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# 3-Chloro-4-hydroxy-4′-methylbenzophenone

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**Key indicators**

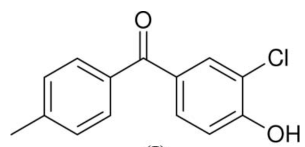
Single-crystal X-ray study
*T* = 120 K
Mean σ(C–C) = 0.002 Å
*R* factor = 0.041
*wR* factor = 0.115
Data-to-parameter ratio = 17.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{14}H_{11}ClO_2$, possesses normal geometrical parameters. The two benzene rings are twisted by 54.70 (4)°, perhaps as a result of steric repulsion between H atoms. The crystal packing is consolidated by an O—H···O hydrogen bond, $\pi$–$\pi$ stacking and C—H···O and C—H···$\pi$ interactions, resulting in a two-dimensional network.

## Comment

The title compound, (I) (Fig. 1), is an intermediate for the synthesis of podophyllotoxin and its derivatives which have pharmaceutical applications (Basavaraju & Devaraju, 2002). More generally, benzophenone derivatives have many applications in organic chemistry (Sieron *et al.*, 2004; Khanum *et al.*, 2005).




(I)

Compound (I) possesses normal geometrical parameters (Allen *et al.*, 1995). The dihedral angle, $\delta$, between the mean planes of the two benzene rings (atoms C1–C6 and C8–C13) is 54.70 (4)°. The C—$C_c$ ($c$ = carbonyl) C6—C7 [1.480 (2) Å] and C7—C8 [1.482 (2) Å] bond lengths are only slightly shorter than normal C—C single bonds, indicating negligible conjugation between the two aromatic ring systems. The rings may be twisted as a result of steric repulsion between the C5 and C9 H atoms (H5···H9 = 2.40 Å; van der Waals contact distance = 2.40 Å), although we note that H9 also participates in a C—H···O interaction (see below). Many other substituted benzophenones possess similar geometrical parameters for the equivalent distances and angles. For example, in 4-dimethylamino-4′-[bis(2-hydroxyethyl)amino]benzophenone

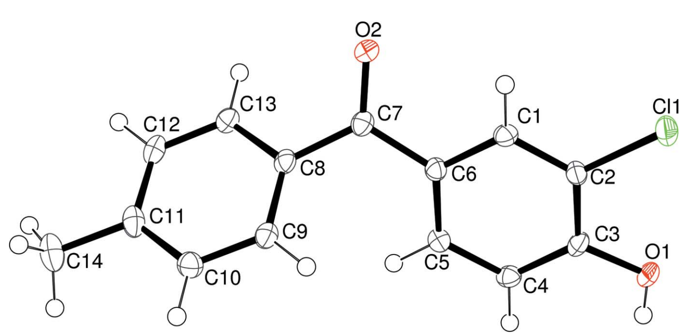



**Figure 1**
The molecular structure of (I), with 50% probability displacement ellipsoids (arbitrary spheres for the H atoms).

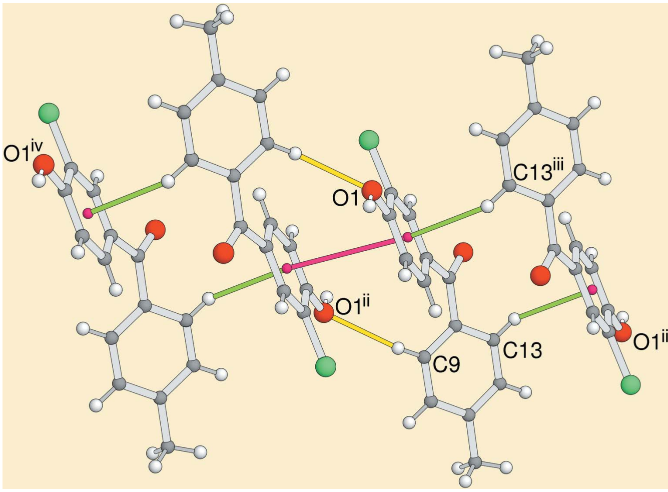



**Figure 2**
Detail of (I) showing how $\pi$–$\pi$ stacking (pink line) and C—H$\cdots$O (yellow lines) and C—H$\cdots\pi$ (green lines) weak intermolecular interactions help to establish the crystal packing. Symmetry codes as in Table 1; additionally (iv) $1 - x, 1 - y, -z$.

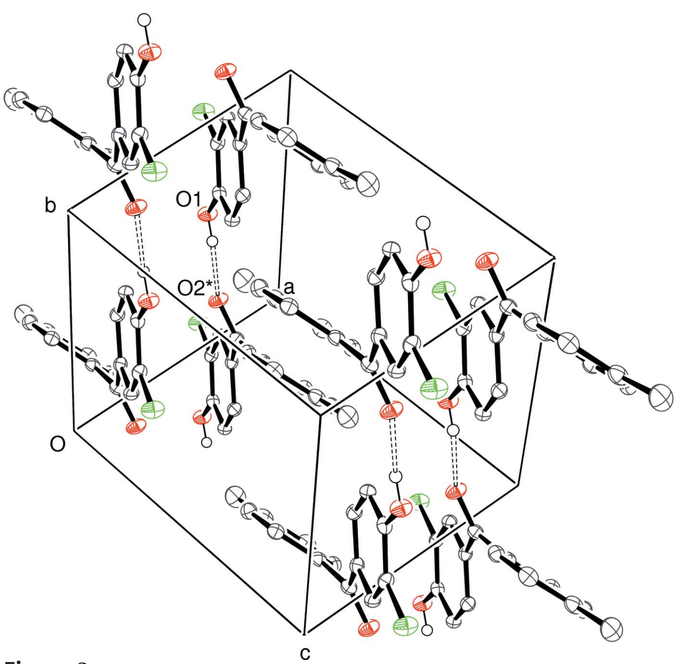



**Figure 3**
The packing for (I), with all H atoms except H1 omitted for clarity. The O—H$\cdots$O hydrogen bond is indicated by a dashed line. The molecule containing O2* is generated by the symmetry code ($x$, $1 + y$, $z$).

(El Sayed *et al.*, 2001), H$\cdots$H = 2.38 Å, C—$C_c$ = 1.460 (3) and 1.484 (3) Å, and $\delta$ = 47.4 (1)°, and in (3-chlorophenyl)(2-hydroxy-5-methylphenyl)methanone (Khanum *et al.*, 2005) H$\cdots$H = 2.52 Å, C—$C_c$ = 1.468 (3) and 1.493 (3) Å, and $\delta$ = 57.37 (12)°.

As well as van der Waals forces, the crystal packing in (I) appears to be controlled by several different intermolecular interactions (Table 1). The most clearcut is an O—H$\cdots$O hydrogen bond that links adjacent molecules of (I) in the *b*-axis direction. Fig. 2 shows that $\pi$–$\pi$ stacking occurs between adjacent inversion-related C1–C6 benzene rings, with a centroid–centroid separation of 3.7642 (10) Å and an interplanar distance of 3.357 Å. Additionally, a *PLATON* (Spek, 2003) analysis of (I) identified probable C—H$\cdots$O and C—H$\cdots\pi$ interactions (Table 1). Together, these interactions lead to a two-dimensional network that propagates in the *ab* plane. The packing is shown in Fig. 3.

## Experimental

A solution of *o*-chlorophenol (1 g, 0.0077 mol) in dry dichloromethane (10 ml) was treated with anhydrous aluminium chloride (1.037 g, 0.0077 mol). The reaction mixture was stirred continuously for 30 min and then cooled. To this, a solution of toluoyl chloride (1.203 g, 0.0077 mol) in methylene chloride (10 ml) was added dropwise and the mixture kept overnight. After 24 h, about 5 ml of concentrated HCl was added and the reaction mixture was stirred for another 24 h. Aqueous NaCl solution (10%) was added to break the emulsion and the lower organic layer was separated and washed with 10% brine. Excess dichloromethane was distilled off on a water bath. The concentrated solution was kept overnight, resulting in a pale-brown solid (yield: 89.2%; m.p. 352 K). Colourless single crystals of (I) were recrystallized from a 1:1 mixture of acetone and acetonitrile.

*Crystal data*

$C_{14}H_{11}ClO_2$
$M_r$ = 246.68
Triclinic, $P\overline{1}$
$a$ = 7.1062 (3) Å
$b$ = 8.5441 (5) Å
$c$ = 9.8766 (6) Å
$\alpha$ = 86.124 (3)°
$\beta$ = 83.804 (3)°
$\gamma$ = 77.290 (3)°
$V$ = 580.96 (5) Å$^3$
$Z$ = 2
$D_x$ = 1.410 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 2534 reflections
$\theta$ = 2.9–27.5°
$\mu$ = 0.31 mm$^{-1}$
$T$ = 120 (2) K
Cut block, colourless
0.32 × 0.16 × 0.10 mm

*Data collection*

Nonius KappaCCD diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
$T_{min}$ = 0.906, $T_{max}$ = 0.969
11199 measured reflections
2684 independent reflections
2037 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048
$\theta_{max}$ = 27.8°
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -12 \rightarrow 12$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.115
$S$ = 1.05
2684 reflections
158 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0595P)^2 + 0.1677P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| O1—H1$\cdots$O2$^{i}$ | 0.78 (2) | 1.93 (2) | 2.6418 (17) | 150 (2) |
| C9—H9$\cdots$O1$^{ii}$ | 0.95 | 2.48 | 3.375 (2) | 157 |
| C13—H13$\cdots$$Cg1^{iii}$ | 0.95 | 2.59 | 3.3908 (17) | 142 |

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+2, -y+1, -z$; (iii) $-x+1, -y+2, -z$. $Cg1$ is the centroid of the C1–C6 ring

The hydroxy H atom was located in a difference map and its position was freely refined with the constraint $U_{iso}(H) = 1.2U_{eq}(O)$. Other H atoms were placed in calculated positions (C—H = 0.95–0.98 Å) and refined as riding, with $U_{iso}(H) = 1.2U_{eq}$(carrier) or $1.5U_{eq}$(methyl carrier). The $-CH_3$ group was rotated to fit the electron density.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997) and *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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# supporting information

*Acta Cryst.* (2005). E**61**, o4146–o4148 [https://doi.org/10.1107/S1600536805036780]

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$Z$ = 2
$F$(000) = 256
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Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2534 reflections
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$T$ = 120 K
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*Data collection*

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Radiation source: fine-focus sealed tube
Graphite monochromator
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Absorption correction: multi-scan (SADABS; Bruker, 2003)
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11199 measured reflections
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$\theta_{max}$ = 27.8°, $\theta_{min}$ = 3.3°
$h$ = −9→9
$k$ = −11→11
$l$ = −12→12

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.115
$S$ = 1.05
2684 reflections
158 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difmap (O-H) and geom (others)
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0595P)^2 + 0.1677P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 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.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted $R$-factor $wR$ and goodness 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 threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating $R$-factors(gt) *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)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.8691 (2) | 0.7775 (2) | −0.13871 (18) | 0.0173 (4) |
| H2 | 0.9198 | 0.8558 | −0.1953 | 0.021* |
| C2 | 0.8806 (2) | 0.6279 (2) | −0.18629 (17) | 0.0169 (4) |
| C3 | 0.8048 (2) | 0.5108 (2) | −0.10592 (18) | 0.0171 (4) |
| C4 | 0.7215 (2) | 0.5473 (2) | 0.02553 (18) | 0.0179 (4) |
| H4 | 0.6712 | 0.4686 | 0.0820 | 0.021* |
| C5 | 0.7113 (2) | 0.6977 (2) | 0.07467 (18) | 0.0176 (4) |
| H5 | 0.6550 | 0.7208 | 0.1647 | 0.021* |
| C6 | 0.7830 (2) | 0.8149 (2) | −0.00730 (17) | 0.0164 (4) |
| C7 | 0.7567 (2) | 0.9819 (2) | 0.03481 (18) | 0.0175 (4) |
| C8 | 0.7257 (2) | 1.0217 (2) | 0.18041 (18) | 0.0171 (4) |
| C9 | 0.8176 (3) | 0.9232 (2) | 0.28295 (18) | 0.0188 (4) |
| H9 | 0.8970 | 0.8213 | 0.2621 | 0.023* |
| C10 | 0.7929 (3) | 0.9743 (2) | 0.41554 (19) | 0.0213 (4) |
| H10 | 0.8573 | 0.9070 | 0.4845 | 0.026* |
| C11 | 0.6753 (3) | 1.1224 (2) | 0.44931 (19) | 0.0225 (4) |
| C12 | 0.5813 (3) | 1.2185 (2) | 0.34659 (19) | 0.0219 (4) |
| H12 | 0.4984 | 1.3189 | 0.3680 | 0.026* |
| C13 | 0.6067 (2) | 1.1701 (2) | 0.21448 (18) | 0.0186 (4) |
| H13 | 0.5428 | 1.2382 | 0.1457 | 0.022* |
| C14 | 0.6528 (3) | 1.1784 (3) | 0.5928 (2) | 0.0324 (5) |
| H14A | 0.5353 | 1.2631 | 0.6058 | 0.049* |
| H14B | 0.7659 | 1.2207 | 0.6083 | 0.049* |
| H14C | 0.6426 | 1.0879 | 0.6576 | 0.049* |
| O1 | 0.81397 (19) | 0.36984 (15) | −0.16234 (13) | 0.0220 (3) |
| H1 | 0.780 (3) | 0.308 (3) | −0.108 (2) | 0.026* |
| O2 | 0.75791 (19) | 1.09033 (14) | −0.05454 (13) | 0.0235 (3) |
| Cl1 | 0.99046 (7) | 0.58148 (5) | −0.34839 (5) | 0.02638 (17) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0197 (9) | 0.0155 (8) | 0.0175 (9) | −0.0062 (7) | −0.0020 (7) | 0.0008 (7) |
| C2 | 0.0189 (9) | 0.0175 (9) | 0.0138 (9) | −0.0020 (7) | −0.0013 (7) | −0.0027 (7) |
| C3 | 0.0182 (8) | 0.0122 (8) | 0.0215 (9) | −0.0023 (7) | −0.0055 (7) | −0.0035 (7) |
| C4 | 0.0195 (9) | 0.0163 (9) | 0.0191 (9) | −0.0066 (7) | −0.0029 (7) | 0.0017 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C5 | 0.0188 (9) | 0.0182 (9) | 0.0157 (9) | −0.0037 (7) | −0.0015 (7) | −0.0012 (7) |
| C6 | 0.0176 (9) | 0.0162 (8) | 0.0156 (9) | −0.0029 (7) | −0.0034 (7) | −0.0020 (7) |
| C7 | 0.0174 (9) | 0.0164 (9) | 0.0196 (9) | −0.0051 (7) | −0.0010 (7) | −0.0025 (7) |
| C8 | 0.0188 (8) | 0.0157 (8) | 0.0188 (9) | −0.0078 (7) | −0.0015 (7) | −0.0027 (7) |
| C9 | 0.0202 (9) | 0.0167 (9) | 0.0203 (9) | −0.0053 (7) | −0.0008 (7) | −0.0033 (7) |
| C10 | 0.0236 (9) | 0.0219 (9) | 0.0203 (10) | −0.0077 (8) | −0.0047 (7) | −0.0002 (7) |
| C11 | 0.0224 (9) | 0.0277 (10) | 0.0203 (10) | −0.0114 (8) | 0.0019 (7) | −0.0082 (8) |
| C12 | 0.0221 (9) | 0.0171 (9) | 0.0266 (10) | −0.0040 (8) | 0.0006 (8) | −0.0079 (8) |
| C13 | 0.0189 (9) | 0.0160 (8) | 0.0217 (10) | −0.0045 (7) | −0.0029 (7) | −0.0023 (7) |
| C14 | 0.0344 (11) | 0.0406 (12) | 0.0239 (11) | −0.0101 (10) | 0.0013 (9) | −0.0137 (9) |
| O1 | 0.0331 (8) | 0.0122 (6) | 0.0218 (7) | −0.0071 (6) | −0.0003 (6) | −0.0035 (5) |
| O2 | 0.0368 (8) | 0.0146 (6) | 0.0192 (7) | −0.0063 (6) | −0.0012 (6) | 0.0000 (5) |
| Cl1 | 0.0371 (3) | 0.0229 (3) | 0.0189 (3) | −0.0084 (2) | 0.00578 (19) | −0.00673 (18) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.374 (2) | C8—C13 | 1.400 (2) |
| C1—C6 | 1.400 (2) | C9—C10 | 1.389 (3) |
| C1—H2 | 0.9500 | C9—H9 | 0.9500 |
| C2—C3 | 1.400 (2) | C10—C11 | 1.393 (3) |
| C2—Cl1 | 1.7349 (17) | C10—H10 | 0.9500 |
| C3—O1 | 1.346 (2) | C11—C12 | 1.394 (3) |
| C3—C4 | 1.393 (2) | C11—C14 | 1.507 (3) |
| C4—C5 | 1.388 (2) | C12—C13 | 1.377 (3) |
| C4—H4 | 0.9500 | C12—H12 | 0.9500 |
| C5—C6 | 1.395 (2) | C13—H13 | 0.9500 |
| C5—H5 | 0.9500 | C14—H14A | 0.9800 |
| C6—C7 | 1.480 (2) | C14—H14B | 0.9800 |
| C7—O2 | 1.236 (2) | C14—H14C | 0.9800 |
| C7—C8 | 1.482 (2) | O1—H1 | 0.78 (2) |
| C8—C9 | 1.395 (2) | | |
| | | | |
| C2—C1—C6 | 120.31 (16) | C13—C8—C7 | 117.82 (15) |
| C2—C1—H2 | 119.8 | C10—C9—C8 | 119.97 (17) |
| C6—C1—H2 | 119.8 | C10—C9—H9 | 120.0 |
| C1—C2—C3 | 121.09 (16) | C8—C9—H9 | 120.0 |
| C1—C2—Cl1 | 120.04 (14) | C9—C10—C11 | 121.24 (17) |
| C3—C2—Cl1 | 118.87 (13) | C9—C10—H10 | 119.4 |
| O1—C3—C4 | 124.00 (16) | C11—C10—H10 | 119.4 |
| O1—C3—C2 | 117.39 (16) | C10—C11—C12 | 118.31 (17) |
| C4—C3—C2 | 118.60 (15) | C10—C11—C14 | 120.88 (18) |
| C5—C4—C3 | 120.55 (16) | C12—C11—C14 | 120.80 (17) |
| C5—C4—H4 | 119.7 | C13—C12—C11 | 120.97 (17) |
| C3—C4—H4 | 119.7 | C13—C12—H12 | 119.5 |
| C4—C5—C6 | 120.45 (16) | C11—C12—H12 | 119.5 |
| C4—C5—H5 | 119.8 | C12—C13—C8 | 120.71 (17) |
| C6—C5—H5 | 119.8 | C12—C13—H13 | 119.6 |
| C5—C6—C1 | 118.97 (15) | C8—C13—H13 | 119.6 |

| | | | |
|---|---|---|---|
| C5—C6—C7 | 122.40 (16) | C11—C14—H14A | 109.5 |
| C1—C6—C7 | 118.42 (15) | C11—C14—H14B | 109.5 |
| O2—C7—C6 | 118.64 (15) | H14A—C14—H14B | 109.5 |
| O2—C7—C8 | 119.70 (15) | C11—C14—H14C | 109.5 |
| C6—C7—C8 | 121.65 (15) | H14A—C14—H14C | 109.5 |
| C9—C8—C13 | 118.79 (16) | H14B—C14—H14C | 109.5 |
| C9—C8—C7 | 123.28 (16) | C3—O1—H1 | 110.8 (17) |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | 0.8 (3) | C1—C6—C7—C8 | −160.64 (15) |
| C6—C1—C2—Cl1 | −179.11 (12) | O2—C7—C8—C9 | −144.16 (17) |
| C1—C2—C3—O1 | 177.04 (16) | C6—C7—C8—C9 | 37.0 (2) |
| Cl1—C2—C3—O1 | −3.0 (2) | O2—C7—C8—C13 | 32.0 (2) |
| C1—C2—C3—C4 | −1.7 (3) | C6—C7—C8—C13 | −146.81 (16) |
| Cl1—C2—C3—C4 | 178.26 (13) | C13—C8—C9—C10 | −1.1 (2) |
| O1—C3—C4—C5 | −177.62 (16) | C7—C8—C9—C10 | 175.03 (16) |
| C2—C3—C4—C5 | 1.0 (3) | C8—C9—C10—C11 | 0.8 (3) |
| C3—C4—C5—C6 | 0.5 (3) | C9—C10—C11—C12 | 0.4 (3) |
| C4—C5—C6—C1 | −1.4 (3) | C9—C10—C11—C14 | −178.65 (17) |
| C4—C5—C6—C7 | 173.28 (16) | C10—C11—C12—C13 | −1.3 (3) |
| C2—C1—C6—C5 | 0.7 (3) | C14—C11—C12—C13 | 177.77 (17) |
| C2—C1—C6—C7 | −174.16 (15) | C11—C12—C13—C8 | 1.0 (3) |
| C5—C6—C7—O2 | −154.18 (17) | C9—C8—C13—C12 | 0.3 (3) |
| C1—C6—C7—O2 | 20.5 (2) | C7—C8—C13—C12 | −176.10 (15) |
| C5—C6—C7—C8 | 24.7 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···O2$^{i}$ | 0.78 (2) | 1.93 (2) | 2.6418 (17) | 150 (2) |
| C9—H9···O1$^{ii}$ | 0.95 | 2.48 | 3.375 (2) | 157 |
| C13—H13···*Cg*1$^{iii}$ | 0.95 | 2.59 | 3.3908 (17) | 142 |

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) −*x*+2, −*y*+1, −*z*; (iii) −*x*+1, −*y*+2, −*z*.