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Crystal structure of 7,8,9,10-tetrahydrobenzo[*b*]-naphtho[2,1-*d*]furan

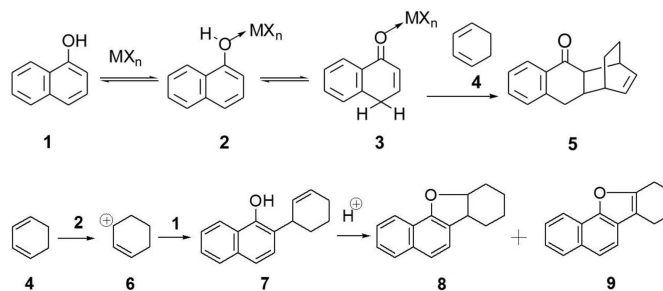
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In the title compound, C₁₆H₁₄O, the cyclohexene ring has a half-chair conformation. The mean plane, calculated through all non-H atoms of the molecule, except for the central CH₂ atoms of the cyclohexene ring, which deviate by 0.340 (3) and −0.369 (3) Å from this mean plane, has an r.m.s. deviation of 0.012 Å. In the crystal, there are C—H... π contacts present, resulting in the formation of zigzag chains propagating along the [010] direction.

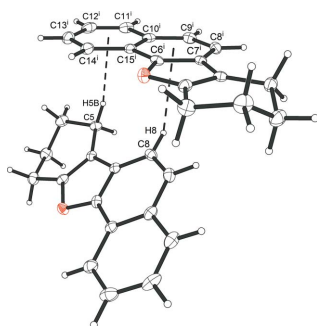
1. Chemical context

The interaction of Lewis acids with 1-naphthol **1** can be expected to induce metal coordination at the hydroxy function with concomitant increase in Brønsted-acidity (**2**) (Yamamoto & Futatsugi, 2005; Goering, 1995). It is conceivable that the proton, once released from this intermediate **2**, adds reversibly to the 4-position with formation of adduct **3**, which is the Lewis acid coordinated form of the keto-tautomer of **1**. Even if only minute amounts of **3** were to be formed, this intermediate should be a highly reactive dienophile in Diels–Alder reactions with such dienes as cyclohexadiene **4** leading to adduct **5** (see Scheme). Such a transformation implies de-aromatization of 1-naphthol **1**.



Alternatively, protonation of diene **4** leading to carbocation **6** would set the stage for Friedel–Crafts reaction with formation of the alkylation product **7**, which could continue to react acid catalyzed, leading to adduct **8** and possibly to the aromatized furan product **9**. In a previous study, Novák and coworkers reported the reaction of **1** with **4** in the presence of TsOH·H₂O in boiling toluene (26 h) or at room temperature (7 d), furan derivative **9** being formed in 58% yield, presumably *via* the intermediacy of **7** and **8** (Orovecz *et al.*, 2003; Novák *et al.*, 2000).

In exploratory experiments, we tested Et₂O·BF₃, FeCl₃, TiCl₄ and ZrCl₄ as Lewis acids in the reaction of **1** and **4** at room temperature in CH₂Cl₂. Essentially only products derived from formal Friedel–Crafts alkylation were identified



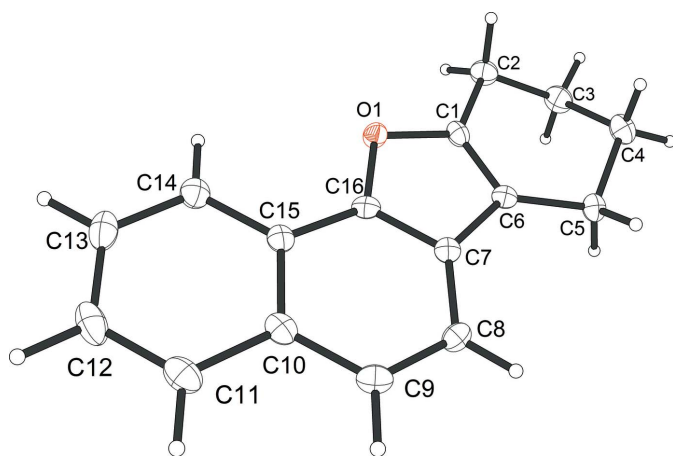


Figure 1
The molecular structure of compound **9**, showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

following column chromatographic separation. Small amounts of unidentified compounds which could not be separated were also formed. A general protocol is provided. If a 2.5-fold excess of cyclohexadiene **4** is used in these reactions, only small amounts of Friedel–Crafts products are formed (3–4%). Rather, acid-mediated oligomerization of diene **4** occurs.

In contrast to the acidic conditions employed by Novák and coworkers, using the present protocol we isolated compound **8** and characterized it for the first time. We report herein on the crystal structure of the final product, furan **9**.

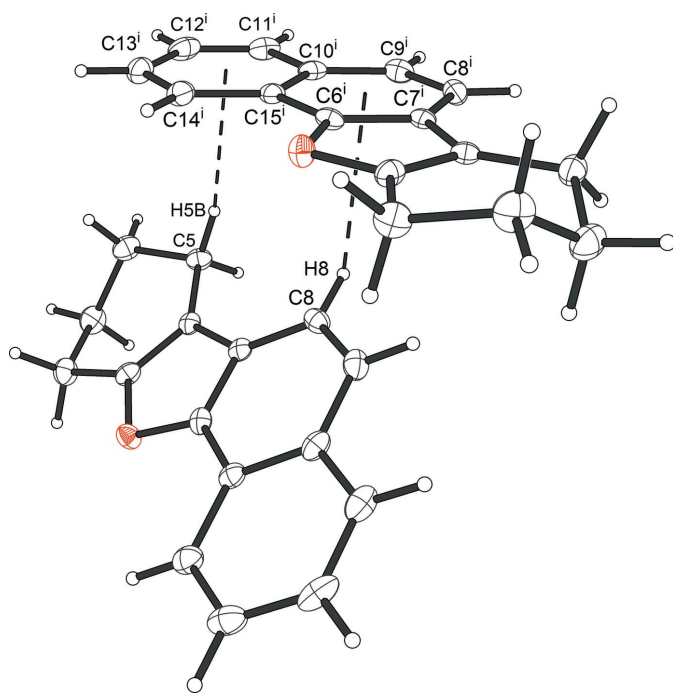


Figure 2
A view of the nearest C–H...ring centroid distances, shown as dashed lines [see Table 1; symmetry code: (i) $-x, -y + 2, z - \frac{1}{2}$].

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

$Cg3$ and $Cg4$ are the centroids of rings C7–C10/C15/C16 and C10–C15, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C5-H5B\cdots Cg4^i$	0.99	2.69	3.664 (3)	167
$C8-H8\cdots Cg3^i$	0.95	2.93	3.650 (3)	134

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

2. Structural commentary

In the title compound **9**, illustrated in Fig. 1, the cyclohexene ring (C1–C6) has a half-chair conformation. The mean plane, calculated through all non-hydrogen atoms of the molecule (O1/C1/C2/C5–C16), except atoms C3 and C4 of the cyclohexene ring that deviate by 0.340 (3) and -0.369 (3) Å from this mean plane, has an r.m.s. deviation of 0.012 Å. The other C and O atoms lie in this mean plane with a maximum deviation of -0.051 (3) Å for atom C2.

3. Supramolecular features

In the crystal of **9**, there are C–H... π contacts present (Table 1 and Fig. 2), but no classical hydrogen bonds and no π – π interactions present. Intermolecular contacts thus appear to be limited to van der Waals interactions. The two rather short intermolecular C–H...ring centroid distances are: H5B...centroid of ring (C10–C15) = 2.69 Å, H8...centroid of ring (C7–C10/C15/C16) = 2.93 Å. These interactions result in the formation of zigzag chains propagating along the b -axis direction.

4. Database survey

Only one structure of a tetrahydrobenzophenanthofuran (Refcode PEBDAD; Scully & Porco, 2012) is present in the current version 5.36 of the CSD (Groom & Allen, 2014), and the cyclohexene ring also has a half-chair conformation.

5. Synthesis and crystallization

General Procedure: To a mixture of 1-naphthol (6.48 g, 45 mmol), catalyst (2.25 mmol) in CH_2Cl_2 (10 ml), 1,3-cyclohexadiene (0.7 ml, 22.5 mmol) in CH_2Cl_2 (30 ml) was added drop wise, and the resulting solution was stirred at 273 K for 5 h. After completion of the reaction (TLC) at room temperature, a cold aqueous solution of $NaHCO_3$ (5%, 20 ml) was added and the mixture was extracted with CH_2Cl_2 (3×10 ml). The organic extracts were washed with water (2×10 mL) and dried over anhydrous Na_2SO_4 , and concentrated in vacuum. The crude product was purified by silica column chromatography (petroleum ether) to give the desired product, which was identified by NMR spectroscopic comparison with authentic samples of **1**, **2** and by X-ray diffraction analysis (Fig. 1).

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₆ H ₁₄ O
<i>M</i> _r	222.27
Crystal system, space group	Orthorhombic, <i>Pna</i> 2 ₁
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	13.8369 (9), 12.2202 (8), 6.8468 (4)
<i>V</i> (Å ³)	1157.72 (13)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.08
Crystal size (mm)	0.16 × 0.05 × 0.04
Data collection	
Diffractometer	Bruker D8 QUEST area detector
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2014)
<i>T</i> _{min} , <i>T</i> _{max}	0.94, 1.00
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	5983, 2024, 1808
<i>R</i> _{int}	0.038
(sin θ/λ) _{max} (Å ⁻¹)	0.601
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.038, 0.081, 1.09
No. of reflections	2024
No. of parameters	154
No. of restraints	1
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.16, -0.24

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b), *DIAMOND* (Brandenburg, 2006), *publCIF* (Westrip, 2010) and *PLATON* (Spek, 2009).

Compound **8**: ¹H NMR (300 MHz, CDCl₃, p.p.m.): δ 1.19–1.27 (*m*, 1H), 1.34–1.48 (*m*, 4H), 1.69–1.84 (*m*, 2H), 1.92–2.02 (*m*, 1H), 3.17–3.24 (*m*, 1H), 4.71–4.77 (*m*, 1H), 7.16–7.18 (*m*, 1H), 7.24–7.32 (*m*, 3H), 7.66–7.69 (*m*, 1H), 7.87–7.90 (*m*, 1H); ¹³C NMR (300 MHz, CDCl₃, p.p.m.): δ 20.50, 21.86, 27.64,

28.38, 41.41, 83.44, 120.16, 121.16, 121.60, 121.92, 125.13, 125.48, 126.55, 128.01, 134.11, 155.07.

High Resolution Mass Spectrum: (*M* + H⁺) calculated for C₁₆H₁₆O 225.1274; found (*M* + H⁺) 225.1275.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were located in difference Fourier maps, but subsequently included in the refinement using a riding model: C–H = 0.95–0.99 Å with *U*_{iso}(H) = 1.2*U*_{eq}(C).

Acknowledgements

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Crystal structure of 7,8,9,10-tetrahydrobenzo[*b*]naphtho[2,1-*d*]furan

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Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010) and *PLATON* (Spek, 2009).

7,8,9,10-Tetrahydrobenzo[*b*]naphtho[2,1-*d*]furan

Crystal data

$C_{16}H_{14}O$

$M_r = 222.27$

Orthorhombic, *Pna*2₁

$a = 13.8369$ (9) Å

$b = 12.2202$ (8) Å

$c = 6.8468$ (4) Å

$V = 1157.72$ (13) Å³

$Z = 4$

$F(000) = 472$

$D_x = 1.275$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2867 reflections

$\theta = 2.2$ – 25.2°

$\mu = 0.08$ mm⁻¹

$T = 100$ K

Prism, colourless

$0.16 \times 0.05 \times 0.04$ mm

Data collection

Bruker D8 QUEST area-detector
diffractometer

Radiation source: microfocus sealed X-ray tube

Detector resolution: 7.9 pixels mm⁻¹

ω and ϕ scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2014)

$T_{\min} = 0.94$, $T_{\max} = 1.00$

5983 measured reflections

2024 independent reflections

1808 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.038$

$\theta_{\max} = 25.3^\circ$, $\theta_{\min} = 2.2^\circ$

$h = -16 \rightarrow 16$

$k = -14 \rightarrow 14$

$l = -8 \rightarrow 8$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.038$

$wR(F^2) = 0.081$

$S = 1.09$

2024 reflections

154 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-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 0.0066P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.16$ e Å⁻³

$\Delta\rho_{\min} = -0.24$ e Å⁻³

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.03747 (16)	0.7566 (2)	0.3738 (4)	0.0159 (5)
O1	0.09729 (11)	0.83253 (13)	0.4640 (2)	0.0165 (4)
C2	0.00207 (19)	0.6599 (2)	0.4844 (4)	0.0207 (6)
H2A	-0.0492	0.6822	0.5770	0.025*
H2B	0.0557	0.6267	0.5596	0.025*
C3	-0.03802 (19)	0.5773 (2)	0.3369 (4)	0.0237 (6)
H3A	-0.0767	0.5215	0.4070	0.028*
H3B	0.0164	0.5395	0.2716	0.028*
C4	-0.10145 (19)	0.6329 (2)	0.1823 (4)	0.0232 (6)
H4A	-0.1300	0.5763	0.0964	0.028*
H4B	-0.1551	0.6719	0.2480	0.028*
C5	-0.04412 (18)	0.7140 (2)	0.0581 (4)	0.0179 (6)
H5A	-0.0036	0.6738	-0.0369	0.021*
H5B	-0.0891	0.7616	-0.0156	0.021*
C6	0.01857 (16)	0.78260 (19)	0.1870 (4)	0.0138 (5)
C7	0.06900 (16)	0.8841 (2)	0.1498 (3)	0.0137 (5)
C8	0.07806 (17)	0.9549 (2)	-0.0120 (4)	0.0165 (6)
H8	0.0475	0.9381	-0.1326	0.020*
C9	0.13190 (18)	1.0484 (2)	0.0084 (4)	0.0187 (6)
H9	0.1371	1.0973	-0.0991	0.022*
C10	0.18051 (17)	1.07448 (19)	0.1866 (4)	0.0171 (6)
C11	0.23745 (18)	1.1700 (2)	0.2054 (4)	0.0215 (6)
H11	0.2441	1.2179	0.0969	0.026*
C12	0.28309 (18)	1.1947 (2)	0.3768 (4)	0.0243 (7)
H12	0.3209	1.2593	0.3862	0.029*
C13	0.27444 (18)	1.1254 (2)	0.5383 (4)	0.0234 (6)
H13	0.3060	1.1438	0.6571	0.028*
C14	0.22067 (17)	1.0308 (2)	0.5271 (4)	0.0191 (6)
H14	0.2157	0.9837	0.6371	0.023*
C15	0.17295 (17)	1.0040 (2)	0.3507 (4)	0.0151 (5)
C16	0.11541 (17)	0.9100 (2)	0.3225 (3)	0.0141 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0135 (11)	0.0131 (13)	0.0211 (13)	-0.0013 (10)	0.0009 (11)	-0.0021 (11)
O1	0.0202 (8)	0.0147 (9)	0.0144 (8)	-0.0019 (8)	-0.0021 (7)	0.0019 (7)
C2	0.0232 (13)	0.0180 (14)	0.0210 (14)	-0.0019 (11)	0.0019 (12)	0.0042 (12)
C3	0.0263 (14)	0.0171 (14)	0.0277 (14)	-0.0048 (12)	0.0018 (13)	0.0035 (12)

C4	0.0197 (13)	0.0213 (15)	0.0286 (15)	-0.0056 (12)	-0.0006 (12)	-0.0007 (13)
C5	0.0164 (12)	0.0169 (14)	0.0203 (13)	-0.0010 (11)	-0.0023 (11)	-0.0023 (12)
C6	0.0126 (11)	0.0128 (13)	0.0159 (12)	0.0037 (10)	0.0024 (10)	-0.0007 (11)
C7	0.0119 (12)	0.0132 (13)	0.0158 (12)	0.0041 (10)	0.0022 (11)	-0.0027 (11)
C8	0.0185 (12)	0.0172 (14)	0.0140 (12)	0.0036 (11)	-0.0010 (11)	-0.0012 (11)
C9	0.0200 (12)	0.0174 (13)	0.0186 (13)	0.0036 (11)	0.0040 (11)	0.0030 (12)
C10	0.0127 (11)	0.0153 (13)	0.0233 (14)	0.0024 (10)	0.0046 (11)	-0.0019 (12)
C11	0.0168 (13)	0.0174 (15)	0.0303 (15)	0.0005 (11)	0.0056 (13)	0.0015 (13)
C12	0.0140 (12)	0.0199 (15)	0.0391 (17)	-0.0041 (11)	0.0037 (13)	-0.0069 (14)
C13	0.0167 (12)	0.0257 (16)	0.0278 (15)	-0.0006 (12)	-0.0023 (12)	-0.0106 (14)
C14	0.0149 (12)	0.0209 (14)	0.0216 (13)	0.0012 (11)	0.0002 (11)	-0.0020 (13)
C15	0.0115 (11)	0.0159 (13)	0.0180 (12)	0.0020 (10)	0.0021 (10)	-0.0026 (11)
C16	0.0155 (12)	0.0117 (13)	0.0152 (13)	0.0035 (10)	0.0039 (11)	0.0003 (11)

Geometric parameters (Å, °)

C1—C6	1.343 (3)	C7—C16	1.383 (3)
C1—O1	1.388 (3)	C7—C8	1.411 (3)
C1—C2	1.486 (3)	C8—C9	1.371 (3)
O1—C16	1.377 (3)	C8—H8	0.9500
C2—C3	1.532 (4)	C9—C10	1.429 (4)
C2—H2A	0.9900	C9—H9	0.9500
C2—H2B	0.9900	C10—C11	1.414 (4)
C3—C4	1.534 (4)	C10—C15	1.419 (3)
C3—H3A	0.9900	C11—C12	1.366 (4)
C3—H3B	0.9900	C11—H11	0.9500
C4—C5	1.528 (4)	C12—C13	1.398 (4)
C4—H4A	0.9900	C12—H12	0.9500
C4—H4B	0.9900	C13—C14	1.377 (3)
C5—C6	1.494 (3)	C13—H13	0.9500
C5—H5A	0.9900	C14—C15	1.415 (4)
C5—H5B	0.9900	C14—H14	0.9500
C6—C7	1.446 (3)	C15—C16	1.411 (3)
C6—C1—O1	112.4 (2)	C16—C7—C8	119.4 (2)
C6—C1—C2	127.5 (2)	C16—C7—C6	105.6 (2)
O1—C1—C2	120.1 (2)	C8—C7—C6	135.0 (2)
C16—O1—C1	104.80 (18)	C9—C8—C7	118.6 (2)
C1—C2—C3	107.9 (2)	C9—C8—H8	120.7
C1—C2—H2A	110.1	C7—C8—H8	120.7
C3—C2—H2A	110.1	C8—C9—C10	121.9 (2)
C1—C2—H2B	110.1	C8—C9—H9	119.1
C3—C2—H2B	110.1	C10—C9—H9	119.1
H2A—C2—H2B	108.4	C11—C10—C15	118.0 (2)
C2—C3—C4	111.7 (2)	C11—C10—C9	121.6 (2)
C2—C3—H3A	109.3	C15—C10—C9	120.4 (2)
C4—C3—H3A	109.3	C12—C11—C10	121.2 (3)
C2—C3—H3B	109.3	C12—C11—H11	119.4

C4—C3—H3B	109.3	C10—C11—H11	119.4
H3A—C3—H3B	107.9	C11—C12—C13	120.4 (2)
C5—C4—C3	112.0 (2)	C11—C12—H12	119.8
C5—C4—H4A	109.2	C13—C12—H12	119.8
C3—C4—H4A	109.2	C14—C13—C12	120.7 (3)
C5—C4—H4B	109.2	C14—C13—H13	119.6
C3—C4—H4B	109.2	C12—C13—H13	119.6
H4A—C4—H4B	107.9	C13—C14—C15	119.6 (2)
C6—C5—C4	109.7 (2)	C13—C14—H14	120.2
C6—C5—H5A	109.7	C15—C14—H14	120.2
C4—C5—H5A	109.7	C16—C15—C14	124.6 (2)
C6—C5—H5B	109.7	C16—C15—C10	115.3 (2)
C4—C5—H5B	109.7	C14—C15—C10	120.1 (2)
H5A—C5—H5B	108.2	O1—C16—C7	111.1 (2)
C1—C6—C7	106.1 (2)	O1—C16—C15	124.5 (2)
C1—C6—C5	122.8 (2)	C7—C16—C15	124.4 (2)
C7—C6—C5	131.1 (2)		
C6—C1—O1—C16	0.3 (2)	C15—C10—C11—C12	-0.7 (4)
C2—C1—O1—C16	-179.7 (2)	C9—C10—C11—C12	179.5 (2)
C6—C1—C2—C3	15.0 (3)	C10—C11—C12—C13	0.1 (4)
O1—C1—C2—C3	-165.0 (2)	C11—C12—C13—C14	0.6 (4)
C1—C2—C3—C4	-44.6 (3)	C12—C13—C14—C15	-0.6 (4)
C2—C3—C4—C5	63.3 (3)	C13—C14—C15—C16	-179.5 (2)
C3—C4—C5—C6	-45.0 (3)	C13—C14—C15—C10	-0.1 (4)
O1—C1—C6—C7	-0.5 (3)	C11—C10—C15—C16	-179.8 (2)
C2—C1—C6—C7	179.5 (2)	C9—C10—C15—C16	0.0 (3)
O1—C1—C6—C5	-179.9 (2)	C11—C10—C15—C14	0.7 (3)
C2—C1—C6—C5	0.0 (4)	C9—C10—C15—C14	-179.5 (2)
C4—C5—C6—C1	14.8 (3)	C1—O1—C16—C7	0.0 (2)
C4—C5—C6—C7	-164.5 (2)	C1—O1—C16—C15	179.4 (2)
C1—C6—C7—C16	0.4 (2)	C8—C7—C16—O1	179.21 (19)
C5—C6—C7—C16	179.8 (2)	C6—C7—C16—O1	-0.2 (3)
C1—C6—C7—C8	-178.9 (3)	C8—C7—C16—C15	-0.2 (3)
C5—C6—C7—C8	0.5 (4)	C6—C7—C16—C15	-179.6 (2)
C16—C7—C8—C9	-0.9 (3)	C14—C15—C16—O1	0.8 (4)
C6—C7—C8—C9	178.4 (2)	C10—C15—C16—O1	-178.7 (2)
C7—C8—C9—C10	1.4 (3)	C14—C15—C16—C7	-179.9 (2)
C8—C9—C10—C11	178.8 (2)	C10—C15—C16—C7	0.6 (3)
C8—C9—C10—C15	-1.0 (4)		

Hydrogen-bond geometry (\AA , $^\circ$)

Cg3 and Cg4 are the centroids of rings C7—C10/C15/C16 and C10—C15, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C5—H5B \cdots Cg4 ⁱ	0.99	2.69	3.664 (3)	167

C8—H8 \cdots Cg3 ⁱ	0.95	2.93	3.650 (3)	134
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Symmetry code: (i) $-x, -y+2, z-1/2$.