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3,3-Dimethyl-2-benzofuran-1(3H)-one

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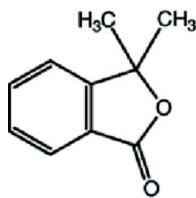
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 Key indicators: single-crystal X-ray study; $T = 123$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.052; wR factor = 0.133; data-to-parameter ratio = 25.9.

In the title compound, $\text{C}_{10}\text{H}_{10}\text{O}_2$, all the non-H atoms except the methyl C atoms lie on a crystallographic mirror plane. In the crystal, $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules into zigzag chains running parallel to [100]. Weak $\pi-\pi$ stacking interactions between the benzene rings [centroid-centroid distance = 3.9817 (5) Å] link the chains in the [010] direction.

Related literature

 For related structures, see: Fun *et al.* (2010, 2011).


Experimental

Crystal data

 $\text{C}_{10}\text{H}_{10}\text{O}_2$
 $M_r = 162.18$
 Orthorhombic, $Pnma$
 $a = 14.3537$ (9) Å

 $b = 7.0069$ (5) Å
 $c = 8.2605$ (5) Å
 $V = 830.80$ (9) Å³
 $Z = 4$

 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 123$ K
 $0.55 \times 0.44 \times 0.30$ mm

Data collection

 Oxford Diffraction Xcalibur Ruby Gemini diffractometer
 Absorption correction: refined from ΔF (XABS2; Parkin *et al.*, 1995)
 $T_{\min} = 0.952$, $T_{\max} = 0.974$

 1840 measured reflections
 1840 independent reflections
 1454 reflections with $I > 2\sigma(I)$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.133$
 $S = 1.09$
 1840 reflections

 71 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.34$ e Å⁻³
 $\Delta\rho_{\min} = -0.30$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C}2-\text{H}2\cdots\text{O}2^i$	0.93	2.43	3.3072 (17)	158

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6560).

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supporting information

Acta Cryst. (2012). E68, o113 [doi:10.1107/S1600536811052913]

3,3-Dimethyl-2-benzofuran-1(3*H*)-one

M. S. Siddegowda, Ray J. Butcher, Sema Ozturk Yıldırım, Mehmet Akkurt, H. S. Yathirajan and A. R. Ramesha

S1. Comment

3,3-Dimethylisobenzofuran-1(3*H*)-one, (I), is used to synthesize 10,10-dimethylanthrone (Fun *et al.*, 2010). It is one of the intermediate for melitraceniium chloride (Fun *et al.*, 2011). We now report its structure.

In the title molecule (I), (Fig. 1), a mirror plane passes through the remaining atoms of the molecule, except the atoms of two methyl groups which are *mirror images of each other*.

In the crystal, intermolecular C—H \cdots O hydrogen bonds link molecules forming zigzag chains in the layer parallel to the (101) plane and along the *a* axis (Table 1, Fig. 2a,b,c). Furthermore, there exist weak π - π stacking interactions [$Cg2 \cdots Cg2(2-x, -1/2+y, -z) = 3.9817(5) \text{ \AA}$, $Cg2 \cdots Cg2(2-x, 1/2+y, -z) = 3.9817(5) \text{ \AA}$, $Cg2 \cdots Cg2(2-x, -y, -z) = 3.9817(5) \text{ \AA}$, $Cg2 \cdots Cg2(2-x, 1-y, -z) = 3.9817(5) \text{ \AA}$] between the C1–C6 benzene rings along the [010] direction.

S2. Experimental

The title compound was obtained as a gift sample from *R. L. Fine Chemicals*, Bengaluru, India. Colourless prisms of (I) were grown from toluene solution by slow evaporation (m.p.: 337–340 K).

S3. Refinement

All H atoms were added in calculated positions and refined as riding with C–H distances of 0.93 and 0.96 \AA . The isotropic atomic displacement parameters of H atoms were fixed to 1.2 or 1.5 $\times U_{eq}$ of the parent atom.

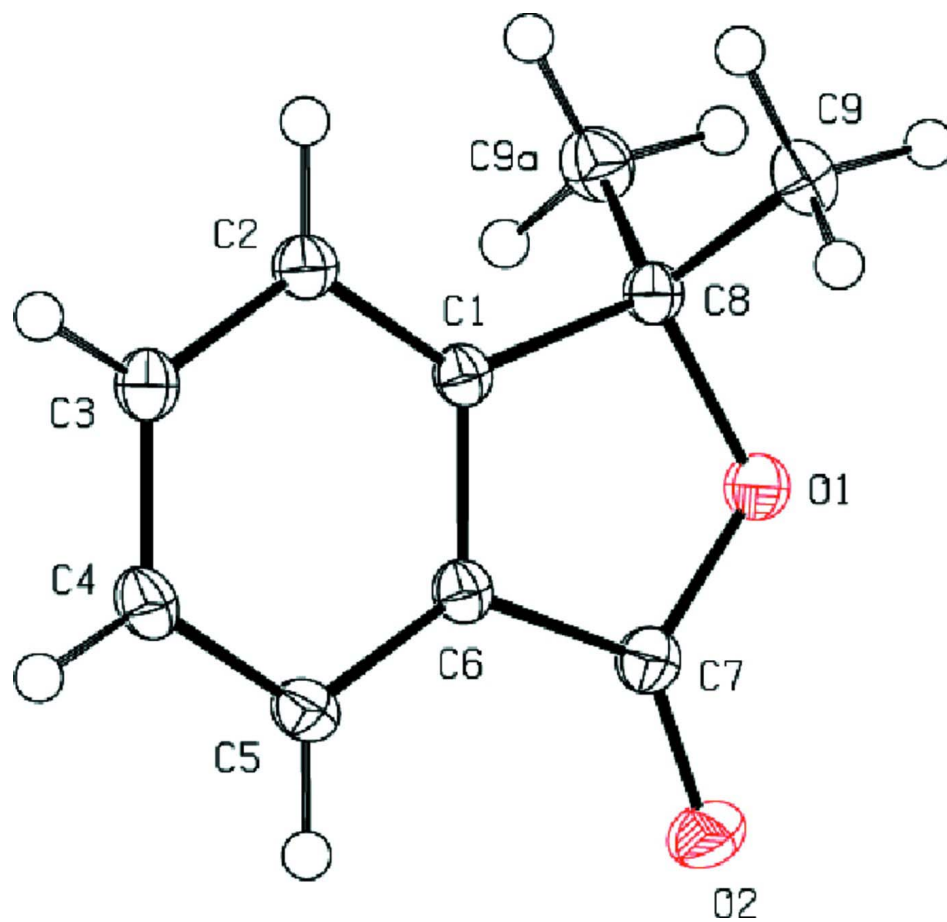


Figure 1

The title molecule (I) showing displacement ellipsoids for non-H atoms drawn at the 50% probability level.

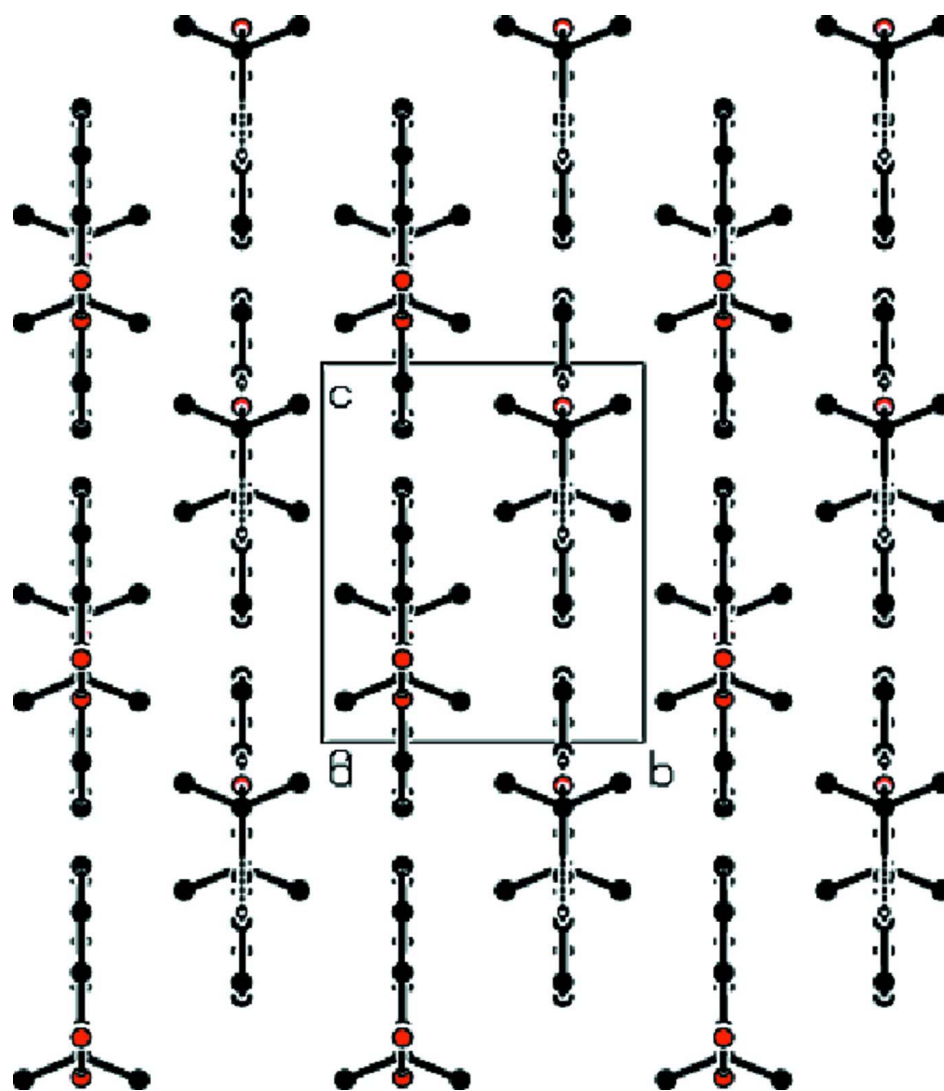


Figure 2

View of the packing and hydrogen bonding of (I) down *a* axis.

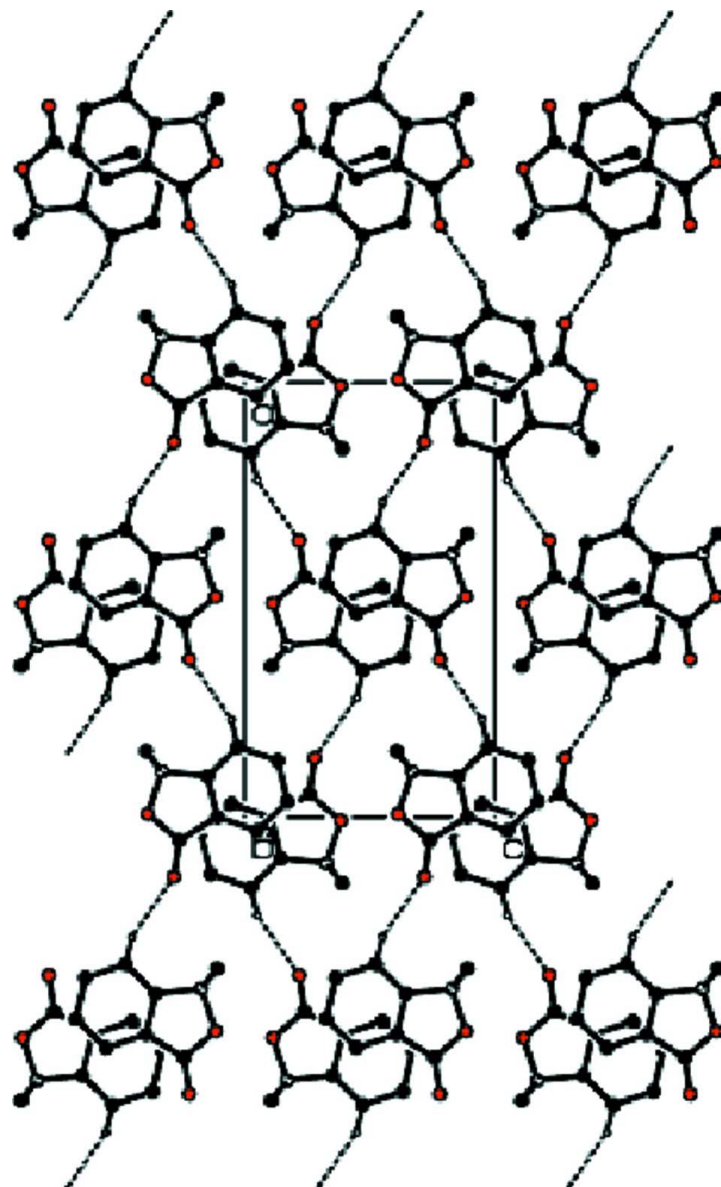


Figure 3

View of the packing and hydrogen bonding of (I) down *b* axis.

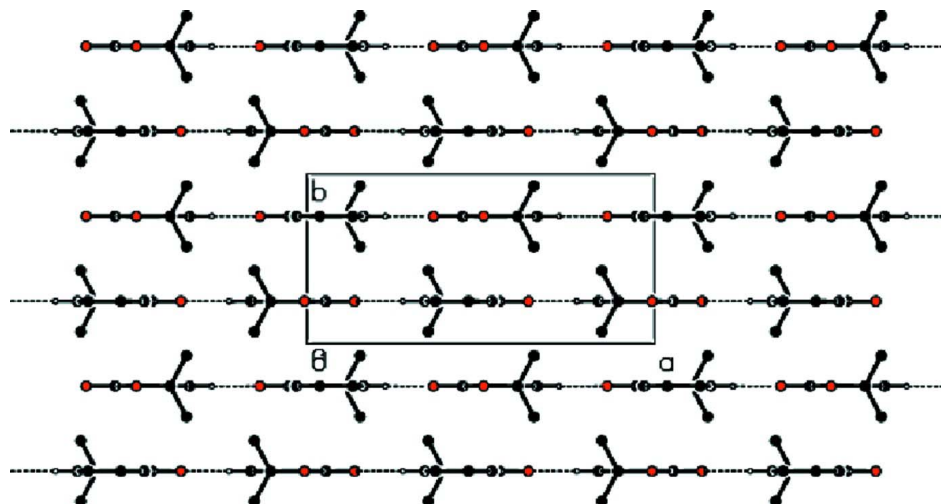


Figure 4

View of the packing and hydrogen bonding of (I) down c axis.

3,3-Dimethyl-2-benzofuran-1(3H)-one

Crystal data

$C_{10}H_{10}O_2$

$M_r = 162.18$

Orthorhombic, $Pnma$

Hall symbol: $-P\ 2ac\ 2n$

$a = 14.3537\ (9)\ \text{\AA}$

$b = 7.0069\ (5)\ \text{\AA}$

$c = 8.2605\ (5)\ \text{\AA}$

$V = 830.80\ (9)\ \text{\AA}^3$

$Z = 4$

$F(000) = 344$

$D_x = 1.297\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1444 reflections

$\theta = 2.8\text{--}35.2^\circ$

$\mu = 0.09\ \text{mm}^{-1}$

$T = 123\ \text{K}$

Prism, colourless

$0.55 \times 0.44 \times 0.30\ \text{mm}$

Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer

Radiation source: Enhance (Mo) X-ray Source

Graphite monochromator

Detector resolution: $10.5081\ \text{pixels mm}^{-1}$

ω scans

Absorption correction: part of the refinement

model (ΔF)

($XABS2$; Parkin *et al.*, 1995)

$T_{\min} = 0.952$, $T_{\max} = 0.974$

1840 measured reflections

1840 independent reflections

1454 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.000$

$\theta_{\max} = 35.2^\circ$, $\theta_{\min} = 2.8^\circ$

$h = 0 \rightarrow 22$

$k = 0 \rightarrow 11$

$l = 0 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.052$

$wR(F^2) = 0.133$

$S = 1.09$

1840 reflections

71 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

$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 0.0987P]$

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

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

$\Delta\rho_{\max} = 0.34\ \text{e \AA}^{-3}$

$\Delta\rho_{\min} = -0.30\ \text{e \AA}^{-3}$

Special details

Experimental. Absorption correction: XABS2 (Parkin *et al.*, 1995); cubic fit to $\sin\theta/\lambda$ - 24 parameters

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.99217 (7)	0.25000	0.38584 (11)	0.0216 (3)
O2	1.13652 (7)	0.25000	0.28045 (13)	0.0260 (3)
C1	0.90567 (9)	0.25000	0.14603 (15)	0.0159 (3)
C2	0.83829 (9)	0.25000	0.02623 (16)	0.0193 (3)
C3	0.86910 (10)	0.25000	-0.13404 (16)	0.0211 (3)
C4	0.96384 (10)	0.25000	-0.17273 (16)	0.0208 (3)
C5	1.03071 (9)	0.25000	-0.05143 (16)	0.0192 (3)
C6	0.99948 (9)	0.25000	0.10807 (15)	0.0165 (3)
C7	1.05334 (9)	0.25000	0.25962 (15)	0.0189 (3)
C8	0.89464 (9)	0.25000	0.32851 (15)	0.0175 (3)
C9	0.84773 (7)	0.07067 (15)	0.39183 (12)	0.0229 (3)
H2	0.77510	0.25000	0.05140	0.0230*
H3	0.82540	0.25000	-0.21720	0.0250*
H4	0.98220	0.25000	-0.28070	0.0250*
H5	1.09400	0.25000	-0.07580	0.0230*
H9A	0.88010	-0.03960	0.35190	0.0340*
H9B	0.78420	0.06740	0.35560	0.0340*
H9C	0.84920	0.07080	0.50800	0.0340*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0185 (4)	0.0326 (5)	0.0136 (4)	0.0000	-0.0019 (4)	0.0000
O2	0.0169 (4)	0.0368 (6)	0.0242 (5)	0.0000	-0.0042 (4)	0.0000
C1	0.0169 (5)	0.0170 (5)	0.0137 (5)	0.0000	0.0004 (4)	0.0000
C2	0.0176 (5)	0.0251 (6)	0.0153 (5)	0.0000	-0.0002 (5)	0.0000
C3	0.0220 (6)	0.0270 (6)	0.0143 (5)	0.0000	-0.0021 (5)	0.0000
C4	0.0246 (6)	0.0248 (6)	0.0131 (5)	0.0000	0.0025 (5)	0.0000
C5	0.0185 (5)	0.0213 (5)	0.0177 (5)	0.0000	0.0031 (5)	0.0000
C6	0.0176 (5)	0.0173 (5)	0.0147 (5)	0.0000	0.0003 (4)	0.0000
C7	0.0182 (6)	0.0214 (5)	0.0172 (5)	0.0000	-0.0011 (5)	0.0000
C8	0.0164 (5)	0.0232 (6)	0.0130 (5)	0.0000	-0.0007 (4)	0.0000
C9	0.0259 (5)	0.0244 (4)	0.0185 (4)	-0.0011 (4)	0.0028 (3)	0.0028 (3)

Geometric parameters (Å, °)

O1—C7	1.3631 (16)	C6—C7	1.4714 (18)
O1—C8	1.4779 (16)	C8—C9	1.5185 (13)
O2—C7	1.2063 (16)	C8—C9 ⁱ	1.5185 (13)
C1—C2	1.3837 (18)	C2—H2	0.9300
C1—C6	1.3826 (18)	C3—H3	0.9300
C1—C8	1.5157 (18)	C4—H4	0.9300
C2—C3	1.3958 (19)	C5—H5	0.9300
C3—C4	1.397 (2)	C9—H9A	0.9600
C4—C5	1.3875 (19)	C9—H9B	0.9600
C5—C6	1.3917 (18)	C9—H9C	0.9600
C7—O1—C8	111.41 (9)	C1—C8—C9	112.89 (7)
C2—C1—C6	121.23 (12)	C1—C8—C9 ⁱ	112.89 (7)
C2—C1—C8	129.66 (12)	C9—C8—C9 ⁱ	111.68 (10)
C6—C1—C8	109.11 (11)	C1—C2—H2	121.00
C1—C2—C3	117.19 (12)	C3—C2—H2	121.00
C2—C3—C4	121.70 (12)	C2—C3—H3	119.00
C3—C4—C5	120.54 (12)	C4—C3—H3	119.00
C4—C5—C6	117.44 (12)	C3—C4—H4	120.00
C1—C6—C5	121.90 (12)	C5—C4—H4	120.00
C1—C6—C7	108.59 (11)	C4—C5—H5	121.00
C5—C6—C7	129.51 (12)	C6—C5—H5	121.00
O1—C7—O2	121.90 (12)	C8—C9—H9A	109.00
O1—C7—C6	108.20 (11)	C8—C9—H9B	109.00
O2—C7—C6	129.90 (12)	C8—C9—H9C	110.00
O1—C8—C1	102.69 (10)	H9A—C9—H9B	109.00
O1—C8—C9	108.04 (7)	H9A—C9—H9C	109.00
O1—C8—C9 ⁱ	108.04 (7)	H9B—C9—H9C	109.00
C7—O1—C8—C9	119.51 (7)	C8—C1—C6—C5	180.00
C8—O1—C7—O2	180.00	C2—C1—C8—C9	63.92 (8)
C8—O1—C7—C6	0.00	C1—C2—C3—C4	0.00
C7—O1—C8—C1	0.00	C2—C3—C4—C5	0.00
C8—C1—C2—C3	180.00	C3—C4—C5—C6	0.00
C2—C1—C6—C5	0.00	C4—C5—C6—C1	0.00
C2—C1—C6—C7	180.00	C4—C5—C6—C7	180.00
C6—C1—C2—C3	0.00	C1—C6—C7—O2	180.00
C6—C1—C8—O1	0.00	C5—C6—C7—O1	180.00
C6—C1—C8—C9	-116.08 (8)	C5—C6—C7—O2	0.00
C8—C1—C6—C7	0.00	C1—C6—C7—O1	0.00
C2—C1—C8—O1	180.00		

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C2—H2 \cdots O2 ⁱⁱ	0.93	2.43	3.3072 (17)	158

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