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

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–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.

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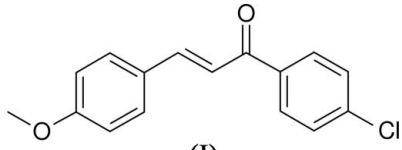
The geometrical parameters for the title compound, $C_{16}H_{13}ClO_2$, are normal. Packing in a non-centrosymmetric space group, which is consistent with the non-zero second harmonic generation response, may be influenced by a C—H···O interaction.

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).



(I)

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* = OH (Moorthi *et al.*, 2005), (III) with *X* = CH_3 (Wang *et al.*, 2005), (IV) with *X* = H (Rabinovich & Schmidt, 1970), and (V) with *X* = 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 C6—C7 and the C7—C8 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 (C1–C6 and C10–C15) in (I) is 21.82 (6)°. Cl1, C7 and O1 deviate from the former mean plane by 0.031 (3), 0.022 (3) and 0.346 (3) Å, respectively. The deviations of C9, O2 and C16 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 C9—H9···O1 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).

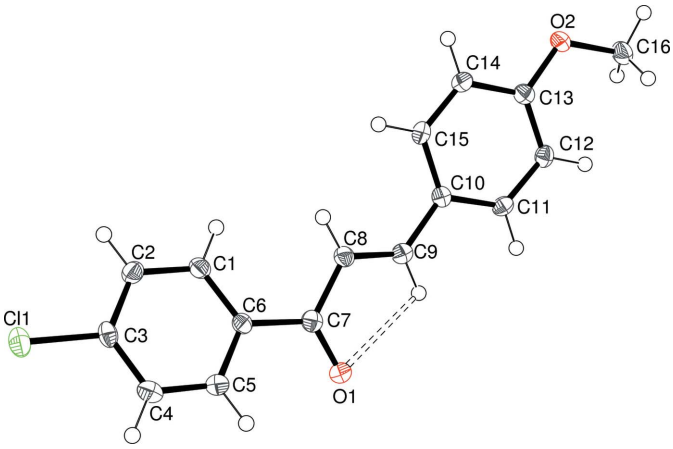


Figure 1
View of (I), showing 50% displacement ellipsoids (arbitrary spheres for the H atoms). The possible intramolecular C—H···O interaction is indicated by a dashed line.

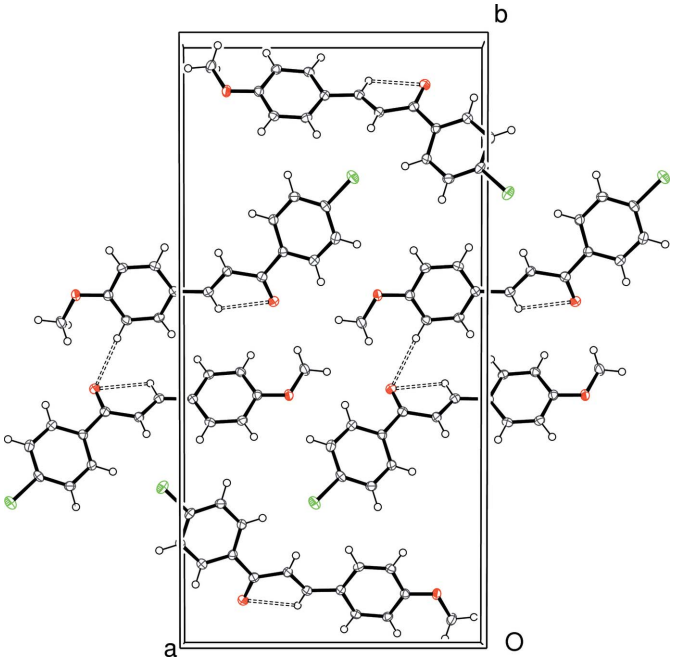


Figure 2
The packing for (I), viewed down [001], with C—H···O interactions shown as dashed lines.

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^3
Z = 4
D_x = 1.412 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1708 reflections
θ = 2.9–27.5°
μ = 0.29 mm^{-1}
T = 120 (2) K
Slab, colourless
0.50 × 0.40 × 0.20 mm

Data collection

Nonius KappaCCD diffractometer
ω and φ 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_{int} = 0.028
θ_{max} = 27.5°
$h = -9 \rightarrow 16$
$k = -33 \rightarrow 32$
$l = -5 \rightarrow 5$

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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
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···A	D—H	H···A	D···A	D—H···A
C9—H9···O1	0.95	2.46	2.8065 (19)	102
C12—H12···O1^{i}	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_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(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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Hall symbol: P 2c -2n
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$V = 1283.22$ (6) Å^3
$Z = 4$
$F(000) = 568$
$D_x = 1.412$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1708 reflections
$\theta = 2.9$–$27.5°$
$\mu = 0.29$ mm^{-1}
$T = 120$ K
Slab, colourless
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Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2003)
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2569 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -9 \rightarrow 16$
$k = -33 \rightarrow 32$
$l = -5 \rightarrow 5$

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^{-3}
$\Delta\rho_{min} = -0.22$ e Å^{-3}
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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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, º)

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—Cl1	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—Cl1	119.04 (12)	C11—C12—C13	118.51 (14)
C2—C3—Cl1	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—Cl1	−179.03 (13)	C8—C9—C10—C15	−8.4 (3)
C2—C3—C4—C5	−0.7 (3)	C15—C10—C11—C12	2.2 (3)
Cl1—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 (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O1	0.95	2.46	2.8065 (19)	102
C12—H12···O1^{i}	0.95	2.54	3.4828 (18)	175

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