Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2*E*)-3-(2-Bromo-5-methoxyphenyl)-1-(2,4-dichlorophenyl)prop-2-en-1-one

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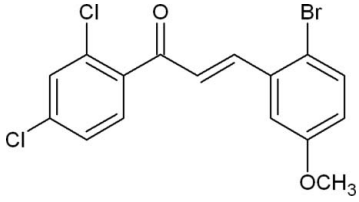
Received 12 September 2007; accepted 2 October 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.053; wR factor = 0.126; data-to-parameter ratio = 24.0.

In the title molecule, $C_{16}H_{11}BrCl_2O_2$, the angle between the mean planes of the 2,4-dichlorophenyl and 2-bromophenyl groups is 45.3 (5)°. The 5-methoxy group, with a torsion angle of 175.4 (4)°, is twisted slightly away from the plane of the 2-bromophenyl ring in an antiperiplanar conformation. The ketone oxygen of the prop-2-en-1-one group is twisted in a synclinal arrangement with respect to the 2,4-dichlorophenyl group, with a torsion angle of 54.1 (5)°. Molecules pack in a chain-like fashion, in an alternate inverted pattern parallel to the *bc* face of the unit cell, along the *c* axis.

Related literature

For related structures, see: Sarojini *et al.*, 2007; Yathirajan *et al.* (2007*a*,*b*,*c*,*d*,*e*); Butcher *et al.*, (2007*a*,*b*,*c*,*d*). For related literature, see: Dhar, (1981); Fichou *et al.* (1988); Tam *et al.* (1989); Goto *et al.* (1991); Cho *et al.* (1996); Uchida *et al.* (1998); Di Carlo *et al.* (1999); Dimmock *et al.* (1999); Opletalova & Sedivy, (1999); Lawrence *et al.* (2001); Indira *et al.* (2002); Lin *et al.* (2002); Zhao *et al.* (2002); Bhat *et al.* (2005); Pandey *et al.* (2005); Sarojini *et al.* (2006).



Experimental

Crystal data

$C_{16}H_{11}BrCl_2O_2$
M_r = 386.06
Triclinic, $P\overline{1}$
a = 7.7836 (13) Å
b = 7.8829 (8) Å
c = 13.0927 (19) Å
α = 83.050 (10)°
β = 88.899 (13)°
γ = 78.596 (11)°
V = 781.68 (19) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.97 mm^{-1}
T = 296 K
0.45 × 0.37 × 0.17 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.305, T_{max} = 1.000 (expected range = 0.184–0.603)
8869 measured reflections
4577 independent reflections
2880 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.126
S = 1.08
4577 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro* (Oxford Diffraction, 2007); 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*.

ANM thanks the Department of Studies in Chemistry, University of Mysore, for use of their research facilities. RJB acknowledges the NSF MRI program (grant No. CHE-0619278) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2098).

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supplementary materials

Acta Cryst. (2007). E**63**, o4253-o4254 [**doi:10.1107/S1600536807048271**]

(2*E*)-3-(2-Bromo-5-methoxyphenyl)-1-(2,4-dichlorophenyl)prop-2-en-1-one

R. J. Butcher, J. P. Jasinski, H. S. Yathirajan, B. Narayana and A. N. Mayekar

Comment

Chalcones are one of the major classes of natural products with widespread distribution in fruits, vegetables, spices, tea and soy based foodstuff have been recently subjects of great interest for their interesting pharmacological activities (Di Carlo *et al.*, 1999). 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). Chalcones can be easily obtained from the aldol condensation of aromatic aldehydes and aromatic ketones. This class of compounds presents interesting biological properties such as cytotoxicity (Pandey *et al.*, 2005; Bhat *et al*., 2005) and antiherpes activity and antitumour activity and may be useful for the chemotherapy of leishmaniasis among others (Lawrence *et al.*, 2001). A review on the bioactivities of chalcones is described (Dimmock *et al.*, 1999). Chalcones and their heterocyclic analogs as potential antifungal chemotherapeutic agents is published (Opletalova & Sedivy, 1999). Chalcones and flavonoids as anti-tuberculosis agents is reported (Lin *et al.*, 2002). Among several organic compounds reported for NLO property, chalcone derivatives are noticeable materials for their excellent blue light transmittance and good crystallizability. They provide a necessary configuration to show NLO property with two planar rings connected through a conjugated double bond (Goto *et al.*, 1991; Uchida *et al.*, 1998; Tam *et al.*, 1989; Indira *et al.*, 2002, Sarojini *et al.*, 2006). Substitution on either of the phenyl rings greatly influence non-centrosymmetric crystal packing. It is speculated that in order to improve the activity, more bulky substituents should be introduced to increase the spontaneous polarization of noncentrosymmetric crystal (Fichou *et al.*, 1988). The molecular hyperpolarizability β are strongly influenced not only by the electronic effect but also by the steric effect of the substituent (Cho *et al.*, 1996). Bromo groups can obviously improve the molecular first order hyperpolarizabilities and can effectively reduce the dipole-dipole interactions between the molecules (Zhao *et al.*, 2002). The crystal structures of chalcones containing structures of a few dichloro and bromo substituted chalcones *viz*., (2E)-1-(2,4-dichlorophenyl)-3-(quinolin-8-yl)prop-2-en-1-one (Sarojini *et al.*, 2007), (2E)-1-(2,4-dichlorophenyl)-3-(4,5-dimethoxy-2-nitrophenyl) prop-2-en-1-one (Yathirajan *et al.*, 2007*a*), (2E)-1-(2,4-dichlorophenyl)-3-(6-methoxy-2-naphthyl) prop-2-en-1-one (Yathirajan *et al.*, 2007*b*), (2E)-1-(2,4-dichlorophenyl)-3-(2-hydroxy-3-methoxyphenyl) prop-2-en-1-one (Yathirajan *et al.*, 2007*c*), (2E)-1-(2,4-dichlorophenyl)-3-(4-nitrophenyl)prop-2-en-1-one (Yathirajan *et al.*, 2007 d), (2E)-1-(2,4-dichlorophenyl)-3-(2-hydroxyphenyl)prop-2-en-1-one (Yathirajan *et al.*, 2007 e), (2E)-1-(3-bromo-2-thienyl)-3-[4-(dimethylamino)phenyl] prop-2-en-1-one (Butcher *et al.*, 2007*a*), (2E)-1-(3-bromo-2-thienyl)-3-(4-butoxyphenyl)prop-2-en-1-one (Butcher *et al.*, 2007*b*), (2E)-1-(3-bromo-2-thienyl)-3-(6-methoxy-2-naphthyl)prop-2-en-1-one (Butcher *et al.*, 2007*c*) and (2E)-1-(3-bromothien-2-yl)-3-phenylprop-2-en-1-one (Butcher *et al.*, 2007 d) have been reported. In continuation of our work on chalcones, a new chalcone, (I), $C_{16}H_{11}BrCl_2O_2$ is synthesized and its crystal structure is reported.

The angle between the mean planes of the 2,4-dichlorophenyl and 2-bromophenyl groups is 45.3 (5)° (Fig. 1). The 5-methoxy group, with a torsion angle [C16–O2–C14–C13] of 175.4 (4)°, is twisted slightly away from the plane of the 2-bromophenyl ring in an anti-periplanar formation. The ketone oxygen of the prop-2-en-1-one group, with a 54.1 (5)° torsion angle [C2–C1–C7–O1], is twisted in a *syn*-clinal arrangement with the 2,4-dichlorophenyl group. Molecules in the asymmetric unit pack themselves in a chain-like fashion in an alternate inverted pattern parallel to the *bc* face of the unit

cell along the *c* axis (Fig. 2). Crystal packing is stabilized by van der Waals forces as well as by interactions between π ring orbitals from a nearby 2-bromo-5-methoxyphenyl ring [C10^{i}–C15^{i} (*Cg*1^{i}); where *Cg* = ring center of gravity] and H6A from the 2,4-dichlorophenyl ring [C6–H6A···*Cg*1^{i}: 2.78 (0)Å (symmetry code ^{i}: 1 − *x*, 1 − *y*, 1 − *z*)].

Experimental

2-Bromo-5-methoxybenzaldehyde (2.15 g, 0.01 mol) in ethanol (30 ml) was mixed with 1-(2,4-dichlorophenyl)ethanone (1.89 g, 0.01 mol) in ethanol (20 ml) and the mixture was treated with 7 ml of 10% KOH solution (Fig. 3). The reaction mixture was then kept for constant stirring for 10 h. The solid precipitate obtained was filtered, washed with ethanol and dried. The crystal growth was carried out from a 1:1 mixture of acetone and toluene by the slow evaporation technique (m.p.: 367–369 K). Analysis found: C 49.71, H 2.83%; $C_{16}H_{11}BrCl_2O_2$ requires: C 49.78, H 2.87%.

Refinement

All H atoms were placed in their calculated places and all H atoms were refined using a riding model with C—H = 0.93 Å, and with U_{iso}(H) = 1.18–1.50U_{eq}(C).

Figures

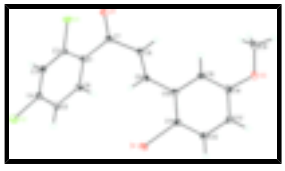


Fig. 1. Molecular structure of the title compound, showing atom labeling and 50% probability displacement ellipsoids.

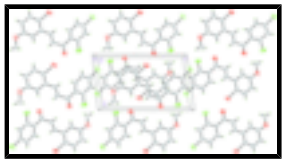


Fig. 2. Packing diagram of the title compound, viewed down the *a* axis and showing 50% probability displacement ellipsoids.

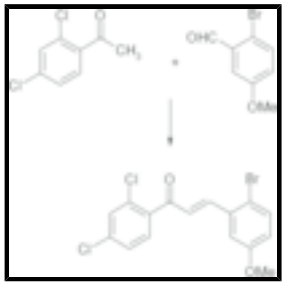


Fig. 3. Synthetic scheme for $C_{16}H_{11}BrCl_2O_2$.

(2E)-3-(2-Bromo-5-methoxyphenyl)-1-(2,4-dichlorophenyl)prop-2-en-1-one

Crystal data

$C_{16}H_{11}BrCl_2O_2$	$Z = 2$
$M_r = 386.06$	$F_{000} = 384$
Triclinic, $P\overline{1}$	$D_x = 1.640$ Mg m^{-3}

Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.7836 (13) Å	Cell parameters from 4266 reflections
b = 7.8829 (8) Å	θ = 4.7–32.4º
c = 13.0927 (19) Å	μ = 2.97 mm^{-1}
α = 83.050 (10)º	T = 296 K
β = 88.899 (13)º	Plate, pale yellow
γ = 78.596 (11)º	0.45 × 0.37 × 0.17 mm
V = 781.68 (19) Å^3	

Data collection

Oxford Diffraction Gemini R CCD diffractometer	4577 independent reflections
Radiation source: fine-focus sealed tube	2880 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.030
Detector resolution: 10.5081 pixels mm^{-1}	θ_{max} = 32.4º
T = 296 K	θ_{min} = 4.7º
φ and ω scans	h = −11→10
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	k = −11→11
T_{min} = 0.305, T_{max} = 1.000	l = −18→19
8869 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
$R[F^2 > 2\sigma(F^2)]$ = 0.053	H-atom parameters constrained
$wR(F^2)$ = 0.126	$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 0.6258P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.08	$(\Delta/\sigma)_{max}$ = 0.002
4577 reflections	$\Delta\rho_{max}$ = 0.74 e Å^{-3}
191 parameters	$\Delta\rho_{min}$ = −0.43 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 $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing *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}
Br	0.19344 (6)	0.81176 (4)	0.43646 (3)	0.06201 (16)
Cl1	0.24366 (16)	0.09035 (12)	0.15596 (9)	0.0728 (3)
Cl2	0.25624 (19)	0.73128 (14)	−0.02982 (8)	0.0837 (4)
O1	0.5150 (4)	0.0495 (3)	0.3339 (2)	0.0678 (8)
O2	0.1303 (4)	0.3275 (3)	0.82251 (18)	0.0643 (7)
C1	0.3892 (4)	0.3245 (4)	0.2449 (2)	0.0378 (6)
C2	0.3062 (5)	0.2898 (4)	0.1586 (2)	0.0441 (7)
C3	0.2649 (5)	0.4133 (4)	0.0736 (2)	0.0537 (9)
H3A	0.2066	0.3893	0.0173	0.064*
C4	0.3121 (5)	0.5721 (4)	0.0743 (2)	0.0513 (8)
C5	0.3987 (5)	0.6101 (4)	0.1559 (3)	0.0504 (8)
H5A	0.4322	0.7172	0.1543	0.060*
C6	0.4354 (4)	0.4865 (4)	0.2408 (2)	0.0437 (7)
H6A	0.4928	0.5125	0.2968	0.052*
C7	0.4314 (4)	0.1950 (4)	0.3399 (2)	0.0432 (7)
C8	0.3722 (4)	0.2515 (4)	0.4402 (2)	0.0417 (7)
H8A	0.4111	0.1766	0.4992	0.050*
C9	0.2675 (4)	0.4020 (4)	0.4518 (2)	0.0388 (6)
H9A	0.2245	0.4717	0.3917	0.047*
C10	0.2116 (4)	0.4711 (4)	0.5489 (2)	0.0374 (6)
C11	0.1705 (4)	0.6497 (4)	0.5541 (2)	0.0425 (7)
C12	0.1197 (5)	0.7168 (4)	0.6455 (3)	0.0496 (8)
H12A	0.0946	0.8367	0.6476	0.060*
C13	0.1066 (5)	0.6045 (5)	0.7330 (3)	0.0518 (8)
H13A	0.0708	0.6490	0.7943	0.062*
C14	0.1467 (5)	0.4245 (4)	0.7307 (2)	0.0455 (7)
C15	0.1996 (4)	0.3585 (4)	0.6394 (2)	0.0395 (6)
H15A	0.2274	0.2385	0.6379	0.047*
C16	0.1558 (8)	0.1460 (6)	0.8250 (3)	0.0852 (15)
H16A	0.1342	0.0951	0.8932	0.128*
H16B	0.2743	0.1011	0.8059	0.128*
H16C	0.0765	0.1175	0.7775	0.128*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br	0.0796 (3)	0.03977 (19)	0.0635 (2)	−0.01194 (17)	−0.00880 (19)	0.00831 (14)
Cl1	0.0965 (8)	0.0418 (4)	0.0858 (7)	−0.0191 (5)	−0.0089 (6)	−0.0200 (4)
Cl2	0.1286 (11)	0.0601 (6)	0.0499 (5)	0.0004 (6)	−0.0125 (6)	0.0143 (4)
O1	0.090 (2)	0.0433 (13)	0.0573 (15)	0.0139 (13)	0.0105 (14)	−0.0001 (11)
O2	0.090 (2)	0.0597 (15)	0.0413 (13)	−0.0130 (14)	0.0090 (13)	−0.0039 (11)
C1	0.0424 (18)	0.0345 (14)	0.0339 (14)	−0.0026 (12)	0.0044 (12)	−0.0023 (11)

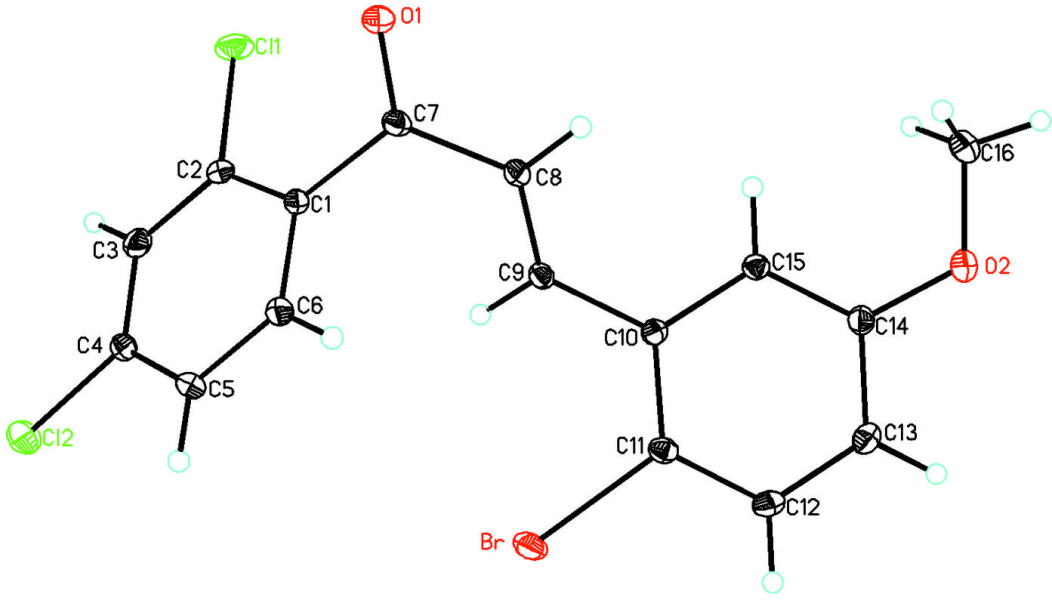
C2	0.056 (2)	0.0323 (14)	0.0449 (17)	−0.0071 (13)	0.0032 (14)	−0.0098 (12)
C3	0.069 (3)	0.0518 (19)	0.0388 (17)	−0.0036 (17)	−0.0066 (16)	−0.0114 (14)
C4	0.070 (2)	0.0410 (16)	0.0366 (16)	−0.0006 (16)	0.0016 (15)	0.0014 (12)
C5	0.066 (2)	0.0354 (15)	0.0494 (18)	−0.0140 (15)	0.0068 (16)	0.0003 (13)
C6	0.050 (2)	0.0421 (15)	0.0399 (16)	−0.0110 (14)	0.0002 (13)	−0.0046 (12)
C7	0.0457 (19)	0.0350 (14)	0.0456 (17)	−0.0033 (13)	0.0016 (13)	0.0003 (12)
C8	0.0462 (19)	0.0387 (15)	0.0366 (15)	−0.0026 (13)	−0.0030 (13)	0.0016 (11)
C9	0.0443 (18)	0.0368 (14)	0.0341 (14)	−0.0080 (13)	−0.0045 (12)	0.0017 (11)
C10	0.0361 (16)	0.0377 (14)	0.0378 (15)	−0.0049 (12)	−0.0044 (12)	−0.0047 (11)
C11	0.0414 (18)	0.0369 (14)	0.0487 (17)	−0.0083 (13)	−0.0080 (14)	−0.0011 (12)
C12	0.049 (2)	0.0382 (15)	0.061 (2)	−0.0019 (14)	−0.0048 (16)	−0.0122 (14)
C13	0.051 (2)	0.056 (2)	0.0474 (18)	−0.0043 (16)	0.0009 (15)	−0.0164 (15)
C14	0.049 (2)	0.0483 (17)	0.0397 (16)	−0.0110 (14)	−0.0007 (14)	−0.0051 (13)
C15	0.0413 (18)	0.0366 (14)	0.0414 (15)	−0.0091 (12)	−0.0028 (13)	−0.0050 (11)
C16	0.141 (5)	0.059 (2)	0.053 (2)	−0.021 (3)	0.018 (3)	0.0067 (18)

Geometric parameters (Å, °)

Br—C11	1.908 (3)	C8—C9	1.323 (4)
Cl1—C2	1.739 (3)	C8—H8A	0.9300
Cl2—C4	1.737 (3)	C9—C10	1.468 (4)
O1—C7	1.213 (4)	C9—H9A	0.9300
O2—C14	1.363 (4)	C10—C11	1.390 (4)
O2—C16	1.401 (5)	C10—C15	1.405 (4)
C1—C6	1.388 (4)	C11—C12	1.386 (5)
C1—C2	1.394 (4)	C12—C13	1.376 (5)
C1—C7	1.507 (4)	C12—H12A	0.9300
C2—C3	1.385 (4)	C13—C14	1.395 (5)
C3—C4	1.374 (5)	C13—H13A	0.9300
C3—H3A	0.9300	C14—C15	1.384 (4)
C4—C5	1.368 (5)	C15—H15A	0.9300
C5—C6	1.380 (4)	C16—H16A	0.9600
C5—H5A	0.9300	C16—H16B	0.9600
C6—H6A	0.9300	C16—H16C	0.9600
C7—C8	1.474 (4)		
C14—O2—C16	118.4 (3)	C8—C9—H9A	116.4
C6—C1—C2	117.2 (3)	C10—C9—H9A	116.4
C6—C1—C7	119.7 (3)	C11—C10—C15	118.2 (3)
C2—C1—C7	123.2 (3)	C11—C10—C9	121.0 (3)
C3—C2—C1	121.8 (3)	C15—C10—C9	120.9 (3)
C3—C2—Cl1	117.5 (3)	C12—C11—C10	121.6 (3)
C1—C2—Cl1	120.7 (2)	C12—C11—Br	117.4 (2)
C4—C3—C2	118.4 (3)	C10—C11—Br	120.9 (2)
C4—C3—H3A	120.8	C13—C12—C11	119.4 (3)
C2—C3—H3A	120.8	C13—C12—H12A	120.3
C5—C4—C3	121.8 (3)	C11—C12—H12A	120.3
C5—C4—Cl2	118.9 (3)	C12—C13—C14	120.6 (3)
C3—C4—Cl2	119.3 (3)	C12—C13—H13A	119.7
C4—C5—C6	118.8 (3)	C14—C13—H13A	119.7

C4—C5—H5A	120.6	O2—C14—C15	125.4 (3)
C6—C5—H5A	120.6	O2—C14—C13	114.9 (3)
C5—C6—C1	121.9 (3)	C15—C14—C13	119.6 (3)
C5—C6—H6A	119.0	C14—C15—C10	120.6 (3)
C1—C6—H6A	119.0	C14—C15—H15A	119.7
O1—C7—C8	121.0 (3)	C10—C15—H15A	119.7
O1—C7—C1	120.7 (3)	O2—C16—H16A	109.5
C8—C7—C1	118.3 (3)	O2—C16—H16B	109.5
C9—C8—C7	124.2 (3)	H16A—C16—H16B	109.5
C9—C8—H8A	117.9	O2—C16—H16C	109.5
C7—C8—H8A	117.9	H16A—C16—H16C	109.5
C8—C9—C10	127.2 (3)	H16B—C16—H16C	109.5
C6—C1—C2—C3	−2.5 (5)	C7—C8—C9—C10	−176.2 (3)
C7—C1—C2—C3	178.2 (3)	C8—C9—C10—C11	151.1 (3)
C6—C1—C2—Cl1	179.8 (2)	C8—C9—C10—C15	−28.3 (5)
C7—C1—C2—Cl1	0.4 (4)	C15—C10—C11—C12	0.3 (5)
C1—C2—C3—C4	1.8 (5)	C9—C10—C11—C12	−179.2 (3)
Cl1—C2—C3—C4	179.6 (3)	C15—C10—C11—Br	177.1 (2)
C2—C3—C4—C5	0.4 (6)	C9—C10—C11—Br	−2.3 (4)
C2—C3—C4—Cl2	−178.2 (3)	C10—C11—C12—C13	−1.1 (5)
C3—C4—C5—C6	−1.7 (5)	Br—C11—C12—C13	−178.0 (3)
Cl2—C4—C5—C6	176.9 (3)	C11—C12—C13—C14	1.0 (5)
C4—C5—C6—C1	0.9 (5)	C16—O2—C14—C15	−5.0 (6)
C2—C1—C6—C5	1.1 (5)	C16—O2—C14—C13	175.4 (4)
C7—C1—C6—C5	−179.5 (3)	C12—C13—C14—O2	179.4 (3)
C6—C1—C7—O1	−125.2 (4)	C12—C13—C14—C15	−0.2 (5)
C2—C1—C7—O1	54.1 (5)	O2—C14—C15—C10	179.8 (3)
C6—C1—C7—C8	53.3 (4)	C13—C14—C15—C10	−0.6 (5)
C2—C1—C7—C8	−127.4 (3)	C11—C10—C15—C14	0.6 (5)
O1—C7—C8—C9	−173.6 (3)	C9—C10—C15—C14	−180.0 (3)
C1—C7—C8—C9	8.0 (5)		

Fig. 1


O1
Cl1
C7
C2
C8
C1
C3
C9
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C6
C4
C10
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C5
Cl2
C11
C13
C12
Br
C16

Fig. 2

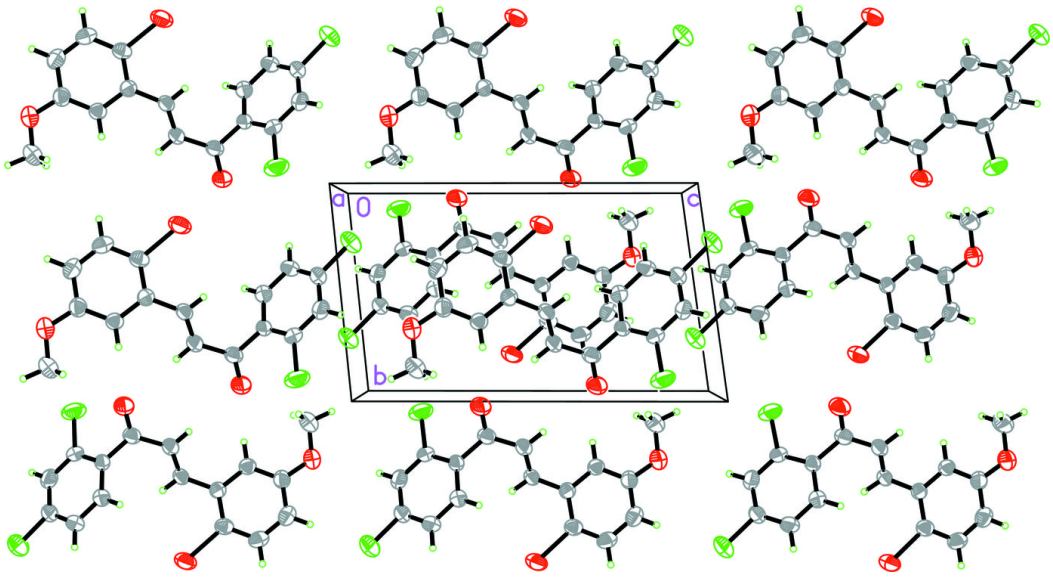
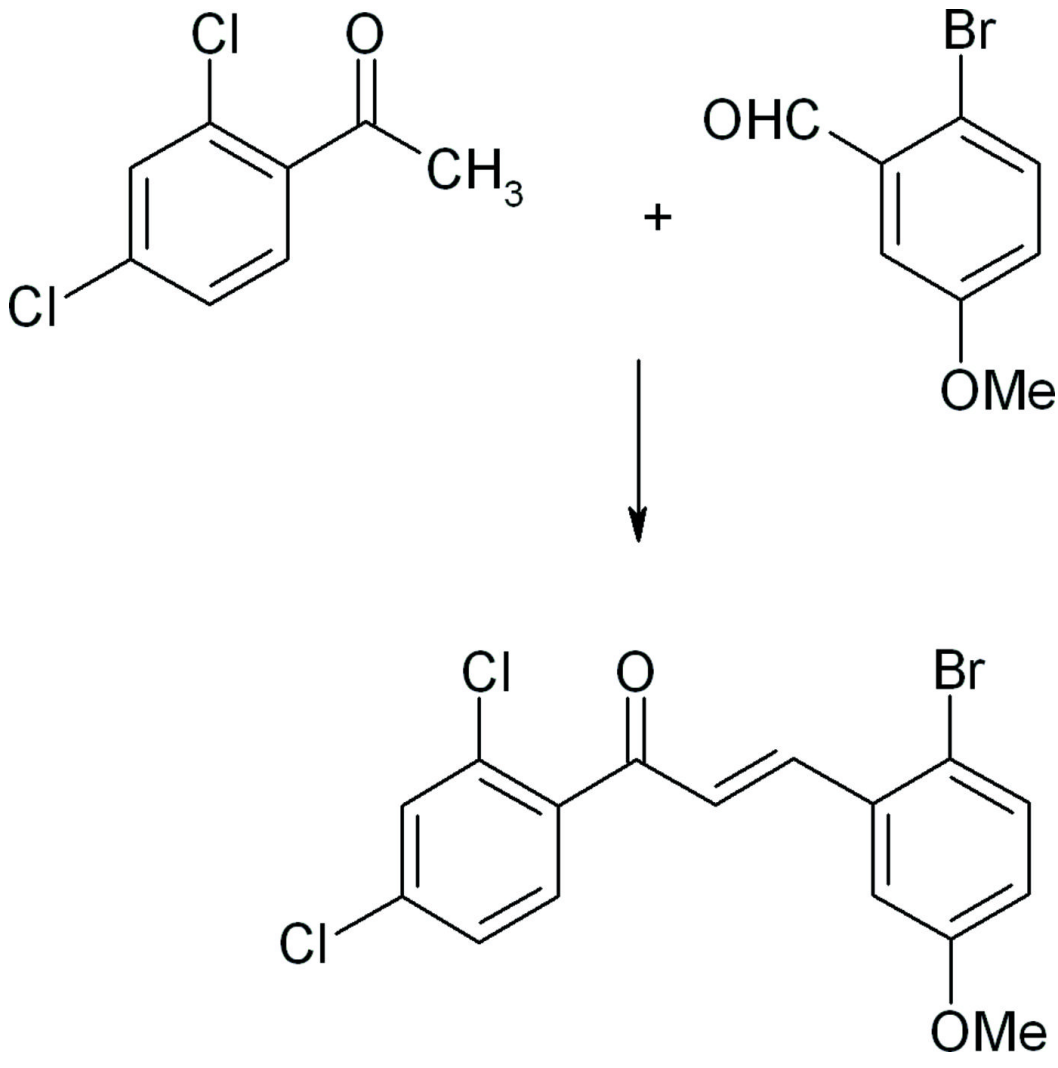
Fig. 3