organic compounds

(E)-1-(4-Chlorophenyl)-3-(4-methylphenyl)prop-2-en-1-one

Hoong-Kun Fun,[a]* **Samuel Robinson Jebas,**[a]‡ **P. S. Patil**[b]
and S. M. Dharmaprakash[c]

[a]X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, [b]Department of Studies in Physics, Mangalore University, Mangalagangotri, Mangalore 574 199, India, and [c]Department of Studies in Physics, Mangalore University, Mangalagangotri, Mangalore 574 199, India.
Correspondence e-mail: hkfun@usm.my

The title compound, $C_{16}H_{13}ClO$, adopts an E configuration with respect to the C=C double bond of the propenone unit. The dihedral angle between the two benzene rings is 45.9 (2)°. In the crystal structure, molecules are arranged into sheets parallel to the ac plane and the sheets are stacked along the b axis. This arrangement is stabilized by weak intermolecular C—H···π interactions involving both aromatic rings.

Related literature

For applications of chalcones in non-linear optics, see: Agrinskaya *et al.* (1999). For related structures, see: Patil, Dharmaprakash *et al.* (2007); Patil, Fun *et al.* (2007); Patil, Rosli *et al.* (2007).
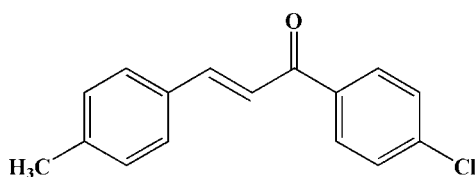
Experimental

Crystal data

C₁₆H₁₃ClO
$M_r = 256.71$
Monoclinic, $P2_1/c$
$a = 15.2632$ (3) Å
$b = 14.0146$ (3) Å
$c = 5.8487$ (1) Å
$\beta = 92.154$ (1)°

$V = 1250.20$ (4) Å³
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.29$ mm⁻¹
$T = 100.0$ (1) K
$0.34 \times 0.18 \times 0.05$ mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.908$, $T_{max} = 0.986$

15494 measured reflections
3661 independent reflections
2534 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.129$
$S = 1.04$
3661 reflections

164 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.41$ e Å⁻³
$\Delta\rho_{min} = -0.27$ e Å⁻³

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O1	0.93	2.50	2.820 (2)	100
C5—H5···$Cg1^i$	0.93	2.98	3.525	119
C2—H2···$Cg2^{ii}$	0.93	2.93	3.563	127
C14—H14···$Cg2^{iii}$	0.93	2.80	3.495	132

Symmetry codes: (i) $x, -y - \frac{1}{2}, z - \frac{3}{2}$; (ii) $-x, -y, -z + 1$; (iii) $x, -y - \frac{1}{2}, z - \frac{1}{2}$. $Cg1$ and $Cg2$ are the centroids of the C1–C6 and C10–C15 rings, respectively.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

References

Agrinskaya, N. V., Lukoshkin, V. A., Kudryavtsev, V. V., Nosova, G. I., Solovskaya, N. A. & Yakimanski, A. V. (1999). *Phys. Solid State*, **41**, 1914–1917.
Bruker (2005). *APEX2, SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Patil, P. S., Dharmaprakash, S. M., Ramakrishna, K., Fun, H.-K., Sai Santosh Kumar, R. & Rao, D. N. (2007). *J. Cryst. Growth*, **303**, 520–524.
Patil, P. S., Fun, H.-K., Chantrapromma, S. & Dharmaprakash, S. M. (2007). *Acta Cryst.* E**63**, o2497–o2498.
Patil, P. S., Rosli, M. M., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2007). *Acta Cryst.* E**63**, o3238.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

‡ Permanent address : Department of Physics, Karunya University, Karunya Nagar, Coimbatore 641 114, India.

supporting information

(*E*)-1-(4-Chlorophenyl)-3-(4-methylphenyl)prop-2-en-1-one

Hoong-Kun Fun, Samuel Robinson Jebas, P. S. Patil and S. M. Dharmaprakash

S1. Comment

Recently, significant progress has been achieved in the growth of noncentrosymmetric crystals for second harmonic generation (SHG), mostly that of chalcone derivatives substituted with different donor/acceptor substituents (Agrinskaya *et al.*, 1999; Patil, Dharmaprakash *et al.*, 2007; Patil, Fun *et al.*, 2007; Patil, Rosli *et al.*, 2007). Herein we report the crystal structure of the title compound.

The title molecule (Fig.1) exhibits an E configuration with respect to the C8?C9 double bond, with the C7—C8—C9—C10 torsion angle being -175.3 (2)°. The bond lengths and angles are comparable to those observed in related structures (Patil, Dharmaprakash *et al.*, 2007; Patil, Fun *et al.*, 2007; Patil, Rosli *et al.*, 2007). The dihedral angle between the two benzene rings is 45.9 (1)°.
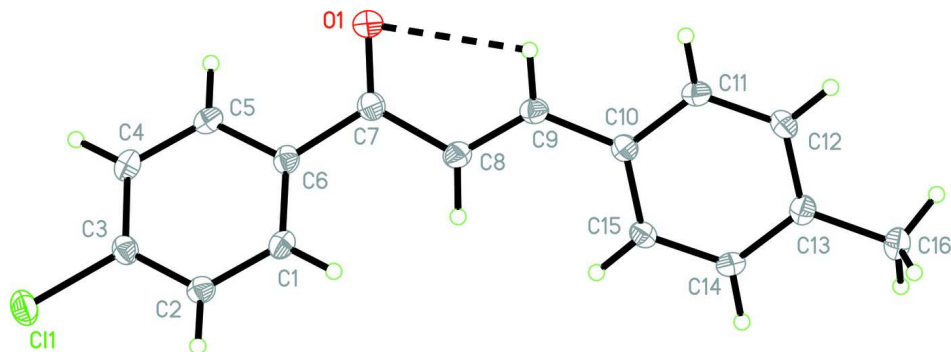
In the molecular structure, an intramolecular C—H⋯O hydrogen bond generates an S(5) ring motif. In the crystal structure, the molecules are arranged into sheets parallel to the *ac* plane and the sheets are stacked along the *b* axis (Fig. 2). This arrangement is stabilized by weak intermolecular C—H⋯π interactions involving both aromatic rings, Table 1.

S2. Experimental

The title compound was synthesized by the condensation of *p*-tolualdehyde (0.01 mol) with 4-chloroacetophenone (0.01 mol) in methanol (60 ml) in the presence of a catalytic amount of sodium hydroxide solution (5 ml, 30%). After stirring for 6 h, the contents of the flask were poured into ice-cold water (500 ml) and left to stand for 12 h. The resulting crude solid was filtered and dried. Single crystals suitable for X-ray diffraction were grown by slow evaporation of an acetone solution at room temperature.

S3. Refinement

H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å for aromatic H and 0.96 Å for methyl H atoms. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for the methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating-group model was used for the methyl group.

Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme. The intramolecular hydrogen bond is shown as a dashed line.
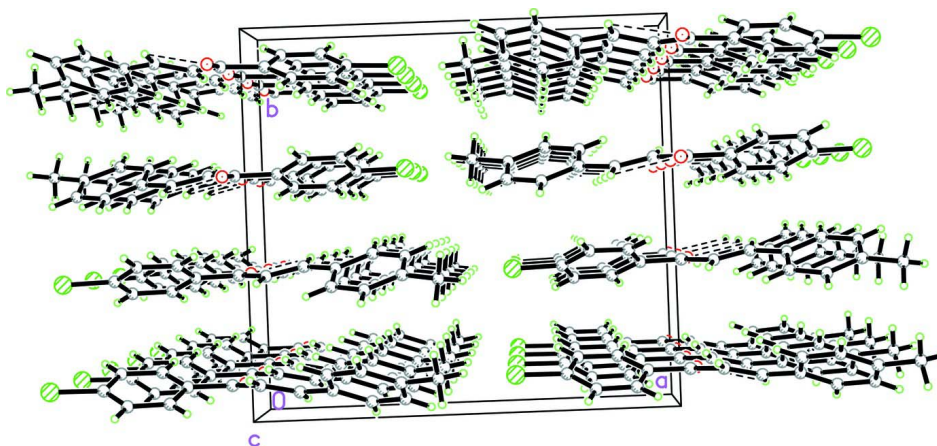
Figure 2

The crystal packing of the title compound, viewed along the *c* axis. Hydrogen bonds are shown as dashed lines.

(*E*)-1-(4-Chlorophenyl)-3-(4-methylphenyl)prop-2-en-1-one

Crystal data

$C_{16}H_{13}ClO$	$F(000) = 536$
$M_r = 256.71$	$D_x = 1.364$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2431 reflections
$a = 15.2632$ (3) Å	$\theta = 2.7–29.9°$
$b = 14.0146$ (3) Å	$\mu = 0.29$ mm^{-1}
$c = 5.8487$ (1) Å	$T = 100$ K
$\beta = 92.154$ (1)°	Plate, colourless
$V = 1250.20$ (4) Å^3	$0.34 \times 0.18 \times 0.05$ mm
$Z = 4$	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
Radiation source: fine-focus sealed tube	$T_{min} = 0.908$, $T_{max} = 0.986$
Graphite monochromator	15494 measured reflections
φ and ω scans	3661 independent reflections
	2534 reflections with $I > 2\sigma(I)$

$R_{int} = 0.055$	$k = -19 \rightarrow 19$
$\theta_{max} = 30.1°$, $\theta_{min} = 1.3°$	$l = -6 \rightarrow 8$
$h = -21 \rightarrow 21$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.053$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.129$	
$S = 1.04$	H-atom parameters constrained
3661 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 0.9337P]$
164 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} = 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.41$ e Å^{-3}
	$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

Experimental. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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 (Å^2)

	x	y	z	$U_{iso}*/U_{eq}$
Cl1	−0.37993 (3)	0.37197 (4)	0.72301 (10)	0.02546 (15)
O1	0.01956 (10)	0.38013 (12)	0.3019 (2)	0.0258 (4)
C1	−0.12084 (13)	0.40835 (14)	0.7779 (3)	0.0177 (4)
H1	−0.0797	0.4295	0.8878	0.021*
C2	−0.20925 (13)	0.40915 (14)	0.8251 (3)	0.0178 (4)
H2	−0.2279	0.4322	0.9643	0.021*
C3	−0.26921 (13)	0.37513 (14)	0.6615 (3)	0.0178 (4)
C4	−0.24374 (13)	0.34215 (14)	0.4505 (4)	0.0192 (4)
H4	−0.2850	0.3196	0.3425	0.023*
C5	−0.15563 (13)	0.34352 (14)	0.4044 (3)	0.0178 (4)
H5	−0.1375	0.3225	0.2630	0.021*
C6	−0.09327 (12)	0.37615 (14)	0.5676 (3)	0.0166 (4)
C7	0.00093 (13)	0.37789 (14)	0.5041 (4)	0.0183 (4)
C8	0.06927 (13)	0.37523 (15)	0.6898 (3)	0.0190 (4)
H8	0.0541	0.3596	0.8377	0.023*
C9	0.15291 (13)	0.39512 (14)	0.6470 (3)	0.0170 (4)
H9	0.1641	0.4150	0.4992	0.020*
C10	0.22861 (13)	0.38904 (13)	0.8071 (3)	0.0160 (4)
C11	0.31013 (13)	0.42159 (14)	0.7374 (3)	0.0172 (4)
H11	0.3144	0.4494	0.5939	0.021*
C12	0.38450 (13)	0.41295 (14)	0.8791 (4)	0.0187 (4)

H12	0.4378	0.4358	0.8299	0.022*
C13	0.38079 (13)	0.37070 (14)	1.0938 (3)	0.0180 (4)
C14	0.29931 (13)	0.33856 (14)	1.1634 (3)	0.0174 (4)
H14	0.2953	0.3101	1.3063	0.021*
C15	0.22434 (13)	0.34813 (14)	1.0242 (3)	0.0167 (4)
H15	0.1708	0.3271	1.0757	0.020*
C16	0.46114 (13)	0.35970 (16)	1.2478 (4)	0.0241 (5)
H16A	0.5117	0.3523	1.1567	0.036*
H16B	0.4549	0.3044	1.3428	0.036*
H16C	0.4682	0.4153	1.3425	0.036*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0154 (2)	0.0311 (3)	0.0299 (3)	0.0011 (2)	0.00166 (19)	−0.0017 (2)
O1	0.0214 (7)	0.0393 (9)	0.0169 (8)	−0.0012 (7)	0.0016 (6)	0.0010 (7)
C1	0.0183 (9)	0.0173 (9)	0.0171 (10)	−0.0015 (8)	−0.0029 (8)	0.0006 (8)
C2	0.0194 (9)	0.0177 (10)	0.0162 (10)	0.0015 (8)	0.0004 (8)	−0.0004 (8)
C3	0.0154 (9)	0.0166 (9)	0.0214 (10)	0.0007 (8)	0.0010 (8)	0.0031 (8)
C4	0.0195 (10)	0.0183 (10)	0.0195 (10)	0.0000 (8)	−0.0047 (8)	−0.0006 (8)
C5	0.0214 (10)	0.0171 (9)	0.0148 (10)	0.0022 (8)	−0.0013 (8)	−0.0002 (8)
C6	0.0161 (9)	0.0150 (9)	0.0185 (10)	0.0014 (8)	−0.0011 (7)	0.0032 (8)
C7	0.0179 (9)	0.0178 (9)	0.0192 (10)	0.0005 (8)	0.0009 (8)	−0.0001 (8)
C8	0.0196 (10)	0.0214 (10)	0.0161 (10)	0.0019 (8)	0.0004 (8)	0.0023 (8)
C9	0.0194 (9)	0.0165 (10)	0.0152 (10)	0.0023 (8)	0.0017 (8)	0.0010 (8)
C10	0.0162 (9)	0.0147 (9)	0.0171 (10)	0.0035 (7)	0.0013 (7)	−0.0015 (8)
C11	0.0205 (10)	0.0168 (10)	0.0144 (10)	0.0018 (8)	0.0022 (8)	0.0012 (8)
C12	0.0153 (9)	0.0197 (10)	0.0212 (11)	−0.0007 (8)	0.0037 (8)	0.0010 (8)
C13	0.0171 (9)	0.0177 (9)	0.0191 (10)	0.0012 (8)	−0.0012 (8)	−0.0021 (8)
C14	0.0207 (10)	0.0185 (10)	0.0129 (9)	−0.0004 (8)	0.0010 (8)	0.0006 (8)
C15	0.0160 (9)	0.0167 (10)	0.0175 (10)	−0.0010 (8)	0.0033 (8)	−0.0018 (8)
C16	0.0175 (10)	0.0309 (12)	0.0235 (11)	0.0004 (9)	−0.0030 (8)	0.0027 (9)

Geometric parameters (Å, º)

Cl1—C3	1.742 (2)	C9—C10	1.462 (3)
O1—C7	1.227 (2)	C9—H9	0.93
C1—C2	1.388 (3)	C10—C15	1.397 (3)
C1—C6	1.390 (3)	C10—C11	1.400 (3)
C1—H1	0.93	C11—C12	1.385 (3)
C2—C3	1.384 (3)	C11—H11	0.93
C2—H2	0.93	C12—C13	1.391 (3)
C3—C4	1.387 (3)	C12—H12	0.93
C4—C5	1.382 (3)	C13—C14	1.397 (3)
C4—H4	0.93	C13—C16	1.502 (3)
C5—C6	1.399 (3)	C14—C15	1.386 (3)
C5—H5	0.93	C14—H14	0.93
C6—C7	1.499 (3)	C15—H15	0.93

C7—C8	1.478 (3)	C16—H16A	0.96
C8—C9	1.340 (3)	C16—H16B	0.96
C8—H8	0.93	C16—H16C	0.96
C2—C1—C6	120.50 (19)	C10—C9—H9	116.4
C2—C1—H1	119.7	C15—C10—C11	118.07 (18)
C6—C1—H1	119.7	C15—C10—C9	122.91 (18)
C3—C2—C1	118.86 (19)	C11—C10—C9	118.95 (18)
C3—C2—H2	120.6	C12—C11—C10	120.97 (18)
C1—C2—H2	120.6	C12—C11—H11	119.5
C2—C3—C4	122.00 (18)	C10—C11—H11	119.5
C2—C3—Cl1	119.19 (16)	C11—C12—C13	121.12 (19)
C4—C3—Cl1	118.81 (15)	C11—C12—H12	119.4
C5—C4—C3	118.44 (19)	C13—C12—H12	119.4
C5—C4—H4	120.8	C12—C13—C14	117.82 (18)
C3—C4—H4	120.8	C12—C13—C16	121.66 (18)
C4—C5—C6	120.91 (19)	C14—C13—C16	120.52 (18)
C4—C5—H5	119.5	C15—C14—C13	121.47 (19)
C6—C5—H5	119.5	C15—C14—H14	119.3
C1—C6—C5	119.27 (18)	C13—C14—H14	119.3
C1—C6—C7	122.63 (18)	C14—C15—C10	120.54 (18)
C5—C6—C7	118.07 (18)	C14—C15—H15	119.7
O1—C7—C8	121.77 (18)	C10—C15—H15	119.7
O1—C7—C6	119.90 (18)	C13—C16—H16A	109.5
C8—C7—C6	118.32 (18)	C13—C16—H16B	109.5
C9—C8—C7	120.57 (19)	H16A—C16—H16B	109.5
C9—C8—H8	119.7	C13—C16—H16C	109.5
C7—C8—H8	119.7	H16A—C16—H16C	109.5
C8—C9—C10	127.16 (19)	H16B—C16—H16C	109.5
C8—C9—H9	116.4		
C6—C1—C2—C3	1.6 (3)	C6—C7—C8—C9	−166.97 (19)
C1—C2—C3—C4	−1.3 (3)	C7—C8—C9—C10	−175.30 (19)
C1—C2—C3—Cl1	177.78 (15)	C8—C9—C10—C15	9.1 (3)
C2—C3—C4—C5	0.1 (3)	C8—C9—C10—C11	−173.9 (2)
Cl1—C3—C4—C5	−179.00 (15)	C15—C10—C11—C12	0.4 (3)
C3—C4—C5—C6	0.9 (3)	C9—C10—C11—C12	−176.80 (18)
C2—C1—C6—C5	−0.7 (3)	C10—C11—C12—C13	0.8 (3)
C2—C1—C6—C7	177.19 (18)	C11—C12—C13—C14	−1.0 (3)
C4—C5—C6—C1	−0.6 (3)	C11—C12—C13—C16	179.17 (19)
C4—C5—C6—C7	−178.54 (18)	C12—C13—C14—C15	0.0 (3)
C1—C6—C7—O1	−155.5 (2)	C16—C13—C14—C15	179.90 (19)
C5—C6—C7—O1	22.4 (3)	C13—C14—C15—C10	1.1 (3)
C1—C6—C7—C8	25.5 (3)	C11—C10—C15—C14	−1.3 (3)
C5—C6—C7—C8	−156.65 (18)	C9—C10—C15—C14	175.76 (18)
O1—C7—C8—C9	14.0 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9···O1	0.93	2.50	2.820 (2)	100
C5—H5···*Cg*1[i]	0.93	2.98	3.525	119
C2—H2···*Cg*2[ii]	0.93	2.93	3.563	127
C14—H14···*Cg*2[iii]	0.93	2.80	3.495	132

Symmetry codes: (i) *x*, −*y*−1/2, *z*−3/2; (ii) −*x*, −*y*, −*z*+1; (iii) *x*, −*y*−1/2, *z*−1/2.