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(*E*)-3-(2,3-Dichlorophenyl)-1-phenylprop-2-en-1-one

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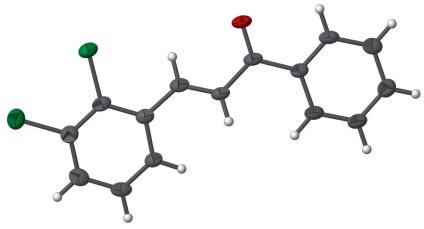
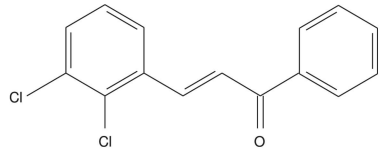
In the title compound, $C_{15}H_{10}Cl_2O$, the dihedral angle between the aromatic rings is 5.59 (15)° and the C—C═C—C torsion angle is 177.5 (3)°. In the crystal, molecules are linked *via* pairs of C—H···O hydrogen bonds, forming inversion dimers with $R_2^2(10)$ ring motifs.

3D view



Chemical scheme



Structure description

As part of our ongoing studies of chalcone derivatives (Tejkiran *et al.*, 2016; Kumara *et al.*, 2017), we now report herein on the synthesis and crystal structure of the title compound.

The structure of the molecule is shown in Fig. 1. The molecule is nearly planar, with a dihedral angle of 5.59 (15)° between the aromatic rings that are bridged by the enone unit. This value is less than the value of 19.13 (15)° reported earlier between the aromatic rings in the related chalcone derivative (*E*)-3-(2,3-dichlorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one (Naveen *et al.*, 2016). The *trans* conformation about the C7═C8 double bond in the central enone group is confirmed by the C2—C7═C8—C9 torsion angle of 177.5 (3)°. The carbonyl group at atom C9 lies almost in the plane of the olefinic double bond and phenyl ring as indicated by the O1—C9—C10—C11 and O1—C9—C8—C7 torsion angles of 2.9 (5) and 11.1 (5)°, respectively. The double-bond length in the propene unit [C7═C8 = 1.336 (4)°] is significantly longer than the value reported earlier for (2*E*)-1-(5-chlorothiophen-2-yl)-3-[4-(dimethylamino)phenyl]prop-2-en-1-one (Rodríguez-Lugo *et al.*, 2015).

In the crystal, molecules are linked *via* pairs of weak C—H···O hydrogen bonds, forming inversion dimers with $R_2^2(10)$ ring motifs (Table 1, Fig. 2).

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···O1^{i}	0.93	2.48	3.360 (4)	159

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

Synthesis and crystallization

A mixture of 2,3-dichlorobenzaldehyde (0.05 mmol), acetophenone (0.05 mmol) and sodium hydroxide (0.05 mmol) in 80% ethyl alcohol (25 ml) was stirred at room temperature for 3 h. The progress of the reaction was monitored by TLC. After the completion of the reaction, the mixture was poured into ice-cold water and kept in the refrigerator for 18 h. The solid formed was filtered, and washed with cold acetic acid (5%). The single crystals were obtained by recrystallization from a solution of the title compound in dichloromethane and 3–4 drops of acetonitrile (m.p. 391–392 K).

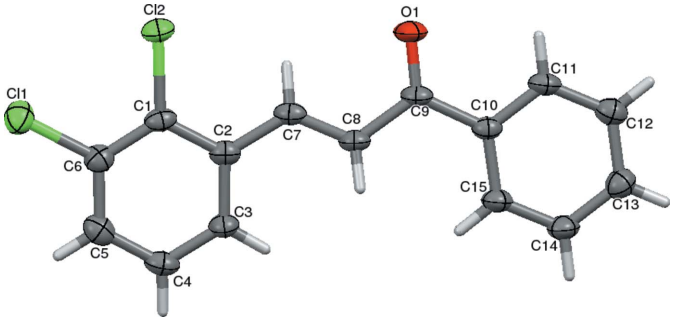


Figure 1
The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

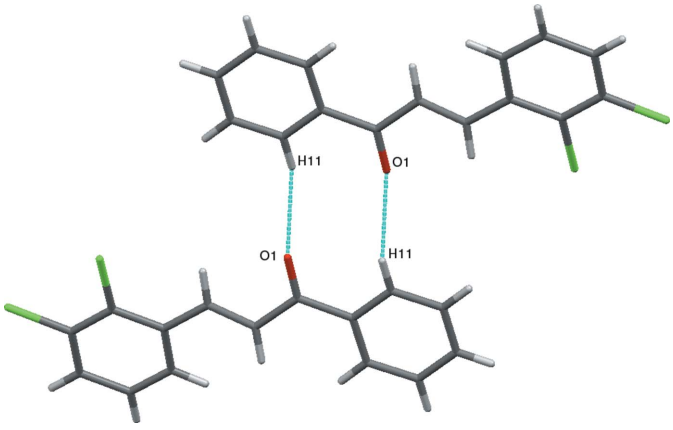


Figure 2
C—H···O hydrogen bonds forming inversion dimers with $R_2^2(10)$ ring motifs.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{10}Cl_2O$
M_r	277.13
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	13.7594 (19), 11.3610 (16), 8.0912 (11)
β (°)	97.139 (9)
V (Å^3)	1255.0 (3)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	4.51
Crystal size (mm)	0.28 × 0.27 × 0.25
Data collection	
Diffractometer	Bruker X8 Proteum
Absorption correction	Multi-scan (*SADABS*; Bruker, 2013)
T_{min}, T_{max}	0.365, 0.399
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6357, 2010, 1748
R_{int}	0.056
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.584
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.070, 0.193, 1.06
No. of reflections	2010
No. of parameters	163
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.56, −0.62

Computer programs: *APEX2* and *SAINT* (Bruker, 2013), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170126 [https://doi.org/10.1107/S2414314617001262]

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(*E*)-3-(2,3-Dichlorophenyl)-1-phenylprop-2-en-1-one

Crystal data

$C_{15}H_{10}Cl_2O$
M_r = 277.13
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 13.7594 (19) Å
b = 11.3610 (16) Å
c = 8.0912 (11) Å
β = 97.139 (9)°
V = 1255.0 (3) Å^3
Z = 4
$F(000)$ = 568
D_x = 1.467 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 1748 reflections
θ = 6.5–64.3°
μ = 4.51 mm^{-1}
T = 296 K
Rectangle, yellow
0.28 × 0.27 × 0.25 mm

Data collection

Bruker X8 Proteum diffractometer
Radiation source: Bruker MicroStar microfocus rotating anode
Helios multilayer optics monochromator
Detector resolution: 18.4 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2013)
T_{min} = 0.365, T_{max} = 0.399
6357 measured reflections
2010 independent reflections
1748 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 64.3°, θ_{min} = 6.5°
h = −15→16
k = −12→12
l = −9→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.193
S = 1.06
2010 reflections
163 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1509P)^2 + 0.1324P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.56 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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}
Cl1	1.04081 (6)	0.24127 (8)	0.72918 (10)	0.0411 (3)
Cl2	0.87488 (6)	0.09212 (6)	0.52852 (9)	0.0337 (3)
O1	0.5691 (2)	0.09538 (18)	0.1522 (3)	0.0397 (8)
C1	0.8669 (2)	0.2440 (3)	0.5286 (4)	0.0276 (9)
C2	0.7861 (2)	0.3004 (3)	0.4371 (4)	0.0270 (9)
C3	0.7826 (2)	0.4231 (3)	0.4453 (4)	0.0289 (9)
C4	0.8556 (2)	0.4871 (3)	0.5380 (4)	0.0338 (10)
C5	0.9341 (2)	0.4310 (3)	0.6275 (4)	0.0340 (10)
C6	0.9394 (2)	0.3097 (3)	0.6213 (4)	0.0309 (10)
C7	0.7101 (2)	0.2341 (3)	0.3350 (4)	0.0280 (9)
C8	0.6215 (2)	0.2747 (3)	0.2755 (4)	0.0276 (9)
C9	0.5519 (2)	0.2003 (3)	0.1673 (4)	0.0276 (9)
C10	0.4623 (2)	0.2540 (2)	0.0750 (4)	0.0258 (9)
C11	0.3971 (2)	0.1808 (3)	−0.0221 (4)	0.0291 (9)
C12	0.3129 (2)	0.2265 (3)	−0.1114 (4)	0.0336 (10)
C13	0.2927 (2)	0.3456 (3)	−0.1034 (4)	0.0353 (10)
C14	0.3576 (3)	0.4189 (3)	−0.0083 (4)	0.0347 (10)
C15	0.4414 (2)	0.3744 (3)	0.0803 (4)	0.0313 (9)
H3	0.73000	0.46270	0.38700	0.0350*
H4	0.85170	0.56880	0.54000	0.0410*
H5	0.98270	0.47410	0.69100	0.0410*
H7	0.72470	0.15680	0.30900	0.0340*
H8	0.60340	0.35050	0.30250	0.0330*
H11	0.41010	0.10070	−0.02710	0.0350*
H12	0.27010	0.17710	−0.17680	0.0400*
H13	0.23580	0.37620	−0.16160	0.0420*
H14	0.34440	0.49910	−0.00410	0.0420*
H15	0.48440	0.42460	0.14390	0.0380*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0359 (6)	0.0413 (6)	0.0449 (6)	−0.0008 (3)	0.0001 (4)	0.0089 (4)
Cl2	0.0406 (6)	0.0214 (5)	0.0391 (5)	0.0029 (3)	0.0055 (4)	0.0040 (3)
O1	0.0523 (15)	0.0163 (13)	0.0480 (14)	0.0031 (9)	−0.0036 (11)	−0.0023 (9)
C1	0.0343 (17)	0.0208 (16)	0.0299 (16)	0.0018 (12)	0.0128 (14)	0.0046 (11)
C2	0.0337 (16)	0.0233 (15)	0.0257 (15)	0.0004 (13)	0.0102 (12)	0.0003 (12)
C3	0.0344 (17)	0.0210 (15)	0.0317 (16)	0.0005 (12)	0.0054 (13)	0.0038 (12)
C4	0.0436 (18)	0.0219 (16)	0.0375 (17)	−0.0045 (13)	0.0120 (14)	−0.0009 (13)

C5	0.0366 (18)	0.0348 (17)	0.0323 (16)	−0.0081 (14)	0.0114 (14)	−0.0011 (14)
C6	0.0331 (17)	0.0298 (17)	0.0305 (16)	−0.0009 (13)	0.0068 (13)	0.0048 (13)
C7	0.0400 (19)	0.0196 (15)	0.0259 (15)	−0.0003 (12)	0.0099 (13)	0.0010 (12)
C8	0.0365 (17)	0.0167 (14)	0.0304 (16)	0.0012 (12)	0.0078 (13)	0.0003 (12)
C9	0.0391 (17)	0.0156 (16)	0.0293 (16)	−0.0002 (13)	0.0087 (13)	0.0016 (11)
C10	0.0314 (17)	0.0204 (15)	0.0269 (15)	−0.0004 (12)	0.0093 (12)	0.0013 (11)
C11	0.0375 (17)	0.0182 (15)	0.0338 (16)	−0.0021 (12)	0.0133 (14)	−0.0024 (12)
C12	0.0377 (18)	0.0292 (18)	0.0351 (17)	−0.0037 (13)	0.0091 (14)	−0.0017 (14)
C13	0.0346 (17)	0.0331 (18)	0.0387 (17)	0.0024 (14)	0.0068 (13)	0.0054 (14)
C14	0.0378 (18)	0.0208 (16)	0.0460 (19)	0.0014 (13)	0.0073 (15)	0.0009 (14)
C15	0.0357 (17)	0.0194 (15)	0.0398 (16)	−0.0010 (13)	0.0083 (14)	−0.0022 (13)

Geometric parameters (Å, º)

Cl1—C6	1.735 (3)	C11—C12	1.388 (4)
Cl2—C1	1.729 (3)	C12—C13	1.385 (5)
O1—C9	1.224 (4)	C13—C14	1.383 (5)
C1—C2	1.411 (4)	C14—C15	1.376 (5)
C1—C6	1.389 (4)	C3—H3	0.9300
C2—C3	1.397 (5)	C4—H4	0.9300
C2—C7	1.459 (4)	C5—H5	0.9300
C3—C4	1.383 (4)	C7—H7	0.9300
C4—C5	1.379 (4)	C8—H8	0.9300
C5—C6	1.381 (5)	C11—H11	0.9300
C7—C8	1.336 (4)	C12—H12	0.9300
C8—C9	1.480 (4)	C13—H13	0.9300
C9—C10	1.490 (4)	C14—H14	0.9300
C10—C11	1.392 (4)	C15—H15	0.9300
C10—C15	1.400 (4)		
Cl2—C1—C2	119.9 (2)	C13—C14—C15	120.7 (3)
Cl2—C1—C6	119.7 (2)	C10—C15—C14	120.3 (3)
C2—C1—C6	120.4 (3)	C2—C3—H3	119.00
C1—C2—C3	117.3 (3)	C4—C3—H3	119.00
C1—C2—C7	121.7 (3)	C3—C4—H4	120.00
C3—C2—C7	121.0 (3)	C5—C4—H4	120.00
C2—C3—C4	121.6 (3)	C4—C5—H5	121.00
C3—C4—C5	120.7 (3)	C6—C5—H5	121.00
C4—C5—C6	118.9 (3)	C2—C7—H7	117.00
Cl1—C6—C1	120.6 (3)	C8—C7—H7	117.00
Cl1—C6—C5	118.1 (2)	C7—C8—H8	120.00
C1—C6—C5	121.2 (3)	C9—C8—H8	120.00
C2—C7—C8	125.7 (3)	C10—C11—H11	120.00
C7—C8—C9	120.7 (3)	C12—C11—H11	120.00
O1—C9—C8	119.8 (3)	C11—C12—H12	120.00
O1—C9—C10	120.4 (3)	C13—C12—H12	120.00
C8—C9—C10	119.8 (3)	C12—C13—H13	120.00
C9—C10—C11	118.2 (2)	C14—C13—H13	120.00

C9—C10—C15	123.0 (3)	C13—C14—H14	120.00
C11—C10—C15	118.7 (3)	C15—C14—H14	120.00
C10—C11—C12	120.5 (3)	C10—C15—H15	120.00
C11—C12—C13	120.1 (3)	C14—C15—H15	120.00
C12—C13—C14	119.7 (3)		

Cl2—C1—C2—C3	178.5 (2)	C2—C7—C8—C9	177.5 (3)
Cl2—C1—C2—C7	−2.8 (4)	C7—C8—C9—O1	11.1 (5)
C6—C1—C2—C3	−0.4 (4)	C7—C8—C9—C10	−167.8 (3)
C6—C1—C2—C7	178.3 (3)	O1—C9—C10—C11	2.9 (5)
Cl2—C1—C6—Cl1	3.0 (4)	O1—C9—C10—C15	−176.5 (3)
Cl2—C1—C6—C5	−178.4 (2)	C8—C9—C10—C11	−178.3 (3)
C2—C1—C6—Cl1	−178.1 (2)	C8—C9—C10—C15	2.4 (5)
C2—C1—C6—C5	0.5 (5)	C9—C10—C11—C12	−179.6 (3)
C1—C2—C3—C4	0.5 (5)	C15—C10—C11—C12	−0.2 (5)
C7—C2—C3—C4	−178.2 (3)	C9—C10—C15—C14	179.7 (3)
C1—C2—C7—C8	163.8 (3)	C11—C10—C15—C14	0.4 (5)
C3—C2—C7—C8	−17.5 (5)	C10—C11—C12—C13	−0.5 (5)
C2—C3—C4—C5	−0.8 (5)	C11—C12—C13—C14	1.1 (5)
C3—C4—C5—C6	0.9 (5)	C12—C13—C14—C15	−0.9 (5)
C4—C5—C6—Cl1	177.9 (2)	C13—C14—C15—C10	0.2 (5)
C4—C5—C6—C1	−0.7 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O1^{i}	0.93	2.48	3.360 (4)	159

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