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# Synthesis and crystal structure of 2-chloro-1-(3-hydroxyphenyl)ethanone

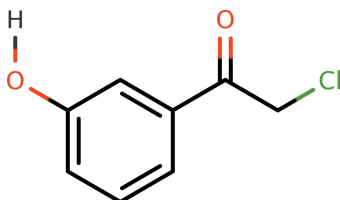
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The structure of 2-chloro-1-(3-hydroxyphenyl)ethanone, C<sub>8</sub>H<sub>7</sub>ClO<sub>2</sub>, an  $\alpha$ -haloketone is described. The molecule is planar (r.m.s. deviation = 0.0164 Å) and in the crystal, inversion-symmetric dimers are formed as a result of pairs of strong O—H...O and weak C—H...O hydrogen bonds. A brief comparison is made with structurally related compounds deposited in the CSD. In addition, the synthesis and some spectroscopic details are presented.

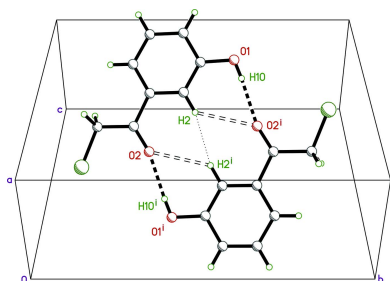
## 1. Chemical context

$\alpha$ -Haloketones have proven to be useful building blocks for the preparation of compounds of various classes because of their high reactivity and selective transformations with a variety of reagents (Erian *et al.*, 2003). Chlorinated acetophenones are widely used in organic synthesis as intermediates for the manufacture of active pharmaceutical ingredients (Ott-Dombrowski *et al.*, 2019). For example, 2-chloro-1-(4-hydroxyphenyl)ethanone is a reagent that is used in the preparation of hydroxypyrimidine derivatives for their HDAC (histone deacetylase) inhibitory activity (Kemp *et al.*, 2011). In light of the importance of  $\alpha$ -haloketones, this paper reports the synthesis, crystal structure, and some spectroscopic details for the title compound, C<sub>8</sub>H<sub>7</sub>O<sub>2</sub>Cl, (**I**).



## 2. Structural commentary

The molecule of **I** (Fig. 1) is planar (r.m.s. deviation = 0.0164 Å), with the largest deviation being for Cl1, which is 0.0346 (5) Å from the mean plane through all non-H atoms due to the O2—C7—C8—Cl1 torsion angle of  $-2.07$  (14)°. The hydroxyl hydrogen atom, H1O, which was refined freely, lies 0.045 (16) Å out of the mean plane, with a C2—C3—O1—H1O torsion angle of  $1.8$  (12)°, its position being mandated by intermolecular hydrogen bonding (see section 3, *Supramolecular details*). All bond lengths and angles fall within the expected ranges for organic structures.



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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1-H1O\cdots O2^i$	0.803 (17)	2.004 (18)	2.8029 (12)	173.4 (16)
$C2-H2\cdots O2^i$	0.945 (15)	2.547 (15)	3.2633 (14)	132.7 (11)
$C8-H8A\cdots O1^{ii}$	0.99	2.36	3.3485 (14)	176

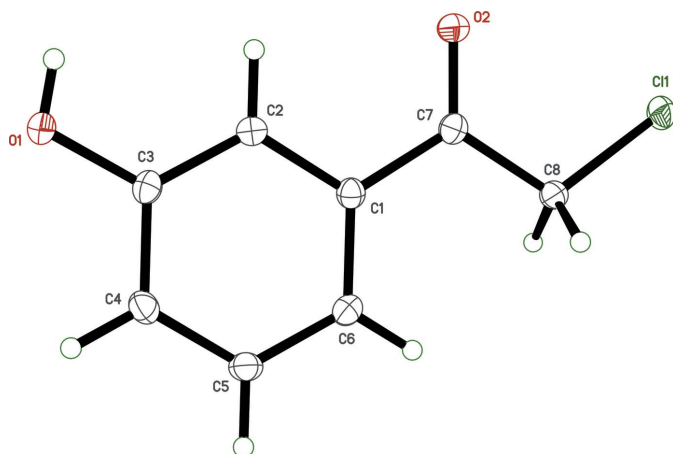
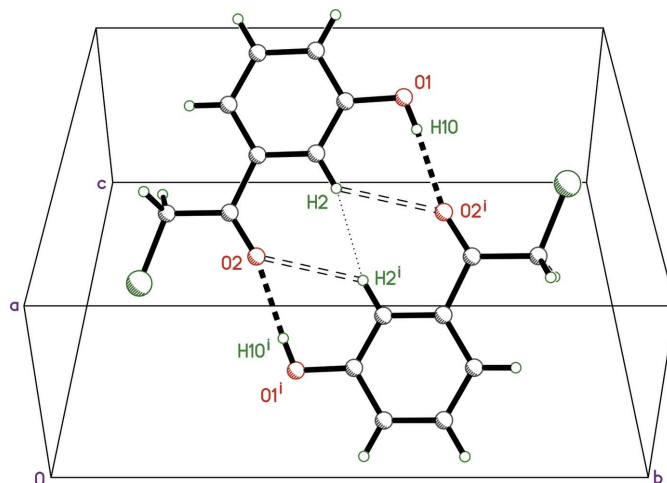
 Symmetry codes: (i)  $-x + 1, -y + 1, -z + 1$ ; (ii)  $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ .

### 3. Supramolecular features

The main supramolecular feature is an inversion dimer resulting from a pair of symmetrically equivalent hydrogen bonds,  $O1-H1O\cdots O2^i$  and  $O1^i-H1O^i\cdots O2$  [symmetry code: (i)  $-x + 1, -y + 1, -z + 1$ ], giving an  $R_2^2(14)$  motif. The cohesion of this dimer is augmented by a pair of weak hydrogen bonds,  $C2-H2\cdots O2^i$  and  $C2^i-H2^i\cdots O2$  (Table 1). It also, however, brings inversion-related H2 atoms into unfavourably close proximity [ $H2\cdots H2^i = 2.22$  (3) Å]. These interactions are all illustrated in Fig. 2. Other noteworthy intermolecular contacts are weak  $C8-H8\cdots O1^{ii}$  [symmetry code: (ii)  $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ] interactions between  $2_1$  screw-related molecules, which loosely connect the dimers into layers parallel to  $(10\bar{1})$ . Almost all of the atom–atom contact coverages quantified in a Hirshfeld-surface analysis using *CrystalExplorer* (Spackman *et al.*, 2021) involve hydrogen ( $H\cdots H = 26.6\%$ ,  $H\cdots O/O\cdots H = 23.7\%$ ,  $H\cdots Cl/Cl\cdots H = 21.2\%$ ,  $H\cdots C/C\cdots H = 15.8\%$ ), with all other contact types being <5%. Further details are given in individual Hirshfeld-surface fingerprint plots (Fig. 3).

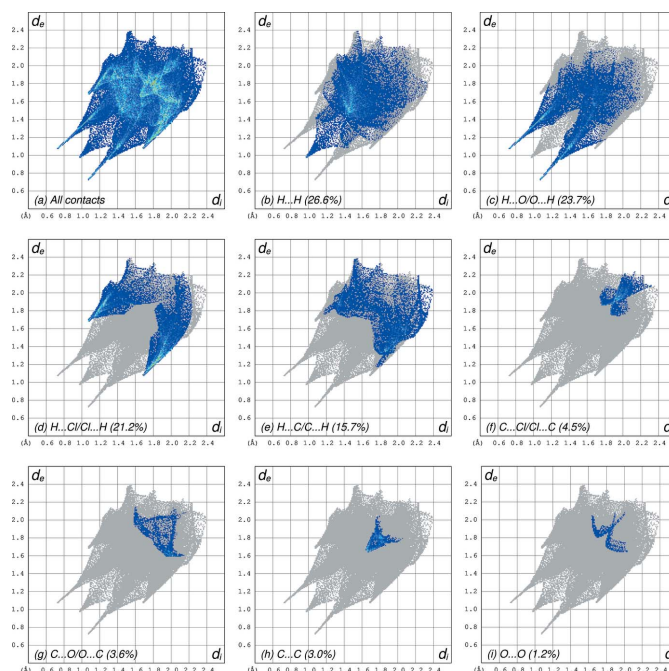
### 4. Database survey

A search of the Cambridge Structure Database (v5.43 with updates as of June 2022; Groom *et al.*, 2016) for a search fragment consisting of the structure of **I** but with the OH and Cl groups replaced by ‘any non-H’ gave 71 hits. If the Cl site is specified as ‘any halogen’, there are just four hits, only three of which are unique, and all have Br as the halogen. Structure


**Figure 1**  
 An ellipsoid plot (50% probability) of **I**. Hydrogen atoms are drawn as small circles.

**Figure 2**

A partial packing plot showing the main supramolecular motif in **I**: a hydrogen-bonded dimer between inversion-related [symmetry code: (i)  $-x + 1, -y + 1, -z + 1$ ] molecules. Strong  $O-H\cdots O$  hydrogen bonds are shown as thick dashed lines, weaker  $C-H\cdots O$  interactions as open dashed lines, and an unfavourable, forced close contact between hydrogen atoms as a dotted line.

AWOCAS (Aldeborgh *et al.*, 2014) is chemically a Br analogue of **I**, but its crystal structure is quite different (triclinic  $P\bar{1}$  vs  $P2_1/n$  for **I**). QAJNAS (Jasinski *et al.*, 2011) [and QAJNAS01 (Mounir *et al.*, 2013)] has  $NO_2$  in place of the hydroxyl. Lastly,


**Figure 3**

Hirshfeld surface fingerprint plots showing the relative contributions of various atom–atom contacts in the packing of **I**. (a) All contacts, (b)  $H\cdots H$  (26.6%), (c)  $H\cdots O/O\cdots H$  (23.7%), (d)  $H\cdots Cl/Cl\cdots H$  (21.2%), (e)  $H\cdots C/C\cdots H$  (15.7%), (f)  $C\cdots Cl/Cl\cdots C$  (4.5%), (g)  $C\cdots O/O\cdots C$  (3.6%), (h)  $C\cdots C$  (3.0%), (i)  $O\cdots O$  (1.2%). All other contact types are <1%.

**Table 2**  
Experimental details.

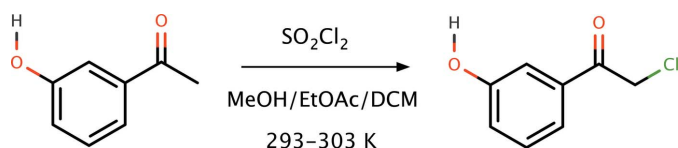
Crystal data	
Chemical formula	C <sub>8</sub> H <sub>7</sub> ClO <sub>2</sub>
<i>M<sub>r</sub></i>	170.59
Crystal system, space group	Monoclinic, <i>P</i> <sub>2</sub> <sub>1</sub> / <i>n</i>
Temperature (K)	90
<i>a</i> , <i>b</i> , <i>c</i> (Å)	4.9172 (2), 12.7016 (4), 11.8573 (3)
β (°)	96.294 (1)
<i>V</i> (Å <sup>3</sup> )	736.10 (4)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm <sup>-1</sup> )	0.46
Crystal size (mm)	0.25 × 0.22 × 0.19
Data collection	
Diffractometer	Bruker D8 Venture dual source
Absorption correction	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.855, 0.971
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	12264, 1685, 1569
<i>R</i> <sub>int</sub>	0.028
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.650
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.024, 0.067, 1.04
No. of reflections	1685
No. of parameters	106
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	0.35, -0.18

Computer programs: *APEX3* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL2019/2* (Sheldrick, 2015b), *XP* in *SHELXTL* and *SHELX* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

MEXCOJ (Ambekar *et al.*, 2013) has OC=Oph in place of the OH in **I**. Other similar structures in the literature include: LEFNAN (Fun *et al.*, 2012), which is the 4-hydroxyphenyl analogue of **I** and crystallizes with the symmetry of *P*<sub>2</sub><sub>1</sub>/*c*; FUHHOG (Qing & Zhang, 2009), which is the bromo analogue of LEFNAN; and CUYDOR (Mei *et al.*, 2015), which has 4-fluorophenyl in place of the halogen of LEFNAN and FUHHOG.

## 5. Synthesis, crystallization and spectroscopic details

**Synthesis and crystallization:** For the synthesis of **I**, sulfuryl chloride (150 mg, 1.1 mmol) was added dropwise to a stirred mixture of 3-hydroxyacetophenone (100 mg, 0.74 mmol) in 5 ml of methanol and 10 ml of ethyl acetate/dichloromethane at 293–303 K. After completion of the addition, it was allowed to return to RT with stirring for 1 h. The reaction was monitored by TLC. Then the solvent was removed under reduced



**Figure 4**  
The overall reaction scheme for the synthesis of **I**.

pressure by rotary evaporation to give the desired product in 95% yield. An overall reaction scheme is depicted in Fig. 4. X-ray quality crystals were obtained by crystallization from ethanol (m.p. 352–354 K).

**Spectroscopic data:** Infrared and NMR spectroscopic details are as follows.

FTIR (γ in cm<sup>-1</sup>): 3400 (Ar–OH, broad), 2987 (C–H stretching), 1694 (C=C stretching), 1789 (*s*, C=O stretching), 832 (*s*, Ar–C–H bending).

<sup>1</sup>H NMR: CDCl<sub>3</sub> (400 MHz, δ ppm): 4.7 (*s*, 2H, –CH<sub>2</sub>), 5.671 (*s*, 1H, –OH), 7.14 (*d*, 1H, Ar–H, *J* = 4.8 Hz), 7.36–7.4 (*t*, 2H, Ar–H, *J* = 16 Hz), 7.493–7.51 (*m*, 1H, Ar–H, *J* = 6.4 Hz).

## 6. Refinement

Crystal data, data collection, and structure refinement details are given in Table 2. All hydrogen atoms were found in difference-Fourier maps, but subsequently, the carbon-bound hydrogens were included using riding models, with constrained distances set to 0.95 Å (Csp<sup>2</sup>–H) and 0.99 Å (R<sub>2</sub>CH<sub>2</sub>). The hydroxyl hydrogen atom coordinates were refined freely. In all cases, *U*<sub>iso</sub>(H) values were set to 1.2*U*<sub>eq</sub> of the attached atom.

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## References

- Aldeborgh, H., George, K., Howe, M., Lowman, H., Moustakas, H., Strunsky, N. & Tanski, J. M. (2014). *J. Chem. Crystallogr.* **44**, 70–81.
- Ambekar, S. P., Devarajegowda, H. C., ShylajaKumari, J., Kumar, K. M. & Kotresh, O. (2013). *Acta Cryst.* **E69**, o322.
- Bruker (2016). *APEX3*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Erian, A. W., Sherif, S. M. & Gaber, H. M. (2003). *Molecules*, **8**, 793–865.
- Fun, H.-K., Quah, C. K., Shetty, D. N., Narayana, B. & Sarojini, B. K. (2012). *Acta Cryst.* **E68**, o2424.
- Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* **B72**, 171–179.
- Jasinski, J. P., Butcher, R. J., Praveen, A. S., Yathirajan, H. S. & Narayana, B. (2011). *Acta Cryst.* **E67**, o29–o30.
- Kemp, M. M., Wang, Q., Fuller, J. H., West, N., Martinez, N. M., Morse, E. M., Weïwer, M., Schreiber, S. L., Bradner, J. E. & Koehler, A. N. (2011). *Bioorg. Med. Chem. Lett.* **21**, 4164–4169.
- Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
- Mei, Q., Liu, H. & Han, B. (2015). *CSD Communication* (refcode CUYDOR). CCDC, Cambridge, England.
- Mounir, F., Gandour, R. D. & Fronczek, F. (2013). *CSD Communication* (refcode QAJNAS01). CCDC, Cambridge, England.
- Ott-Dombrowski, S., Rüter, H. & Ulrich, R. (2019). European patent EP3498687A1.

Qing, W.-X. & Zhang, W. (2009). *Acta Cryst.* **E65**, o2837.  
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.  
Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.

Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.  
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

## supporting information

*Acta Cryst.* (2022). E78, 1127-1130 [https://doi.org/10.1107/S2056989022009835]

## Synthesis and crystal structure of 2-chloro-1-(3-hydroxyphenyl)ethanone

**Prabhakar Priyanka, Bidarur K. Jayanna, Vinaya, Holehundi J. Shankara Prasad, Thayamma R. Divakara, Hemmige S. Yathirajan and Sean Parkin**

### Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *APEX3* (Bruker, 2016); data reduction: *APEX3* (Bruker, 2016); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2019/2* (Sheldrick, 2015b); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELX* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

### 2-Chloro-1-(3-hydroxyphenyl)ethanone

#### Crystal data

$C_8H_7ClO_2$

$M_r = 170.59$

Monoclinic,  $P2_1/n$

$a = 4.9172$  (2) Å

$b = 12.7016$  (4) Å

$c = 11.8573$  (3) Å

$\beta = 96.294$  (1)°

$V = 736.10$  (4) Å<sup>3</sup>

$Z = 4$

$F(000) = 352$

$D_x = 1.539$  Mg m<sup>-3</sup>

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

Cell parameters from 9994 reflections

$\theta = 2.4$ – $27.5$ °

$\mu = 0.46$  mm<sup>-1</sup>

$T = 90$  K

Cut block, colourless

$0.25 \times 0.22 \times 0.19$  mm

#### Data collection

Bruker D8 Venture dual source  
diffractometer

Radiation source: microsource

Detector resolution: 7.41 pixels mm<sup>-1</sup>

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(*SADABS*; Krause *et al.*, 2015)

$T_{\min} = 0.855$ ,  $T_{\max} = 0.971$

12264 measured reflections

1685 independent reflections

1569 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.028$

$\theta_{\max} = 27.5$ °,  $\theta_{\min} = 2.4$ °

$h = -6 \rightarrow 6$

$k = -15 \rightarrow 16$

$l = -15 \rightarrow 15$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.067$

$S = 1.04$

1685 reflections

106 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

Hydrogen site location: mixed

H atoms treated by a mixture of independent  
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0323P)^2 + 0.366P]$

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

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

$\Delta\rho_{\max} = 0.35$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.18$  e Å<sup>-3</sup>

*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.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	1.05641 (18)	0.59830 (6)	0.66167 (7)	0.01786 (19)
H1O	0.938 (3)	0.6217 (12)	0.6166 (14)	0.021*
O2	0.38728 (17)	0.32908 (6)	0.48648 (7)	0.01810 (19)
Cl1	0.22134 (5)	0.10971 (2)	0.48449 (2)	0.01719 (10)
C1	0.7757 (2)	0.33060 (8)	0.62318 (9)	0.0131 (2)
C2	0.8093 (2)	0.43878 (9)	0.60814 (9)	0.0140 (2)
H2	0.686 (3)	0.4757 (12)	0.5553 (12)	0.017*
C3	1.0190 (2)	0.49212 (9)	0.67174 (9)	0.0139 (2)
C4	1.1997 (2)	0.43790 (9)	0.74969 (9)	0.0151 (2)
H4	1.345037	0.474217	0.792591	0.018*
C5	1.1662 (2)	0.33023 (9)	0.76434 (9)	0.0157 (2)
H5	1.289511	0.293235	0.817524	0.019*
C6	0.9546 (2)	0.27607 (9)	0.70220 (9)	0.0147 (2)
H6	0.931888	0.202668	0.713351	0.018*
C7	0.5426 (2)	0.27915 (8)	0.55286 (9)	0.0133 (2)
C8	0.5108 (2)	0.16148 (9)	0.56861 (10)	0.0148 (2)
H8A	0.493730	0.146717	0.649517	0.018*
H8B	0.677307	0.125426	0.548476	0.018*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0212 (4)	0.0116 (4)	0.0191 (4)	−0.0027 (3)	−0.0048 (3)	0.0006 (3)
O2	0.0185 (4)	0.0146 (4)	0.0198 (4)	−0.0007 (3)	−0.0042 (3)	0.0025 (3)
Cl1	0.01466 (15)	0.01477 (15)	0.02144 (16)	−0.00314 (9)	−0.00114 (11)	−0.00204 (10)
C1	0.0128 (5)	0.0128 (5)	0.0137 (5)	−0.0003 (4)	0.0021 (4)	−0.0010 (4)
C2	0.0143 (5)	0.0132 (5)	0.0141 (5)	0.0006 (4)	−0.0001 (4)	0.0008 (4)
C3	0.0160 (5)	0.0120 (5)	0.0141 (5)	−0.0006 (4)	0.0030 (4)	−0.0012 (4)
C4	0.0142 (5)	0.0162 (5)	0.0146 (5)	−0.0004 (4)	−0.0004 (4)	−0.0032 (4)
C5	0.0159 (5)	0.0157 (5)	0.0150 (5)	0.0033 (4)	−0.0006 (4)	−0.0001 (4)
C6	0.0161 (5)	0.0121 (5)	0.0159 (5)	0.0010 (4)	0.0020 (4)	0.0000 (4)
C7	0.0136 (5)	0.0129 (5)	0.0138 (5)	0.0000 (4)	0.0029 (4)	−0.0006 (4)
C8	0.0125 (5)	0.0126 (5)	0.0184 (5)	−0.0011 (4)	−0.0020 (4)	0.0005 (4)

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

O1—C3	1.3682 (13)	C3—C4	1.3922 (16)
O1—H1O	0.803 (17)	C4—C5	1.3906 (16)
O2—C7	1.2138 (14)	C4—H4	0.9500

C11—C8	1.7725 (11)	C5—C6	1.3892 (16)
C1—C6	1.3967 (15)	C5—H5	0.9500
C1—C2	1.3978 (15)	C6—H6	0.9500
C1—C7	1.4921 (15)	C7—C8	1.5164 (15)
C2—C3	1.3857 (15)	C8—H8A	0.9900
C2—H2	0.945 (15)	C8—H8B	0.9900
C3—O1—H1O	109.2 (11)	C6—C5—H5	119.6
C6—C1—C2	119.91 (10)	C4—C5—H5	119.6
C6—C1—C7	123.12 (10)	C5—C6—C1	119.35 (10)
C2—C1—C7	116.97 (10)	C5—C6—H6	120.3
C3—C2—C1	120.16 (10)	C1—C6—H6	120.3
C3—C2—H2	120.1 (9)	O2—C7—C1	121.59 (10)
C1—C2—H2	119.7 (9)	O2—C7—C8	121.91 (10)
O1—C3—C2	122.25 (10)	C1—C7—C8	116.50 (9)
O1—C3—C4	117.6 (1)	C7—C8—C11	112.57 (8)
C2—C3—C4	120.15 (10)	C7—C8—H8A	109.1
C5—C4—C3	119.57 (10)	C11—C8—H8A	109.1
C5—C4—H4	120.2	C7—C8—H8B	109.1
C3—C4—H4	120.2	C11—C8—H8B	109.1
C6—C5—C4	120.86 (10)	H8A—C8—H8B	107.8
C6—C1—C2—C3	-0.24 (16)	C2—C1—C6—C5	-0.61 (16)
C7—C1—C2—C3	179.06 (10)	C7—C1—C6—C5	-179.86 (10)
C1—C2—C3—O1	-178.62 (10)	C6—C1—C7—O2	178.50 (11)
C1—C2—C3—C4	0.97 (16)	C2—C1—C7—O2	-0.77 (15)
O1—C3—C4—C5	178.75 (10)	C6—C1—C7—C8	-1.61 (15)
C2—C3—C4—C5	-0.85 (16)	C2—C1—C7—C8	179.11 (9)
C3—C4—C5—C6	0.00 (17)	O2—C7—C8—C11	-2.07 (14)
C4—C5—C6—C1	0.73 (17)	C1—C7—C8—C11	178.05 (7)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1O $\cdots$ O2 <sup>i</sup>	0.803 (17)	2.004 (18)	2.8029 (12)	173.4 (16)
C2—H2 $\cdots$ O2 <sup>i</sup>	0.945 (15)	2.547 (15)	3.2633 (14)	132.7 (11)
C8—H8A $\cdots$ O1 <sup>ii</sup>	0.99	2.36	3.3485 (14)	176

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