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

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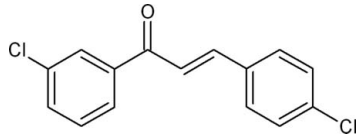
Key indicators: single-crystal X-ray study; T = 110 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.133; data-to-parameter ratio = 14.7.

The title compound, $C_{15}H_{10}Cl_2O$, is a chalcone with 3-chlorophenyl and 4-chlorophenyl substituents bonded at the opposite ends of a propenone group, the biologically active region. The dihedral angle between mean planes of these two chloro-substituted benzene rings is 46.7 (7)° compared to 46.0 (1) and 32.4 (1)° in similar published sructures. The angles between the mean plane of the prop-2-en-1-one group and the mean planes of the 3-chlorophenyl and 4-chlorophenyl rings are 24.1 (2) and 29.63°, respectively. While no classical hydrogen bonds are present, weak intermolecular C—H···π-ring interactions are observed, which contribute to the stability of crystal packing.

Related literature

For the potential use of chalcones or chalcone-rich plant extracts as drugs or food preservatives, see: Dhar (1981). For the biological and pharmaceutical activity of chalcones, see: Dimmock *et al.* (1999); Troeberg *et al.* (2000); Ram *et al.* (2000). For their applications as organic nonlinear optical materials, see: Sarojini *et al.* (2006). For the bis-(4-chlorophenyl) analog, see: Wang *et al.* (2005) and for the (2-chlorophenyl, 4-chlorophenyl) analog, see: Fun *et al.* (2008*b*). For antitumor and antioxidant activity studies and non-linear optical studies, see: Mukherjee *et al.* (2001); Poornesh *et al.* (2009); Shettigar *et al.* (2006, 2008); Wang *et al.* (1997). For related structures, see: Butcher *et al.* (2007); Fischer *et al.* (2007); Fun *et al.* (2008*a*); Harrison *et al.* (2006); Ng *et al.* (2006); Teh *et al.* (2007); Yathirajan *et al.* (2006).



Experimental

Crystal data

$C_{15}H_{10}Cl_2O$
M_r = 277.13
Triclinic, $P\overline{1}$
a = 5.8884 (9) Å
b = 7.3328 (9) Å
c = 14.6752 (16) Å
α = 102.821 (10)°
β = 95.003 (10)°
γ = 92.933 (11)°
V = 613.88 (14) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 4.61 mm^{-1}
T = 110 K
0.53 × 0.33 × 0.28 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlisPro*; Oxford Diffraction, 2007)
T_{min} = 0.067, T_{max} = 0.275
4041 measured reflections
2402 independent reflections
2147 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.133
S = 1.04
2402 reflections
163 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···$Cg2^{i}$	0.95	2.98	3.608 (2)	125
C5—H5A···$Cg2^{ii}$	0.95	2.88	3.488 (2)	126
C14—H14A···$Cg1^{iii}$	0.95	2.77	3.474 (2)	131

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y, -z+1$; (iii) $-x, -y+1, -z+1$. $Cg1$ is the centroid of the C1–C6 ring and $Cg2$ is the centroid of the C10–C15 ring.

Data collection: *CrysAlis Pro* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: ZS2009).

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supplementary materials

Acta Cryst. (2009). E**65**, o2641-o2642 [**doi:10.1107/S1600536809037805**]

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

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

Comment

Chalcones or 1,3-diaryl-2-propen-1-ones, belong to the flavonoid family. Chemically, they consist of open-chain flavonoids in which the two aromatic rings are joined by a three-carbon α, β-unsaturated carbonyl system. A vast number of naturally occurring chalcones are polyhydroxylated in the aryl rings. The radical quenching properties of the phenolic groups present in many chalcones have raised interest in using the compounds or chalcone-rich plant extracts as drugs or food preservatives (Dhar, 1981). Among the many useful properties that chalcones have been reported to possess include anti-inflammatory, antimicrobial, antifungal, antioxidant, cytotoxic and anticancer activities (Dimmock *et al.*, 1999). Many chalcones have been assessed for their high antimalarial activity, which is probably a result of Michael addition of nucleophilic species to the double bond of the enone (Troeberg *et al.*, 2000; Ram *et al.*, 2000). Chalcones are also finding applications as organic non-linear optical (NLO) materials due to their good SHG conversion efficiencies (Sarojini *et al.*, 2006). Owing to the importance of these flavanoid analogs, the title chalcone (I), $C_{15}H_{10}Cl_2O$ has been synthesized and its crystal structure is reported here.

The title compound is a chalcone with 3-chlorophenyl and 4-chlorophenyl rings bonded at the opposite ends of a propen-one group which is the biologically active region. The dihedral angle between mean planes of these two chloro-substituted benzene rings is 46.7 (7)° compared to 46.0 (1)° in the bis-(4-chlorophenyl) analog (Wang *et al.*, 2005) and 32.4 (1)° in the (2-chlorophenyl, 4-chlorophenyl) analog (Fun *et al.*, 2008*b*). The angles between the mean plane of the prop-2-ene-1-one group and the mean planes of the 3-chlorophenyl and 4-chlorophenyl rings are 24.1 (2)° and 29.63°, respectively. While no classical hydrogen bonds are present, weak intermolecular C–H···π-ring interactions are observed which contribute to the stability of crystal packing (Table 1).

Experimental

50% KOH was added to a mixture of 3-chloroacetophenone (0.01 mol) and *p*-chlorobenzaldehyde (0.01 mol) in 25 ml of ethanol. The mixture was stirred for an hour at room temperature and the precipitate was collected by filtration and purified by recrystallization from ethanol: yield 70% . Single crystals (m.p. 406–408 K) were grown from ethyl acetate by the slow evaporation method. Anal. found: C, 64.96; H, 3.61%; calc. for $C_{15}H_{10}Cl_2O$: C 65.01; H, 3.64%.

Refinement

All of the H atoms were placed in their calculated positions and then refined using the riding model with C—H = 0.95 Å, and with U_{iso}(H) = 1.17–1.24U_{eq}(C).

Figures

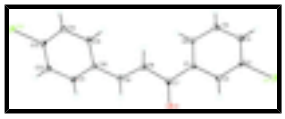

Fig. 1. Molecular structure of the title compound (I) showing the atom labeling scheme and 50% probability displacement ellipsoids.

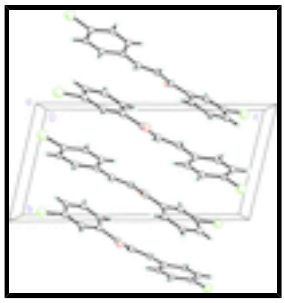

Fig. 2. Packing diagram of the title compound viewed down the *a* axis of the unit cell.

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

Crystal data

$C_{15}H_{10}Cl_2O$	$Z = 2$
$M_r = 277.13$	$F_{000} = 284$
Triclinic, $P\bar{1}$	$D_x = 1.499$ Mg m^{-3}
Hall symbol: -P 1	Melting point = 406–408 K
$a = 5.8884$ (9) Å	Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å
$b = 7.3328$ (9) Å	Cell parameters from 2900 reflections
$c = 14.6752$ (16) Å	$\theta = 6.2$–73.9^o
$\alpha = 102.821$ (10)º	$\mu = 4.61$ mm^{-1}
$\beta = 95.003$ (10)º	$T = 110$ K
$\gamma = 92.933$ (11)º	Block, colorless
$V = 613.88$ (14) Å^3	0.53 × 0.33 × 0.28 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer	2402 independent reflections
Radiation source: Enhance (Cu) X-ray Source	2147 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.035$
Detector resolution: 10.5081 pixels mm^{-1}	$\theta_{max} = 73.9^o$
$T = 110$ K	$\theta_{min} = 6.2^o$
ω scans	$h = -7 \rightarrow 7$
Absorption correction: multi-scan (*CrysAlisPro*; Oxford Diffraction, 2007)	$k = -4 \rightarrow 9$
$T_{min} = 0.067$, $T_{max} = 0.275$	$l = -18 \rightarrow 18$
4041 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.047$	H-atom parameters constrained
$wR(F^2) = 0.133$	$w = 1/[\sigma^2(F_o^2) + (0.0992P)^2 + 0.1931P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.04$	$(\Delta/\sigma)_{max} < 0.001$
2402 reflections	$\Delta\rho_{max} = 0.48$ e Å^{-3}
163 parameters	$\Delta\rho_{min} = -0.38$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.57079 (8)	−0.05763 (7)	0.10784 (3)	0.0235 (2)
Cl2	−0.09011 (9)	0.72931 (8)	0.93921 (3)	0.0286 (2)
O1	0.7088 (2)	0.2250 (2)	0.47821 (10)	0.0233 (4)
C1	0.3892 (3)	0.1004 (3)	0.36950 (14)	0.0161 (4)
C2	0.5165 (3)	0.0748 (3)	0.29158 (14)	0.0154 (4)
H2A	0.6696	0.1269	0.2980	0.019*
C3	0.4159 (3)	−0.0275 (3)	0.20525 (14)	0.0164 (4)
C4	0.1936 (4)	−0.1087 (3)	0.19394 (15)	0.0203 (4)
H4A	0.1276	−0.1790	0.1343	0.024*
C5	0.0704 (3)	−0.0849 (3)	0.27143 (15)	0.0198 (4)
H5A	−0.0810	−0.1409	0.2649	0.024*
C6	0.1652 (3)	0.0201 (3)	0.35873 (14)	0.0179 (4)
H6A	0.0777	0.0371	0.4110	0.021*
C7	0.5008 (3)	0.2095 (3)	0.46235 (14)	0.0177 (4)
C8	0.3516 (3)	0.2980 (3)	0.53315 (14)	0.0191 (4)
H8A	0.1959	0.3100	0.5139	0.023*
C9	0.4301 (3)	0.3613 (3)	0.62341 (14)	0.0169 (4)
H9A	0.5857	0.3439	0.6403	0.020*

C10	0.3008 (3)	0.4551 (3)	0.69935 (14)	0.0161 (4)
C11	0.3922 (3)	0.4779 (3)	0.79294 (14)	0.0174 (4)
H11A	0.5390	0.4357	0.8058	0.021*
C12	0.2738 (3)	0.5603 (3)	0.86707 (14)	0.0202 (4)
H12A	0.3365	0.5729	0.9302	0.024*
C13	0.0614 (4)	0.6243 (3)	0.84698 (14)	0.0189 (4)
C14	−0.0325 (3)	0.6083 (3)	0.75532 (14)	0.0177 (4)
H14A	−0.1765	0.6555	0.7430	0.021*
C15	0.0860 (3)	0.5226 (3)	0.68181 (14)	0.0167 (4)
H15A	0.0213	0.5094	0.6189	0.020*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0286 (3)	0.0275 (3)	0.0145 (3)	0.0029 (2)	0.0075 (2)	0.0028 (2)
Cl2	0.0267 (3)	0.0389 (4)	0.0174 (3)	0.0087 (2)	0.0064 (2)	−0.0026 (2)
O1	0.0188 (7)	0.0308 (9)	0.0191 (7)	0.0014 (6)	0.0024 (6)	0.0028 (6)
C1	0.0191 (9)	0.0144 (9)	0.0156 (10)	0.0038 (7)	0.0033 (7)	0.0041 (7)
C2	0.0154 (9)	0.0139 (9)	0.0177 (10)	0.0025 (7)	0.0025 (7)	0.0045 (7)
C3	0.0193 (10)	0.0154 (9)	0.0154 (9)	0.0045 (7)	0.0053 (7)	0.0035 (7)
C4	0.0231 (10)	0.0164 (10)	0.0196 (10)	0.0005 (8)	−0.0013 (8)	0.0017 (8)
C5	0.0162 (9)	0.0168 (10)	0.0264 (11)	−0.0002 (8)	0.0005 (8)	0.0063 (8)
C6	0.0169 (9)	0.0189 (10)	0.0201 (10)	0.0038 (8)	0.0066 (7)	0.0067 (8)
C7	0.0205 (10)	0.0182 (10)	0.0160 (10)	0.0031 (8)	0.0048 (7)	0.0055 (8)
C8	0.0193 (10)	0.0214 (10)	0.0167 (10)	0.0041 (8)	0.0049 (7)	0.0029 (8)
C9	0.0181 (9)	0.0142 (9)	0.0194 (10)	0.0007 (7)	0.0053 (7)	0.0047 (8)
C10	0.0182 (10)	0.0132 (9)	0.0168 (10)	−0.0016 (7)	0.0038 (7)	0.0031 (7)
C11	0.0183 (10)	0.0147 (10)	0.0183 (10)	−0.0002 (7)	0.0010 (7)	0.0026 (7)
C12	0.0230 (10)	0.0213 (10)	0.0148 (9)	0.0004 (8)	0.0007 (7)	0.0015 (8)
C13	0.0216 (10)	0.0174 (10)	0.0167 (10)	−0.0002 (8)	0.0067 (8)	0.0006 (7)
C14	0.0169 (9)	0.0150 (10)	0.0211 (10)	0.0006 (7)	0.0033 (7)	0.0036 (8)
C15	0.0194 (10)	0.0162 (10)	0.0142 (9)	−0.0004 (8)	0.0014 (7)	0.0034 (7)

Geometric parameters (Å, °)

Cl1—C3	1.7414 (19)	C8—C9	1.335 (3)
Cl2—C13	1.743 (2)	C8—H8A	0.9500
O1—C7	1.221 (2)	C9—C10	1.469 (3)
C1—C6	1.398 (3)	C9—H9A	0.9500
C1—C2	1.405 (3)	C10—C11	1.401 (3)
C1—C7	1.495 (3)	C10—C15	1.405 (3)
C2—C3	1.386 (3)	C11—C12	1.385 (3)
C2—H2A	0.9500	C11—H11A	0.9500
C3—C4	1.391 (3)	C12—C13	1.389 (3)
C4—C5	1.385 (3)	C12—H12A	0.9500
C4—H4A	0.9500	C13—C14	1.386 (3)
C5—C6	1.393 (3)	C14—C15	1.386 (3)
C5—H5A	0.9500	C14—H14A	0.9500
C6—H6A	0.9500	C15—H15A	0.9500

C7—C8	1.480 (3)		
C6—C1—C2	119.42 (18)	C7—C8—H8A	119.1
C6—C1—C7	122.00 (17)	C8—C9—C10	126.68 (19)
C2—C1—C7	118.57 (17)	C8—C9—H9A	116.7
C3—C2—C1	119.19 (17)	C10—C9—H9A	116.7
C3—C2—H2A	120.4	C11—C10—C15	118.27 (19)
C1—C2—H2A	120.4	C11—C10—C9	119.40 (18)
C2—C3—C4	121.81 (18)	C15—C10—C9	122.33 (18)
C2—C3—Cl1	119.60 (15)	C12—C11—C10	121.58 (19)
C4—C3—Cl1	118.59 (16)	C12—C11—H11A	119.2
C5—C4—C3	118.61 (19)	C10—C11—H11A	119.2
C5—C4—H4A	120.7	C11—C12—C13	118.49 (19)
C3—C4—H4A	120.7	C11—C12—H12A	120.8
C4—C5—C6	120.93 (18)	C13—C12—H12A	120.8
C4—C5—H5A	119.5	C14—C13—C12	121.62 (19)
C6—C5—H5A	119.5	C14—C13—Cl2	119.12 (16)
C5—C6—C1	120.02 (18)	C12—C13—Cl2	119.25 (16)
C5—C6—H6A	120.0	C15—C14—C13	119.30 (19)
C1—C6—H6A	120.0	C15—C14—H14A	120.4
O1—C7—C8	121.66 (19)	C13—C14—H14A	120.4
O1—C7—C1	120.42 (18)	C14—C15—C10	120.71 (18)
C8—C7—C1	117.93 (17)	C14—C15—H15A	119.6
C9—C8—C7	121.72 (19)	C10—C15—H15A	119.6
C9—C8—H8A	119.1		
C6—C1—C2—C3	1.0 (3)	C1—C7—C8—C9	164.85 (19)
C7—C1—C2—C3	179.45 (17)	C7—C8—C9—C10	178.46 (18)
C1—C2—C3—C4	−1.3 (3)	C8—C9—C10—C11	166.7 (2)
C1—C2—C3—Cl1	179.19 (14)	C8—C9—C10—C15	−12.9 (3)
C2—C3—C4—C5	0.4 (3)	C15—C10—C11—C12	1.6 (3)
Cl1—C3—C4—C5	179.94 (15)	C9—C10—C11—C12	−178.04 (17)
C3—C4—C5—C6	0.8 (3)	C10—C11—C12—C13	−1.2 (3)
C4—C5—C6—C1	−1.1 (3)	C11—C12—C13—C14	−0.4 (3)
C2—C1—C6—C5	0.2 (3)	C11—C12—C13—Cl2	−179.77 (15)
C7—C1—C6—C5	−178.20 (18)	C12—C13—C14—C15	1.4 (3)
C6—C1—C7—O1	155.76 (19)	Cl2—C13—C14—C15	−179.14 (14)
C2—C1—C7—O1	−22.7 (3)	C13—C14—C15—C10	−1.0 (3)
C6—C1—C7—C8	−24.7 (3)	C11—C10—C15—C14	−0.4 (3)
C2—C1—C7—C8	156.89 (18)	C9—C10—C15—C14	179.15 (17)
O1—C7—C8—C9	−15.6 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2A···Cg2^{i}	0.95	2.98	3.608 (2)	125
C5—H5A···Cg2^{ii}	0.95	2.88	3.488 (2)	126
C14—H14A···Cg1^{iii}	0.95	2.77	3.474 (2)	131

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

Fig. 1

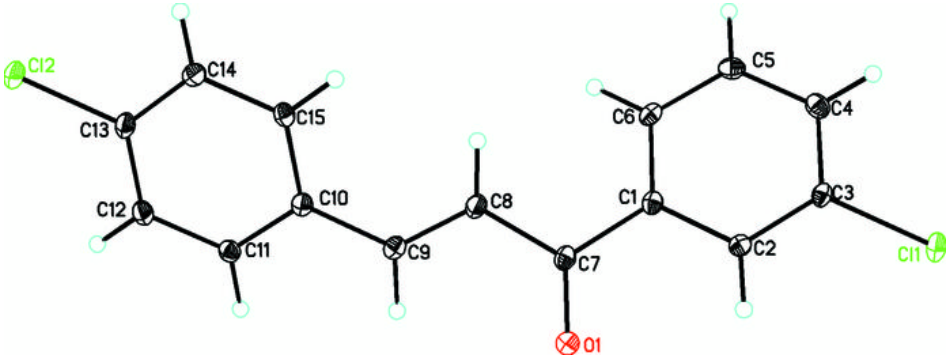

Fig. 2