	−0.8 (4)
C2—C1—C6—C5	−2.2 (3)	C11—C12—C13—C14	174.9 (3)
C10—C5—C6—C1	−176.7 (2)	C13—C12—C17—C16	1.4 (4)
C4—C5—C6—C1	1.4 (3)	C11—C12—C17—C16	−174.2 (2)
C3—C4—C7—C8	−178.1 (2)	C12—C17—C16—C15	−0.7 (4)
C5—C4—C7—C8	0.0 (3)	C12—C13—C14—C15	−0.4 (4)
C4—C3—C2—C1	1.6 (3)	C17—C16—C15—C14	−0.6 (5)
C6—C1—C2—C3	0.7 (3)	C13—C14—C15—C16	1.2 (5)
O1—C1—C2—C3	−178.9 (2)		

Hydrogen-bond geometry (Å, º)

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C1–C6, C4/C5/C7–C10 and C12–C17 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···*Cg*1^{i}	0.93	2.71	3.439 (2)	135

C11—H11*A*···*Cg*2^{ii}	0.97	2.63	3.512 (3)	150
C16—H16···*Cg*3^{iii}	0.93	2.87	3.586 (3)	135

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