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

**M. S. Siddegowda,[a] Ray J. Butcher,[b] Sema Ozturk Yıldırım,[b,c] Mehmet Akkurt,[c]* H. S. Yathirajan[a] and A. R. Ramesha[d]**

[a]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, [b]Department of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA, [c]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, and [d]R. L. Fine Chem, Bengaluru 560 064, India
Correspondence e-mail: akkurt@erciyes.edu.tr

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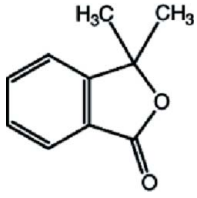
Key indicators: single-crystal X-ray study; $T$ = 123 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.052; $wR$ factor = 0.133; data-to-parameter ratio = 25.9.

In the title compound, $C_{10}H_{10}O_2$, all the non-H atoms except the methyl C atoms lie on a crystallographic mirror plane. In the crystal, C—H···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

$C_{10}H_{10}O_2$
$M_r$ = 162.18
Orthorhombic, *Pnma*
$a$ = 14.3537 (9) Å
$b$ = 7.0069 (5) Å
$c$ = 8.2605 (5) Å
$V$ = 830.80 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 123 K
0.55 × 0.44 × 0.30 mm

### Data collection

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Absorption correction: refined from $\Delta F$ (*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···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C2—H2···O2$^{i}$ | 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).

MSS thanks the University of Mysore for research facilities. RJB wishes to acknowledge the NSF–MRI program (grant CHE-0619278) for funds to purchase the diffractometer.

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

## References

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# supporting information

*Acta Cryst.* (2012). E**68**, 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 a one of the intermediate for melitracenium chloride (Fun *et al.*, 2011). We now report its stucture.

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 ··· 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 $\pi$-$\pi$ stacking interactions [*Cg*2···*Cg*2(2 - *x*, -1/2 + *y*, -*z*) = 3.9817 (5) Å, *Cg*2···*Cg*2(2 - *x*, 1/2 + *y*, -*z*) = 3.9817 (5) Å, *Cg*2···*Cg*2(2 - *x*, -*y*, -*z*) = 3.9817 (5) Å, *Cg*2···*Cg*2(2 - *x*, 1 - *y*, -*z*) = 3.9817 (5) Å] 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 Å. The isotropic atomic displacement parameters of H atoms were fixed to 1.2 or 1.5 $\times U_{eq}$ of the parent atom.

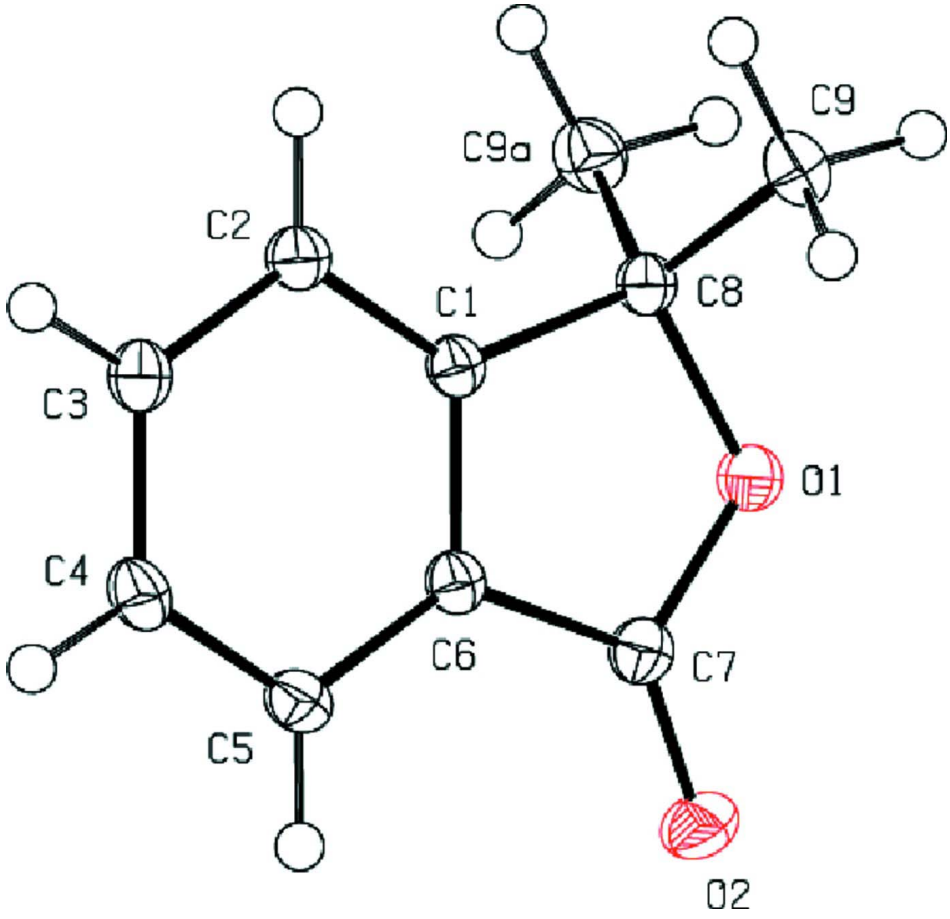


**Figure 1**

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

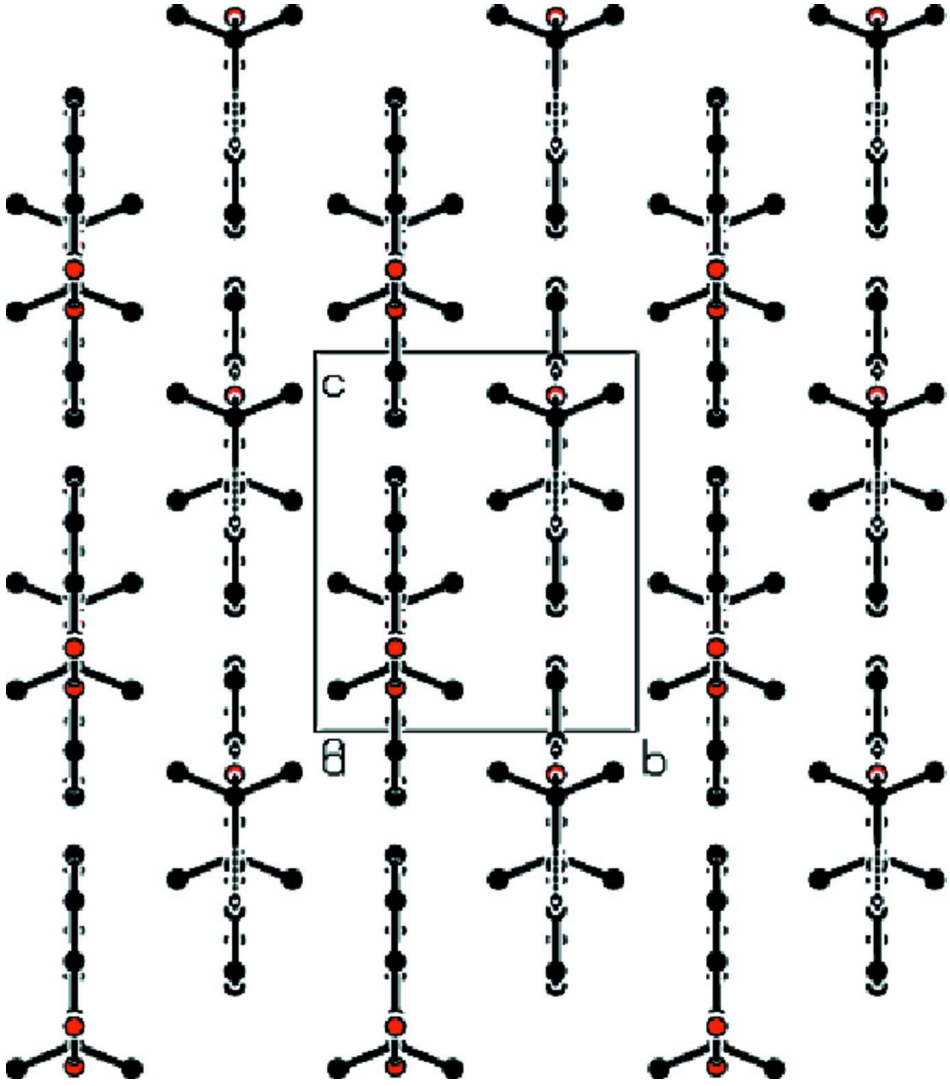


**Figure 2**

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

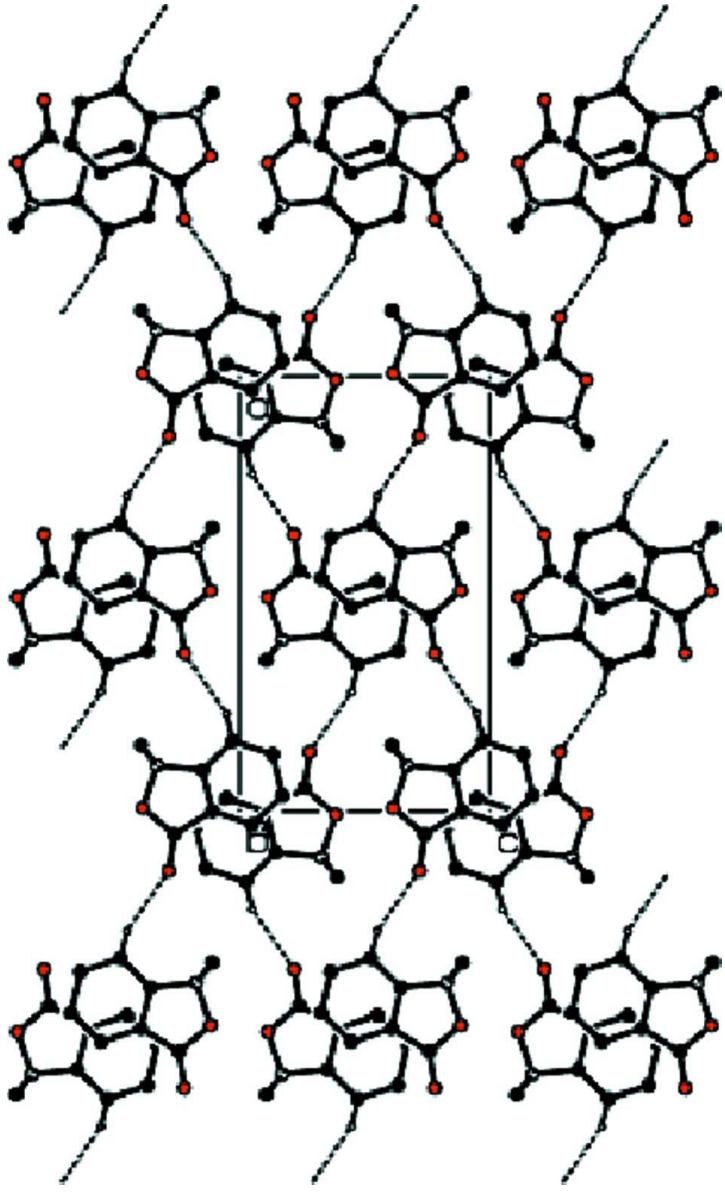

**Figure 3**

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

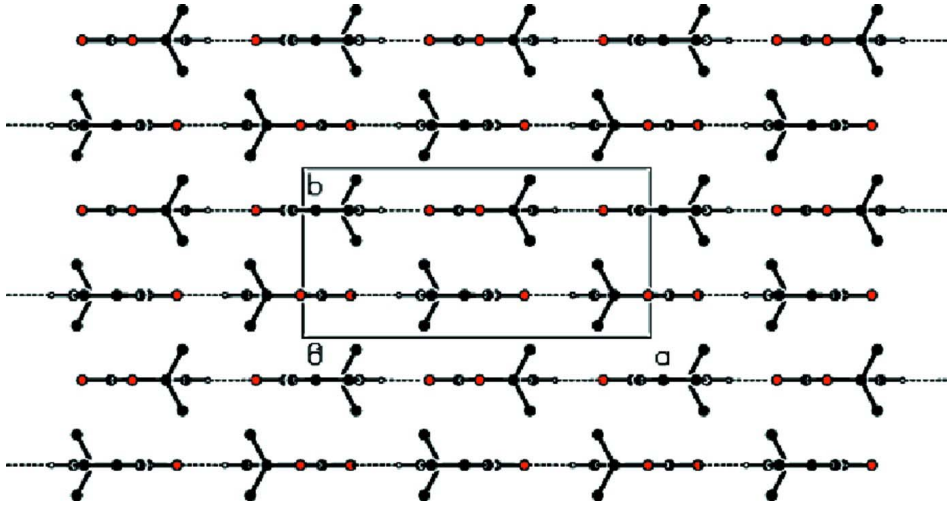


**Figure 4**

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

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

*Crystal data*

$C_{10}H_{10}O_2$
$M_r = 162.18$
Orthorhombic, *Pnma*
Hall symbol: -P 2ac 2n
$a = 14.3537\ (9)$ Å
$b = 7.0069\ (5)$ Å
$c = 8.2605\ (5)$ Å
$V = 830.80\ (9)$ Å$^3$
$Z = 4$
$F(000) = 344$
$D_x = 1.297$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1444 reflections
$\theta = 2.8–35.2°$
$\mu = 0.09$ mm$^{-1}$
$T = 123$ K
Prism, colourless
0.55 × 0.44 × 0.30 mm

*Data collection*

Oxford Diffraction Xcalibur Ruby Gemini diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 10.5081 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: part of the refinement model ($\Delta F$)
(*XABS2*; Parkin *et al.*, 1995)
$T_{min} = 0.952$, $T_{max} = 0.974$
1840 measured reflections
1840 independent reflections
1454 reflections with $I > 2\sigma(I)$
$R_{int} = 0.000$
$\theta_{max} = 35.2°$, $\theta_{min} = 2.8°$
$h = 0\rightarrow22$
$k = 0\rightarrow11$
$l = 0\rightarrow13$

*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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.34$ e Å$^{-3}$
$\Delta\rho_{min} = -0.30$ e Å$^{-3}$

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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 (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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, º)*

| | | | |
|---|---|---|---|
| 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, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C2—H2···O2$^{ii}$ | 0.93 | 2.43 | 3.3072 (17) | 158 |

Symmetry code: (ii) *x*−1/2, −*y*+1/2, −*z*+1/2.