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(2*E*)-1-(4-Chlorophenyl)-3-[4-(propan-2-yl)phenyl]prop-2-en-1-one

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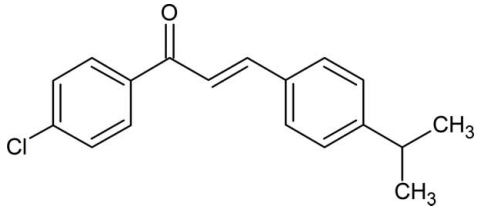
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.006 Å; R factor = 0.093; wR factor = 0.286; data-to-parameter ratio = 15.7.

In the title compound, $C_{18}H_{17}ClO$, the dihedral angle between the benzene rings is 53.5 (1)°. The mean plane of the prop-2-en-1-one group is twisted by 24.5 (8) and 33.5 (3)° from the chloro- and propanyl-substituted rings, respectively.

Related literature

For the non-linear optical properties of the chalcones, see: Sarojini *et al.* (2006); Poornesh *et al.* (2009) and for their biological activity, see: Nielsen *et al.* (1998); Mai *et al.* (2014); Insuasty *et al.* (2013). For related structures, see: Jasinski *et al.* (2009, 2012); Butcher *et al.* (2007); Harrison *et al.* (2006). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{18}H_{17}ClO$
M_r = 284.76
Monoclinic, $P2_1/c$
a = 8.8547 (5) Å
b = 5.8455 (3) Å
c = 28.8034 (17) Å
β = 97.396 (6)°
V = 1478.46 (14) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 2.21 mm^{-1}
T = 173 K
0.41 × 0.32 × 0.14 mm

Data collection

Agilent Eos Gemini diffractometer
Absorption correction: multi-scan *CrysAlis PRO* and *CrysAlis RED* (Agilent, 2012)
T_{min} = 0.370, T_{max} = 1.000
8687 measured reflections
2868 independent reflections
2269 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.093
$wR(F^2)$ = 0.286
S = 1.04
2868 reflections
183 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: *SUPERFLIP* (Palatinus *et al.*, 2012); program(s) used to refine structure: *SHELXL2012* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

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Supporting information for this paper is available from the IUCr electronic archives (Reference: ZS2302).

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supporting information

Acta Cryst. (2014). E**70**, o855 [doi:10.1107/S1600536814015281]

(2*E*)-1-(4-Chlorophenyl)-3-[4-(propan-2-yl)phenyl]prop-2-en-1-one

Badiadka Narayana, Vinutha V. Salian, Balladka K. Sarojini and Jerry P. Jasinski

S1. Comment

Chalcones are an important class of natural compounds and have been widely applied as synthons in synthetic organic chemistry. The nonlinear optical properties of the different chalcone derivatives have been reported (Sarojini *et al.*, 2006; Poornesh *et al.*, 2009). These *α*,*β*-unsaturated ketones also possess a wide variety of biological activities, including anti-leishmanial (Nielsen *et al.*, 1998), anticancer (Mai *et al.*, 2014) and antitumor activity (Insuasty *et al.*, 2013). The crystal structures of some chalcone derivatives viz., a second polymorph of (2*E*)-1-(4-fluorophenyl)-3-(3, 4, 5-trimethoxy-phenyl)prop-2-en- 1-one, (2*E*)-1-(3,4-dichlorophenyl)-3-(2-hydroxyphenyl)prop-2-en- 1-one (Jasinski *et al.*, 2009, 2012), (2*E*)-1-(2,4-dichlorophenyl)-3-[4-(methylsulfanyl)phenyl] prop-2-en-1-one (Butcher *et al.*, 2007) and 2-bromo-1-chloro-phenyl-3-(4-methoxyphenyl) prop-2-en-1-one (Harrison *et al.*, 2006) have been reported. In view of the importance of chalcone derivatives, we report herein the crystal structure of the title compound, $C_{18}H_{17}ClO$.

In the title compound, the dihedral angle between the mean planes of the phenyl rings is 53.5 (1)°. The mean plane of the prop-2-en-1-one group (C1/C2/O1/C8) is twisted away from the two phenyl rings by 24.5 (8)° (C2–C7) and 33.5 (3)° (C10–C15) (Fig. 1). Bond lengths are in normal ranges (Allen *et al.*, 1987). No classical hyrogen bonds are observed.

S2. Experimental

To a mixture of cuminaldehyde (1.5 mL, 0.01 mol) and 4-chloroacetophenone (1.3 mL, 0.01 mol) in ethanol (50 mL), 15 mL of 10 % sodium hydroxide solution was added and stirred at 273–278 K for 3 h (Fig. 2). The precipitate formed was collected by filtration. Single crystals were grown from ethanol by slow the evaporation method (m.p.: 343–345 K).

S3. Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with atom—H bond lengths of 0.95– 1.00 Å or 0.98 Å (CH_3). Isotropic displacement parameters for these atoms were set to 1.2 (CH) or 1.5 (CH_3) times U_{eq} of the parent atom. The Me group was refined as an ideally rotating group. No twinning has been observed.

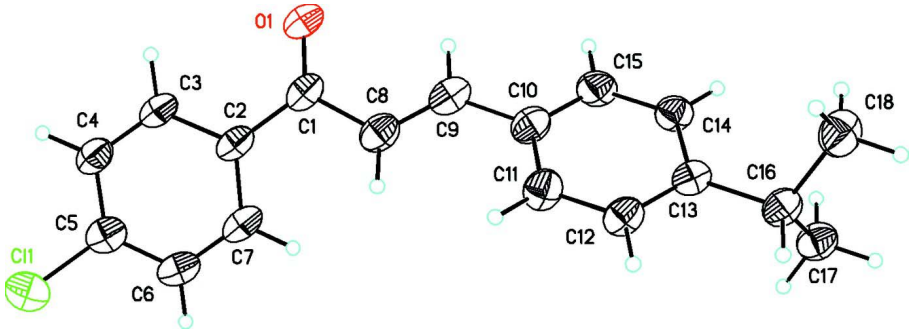

Figure 1

ORTEP drawing of $C_{18}H_{17}ClO$, showing the atom labeling scheme, with 30% probability displacement ellipsoids.

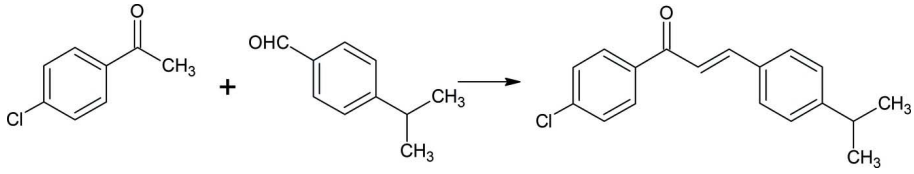

Figure 2

Synthesis of $C_{18}H_{17}ClO$.

(2*E*)-1-(4-Chlorophenyl)-3-[4-(propan-2-yl)phenyl]prop-2-en-1-one

Crystal data

$C_{18}H_{17}ClO$
$M_r = 284.76$
Monoclinic, $P2_1/c$
$a = 8.8547$ (5) Å
$b = 5.8455$ (3) Å
$c = 28.8034$ (17) Å
$\beta = 97.396$ (6)°
$V = 1478.46$ (14) Å^3
$Z = 4$
$F(000) = 600$
$D_x = 1.279$ Mg m^{-3}
Melting point = 343–345 K
Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
Cell parameters from 2529 reflections
$\theta = 4.6$–72.0°
$\mu = 2.21$ mm^{-1}
$T = 173$ K
Prism, colourless
0.41 × 0.32 × 0.14 mm

Data collection

Agilent Eos Gemini diffractometer
Radiation source: Enhance (Cu) X-ray Source
Graphite monochromator
Detector resolution: 16.0416 pixels mm^{-1}
ω scans
Absorption correction: multi-scan *CrysAlis PRO* and *CrysAlis RED* (Agilent, 2012)
$T_{min} = 0.370$, $T_{max} = 1.000$
8687 measured reflections
2868 independent reflections
2269 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 72.1°$, $\theta_{min} = 5.0°$
$h = -10\rightarrow10$
$k = -7\rightarrow6$
$l = -35\rightarrow29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.093$
$wR(F^2) = 0.286$
$S = 1.04$
2868 reflections
183 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1595P)^2 + 1.6733P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.87$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	−0.25150 (13)	0.8390 (2)	0.33097 (5)	0.0819 (5)
O1	0.2335 (4)	0.2755 (5)	0.48768 (11)	0.0695 (8)
C1	0.2184 (5)	0.4826 (7)	0.48178 (13)	0.0576 (10)
C2	0.1070 (4)	0.5752 (6)	0.44409 (14)	0.0550 (9)
C3	0.0602 (5)	0.4451 (7)	0.40431 (15)	0.0625 (10)
H3	0.1034	0.2981	0.4012	0.075*
C4	−0.0468 (5)	0.5249 (8)	0.36970 (16)	0.0675 (11)
H4	−0.0755	0.4358	0.3424	0.081*
C5	−0.1133 (5)	0.7368 (8)	0.37462 (16)	0.0638 (11)
C6	−0.0724 (5)	0.8693 (8)	0.41294 (17)	0.0691 (12)
H6	−0.1192	1.0137	0.4161	0.083*
C7	0.0386 (5)	0.7896 (7)	0.44713 (16)	0.0677 (12)
H7	0.0696	0.8833	0.4736	0.081*
C8	0.3018 (5)	0.6508 (8)	0.51427 (16)	0.0671 (11)
H8	0.3047	0.8073	0.5055	0.080*
C9	0.3719 (5)	0.5833 (8)	0.55524 (17)	0.0676 (11)
H9	0.3598	0.4270	0.5630	0.081*
C10	0.4664 (5)	0.7227 (8)	0.59013 (16)	0.0652 (11)
C11	0.5252 (5)	0.9341 (8)	0.57874 (15)	0.0676 (11)
H11	0.5026	0.9925	0.5478	0.081*
C12	0.6155 (5)	1.0579 (7)	0.61201 (14)	0.0612 (10)
H12	0.6546	1.2016	0.6038	0.073*
C13	0.6505 (4)	0.9774 (6)	0.65722 (13)	0.0529 (9)
C14	0.5907 (5)	0.7645 (7)	0.66783 (15)	0.0613 (10)
H14	0.6116	0.7055	0.6987	0.074*
C15	0.5034 (5)	0.6414 (7)	0.63453 (17)	0.0694 (12)
H15	0.4671	0.4953	0.6424	0.083*
C16	0.7492 (5)	1.1144 (7)	0.69393 (15)	0.0614 (10)
H16	0.7841	1.2548	0.6786	0.074*
C17	0.6624 (6)	1.1896 (8)	0.73356 (16)	0.0706 (12)
H17A	0.5750	1.2834	0.7209	0.106*
H17B	0.7299	1.2794	0.7563	0.106*
H17C	0.6265	1.0545	0.7490	0.106*
C18	0.8911 (5)	0.9757 (10)	0.7134 (2)	0.0834 (14)
H18A	0.8599	0.8406	0.7299	0.125*
H18B	0.9583	1.0709	0.7351	0.125*

H18C	0.9454	0.9273	0.6875	0.125*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0684 (8)	0.0788 (8)	0.1002 (10)	−0.0040 (5)	0.0173 (6)	0.0148 (6)
O1	0.0799 (19)	0.0492 (16)	0.0811 (19)	−0.0082 (14)	0.0161 (15)	−0.0158 (14)
C1	0.064 (2)	0.053 (2)	0.061 (2)	−0.0177 (17)	0.0283 (18)	−0.0123 (17)
C2	0.059 (2)	0.0465 (19)	0.065 (2)	−0.0154 (16)	0.0298 (18)	−0.0121 (16)
C3	0.073 (3)	0.047 (2)	0.071 (2)	−0.0081 (18)	0.022 (2)	−0.0150 (18)
C4	0.081 (3)	0.055 (2)	0.068 (2)	−0.010 (2)	0.016 (2)	−0.0130 (19)
C5	0.059 (2)	0.058 (2)	0.079 (3)	−0.0136 (18)	0.029 (2)	−0.001 (2)
C6	0.066 (3)	0.053 (2)	0.092 (3)	−0.0027 (19)	0.027 (2)	−0.011 (2)
C7	0.077 (3)	0.053 (2)	0.078 (3)	−0.013 (2)	0.028 (2)	−0.022 (2)
C8	0.071 (3)	0.061 (2)	0.073 (3)	−0.011 (2)	0.022 (2)	−0.010 (2)
C9	0.067 (2)	0.059 (2)	0.081 (3)	−0.009 (2)	0.027 (2)	−0.013 (2)
C10	0.065 (2)	0.057 (2)	0.076 (3)	−0.0096 (19)	0.016 (2)	−0.0076 (19)
C11	0.076 (3)	0.064 (3)	0.065 (2)	−0.021 (2)	0.015 (2)	0.0024 (19)
C12	0.066 (2)	0.055 (2)	0.065 (2)	−0.0173 (18)	0.0215 (19)	0.0001 (18)
C13	0.0468 (18)	0.0501 (19)	0.066 (2)	−0.0054 (15)	0.0211 (16)	−0.0031 (16)
C14	0.060 (2)	0.053 (2)	0.071 (2)	−0.0070 (18)	0.0101 (18)	0.0066 (18)
C15	0.072 (3)	0.050 (2)	0.086 (3)	−0.0152 (19)	0.006 (2)	0.013 (2)
C16	0.060 (2)	0.057 (2)	0.069 (2)	−0.0092 (18)	0.0171 (19)	−0.0049 (18)
C17	0.079 (3)	0.066 (3)	0.069 (3)	0.002 (2)	0.020 (2)	−0.008 (2)
C18	0.053 (2)	0.092 (4)	0.105 (4)	−0.004 (2)	0.010 (2)	−0.021 (3)

Geometric parameters (Å, º)

Cl1—C5	1.743 (5)	C10—C15	1.364 (6)
O1—C1	1.228 (5)	C11—H11	0.9500
C1—C2	1.472 (6)	C11—C12	1.372 (6)
C1—C8	1.486 (6)	C12—H12	0.9500
C2—C3	1.393 (5)	C12—C13	1.382 (6)
C2—C7	1.400 (6)	C13—C14	1.401 (5)
C3—H3	0.9500	C13—C16	1.512 (5)
C3—C4	1.366 (6)	C14—H14	0.9500
C4—H4	0.9500	C14—C15	1.358 (6)
C4—C5	1.386 (6)	C15—H15	0.9500
C5—C6	1.359 (6)	C16—H16	1.0000
C6—H6	0.9500	C16—C17	1.521 (6)
C6—C7	1.379 (7)	C16—C18	1.538 (7)
C7—H7	0.9500	C17—H17A	0.9800
C8—H8	0.9500	C17—H17B	0.9800
C8—C9	1.321 (7)	C17—H17C	0.9800
C9—H9	0.9500	C18—H18A	0.9800
C9—C10	1.469 (6)	C18—H18B	0.9800
C10—C11	1.396 (6)	C18—H18C	0.9800

O1—C1—C2	121.0 (3)	C12—C11—H11	119.9
O1—C1—C8	121.9 (4)	C11—C12—H12	119.4
C2—C1—C8	116.9 (4)	C11—C12—C13	121.2 (4)
C3—C2—C1	120.4 (4)	C13—C12—H12	119.4
C3—C2—C7	117.0 (4)	C12—C13—C14	117.6 (4)
C7—C2—C1	122.5 (4)	C12—C13—C16	121.2 (3)
C2—C3—H3	119.4	C14—C13—C16	121.2 (4)
C4—C3—C2	121.3 (4)	C13—C14—H14	119.6
C4—C3—H3	119.4	C15—C14—C13	120.9 (4)
C3—C4—H4	120.2	C15—C14—H14	119.6
C3—C4—C5	119.6 (4)	C10—C15—H15	119.2
C5—C4—H4	120.2	C14—C15—C10	121.6 (4)
C4—C5—Cl1	120.0 (4)	C14—C15—H15	119.2
C6—C5—Cl1	118.7 (4)	C13—C16—H16	108.0
C6—C5—C4	121.3 (4)	C13—C16—C17	112.1 (3)
C5—C6—H6	120.7	C13—C16—C18	110.3 (4)
C5—C6—C7	118.6 (4)	C17—C16—H16	108.0
C7—C6—H6	120.7	C17—C16—C18	110.3 (4)
C2—C7—H7	118.9	C18—C16—H16	108.0
C6—C7—C2	122.1 (4)	C16—C17—H17A	109.5
C6—C7—H7	118.9	C16—C17—H17B	109.5
C1—C8—H8	119.9	C16—C17—H17C	109.5
C9—C8—C1	120.2 (4)	H17A—C17—H17B	109.5
C9—C8—H8	119.9	H17A—C17—H17C	109.5
C8—C9—H9	116.3	H17B—C17—H17C	109.5
C8—C9—C10	127.3 (4)	C16—C18—H18A	109.5
C10—C9—H9	116.3	C16—C18—H18B	109.5
C11—C10—C9	121.8 (4)	C16—C18—H18C	109.5
C15—C10—C9	119.7 (4)	H18A—C18—H18B	109.5
C15—C10—C11	118.5 (4)	H18A—C18—H18C	109.5
C10—C11—H11	119.9	H18B—C18—H18C	109.5
C12—C11—C10	120.3 (4)		

Cl1—C5—C6—C7	−179.1 (3)	C8—C9—C10—C11	−16.7 (7)
O1—C1—C2—C3	−25.1 (5)	C8—C9—C10—C15	165.8 (5)
O1—C1—C2—C7	152.0 (4)	C9—C10—C11—C12	−178.8 (4)
O1—C1—C8—C9	−13.1 (6)	C9—C10—C15—C14	179.8 (4)
C1—C2—C3—C4	177.8 (4)	C10—C11—C12—C13	0.1 (7)
C1—C2—C7—C6	−176.0 (4)	C11—C10—C15—C14	2.3 (7)
C1—C8—C9—C10	176.1 (4)	C11—C12—C13—C14	0.1 (6)
C2—C1—C8—C9	162.2 (4)	C11—C12—C13—C16	−179.6 (4)
C2—C3—C4—C5	−1.7 (6)	C12—C13—C14—C15	0.9 (6)
C3—C2—C7—C6	1.1 (6)	C12—C13—C16—C17	115.4 (4)
C3—C4—C5—Cl1	−179.3 (3)	C12—C13—C16—C18	−121.2 (4)
C3—C4—C5—C6	1.1 (6)	C13—C14—C15—C10	−2.1 (7)
C4—C5—C6—C7	0.5 (6)	C14—C13—C16—C17	−64.3 (5)
C5—C6—C7—C2	−1.7 (6)	C14—C13—C16—C18	59.0 (5)
C7—C2—C3—C4	0.6 (6)	C15—C10—C11—C12	−1.3 (7)

C8—C1—C2—C3	159.6 (4)	C16—C13—C14—C15	−179.4 (4)
C8—C1—C2—C7	−23.4 (5)		