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(2*E*)-3-(2-Chlorophenyl)-1-phenylprop-2-en-1-one

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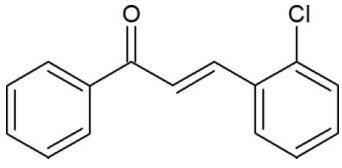
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.086; data-to-parameter ratio = 13.8.

In the title molecule, $C_{15}H_{11}ClO$, the angle between the mean planes of the two rings is 6.6 (8)°. The crystal packing is stabilized by van der Waals interactions, whereby the molecules are aligned in rows in a zigzag pattern.

Related literature

For related structures, see: Teh *et al.* (2006); Butcher, Jasinski *et al.* (2007); Butcher, Yathirajan *et al.* (2007); Yathirajan *et al.* (2007). For related literature, see: Dimmock *et al.* (1999); Go *et al.* (2005); Opletalova & Sedivy, (1999); Opletalova, (2000); Opletalova *et al.*, (2003).



Experimental

Crystal data

$C_{15}H_{11}ClO$
M_r = 242.69
Orthorhombic, $Pca2_1$
a = 19.0061 (7) Å
b = 5.0646 (3) Å
c = 12.6534 (4) Å
V = 1217.99 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 296 K
0.48 × 0.45 × 0.34 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.903, T_{max} = 1.000 (expected range = 0.817–0.905)
7585 measured reflections
2120 independent reflections
1286 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.087
S = 0.96
2120 reflections
154 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack (1983), 2120 Friedel pairs
Flack parameter: 0.02 (7)

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2586).

References

Bruker (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Butcher, R. J., Jasinski, J. P., Yathirajan, H. S., Lakshmana, K. & Narayana, B. (2007). *Acta Cryst.* E**63**, o3661.
Butcher, R. J., Yathirajan, H. S., Narayana, B., Mithun, A. & Sarojini, B. K. (2007). *Acta Cryst.* E**63**, o30–o32.
Dimmock, J. R., Elias, D. W., Beazely, M. A. & Kandepu, N. (1999). *Curr. Med. Chem.* **6**, 1125–1149.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Go, M. L., Wu, X. & Liu, X. L. (2005). *Curr. Med. Chem.* **12**, 481–499.
Opletalova, V. (2000). *Ceska Slov. Farm.* **49**, 278–284.
Opletalova, V., Jahodar, L., Jun, D. & Opletal, L. (2003). *Ceska Slov. Farm.* **52**, 12–19.
Opletalova, V. & Sedivy, D. (1999). *Ceska Slov. Farm.* **48**, 252–255.
Oxford Diffraction (2007). *CrysAlisPro* and *CrysAlis RED*. Versions 1.171.31.8. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Teh, J. B.-J., Patil, P. S., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o890–o892.
Yathirajan, H. S., Mayekar, A. N., Narayana, B., Sarojini, B. K. & Bolte, M. (2007). *Acta Cryst.* E**63**, o540–o541.

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supplementary materials

Acta Cryst. (2007). E**63**, o4715 [**doi:10.1107/S1600536807058011**]

(2*E*)-3-(2-Chlorophenyl)-1-phenylprop-2-en-1-one

J. P. Jasinski, R. J. Butcher, K. Lakshmana, B. Narayana and H. S. Yathirajan

Comment

Chalcone is a unique template molecule that is associated with several biological activities. Chalcone and its analogues are relatively easily available, not only by isolation from natural products but also by classical and combinatorial synthesis. The cytotoxic, anticancer, antiviral, antiprotozoal, insecticidal, chemopreventative, mutagenic and enzyme-inhibitory properties of a number of chalcones have been reviewed (Dimmock *et al.*, 1999; Go *et al.*, 2005). The antifungal and antibacterial activities of these compounds have also been reviewed (Opletalova & Sedivy, 1999; Opletalova, 2000). Chalcones and their analogues are also used as potential therapeutic agents in diseases of the cardiovascular system. The stabilizing action of chalcones on the vascular wall, vasodilating and antioxidative activity have been reported (Opletalova *et al.*, 2003). The crystal structures of 1-phenyl-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one (Teh *et al.*, 2006); 1-(2,4-dichlorophenyl)-3-[4-(methylsalfanyl)phenyl]prop-2-en-1-one (Butcher *et al.* 2007*b*); 1-(2,4-dichlorophenyl)-3-(6-methoxy-2-naphthyl)prop-2-en-1-one, (Yathirajan *et al.*, 2007); 3-(4-chlorophenyl)-1-(3-hydroxyphenyl)prop-2-en-1-one (Butcher *et al.* 2007*a*). As a part of our ongoing studies on chalcones, a new chalcone, $C_{15}H_{11}ClO$, was prepared and the crystal structure is reported.

In the title molecule, $C_{15}H_{11}ClO$, the angle between the mean planes of the 2-chlorophenyl-imino and phenol groups is 6.6 (8)° (Fig 1). Crystal packing is stabilized by van der Waals interactions, whereby the molecules are aligned in rows in a zigzag pattern with the phenyl rings diagonal to the *ac* face of the unit cell (Fig 2).

Experimental

A mixture of acetophenone (1.2 g, 0.01 mol) and 2-chlorobenzaldehyde (1.3 g, 0.01 mol) was stirred well. Sodium hydroxide (4 ml, 5%) was added and the mixture was stirred for 6 hrs. The separated precipitate was washed, dried and recrystallized from ethyl alcohol. (m.p.:318 K). Analysis found: C: 74.10, H: 4.51%; $C_{15}H_{11}ClO$ requires C: 74.23, H: 4.57%.

Refinement

The H atoms were placed in their calculated positions and then refined using the riding model with C—H = 0.93 Å, and with U_{iso}(H) = 1.18–1.20U_{eq}(C).

Figures

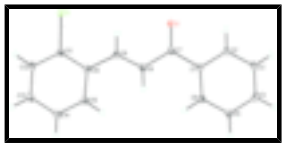

Fig. 1. Molecular structure of the title compound, showing atom labeling and 50% probability displacement ellipsoids.

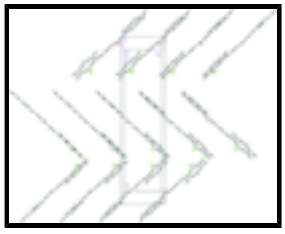

Fig. 2. Packing diagram of the title compound, viewed down the *c* axis.

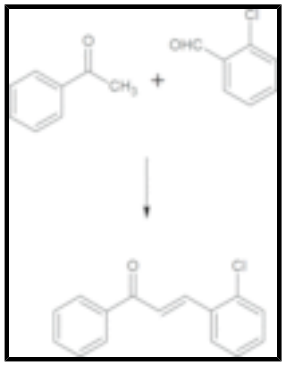

Fig. 3. Synthetic scheme for $C_{15}H_{11}ClO$.

(2E)-3-(2-Chlorophenyl)-1-phenylprop-2-en-1-one

Crystal data

$C_{15}H_{11}ClO$	F_{000} = 504
M_r = 242.69	D_x = 1.323 Mg m^{-3}
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2c -2ac	Cell parameters from 3012 reflections
a = 19.0061 (7) Å	θ = 4.8–32.4º
b = 5.0646 (3) Å	μ = 0.29 mm^{-1}
c = 12.6534 (4) Å	T = 296 K
V = 1217.99 (9) Å^3	Prism, colorless
Z = 4	0.48 × 0.45 × 0.34 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer	2120 independent reflections
Radiation source: fine-focus sealed tube	1286 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.027
Detector resolution: 10.5081 pixels mm^{-1}	θ_{max} = 32.4º
T = 296 K	θ_{min} = 4.8º
φ and ω scans	h = −27→27
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	k = −7→7
T_{min} = 0.903, T_{max} = 1.000	l = −18→17
7585 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.036$	$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.087$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.96$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
2120 reflections	$\Delta\rho_{min} = -0.23$ e Å^{-3}
154 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 2120 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.02 (7)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2$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}
Cl	0.68430 (3)	0.75899 (13)	0.51978 (6)	0.0616 (2)
O	0.49895 (9)	0.0827 (4)	0.52181 (13)	0.0684 (5)
C1	0.44116 (9)	−0.1047 (4)	0.66737 (15)	0.0334 (4)
C2	0.40315 (10)	−0.2764 (4)	0.60322 (17)	0.0388 (5)
H2A	0.4094	−0.2711	0.5304	0.047*
C3	0.35630 (10)	−0.4545 (4)	0.64633 (18)	0.0448 (5)
H3A	0.3310	−0.5676	0.6026	0.054*
C4	0.34697 (11)	−0.4646 (4)	0.7546 (2)	0.0498 (6)
H4A	0.3158	−0.5856	0.7839	0.060*
C5	0.38403 (12)	−0.2949 (4)	0.81904 (18)	0.0482 (5)
H5A	0.3776	−0.3007	0.8919	0.058*
C6	0.43057 (10)	−0.1169 (4)	0.77580 (16)	0.0410 (5)
H6A	0.4553	−0.0031	0.8199	0.049*
C7	0.49182 (9)	0.0816 (4)	0.61733 (15)	0.0388 (5)
C8	0.53307 (11)	0.2646 (4)	0.68406 (16)	0.0399 (5)
H8A	0.5279	0.2545	0.7570	0.048*

C9	0.57618 (10)	0.4390 (4)	0.64553 (17)	0.0422 (5)
H9A	0.5806	0.4423	0.5723	0.051*
C10	0.61854 (9)	0.6302 (4)	0.70391 (15)	0.0356 (4)
C11	0.66921 (10)	0.7863 (4)	0.65482 (17)	0.0394 (5)
C12	0.70887 (10)	0.9688 (4)	0.70996 (18)	0.0445 (5)
H12A	0.7424	1.0700	0.6749	0.053*
C13	0.69862 (10)	1.0003 (5)	0.81699 (18)	0.0471 (5)
H13A	0.7252	1.1226	0.8545	0.057*
C14	0.64873 (11)	0.8496 (5)	0.86826 (17)	0.0482 (5)
H14A	0.6417	0.8703	0.9405	0.058*
C15	0.60925 (11)	0.6678 (4)	0.81245 (16)	0.0422 (5)
H15A	0.5757	0.5680	0.8480	0.051*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0590 (3)	0.0823 (4)	0.0435 (2)	−0.0241 (3)	0.0095 (3)	−0.0010 (3)
O	0.0775 (10)	0.0902 (14)	0.0374 (7)	−0.0422 (10)	0.0054 (9)	−0.0072 (10)
C1	0.0303 (8)	0.0295 (10)	0.0404 (10)	0.0045 (7)	−0.0038 (7)	0.0000 (9)
C2	0.0374 (10)	0.0380 (11)	0.0411 (10)	0.0062 (8)	−0.0063 (8)	−0.0024 (9)
C3	0.0395 (10)	0.0374 (12)	0.0574 (13)	−0.0016 (9)	−0.0087 (10)	−0.0063 (10)
C4	0.0452 (11)	0.0409 (12)	0.0634 (15)	−0.0068 (10)	−0.0008 (11)	0.0077 (12)
C5	0.0526 (13)	0.0512 (14)	0.0409 (10)	−0.0068 (11)	−0.0004 (9)	0.0084 (11)
C6	0.0449 (10)	0.0356 (10)	0.0424 (10)	−0.0037 (9)	−0.0053 (9)	0.0012 (10)
C7	0.0340 (9)	0.0401 (12)	0.0422 (10)	0.0007 (8)	−0.0015 (8)	0.0004 (10)
C8	0.0415 (10)	0.0399 (12)	0.0384 (10)	−0.0030 (9)	−0.0033 (8)	0.0003 (10)
C9	0.0424 (10)	0.0487 (13)	0.0355 (9)	−0.0066 (10)	0.0025 (8)	−0.0022 (9)
C10	0.0307 (9)	0.0358 (10)	0.0403 (10)	0.0022 (8)	−0.0022 (8)	0.0042 (10)
C11	0.0331 (9)	0.0445 (12)	0.0406 (10)	0.0026 (8)	0.0004 (8)	0.0019 (10)
C12	0.0328 (9)	0.0429 (12)	0.0578 (13)	−0.0036 (9)	−0.0041 (10)	0.0024 (11)
C13	0.0415 (11)	0.0409 (11)	0.0590 (13)	0.0028 (10)	−0.0127 (10)	−0.0068 (11)
C14	0.0498 (12)	0.0547 (13)	0.0400 (11)	0.0053 (11)	−0.0068 (10)	−0.0094 (11)
C15	0.0415 (11)	0.0438 (11)	0.0415 (10)	−0.0014 (9)	0.0020 (8)	0.0038 (10)

Geometric parameters (Å, °)

Cl—C11	1.738 (2)	C8—C9	1.300 (3)
O—C7	1.216 (3)	C8—H8A	0.9300
C1—C6	1.388 (3)	C9—C10	1.460 (3)
C1—C2	1.392 (3)	C9—H9A	0.9300
C1—C7	1.489 (3)	C10—C11	1.392 (3)
C2—C3	1.380 (3)	C10—C15	1.398 (3)
C2—H2A	0.9300	C11—C12	1.382 (3)
C3—C4	1.382 (3)	C12—C13	1.377 (3)
C3—H3A	0.9300	C12—H12A	0.9300
C4—C5	1.378 (3)	C13—C14	1.379 (3)
C4—H4A	0.9300	C13—H13A	0.9300
C5—C6	1.376 (3)	C14—C15	1.382 (3)
C5—H5A	0.9300	C14—H14A	0.9300

C6—H6A	0.9300	C15—H15A	0.9300
C7—C8	1.479 (3)		
C6—C1—C2	118.25 (19)	C7—C8—H8A	118.5
C6—C1—C7	122.84 (18)	C8—C9—C10	127.5 (2)
C2—C1—C7	118.91 (18)	C8—C9—H9A	116.3
C3—C2—C1	120.9 (2)	C10—C9—H9A	116.3
C3—C2—H2A	119.6	C11—C10—C15	116.64 (19)
C1—C2—H2A	119.6	C11—C10—C9	122.17 (19)
C2—C3—C4	119.9 (2)	C15—C10—C9	121.19 (18)
C2—C3—H3A	120.0	C12—C11—C10	122.1 (2)
C4—C3—H3A	120.0	C12—C11—Cl	117.37 (16)
C5—C4—C3	119.8 (2)	C10—C11—Cl	120.50 (16)
C5—C4—H4A	120.1	C13—C12—C11	119.8 (2)
C3—C4—H4A	120.1	C13—C12—H12A	120.1
C6—C5—C4	120.1 (2)	C11—C12—H12A	120.1
C6—C5—H5A	119.9	C12—C13—C14	119.7 (2)
C4—C5—H5A	119.9	C12—C13—H13A	120.1
C5—C6—C1	121.0 (2)	C14—C13—H13A	120.1
C5—C6—H6A	119.5	C13—C14—C15	120.1 (2)
C1—C6—H6A	119.5	C13—C14—H14A	119.9
O—C7—C8	120.35 (18)	C15—C14—H14A	119.9
O—C7—C1	119.84 (18)	C14—C15—C10	121.6 (2)
C8—C7—C1	119.80 (17)	C14—C15—H15A	119.2
C9—C8—C7	123.09 (19)	C10—C15—H15A	119.2
C9—C8—H8A	118.5		
C6—C1—C2—C3	−0.1 (3)	C7—C8—C9—C10	179.18 (19)
C7—C1—C2—C3	179.19 (17)	C8—C9—C10—C11	172.1 (2)
C1—C2—C3—C4	−0.3 (3)	C8—C9—C10—C15	−8.8 (3)
C2—C3—C4—C5	0.6 (3)	C15—C10—C11—C12	0.3 (3)
C3—C4—C5—C6	−0.4 (3)	C9—C10—C11—C12	179.46 (19)
C4—C5—C6—C1	−0.1 (3)	C15—C10—C11—Cl	−179.15 (15)
C2—C1—C6—C5	0.3 (3)	C9—C10—C11—Cl	0.0 (3)
C7—C1—C6—C5	−178.96 (18)	C10—C11—C12—C13	−0.1 (3)
C6—C1—C7—O	179.8 (2)	Cl—C11—C12—C13	179.41 (16)
C2—C1—C7—O	0.5 (3)	C11—C12—C13—C14	−0.1 (3)
C6—C1—C7—C8	−0.3 (3)	C12—C13—C14—C15	0.0 (3)
C2—C1—C7—C8	−179.62 (18)	C13—C14—C15—C10	0.3 (3)
O—C7—C8—C9	2.5 (3)	C11—C10—C15—C14	−0.4 (3)
C1—C7—C8—C9	−177.32 (19)	C9—C10—C15—C14	−179.56 (19)

Fig. 1

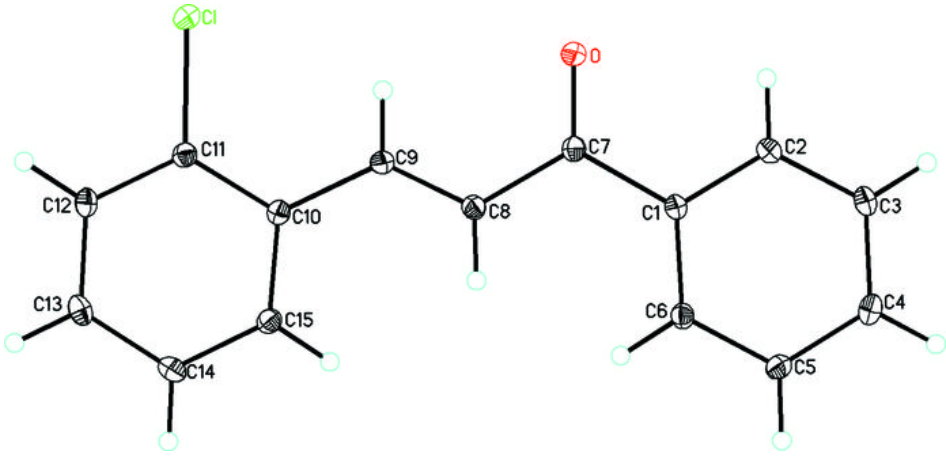

Fig. 2

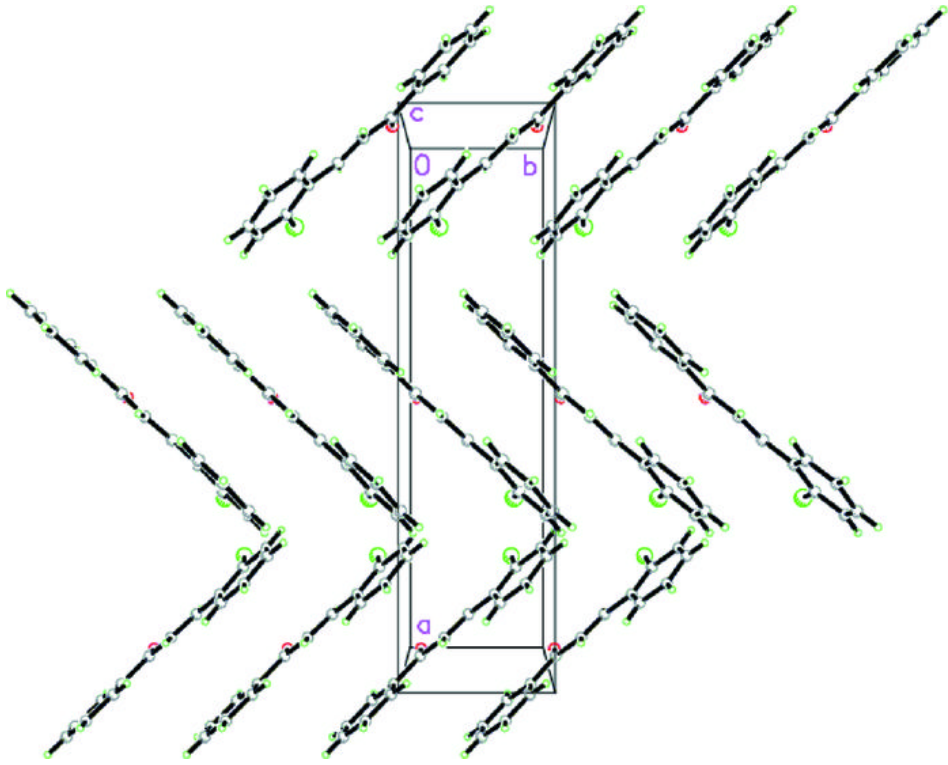

Fig. 3