

William T. A. Harrison,<sup>a\*</sup>  
 H. S. Yathirajan,<sup>b</sup> B. K. Sarojini,<sup>c</sup>  
 B. Narayana<sup>d</sup> and J. Indira<sup>e</sup>

<sup>a</sup>Department of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, Scotland, <sup>b</sup>Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, <sup>c</sup>Department of Chemistry, P. A. College of Engineering, Nadupadavu, Mangalore-574 153, India, <sup>d</sup>Department of Chemistry, Mangalore University, Mangalagangotri 574 199, India, and <sup>e</sup>Department of Physics, University College, Mangalore 575 001, India

Correspondence e-mail:  
 w.harrison@abdn.ac.uk

#### Key indicators

Single-crystal X-ray study  
 $T = 120$  K  
 Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.029  
 $wR$  factor = 0.071  
 Data-to-parameter ratio = 16.3

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

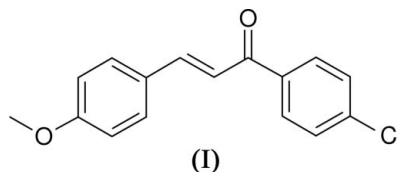
# 1-(4-Chlorophenyl)-3-(4-methoxyphenyl)-prop-2-en-1-one

The geometrical parameters for the title compound,  $\text{C}_{16}\text{H}_{13}\text{ClO}_2$ , are normal. Packing in a non-centrosymmetric space group, which is consistent with the non-zero second harmonic generation response, may be influenced by a  $\text{C}-\text{H} \cdots \text{O}$  interaction.

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#### Comment

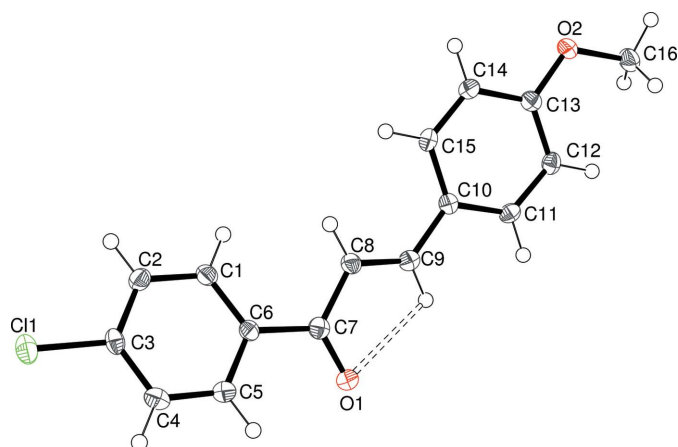
The title compound, (I) (Fig. 1), was prepared as part of our ongoing studies (Indira *et al.*, 2002; Harrison *et al.*, 2005, 2006) of the non-linear optical (NLO) properties of chalcone derivatives (Uchida *et al.*, 1998). The non-centrosymmetric, polar crystal structure of (I) is consistent with its significant second harmonic generation (SHG) response of 0.8 times that of urea (Watson *et al.*, 1993).



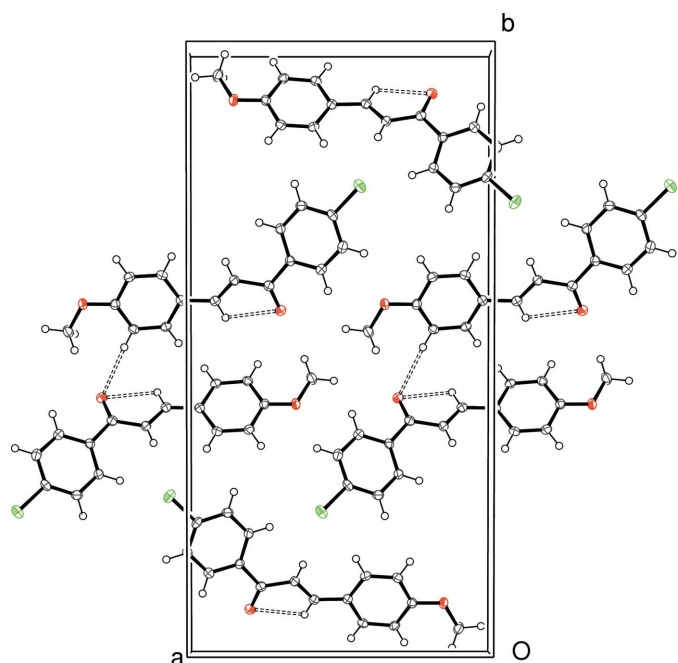
The geometrical parameters for (I) are normal (Allen *et al.*, 1987) and consistent with those of other recently reported chalcone derivatives (Rosli *et al.*, 2006; Patil *et al.*, 2006). Compound (I) complements several closely related molecules with other 4-substituents  $X$  instead of Cl (see scheme), namely (II) with  $X = \text{OH}$  (Moorthi *et al.*, 2005), (III) with  $X = \text{CH}_3$  (Wang *et al.*, 2005), (IV) with  $X = \text{H}$  (Rabinovich & Schmidt, 1970), and (V) with  $X = \text{OCH}_3$  (Zheng *et al.*, 1992). The space groups for (I), (II), (III), (IV) and (V) are  $Pna2_1$ ,  $Pbca$ ,  $P2_1/c$ ,  $P2_1$  and  $P2_12_12_1$ , respectively. The distribution of space groups for this small family is thus consistent with the observation that chalcones are prone to crystallize as non-centrosymmetric structures (Uchida *et al.*, 1998).

The molecule of (I) is distinctly twisted about the  $\text{C}_6-\text{C}_7$  and the  $\text{C}_7-\text{C}_8$  bonds (Table 1), as was also seen for 2-bromo-1-chlorophenyl-3-(4-methoxyphenyl)-2-propen-1-one (Harrison *et al.*, 2006). The dihedral angle between the benzene ring mean planes ( $\text{C}_1-\text{C}_6$  and  $\text{C}_{10}-\text{C}_{15}$ ) in (I) is  $21.82(6)^\circ$ .  $\text{Cl}1$ ,  $\text{C}_7$  and  $\text{O}1$  deviate from the former mean plane by 0.031 (3), 0.022 (3) and 0.346 (3) Å, respectively. The deviations of  $\text{C}_9$ ,  $\text{O}2$  and  $\text{C}_{16}$  from the latter plane are 0.087 (3), 0.038 (3) and 0.049 (3) Å, respectively.

A *PLATON* (Spek, 2003) analysis of (I) indicated a possible intramolecular  $\text{C}_9-\text{H}_9 \cdots \text{O}1$  interaction (Table 2) that might help to maintain the molecular conformation. A similar interaction was proposed for 3-(4-bromophenyl)-1-(4-nitrophenyl)-prop-2-en-1-one (Rosli *et al.*, 2006).



**Figure 1**  
View of (I), showing 50% displacement ellipsoids (arbitrary spheres for the H atoms). The possible intramolecular C—H...O interaction is indicated by a dashed line.



**Figure 2**  
The packing for (I), viewed down [001], with C—H...O interactions shown as dashed lines.

An intermolecular C—H...O hydrogen bond (Fig. 2) appears to help to assemble the molecules of (I) into helical stacks about the  $2_1$  screw axis, propagating in the polar [001] direction.

## Experimental

4-Chloroacetophenone in ethanol (1.54 g, 0.01 mol) (25 ml) was mixed with 4-methoxybenzaldehyde (1.36 g, 0.01 mol) in ethanol (25 ml) and the mixture was treated with an aqueous solution of potassium hydroxide (20 ml, 5%). This mixture was stirred well and left to stand for 24 hr. The resulting crude solid mass was collected by filtration and recrystallized from ethanol, yielding clear blocks of (I).

Yield: 90%, m.p.: 380 K, analysis found (calc.) for  $C_{16}H_{13}ClO_2$ , C 70.5 (70.4%); H 4.72 (4.76%).

## Crystal data

$C_{16}H_{13}ClO_2$   
 $M_r = 272.71$   
Orthorhombic,  $Pna2_1$   
 $a = 12.8179$  (4) Å  
 $b = 25.5550$  (6) Å  
 $c = 3.9175$  (1) Å  
 $V = 1283.22$  (6) Å<sup>3</sup>  
 $Z = 4$   
 $D_x = 1.412$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
Cell parameters from 1708 reflections  
 $\theta = 2.9\text{--}27.5^\circ$   
 $\mu = 0.29$  mm<sup>-1</sup>  
 $T = 120$  (2) K  
Slab, colourless  
 $0.50 \times 0.40 \times 0.20$  mm

## Data collection

Nonius KappaCCD diffractometer  
 $\omega$  and  $\varphi$  scans  
Absorption correction: multi-scan (SADABS; Bruker, 2003)  
 $T_{\min} = 0.868$ ,  $T_{\max} = 0.944$   
8514 measured reflections  
2815 independent reflections

2569 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.028$   
 $\theta_{\text{max}} = 27.5^\circ$   
 $h = -9 \rightarrow 16$   
 $k = -33 \rightarrow 32$   
 $l = -5 \rightarrow 5$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.029$   
 $wR(F^2) = 0.071$   
 $S = 1.04$   
2815 reflections  
173 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2 + 0.2552P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.23$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.22$  e Å<sup>-3</sup>  
Absolute structure: Flack (1983),  
1131 Friedel pairs  
Flack parameter: 0.02 (6)

**Table 1**

Selected geometric parameters (Å, °).

|             |           |             |           |
|-------------|-----------|-------------|-----------|
| C6—C7       | 1.496 (2) | C8—C9       | 1.342 (2) |
| C7—C8       | 1.479 (2) | C9—C10      | 1.461 (2) |
| C5—C6—C7—O1 | 16.7 (2)  | O1—C7—C8—C9 | 6.4 (2)   |

**Table 2**

Hydrogen-bond geometry (Å, °).

| $D-H\cdots A$             | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---------------------------|-------|-------------|-------------|---------------|
| C9—H9...O1                | 0.95  | 2.46        | 2.8065 (19) | 102           |
| C12—H12...O1 <sup>i</sup> | 0.95  | 2.54        | 3.4828 (18) | 175           |

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

H atoms were positioned geometrically (C—H = 0.95–0.98 Å) and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$  or  $1.5U_{\text{eq}}(\text{methyl carrier})$ . The methyl group was rotated to fit the electron density.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor 1997); data reduction: *HKL DENZO* (Otwinowski & Minor 1997), *SCALEPACK* and *SORTAV* (Blessing 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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## supporting information

*Acta Cryst.* (2006). E62, o1647–o1649 [https://doi.org/10.1107/S1600536806010865]

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*Crystal data*

$C_{16}H_{13}ClO_2$

$M_r = 272.71$

Orthorhombic,  $Pna2_1$

Hall symbol: P 2c -2n

$a = 12.8179$  (4) Å

$b = 25.5550$  (6) Å

$c = 3.9175$  (1) Å

$V = 1283.22$  (6) Å<sup>3</sup>

$Z = 4$

$F(000) = 568$

$D_x = 1.412$  Mg m<sup>-3</sup>

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

Cell parameters from 1708 reflections

$\theta = 2.9$ – $27.5^\circ$

$\mu = 0.29$  mm<sup>-1</sup>

$T = 120$  K

Slab, colourless

$0.50 \times 0.40 \times 0.20$  mm

*Data collection*

Nonius KappaCCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

$\omega$  and  $\phi$  scans

Absorption correction: multi-scan

(SADABS; Bruker, 2003)

$T_{\min} = 0.868$ ,  $T_{\max} = 0.944$

8514 measured reflections

2815 independent reflections

2569 reflections with  $I > 2\sigma(I)$

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

$\theta_{\max} = 27.5^\circ$ ,  $\theta_{\min} = 3.2^\circ$

$h = -9 \rightarrow 16$

$k = -33 \rightarrow 32$

$l = -5 \rightarrow 5$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.029$

$wR(F^2) = 0.071$

$S = 1.04$

2815 reflections

173 parameters

1 restraint

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: none

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2 + 0.2552P]$

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

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

$\Delta\rho_{\max} = 0.23$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.22$  e Å<sup>-3</sup>

Absolute structure: Flack (1983), 1131 Friedel

pairs

Absolute structure parameter: 0.02 (6)

*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 ( $\text{\AA}^2$ )*

|      | $x$           | $y$           | $z$          | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|---------------|---------------|--------------|----------------------------------|
| C1   | 0.19574 (12)  | 0.20035 (6)   | 0.2960 (4)   | 0.0205 (4)                       |
| H1   | 0.2650        | 0.2112        | 0.2462       | 0.025*                           |
| C2   | 0.12683 (13)  | 0.23537 (5)   | 0.4453 (5)   | 0.0218 (3)                       |
| H2   | 0.1483        | 0.2700        | 0.4976       | 0.026*                           |
| C3   | 0.02617 (12)  | 0.21890 (6)   | 0.5169 (4)   | 0.0200 (3)                       |
| C4   | -0.00692 (12) | 0.16853 (6)   | 0.4450 (5)   | 0.0236 (3)                       |
| H4   | -0.0760       | 0.1577        | 0.4979       | 0.028*                           |
| C5   | 0.06269 (12)  | 0.13431 (6)   | 0.2947 (4)   | 0.0222 (4)                       |
| H5   | 0.0407        | 0.0997        | 0.2424       | 0.027*                           |
| C6   | 0.16443 (10)  | 0.14935 (5)   | 0.2180 (5)   | 0.0173 (3)                       |
| C7   | 0.23496 (12)  | 0.11027 (6)   | 0.0517 (4)   | 0.0190 (3)                       |
| C8   | 0.34886 (12)  | 0.11936 (6)   | 0.0601 (4)   | 0.0191 (3)                       |
| H8   | 0.3764        | 0.1480        | 0.1861       | 0.023*                           |
| C9   | 0.41349 (11)  | 0.08728 (6)   | -0.1098 (4)  | 0.0185 (3)                       |
| H9   | 0.3813        | 0.0609        | -0.2440      | 0.022*                           |
| C10  | 0.52748 (12)  | 0.08815 (5)   | -0.1131 (4)  | 0.0175 (3)                       |
| C11  | 0.57984 (11)  | 0.04602 (5)   | -0.2616 (4)  | 0.0184 (3)                       |
| H11  | 0.5401        | 0.0193        | -0.3690      | 0.022*                           |
| C12  | 0.68784 (11)  | 0.04173 (5)   | -0.2580 (5)  | 0.0195 (3)                       |
| H12  | 0.7215        | 0.0123        | -0.3569      | 0.023*                           |
| C13  | 0.74565 (12)  | 0.08153 (6)   | -0.1062 (4)  | 0.0190 (3)                       |
| C14  | 0.69544 (12)  | 0.12507 (6)   | 0.0340 (5)   | 0.0210 (3)                       |
| H14  | 0.7355        | 0.1527        | 0.1299       | 0.025*                           |
| C15  | 0.58780 (12)  | 0.12813 (6)   | 0.0338 (4)   | 0.0197 (3)                       |
| H15  | 0.5543        | 0.1575        | 0.1339       | 0.024*                           |
| C16  | 0.90530 (12)  | 0.03755 (6)   | -0.2288 (5)  | 0.0257 (4)                       |
| H16A | 0.9806        | 0.0415        | -0.1942      | 0.039*                           |
| H16B | 0.8903        | 0.0357        | -0.4738      | 0.039*                           |
| H16C | 0.8814        | 0.0054        | -0.1177      | 0.039*                           |
| O1   | 0.19706 (8)   | 0.07117 (4)   | -0.0837 (4)  | 0.0237 (3)                       |
| O2   | 0.85193 (8)   | 0.08157 (4)   | -0.0835 (3)  | 0.0234 (3)                       |
| Cl1  | -0.06159 (3)  | 0.262892 (14) | 0.69857 (14) | 0.02734 (11)                     |

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

|    | $U^{11}$   | $U^{22}$   | $U^{33}$    | $U^{12}$    | $U^{13}$    | $U^{23}$    |
|----|------------|------------|-------------|-------------|-------------|-------------|
| C1 | 0.0165 (7) | 0.0197 (7) | 0.0252 (10) | 0.0001 (6)  | -0.0015 (6) | 0.0032 (6)  |
| C2 | 0.0235 (8) | 0.0168 (6) | 0.0252 (9)  | 0.0001 (6)  | -0.0030 (7) | -0.0002 (6) |
| C3 | 0.0198 (7) | 0.0225 (7) | 0.0179 (8)  | 0.0074 (6)  | -0.0012 (7) | 0.0017 (6)  |
| C4 | 0.0178 (7) | 0.0275 (7) | 0.0256 (9)  | -0.0026 (6) | -0.0001 (7) | 0.0017 (7)  |

|     |              |              |             |              |             |               |
|-----|--------------|--------------|-------------|--------------|-------------|---------------|
| C5  | 0.0202 (7)   | 0.0205 (7)   | 0.0257 (10) | -0.0025 (6)  | -0.0007 (7) | -0.0004 (6)   |
| C6  | 0.0168 (6)   | 0.0186 (6)   | 0.0167 (7)  | 0.0017 (5)   | -0.0036 (7) | 0.0015 (7)    |
| C7  | 0.0206 (8)   | 0.0188 (7)   | 0.0176 (8)  | 0.0009 (6)   | -0.0022 (6) | 0.0047 (6)    |
| C8  | 0.0179 (7)   | 0.0189 (7)   | 0.0204 (8)  | 0.0006 (6)   | -0.0018 (6) | 0.0017 (6)    |
| C9  | 0.0211 (8)   | 0.0182 (6)   | 0.0161 (8)  | -0.0015 (6)  | -0.0007 (7) | 0.0018 (6)    |
| C10 | 0.0182 (7)   | 0.0186 (6)   | 0.0157 (8)  | 0.0011 (6)   | 0.0008 (6)  | 0.0016 (7)    |
| C11 | 0.0223 (7)   | 0.0171 (6)   | 0.0159 (8)  | -0.0025 (5)  | -0.0003 (7) | -0.0013 (6)   |
| C12 | 0.0215 (7)   | 0.0174 (6)   | 0.0198 (9)  | 0.0024 (5)   | 0.0037 (7)  | -0.0005 (6)   |
| C13 | 0.0178 (7)   | 0.0204 (7)   | 0.0189 (8)  | -0.0010 (6)  | 0.0007 (7)  | 0.0030 (6)    |
| C14 | 0.0219 (8)   | 0.0176 (6)   | 0.0234 (9)  | -0.0018 (6)  | -0.0018 (7) | -0.0016 (6)   |
| C15 | 0.0228 (8)   | 0.0163 (7)   | 0.0201 (8)  | 0.0027 (6)   | 0.0012 (7)  | -0.0012 (6)   |
| C16 | 0.0195 (7)   | 0.0276 (7)   | 0.0300 (11) | 0.0052 (6)   | 0.0002 (7)  | -0.0050 (7)   |
| O1  | 0.0211 (6)   | 0.0198 (5)   | 0.0301 (6)  | -0.0011 (4)  | -0.0028 (5) | -0.0037 (5)   |
| O2  | 0.0150 (5)   | 0.0235 (5)   | 0.0318 (7)  | 0.0017 (4)   | -0.0007 (5) | -0.0046 (5)   |
| Cl1 | 0.02487 (18) | 0.03005 (18) | 0.0271 (2)  | 0.00920 (15) | 0.0001 (2)  | -0.00342 (19) |

*Geometric parameters (Å, °)*

|           |             |             |             |
|-----------|-------------|-------------|-------------|
| C1—C2     | 1.387 (2)   | C9—H9       | 0.9500      |
| C1—C6     | 1.3976 (19) | C10—C11     | 1.396 (2)   |
| C1—H1     | 0.9500      | C10—C15     | 1.405 (2)   |
| C2—C3     | 1.386 (2)   | C11—C12     | 1.3888 (19) |
| C2—H2     | 0.9500      | C11—H11     | 0.9500      |
| C3—C4     | 1.384 (2)   | C12—C13     | 1.392 (2)   |
| C3—C11    | 1.7423 (16) | C12—H12     | 0.9500      |
| C4—C5     | 1.381 (2)   | C13—O2      | 1.3653 (18) |
| C4—H4     | 0.9500      | C13—C14     | 1.398 (2)   |
| C5—C6     | 1.392 (2)   | C14—C15     | 1.382 (2)   |
| C5—H5     | 0.9500      | C14—H14     | 0.9500      |
| C6—C7     | 1.496 (2)   | C15—H15     | 0.9500      |
| C7—O1     | 1.2312 (19) | C16—O2      | 1.4344 (19) |
| C7—C8     | 1.479 (2)   | C16—H16A    | 0.9800      |
| C8—C9     | 1.342 (2)   | C16—H16B    | 0.9800      |
| C8—H8     | 0.9500      | C16—H16C    | 0.9800      |
| C9—C10    | 1.461 (2)   |             |             |
| C2—C1—C6  | 120.75 (14) | C10—C9—H9   | 116.1       |
| C2—C1—H1  | 119.6       | C11—C10—C15 | 117.85 (13) |
| C6—C1—H1  | 119.6       | C11—C10—C9  | 118.20 (13) |
| C3—C2—C1  | 118.84 (14) | C15—C10—C9  | 123.91 (14) |
| C3—C2—H2  | 120.6       | C12—C11—C10 | 122.40 (14) |
| C1—C2—H2  | 120.6       | C12—C11—H11 | 118.8       |
| C4—C3—C2  | 121.77 (15) | C10—C11—H11 | 118.8       |
| C4—C3—C11 | 119.04 (12) | C11—C12—C13 | 118.51 (14) |
| C2—C3—C11 | 119.19 (12) | C11—C12—H12 | 120.7       |
| C5—C4—C3  | 118.53 (15) | C13—C12—H12 | 120.7       |
| C5—C4—H4  | 120.7       | O2—C13—C12  | 124.03 (13) |
| C3—C4—H4  | 120.7       | O2—C13—C14  | 115.67 (13) |

|              |              |                 |              |
|--------------|--------------|-----------------|--------------|
| C4—C5—C6     | 121.49 (14)  | C12—C13—C14     | 120.30 (14)  |
| C4—C5—H5     | 119.3        | C15—C14—C13     | 120.29 (14)  |
| C6—C5—H5     | 119.3        | C15—C14—H14     | 119.9        |
| C5—C6—C1     | 118.63 (14)  | C13—C14—H14     | 119.9        |
| C5—C6—C7     | 118.40 (13)  | C14—C15—C10     | 120.58 (14)  |
| C1—C6—C7     | 122.97 (13)  | C14—C15—H15     | 119.7        |
| O1—C7—C8     | 121.77 (14)  | C10—C15—H15     | 119.7        |
| O1—C7—C6     | 119.40 (14)  | O2—C16—H16A     | 109.5        |
| C8—C7—C6     | 118.82 (13)  | O2—C16—H16B     | 109.5        |
| C9—C8—C7     | 120.17 (14)  | H16A—C16—H16B   | 109.5        |
| C9—C8—H8     | 119.9        | O2—C16—H16C     | 109.5        |
| C7—C8—H8     | 119.9        | H16A—C16—H16C   | 109.5        |
| C8—C9—C10    | 127.75 (14)  | H16B—C16—H16C   | 109.5        |
| C8—C9—H9     | 116.1        | C13—O2—C16      | 116.71 (12)  |
| C6—C1—C2—C3  | 0.2 (2)      | C7—C8—C9—C10    | -175.77 (14) |
| C1—C2—C3—C4  | 0.3 (3)      | C8—C9—C10—C11   | 169.56 (16)  |
| C1—C2—C3—C11 | -179.03 (13) | C8—C9—C10—C15   | -8.4 (3)     |
| C2—C3—C4—C5  | -0.7 (3)     | C15—C10—C11—C12 | 2.2 (3)      |
| C11—C3—C4—C5 | 178.70 (13)  | C9—C10—C11—C12  | -175.87 (15) |
| C3—C4—C5—C6  | 0.5 (3)      | C10—C11—C12—C13 | -1.3 (3)     |
| C4—C5—C6—C1  | -0.1 (3)     | C11—C12—C13—O2  | 179.30 (15)  |
| C4—C5—C6—C7  | -179.34 (15) | C11—C12—C13—C14 | -1.0 (3)     |
| C2—C1—C6—C5  | -0.3 (2)     | O2—C13—C14—C15  | -178.00 (15) |
| C2—C1—C6—C7  | 178.96 (16)  | C12—C13—C14—C15 | 2.3 (3)      |
| C5—C6—C7—O1  | 16.7 (2)     | C13—C14—C15—C10 | -1.3 (3)     |
| C1—C6—C7—O1  | -162.55 (15) | C11—C10—C15—C14 | -0.9 (3)     |
| C5—C6—C7—C8  | -162.25 (15) | C9—C10—C15—C14  | 177.08 (15)  |
| C1—C6—C7—C8  | 18.5 (2)     | C12—C13—O2—C16  | 0.4 (2)      |
| O1—C7—C8—C9  | 6.4 (2)      | C14—C13—O2—C16  | -179.36 (14) |
| C6—C7—C8—C9  | -174.69 (15) |                 |              |

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

| $D-H\cdots A$                    | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------------|-------|-------------|-------------|---------------|
| C9—H9 $\cdots$ O1                | 0.95  | 2.46        | 2.8065 (19) | 102           |
| C12—H12 $\cdots$ O1 <sup>i</sup> | 0.95  | 2.54        | 3.4828 (18) | 175           |

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