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interactions; weak C—H...O interactions.**CCDC reference:** 1586885**Supporting information:** this article has
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Crystal structure of a diaryl carbonate: 1,3-phenylene bis(phenyl carbonate)

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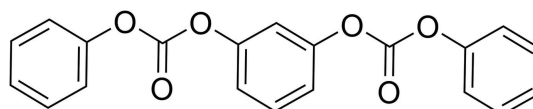
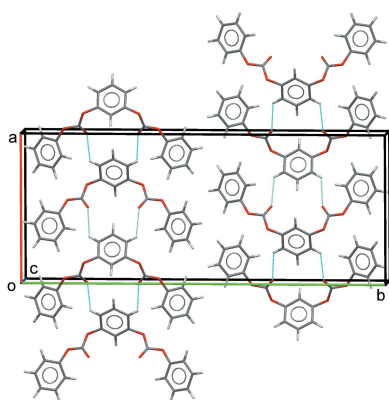
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The whole molecule of the title compound, $C_{20}H_{14}O_6$, is generated by mirror symmetry, the mirror bisecting the central benzene ring. The carbonate groups adopt an *s-cis-s-cis* conformation, with torsion angles of 58.7 (2) and 116.32 (15)°. The crystal structure of 1,3-phenylene bis(phenyl carbonate) contains no strong hydrogen bonds, though weak C—H...O and offset π - π interactions are observed, forming layers parallel to the *ac* plane.

1. Chemical context

Organic carbonates have a wide range of applications as polymers, surfactants, fuel additives, solvents for complex industrial syntheses and extractions, and even medical agents, dyes, and foodstuff (Shukla & Srivastava, 2017). They are commonly synthesized by treating alcohols with phosgene, a rather toxic reagent. Alternative preparatory methods include the reaction of alcohols and carbon monoxide in the presence of a catalyst, direct condensation of alcohols and carbon dioxide (Joe *et al.*, 2012; Zhang *et al.* 2012; Zhao *et al.*, 2009), or the alcoholysis of urea (Ball *et al.*, 1980; Bhanage *et al.*, 2003; Zhang *et al.*, 2016; Mote & Ranade, 2017).

The bis(phenyl carbonate) structure reported herein was identified as an unexpected side product from the attempted recrystallization of 1-(*m*-phenol)-3-phenylurea from ethanol. We surmise this compound formed through a combination of intermolecular 'self-alcoholysis' reactions leading to a carbamate intermediate (Mote & Ranade, 2017), which subsequently over time yields the title compound, 1,3-phenylene bis(phenyl carbonate). Compared to the one-dimensional hydrogen-bonded chain motif so frequently seen in diarylurea crystals (Solomos *et al.*, 2017; Capacci-Daniel *et al.*, 2010, 2015, 2016), diaryl carbonates lack the ability to associate *via* strong intermolecular hydrogen bonds. Analysis of the relatively limited number of diaryl carbonate structures previously reported shows that the title compound shares some of the same structural features.



2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The asymmetric unit consists of half a molecule, as

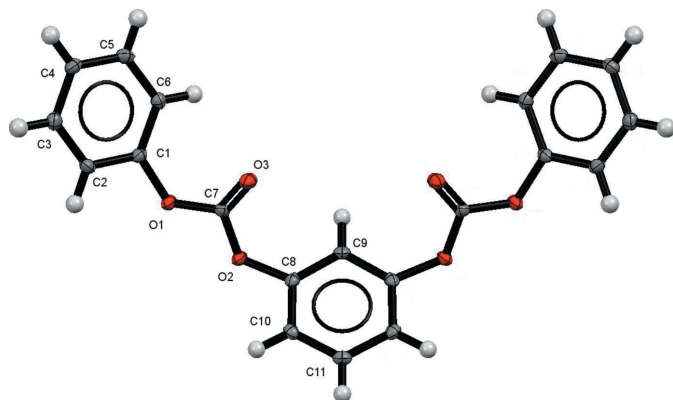


Figure 1
Molecular structure of the title compound, with atom labeling. Displacement ellipsoids are drawn at the 50% probability level. Unlabeled atoms are related to the labeled atoms by mirror symmetry (symmetry operation: $x, -y + \frac{1}{2}, z$).

atoms C9 and C11 sit on a mirror plane. The C7=O3 bond distance [1.1878 (18) Å] and the C7–O1 and C7–O2 bond distances [1.3446 (18) Å and 1.3442 (18) Å, respectively] are in good agreement with values reported for other carbonate structures (Cambridge Structural Database: Version 5.38, Groom *et al.*, 2016). The aromatic rings are both *s-cis* to the carbonate group with C7–O1–C1–C6 and C7–O2–C8–C10 torsion angles of 58.7 (2) and 116.32 (15)°, respectively. The 1,3-substitution of the central aromatic ring imparts the molecule with a bent or ‘U-shape’ conformation and a significant net dipole moment.

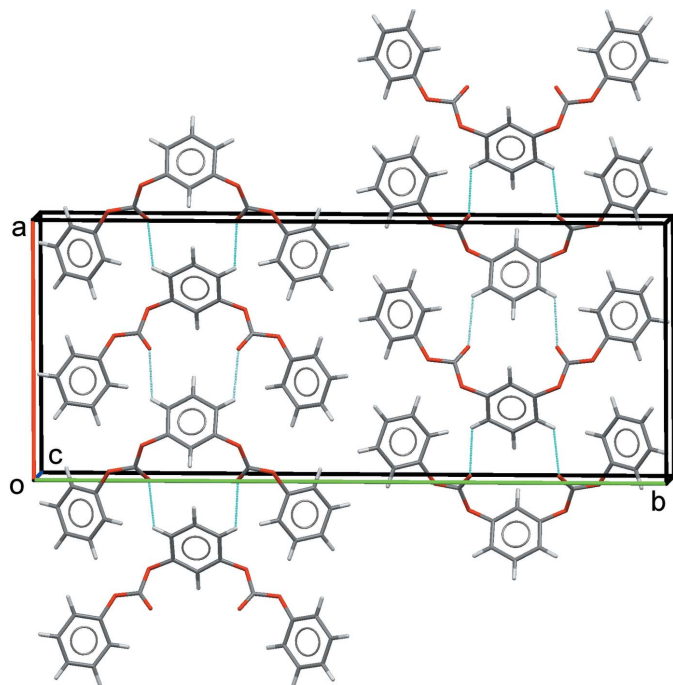


Figure 2
Crystal packing of the title compound viewed along the *c* axis, showing the antiparallel alignment of adjacent rows of molecules, which creates a long *b* axis of 31.548 (3) Å. The C–H···O hydrogen bonds (see Table 1) are shown as dashed line.

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

<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>
C10–H10···O3 ⁱ	0.95	2.59	3.2105 (8)	123

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

3. Supramolecular Features

The lengths of the unit-cell axes in the 1,3-phenylene bis-(phenyl carbonate) structure are strikingly different. Molecules along the *a*-axis direction are related by glide symmetry and assemble into polar chains (Fig. 2). A short intermolecular C=O···H–C contact (2.59 Å; see Table 1) between molecules along this axis may favorably contribute to their assembly. The dipoles of adjacent chains in the *ab* plane adopt an antiparallel alignment, which leads to the very long *b* axis. The very short *c* axis reflects the offset π – π stacking between molecules that are related by translation (Fig. 3). Details: $Cg1 \cdots Cg1^{i,ii} = 3.822$ (1) Å, interplanar distance = 3.438 (1) Å, with a slippage of 1.669 Å [*Cg1* is the centroid of the phenyl ring C1–C6, symmetry codes: (i) $x, y, z - 1$; (ii) $x, y, z + 1$]; $Cg2 \cdots Cg2^{iii,iv} = 3.822$ (1) Å, interplanar distance = 3.398 (1) Å, with a slippage of 1.749 Å [*Cg2* is the centroid of the central benzene ring, symmetry codes: (iii) $x, -y + \frac{1}{2}, z - 1$; (iv) $x, -y + \frac{1}{2}, z + 1$].

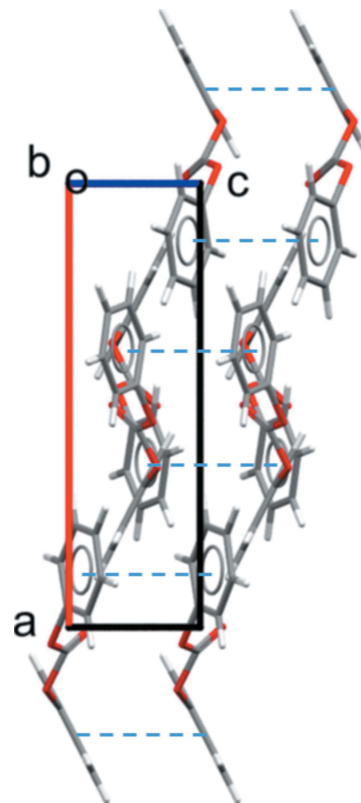


Figure 3
A partial view along the long *b* axis of 31.548 (3) Å of the crystal packing of the title compound, showing the π – π stacking interactions (dashed lines).

4. Database Survey

A search of the Cambridge Structural Database (CSD, Version 5.38 with May 2017 update: Groom *et al.*, 2016) for organic diphenyl carbonates yielded 20 hits. Interestingly, most of the structures have unit-cell parameters with at least one considerably long axis. With a *b*-axis length of 31.548 (3) Å, the structure of 1,3-phenylene bis(phenyl carbonate) is consistent with this trend. Across the 20 structures, the C=O bond lengths range between 1.155 and 1.207 Å [average: 1.178 (11) Å], C–O bond lengths fall within 1.310 and 1.387 Å [average: 1.343 (9) Å], and O–C–O angles average 106 (1)°. However, torsion angles about the C–O–C–C_{arom} bonds are extremely variable.

Only one other acyclic bis(phenyl carbonate) was identified in this search, 4,4'-isopropylidenediphenyl-bis(phenyl-carbonate) (DINWOM10; Perez & Scaringe, 1987). The bond lengths and angles are in good agreement with our structure, with C=O = 1.152 and 1.173 Å; C–O = 1.326–1.337 Å and O–C–O = 106.6 and 105.5°. Also similar is the structure of diphenyl carbonate (ZZZPCA02; Hosten & Betz, 2014), with C=O = 1.188 Å; C–O = 1.343 and 1.337 Å; O–C–O = 104.85°. The aromatic torsion angles for diphenyl carbonate are also similar to the title compound, with C–O–C–C angles of 59.90 and 132.36°.

5. Synthesis and crystallization

Equimolar amounts of 3-aminophenol and phenyl isocyanate were added to benzene under nitrogen and stirred for 24 h. A white precipitate identified as 1-(*m*-phenol)-3-phenylurea was filtered, dried, and recrystallized in assorted organic solvents (ethanol, methanol, acetone, ethyl acetate, benzene, toluene, acetone:hexanes, acetonitrile). Slow evaporation of an ethanolic solution in a 1 dram vial, capped with pierced lids, yielded large colorless plates of 1,3-phenylene bis(phenyl carbonate). Needle-like crystals identified within the same vials corresponded to 1-(*m*-phenol)-3-phenylurea. The appearance of 1,3-phenylene bis(phenyl carbonate) crystals was not consistent across multiple recrystallization experiments, suggesting that select impurities and/or longer, delayed evaporation methods that favor non-equilibrium products may be needed to obtain this material.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were included as riding idealized contributors with C–H = 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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Table 2
Experimental details.

Crystal data	
Chemical formula	C ₂₀ H ₁₄ O ₆
<i>M_r</i>	350.31
Crystal system, space group	Orthorhombic, <i>Pnma</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	12.9597 (12), 31.548 (3), 3.8219 (4)
<i>V</i> (Å ³)	1562.6 (3)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.11
Crystal size (mm)	0.51 × 0.36 × 0.29
Data collection	
Diffractometer	Bruker D8 Quest/Photon 100
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2014)
<i>T</i> _{min} , <i>T</i> _{max}	0.620, 0.746
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	16409, 1625, 1409
<i>R</i> _{int}	0.044
(sin θ/λ) _{max} (Å ⁻¹)	0.625
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.040, 0.093, 1.16
No. of reflections	1625
No. of parameters	121
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.22, −0.28

Computer programs: *APEX2*, *SAINT*, *XCIF* and *XPREP* (Bruker, 2014), *SHELXT2014/4* (Sheldrick, 2015a), *SHELXL2014/6* (Sheldrick, 2015b), *SHELXTL* (Sheldrick, 2008), *Mercury* (Macrae *et al.*, 2008) and *pubCIF* (Westrip, 2010).

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supporting information

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Crystal structure of a diaryl carbonate: 1,3-phenylene bis(phenyl carbonate)

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Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINTE* (Bruker, 2014); data reduction: *SAINTE* (Bruker, 2014) and *XPREP* (Bruker, 2014); program(s) used to solve structure: *SHELXT2014/4* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014/6* (Sheldrick, 2015b); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *XCIF* (Bruker, 2014) and *pubCIF* (Westrip, 2010).

(I)

Crystal data

$C_{20}H_{14}O_6$

$M_r = 350.31$

Orthorhombic, *Pnma*

$a = 12.9597$ (12) Å

$b = 31.548$ (3) Å

$c = 3.8219$ (4) Å

$V = 1562.6$ (3) Å³

$Z = 4$

$F(000) = 728$

$D_x = 1.489$ Mg m⁻³

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

Cell parameters from 6581 reflections

$\theta = 2.6$ – 28.1°

$\mu = 0.11$ mm⁻¹

$T = 100$ K

Prism, colorless

$0.51 \times 0.36 \times 0.29$ mm

Data collection

Bruker D8 Quest/Photon 100

diffractometer

Radiation source: microfocus sealed tube

Multilayer mirrors monochromator

profile data from φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2014)

$T_{\min} = 0.620$, $T_{\max} = 0.746$

16409 measured reflections

1625 independent reflections

1409 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\max} = 26.4^\circ$, $\theta_{\min} = 2.6^\circ$

$h = -16 \rightarrow 16$

$k = -39 \rightarrow 39$

$l = -4 \rightarrow 4$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.093$

$S = 1.16$

1625 reflections

121 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

$w = 1/[\sigma^2(F_o^2) + (0.0297P)^2 + 1.0258P]$

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

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

$\Delta\rho_{\max} = 0.22$ e Å⁻³

$\Delta\rho_{\min} = -0.28$ e Å⁻³

Special details

Experimental. One distinct cell was identified using APEX2 (Bruker, 2014). Four frame series were integrated and filtered for statistical outliers using SAINT (Bruker, 2014) then corrected for absorption by integration using SAINT/SADABS v2014/2 (Bruker, 2014) to sort, merge, and scale the combined data. No decay correction was applied.

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. Structure was phased by direct methods (Sheldrick, 2015). Systematic conditions suggested the ambiguous space group. The space group choice was confirmed by successful convergence of the full-matrix least-squares refinement on F^2 . The final map had no other significant features. A final analysis of variance between observed and calculated structure factors showed some dependence on amplitude and little dependence on resolution.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.53843 (8)	0.37983 (3)	0.6378 (3)	0.0182 (3)
O2	0.64043 (8)	0.32686 (3)	0.6752 (3)	0.0176 (3)
O3	0.49910 (8)	0.32050 (3)	0.3282 (3)	0.0205 (3)
C1	0.45214 (11)	0.40226 (5)	0.5132 (4)	0.0149 (3)
C2	0.47199 (12)	0.44105 (5)	0.3612 (4)	0.0166 (3)
H2	0.5410	0.4506	0.3305	0.020*
C3	0.38982 (12)	0.46595 (5)	0.2539 (4)	0.0185 (3)
H3	0.4022	0.4928	0.1494	0.022*
C4	0.28937 (12)	0.45171 (5)	0.2990 (4)	0.0175 (3)
H4	0.2331	0.4687	0.2238	0.021*
C5	0.27117 (12)	0.41276 (5)	0.4532 (4)	0.0178 (3)
H5	0.2023	0.4031	0.4839	0.021*
C6	0.35262 (12)	0.38772 (5)	0.5632 (4)	0.0159 (3)
H6	0.3404	0.3611	0.6710	0.019*
C7	0.55226 (11)	0.33988 (5)	0.5243 (4)	0.0144 (3)
C8	0.68026 (11)	0.28716 (5)	0.5719 (4)	0.0141 (3)
C9	0.63026 (16)	0.2500	0.6630 (6)	0.0146 (4)
H9	0.5657	0.2500	0.7808	0.018*
C10	0.77487 (11)	0.28802 (5)	0.4077 (4)	0.0152 (3)
H10	0.8068	0.3143	0.3513	0.018*
C11	0.82269 (16)	0.2500	0.3264 (6)	0.0159 (5)
H11	0.8882	0.2500	0.2149	0.019*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0145 (5)	0.0142 (5)	0.0258 (7)	0.0025 (4)	-0.0060 (5)	-0.0041 (5)
O2	0.0132 (5)	0.0147 (5)	0.0250 (6)	0.0033 (4)	-0.0045 (5)	-0.0041 (5)
O3	0.0155 (5)	0.0189 (6)	0.0272 (6)	0.0020 (4)	-0.0062 (5)	-0.0059 (5)
C1	0.0134 (7)	0.0153 (7)	0.0159 (8)	0.0029 (6)	-0.0022 (6)	-0.0035 (6)
C2	0.0142 (7)	0.0162 (8)	0.0193 (8)	-0.0034 (6)	0.0018 (6)	-0.0025 (6)
C3	0.0207 (8)	0.0151 (7)	0.0198 (8)	0.0005 (6)	0.0015 (7)	0.0000 (6)
C4	0.0153 (7)	0.0180 (8)	0.0192 (8)	0.0043 (6)	-0.0014 (6)	-0.0011 (7)

C5	0.0131 (7)	0.0217 (8)	0.0187 (8)	-0.0009 (6)	0.0020 (6)	-0.0035 (7)
C6	0.0176 (8)	0.0141 (7)	0.0161 (8)	-0.0014 (6)	0.0014 (6)	0.0002 (6)
C7	0.0110 (7)	0.0149 (7)	0.0173 (8)	-0.0002 (5)	0.0012 (6)	0.0010 (6)
C8	0.0139 (7)	0.0133 (8)	0.0151 (7)	0.0019 (6)	-0.0043 (6)	-0.0019 (6)
C9	0.0091 (10)	0.0175 (11)	0.0171 (11)	0.000	-0.0008 (8)	0.000
C10	0.0144 (7)	0.0162 (8)	0.0151 (7)	-0.0027 (6)	-0.0024 (6)	0.0010 (6)
C11	0.0116 (10)	0.0211 (11)	0.0150 (11)	0.000	-0.0002 (8)	0.000

Geometric parameters (Å, °)

O1—C7	1.3446 (18)	C4—H4	0.9500
O1—C1	1.4064 (18)	C5—C6	1.384 (2)
O2—C7	1.3442 (18)	C5—H5	0.9500
O2—C8	1.4109 (18)	C6—H6	0.9500
O3—C7	1.1878 (18)	C8—C10	1.377 (2)
C1—C2	1.379 (2)	C8—C9	1.3842 (19)
C1—C6	1.382 (2)	C9—C8 ⁱ	1.3841 (19)
C2—C3	1.385 (2)	C9—H9	0.9500
C2—H2	0.9500	C10—C11	1.3856 (18)
C3—C4	1.388 (2)	C10—H10	0.9500
C3—H3	0.9500	C11—C10 ⁱ	1.3856 (18)
C4—C5	1.383 (2)	C11—H11	0.9500
C7—O1—C1	117.93 (12)	C1—C6—H6	120.6
C7—O2—C8	117.53 (12)	C5—C6—H6	120.6
C2—C1—C6	121.79 (14)	O3—C7—O2	127.33 (14)
C2—C1—O1	116.16 (13)	O3—C7—O1	127.50 (14)
C6—C1—O1	121.89 (14)	O2—C7—O1	105.16 (12)
C1—C2—C3	118.98 (14)	C10—C8—C9	123.23 (14)
C1—C2—H2	120.5	C10—C8—O2	115.82 (13)
C3—C2—H2	120.5	C9—C8—O2	120.67 (14)
C2—C3—C4	120.04 (15)	C8 ⁱ —C9—C8	115.8 (2)
C2—C3—H3	120.0	C8 ⁱ —C9—H9	122.1
C4—C3—H3	120.0	C8—C9—H9	122.1
C5—C4—C3	120.04 (14)	C8—C10—C11	118.90 (15)
C5—C4—H4	120.0	C8—C10—H10	120.5
C3—C4—H4	120.0	C11—C10—H10	120.5
C4—C5—C6	120.43 (14)	C10—C11—C10 ⁱ	119.9 (2)
C4—C5—H5	119.8	C10—C11—H11	120.0
C6—C5—H5	119.8	C10 ⁱ —C11—H11	120.0
C1—C6—C5	118.71 (14)	C8—O2—C7—O1	-173.24 (12)
C7—O1—C1—C2	-125.86 (15)	C1—O1—C7—O3	-0.4 (2)
C7—O1—C1—C6	58.7 (2)	C1—O1—C7—O2	178.35 (12)
C6—C1—C2—C3	-0.4 (2)	C7—O2—C8—C10	116.32 (15)
O1—C1—C2—C3	-175.82 (14)	C7—O2—C8—C9	-69.5 (2)
C1—C2—C3—C4	-0.2 (2)	C10—C8—C9—C8 ⁱ	-1.4 (3)
C2—C3—C4—C5	0.4 (2)		

C3—C4—C5—C6	-0.1 (2)	O2—C8—C9—C8 ⁱ	-175.11 (11)
C2—C1—C6—C5	0.8 (2)	C9—C8—C10—C11	0.5 (3)
O1—C1—C6—C5	175.92 (14)	O2—C8—C10—C11	174.47 (15)
C4—C5—C6—C1	-0.5 (2)	C8—C10—C11—C10 ⁱ	0.5 (3)
C8—O2—C7—O3	5.6 (2)		

Symmetry code: (i) $x, -y+1/2, z$.

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C10—H10 ⁱⁱ ⋯O3 ⁱⁱ	0.95	2.59	3.2105 (8)	123

Symmetry code: (ii) $x+1/2, y, -z+1/2$.