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(2*E*)-3-(3,5-Dichloro-4-methoxy-2,6-dimethylphenyl)-1-(2,4-dichlorophenyl)-prop-2-en-1-one

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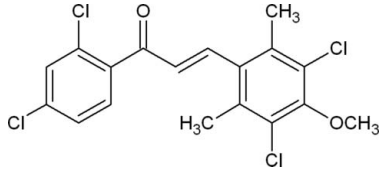
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.011 Å; R factor = 0.081; wR factor = 0.239; data-to-parameter ratio = 18.7.

In the title molecule, $C_{18}H_{14}Cl_4O_2$, the angle between the mean planes of the 3,5-dichloro-4-methoxy-2,6-dimethylphenyl and 2,4-dichlorophenyl groups is 47.6 (2)°. The 4-methoxy group, with a torsion angle of 91.9 (9)°, is twisted away from the plane of the 3,5-dichloro-2,6-dimethylphenyl ring in an anticlinal conformation. The ketone O atom of the prop-2-en-1-one group is twisted in a synclinal conformation with the 2,4-dichlorophenyl group [torsion angle = 45.5 (11)°]. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonding between the ketone O atom from the prop-2-en-1-one group and an H atom from a nearby 2,4-dichlorophenyl group, which link the molecules into chains along the *a* axis. The 3,5-dichloro-4-methoxy-2,6-dimethylphenyl and 2,4-dichlorophenyl groups are aligned obliquely parallel to the *ac* face, with the benzene rings stacked obliquely along the *b* axis for both groups.

Related literature

For related structures, see: Sarojini *et al.* (2007); Yathirajan, Mayekar, Narayana *et al.* (2007*a*,*b*,*c*); Yathirajan, Mayekar, Sarojini *et al.* (2007*a*,*b*). For related literature, see: Goto *et al.* (1991); Indira *et al.* (2002); Lawrence *et al.* (2001); Pandey *et al.* (2005); Sarojini *et al.* (2006).



Experimental

Crystal data

$C_{18}H_{14}Cl_4O_2$
M_r = 404.09
Monoclinic, *Pc*
a = 7.8036 (4) Å
b = 4.3526 (2) Å
c = 26.6839 (11) Å
β = 97.020 (4)°
V = 899.55 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.67 mm^{-1}
T = 296 K
0.37 × 0.31 × 0.23 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.502, T_{max} = 1.000 (expected range = 0.431–0.858)
8039 measured reflections
4142 independent reflections
2501 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.081
$wR(F^2)$ = 0.239
S = 1.03
4142 reflections
221 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3A···O1^{i}	0.93	2.55	3.471 (11)	170

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

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: AT2412).

References

Bruker (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Goto, Y., Hayashi, A., Kimura, Y. & Nakayama, M. (1991). *J. Cryst. Growth*, **108**, 688–698.
Indira, J., Karat, P. P. & Sarojini, B. K. (2002). *J. Cryst. Growth*, **242**, 209–214.
Lawrence, N. J., Rennison, D., McGown, A. T., Ducki, S., Gul, L. A., Hadfield, J. A. & Khan, N. (2001). *J. Comb. Chem.* **3**, 421–426.
Oxford Diffraction (2007). *CrysAlisPro* (Version 171.31.8) and *CrysAlis RED* (Version 1.171.31.8). Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Pandey, S., Suryawanshi, S. N., Gupta, S. & Srivastava, V. M. L. (2005). *Eur. J. Med. Chem.* **40**, 751–756.
Sarojini, B. K., Narayana, B., Ashalatha, B. V., Indira, J. & Lobo, K. G. (2006). *J. Cryst. Growth*, **295**, 54–59.
Sarojini, B. K., Yathirajan, H. S., Mayekar, A. N., Narayana, B. & Bolte, M. (2007). *Acta Cryst.* E**63**, o3488.

 doi:10.1107/S1600536807047654

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Yathirajan, H. S., Mayekar, A. N., Narayana, B., Sarojini, B. K. & Bolte, M. (2007*b*). *Acta Cryst.* E**63**, o540–o541.
Yathirajan, H. S., Mayekar, A. N., Narayana, B., Sarojini, B. K. & Bolte, M. (2007*c*). *Acta Cryst.* E**63**, o2200–o2201.
Yathirajan, H. S., Mayekar, A. N., Narayana, B., Sarojini, & Bolte, M. (2007*a*). *Acta Cryst.* E**63**, o428–o429.
Yathirajan, H. S., Mayekar, A. N., Sarojini, B. K., Narayana, B. & Bolte, M. (2007*a*). *Acta Cryst.* E**63**, o424–o425.
Yathirajan, H. S., Mayekar, A. N., Sarojini, B. K., Narayana, B. & Bolte, M. (2007*b*). *Acta Cryst.* E**63**, o426–o427.

supplementary materials

Acta Cryst. (2007). E**63**, o4229-o4230 [**doi:10.1107/S1600536807047654**]

(2*E*)-3-(3,5-Dichloro-4-methoxy-2,6-dimethylphenyl)-1-(2,4-dichlorophenyl)prop-2-en-1-one

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

Comment

Chalcone is an unique template molecule that is associated with several biological activities. 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), antiherpes activity and antitumour activity and may be useful for the chemotherapy of leishmaniasis among others (Lawrence *et al.* 2001). Among several organic compounds reported to have NLO properties, chalcone derivatives are a recognized material because of their excellent blue light transmittance and good crystallization ability (Goto *et al.* 1991; Indira *et al.* 2002; Sarojini *et al.* 2006). Structures of a few dichloro 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, Mayekar, Narayana *et al.* 2007*c*), (2E)-1-(2,4-dichlorophenyl)-3-(6-methoxy-2-naphthyl)prop-2-en-1-one (Yathirajan, Mayekar, Narayana *et al.* 2007*b*), (2E)-1-(2,4-dichlorophenyl)-3-(2-hydroxy-3-methoxyphenyl) prop-2-en-1-one (Yathirajan, Mayekar, Narayana *et al.* 2007*a*), (2E)-1-(2,4-dichlorophenyl)-3-(4-nitrophenyl)prop-2-en-1-one (Yathirajan, Mayekar, Sarojini *et al.* 2007*a*) and (2E)-1-(2,4-dichlorophenyl)-3-(2-hydroxyphenyl)prop-2-en-1-one (Yathirajan, Mayekar, Sarojini *et al.* 2007*b*) have been published. In continuation of our work on chalcones, a new chalcone $C_{18}H_{14}Cl_4O_2$ was synthesized and its crystal structure is reported.

The angle between the mean planes of the 3,5-dichloro-4-methoxy-2,6-dimethylphenyl and 2,4-dichlorophenyl groups is 47.6 (2)° (Fig. 1). The 4-methoxy group, with a C15–O2–C14–C13 torsion angle of 91.9 (9)°, is twisted away from the plane of the 3,5-dichloro-2,6-dimethylphenyl ring in an anti-clinal conformation. The ketone oxygen of the prop-2-en-1-one group is twisted in a *syn*-clinal conformation with the 2,4-dichlorophenyl group [C6–C1–C7–O1 torsion angle = 45.5 (11)°]. Crystal packing is stabilized by intermolecular C—H···O hydrogen bonding between the ketone oxygen from the prop-2-en-1-one group and a hydrogen atom from a nearby 2,4-dichlorophenyl group [C3–H3A···O1] which link the molecules into chains along the *a* axis of the unit cell (Fig. 2). Both of the 3,5-dichloro-4-methoxy-2,6-dimethylphenyl and 2,4-dichlorophenyl groups are aligned obliquely parallel to the *ac* face with the phenyl rings stacked obliquely along the *b* axis for both groups (Fig. 3).

Experimental

3,5-Dichloro-4-methoxy-2,6-dimethylbenzaldehyde (2.33 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 8 ml of 10% KOH solution (Fig. 4). The reaction mixture was then kept for constant stirring. 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.: 401–403 K). Analysis found: C 53.41, H 3.43%; $C_{18}H_{14}Cl_4O_2$ requires: C 53.50, H 3.49%.

Refinement

All H atoms were placed in their calculated places and refined using a riding model with C—H = 0.93 to 0.96 Å, and with U_{iso}(H) = 1.19–1.50U_{eq}(C).

Figures

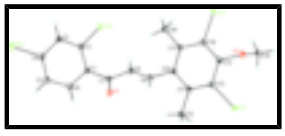

Fig. 1. Molecular structure of the title compound, showing atom labeling and 50% probability displacement ellipsoids.

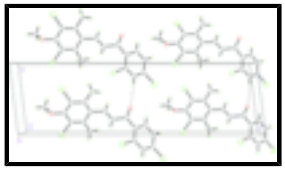

Fig. 2. Packing diagram of the title compound, viewed down the *b* axis.

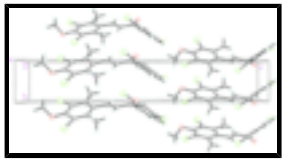

Fig. 3. Packing diagram of the title compound, viewed down the *a* axis.

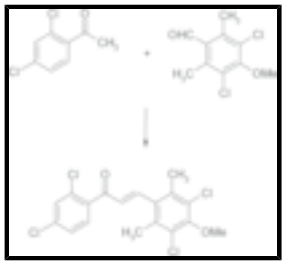

Fig. 4. Synthetic scheme for $C_{18}H_{14}Cl_4O_2$.

(2E)-3-(3,5-Dichloro-4-methoxy-2,6-dimethylphenyl)-1-(2,4-dichlorophenyl)prop- 2-en-1-one

Crystal data

$C_{18}H_{14}Cl_4O_2$	F_{000} = 412
M_r = 404.09	D_x = 1.492 Mg m^{-3}
Monoclinic, *Pc*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P -2yc	Cell parameters from 3151 reflections
a = 7.8036 (4) Å	θ = 4.7–32.4º
b = 4.3526 (2) Å	μ = 0.67 mm^{-1}
c = 26.6839 (11) Å	*T* = 296 K
β = 97.020 (4)º	Chunk, colourless
V = 899.55 (7) Å^3	0.37 × 0.31 × 0.23 mm
Z = 2	

Data collection

Oxford Diffraction Gemini R CCD diffractometer	4142 independent reflections
Radiation source: fine-focus sealed tube	2501 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.045$
Detector resolution: 10.5081 pixels mm^{-1}	$\theta_{max} = 32.5^{o}$
$T = 296$ K	$\theta_{min} = 4.8^{o}$
φ and ω scans	$h = -10 \rightarrow 11$
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	$k = -6 \rightarrow 6$
$T_{min} = 0.502$, $T_{max} = 1.000$	$l = -39 \rightarrow 39$
8039 measured reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.128P)^2 + 0.8404P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.081$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.239$	$\Delta\rho_{max} = 0.80$ e $Å^{-3}$
$S = 1.03$	$\Delta\rho_{min} = -0.55$ e $Å^{-3}$
4142 reflections	Extinction correction: *SHELXL97* (Sheldrick, 1997), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
221 parameters	Extinction coefficient: 0.090 (11)
2 restraints	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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 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	−0.1343 (3)	−0.2032 (6)	0.41662 (8)	0.0672 (6)
Cl2	−0.2962 (4)	0.4321 (8)	0.57611 (11)	0.0929 (9)
Cl3	0.63088 (19)	0.5365 (4)	0.21399 (6)	0.0454 (4)
Cl4	0.0016 (2)	−0.0404 (5)	0.17461 (7)	0.0546 (5)
O1	0.3767 (9)	−0.067 (2)	0.4676 (2)	0.083 (2)
O2	0.3069 (7)	0.3112 (13)	0.15441 (19)	0.0585 (13)
C1	0.1023 (9)	0.1380 (17)	0.4771 (2)	0.0471 (15)
C2	−0.0731 (9)	0.0404 (17)	0.4674 (3)	0.0488 (16)
C3	−0.1907 (10)	0.120 (2)	0.4978 (3)	0.0542 (17)
H3A	−0.3032	0.0465	0.4920	0.065*
C4	−0.1405 (10)	0.317 (2)	0.5384 (3)	0.0590 (19)
C5	0.0273 (13)	0.405 (2)	0.5501 (3)	0.067 (2)
H5A	0.0606	0.5270	0.5782	0.080*
C6	0.1454 (11)	0.309 (2)	0.5198 (3)	0.061 (2)
H6A	0.2606	0.3620	0.5285	0.073*
C7	0.2420 (9)	0.0391 (17)	0.4465 (2)	0.0479 (15)
C8	0.2188 (10)	0.099 (2)	0.3920 (3)	0.0564 (18)
H8A	0.1153	0.1870	0.3780	0.068*
C9	0.3307 (11)	0.038 (2)	0.3625 (3)	0.0554 (18)
H9A	0.4312	−0.0550	0.3777	0.067*
C10	0.3237 (9)	0.0957 (17)	0.3066 (3)	0.0478 (15)
C11	0.4588 (10)	0.2643 (17)	0.2898 (3)	0.0515 (16)
C12	0.6065 (11)	0.383 (2)	0.3266 (3)	0.062 (2)
H12A	0.7138	0.3094	0.3170	0.092*
H12B	0.5936	0.3108	0.3599	0.092*
H12C	0.6060	0.6033	0.3263	0.092*
C13	0.4546 (10)	0.3347 (19)	0.2390 (3)	0.0525 (16)
C14	0.3116 (10)	0.2325 (17)	0.2042 (2)	0.0485 (15)
C15	0.3859 (13)	0.088 (2)	0.1242 (3)	0.062 (2)
H15A	0.3837	0.1642	0.0904	0.093*
H15B	0.3230	−0.1015	0.1238	0.093*
H15C	0.5032	0.0542	0.1386	0.093*
C16	0.1818 (9)	0.0693 (16)	0.2219 (3)	0.0462 (15)
C17	0.1824 (10)	−0.0016 (18)	0.2732 (3)	0.0501 (16)
C18	0.0396 (12)	−0.197 (2)	0.2895 (3)	0.062 (2)
H18A	0.0630	−0.2386	0.3250	0.093*
H18B	0.0332	−0.3872	0.2711	0.093*
H18C	−0.0682	−0.0899	0.2827	0.093*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0663 (12)	0.0760 (14)	0.0580 (10)	−0.0069 (10)	0.0026 (8)	−0.0058 (10)
Cl2	0.0866 (17)	0.123 (2)	0.0776 (14)	0.0037 (16)	0.0454 (13)	−0.0149 (15)
Cl3	0.0402 (8)	0.0484 (8)	0.0485 (8)	−0.0094 (7)	0.0093 (6)	0.0048 (8)
Cl4	0.0430 (9)	0.0764 (13)	0.0439 (8)	−0.0096 (9)	0.0032 (7)	−0.0044 (9)
O1	0.060 (4)	0.135 (6)	0.055 (3)	0.013 (4)	0.012 (3)	0.013 (4)
O2	0.076 (4)	0.053 (3)	0.048 (2)	0.001 (3)	0.013 (2)	0.012 (2)

C1	0.047 (4)	0.057 (4)	0.038 (3)	0.002 (3)	0.010 (3)	0.005 (3)
C2	0.037 (3)	0.063 (4)	0.047 (3)	0.016 (3)	0.003 (3)	0.006 (3)
C3	0.051 (4)	0.066 (4)	0.047 (3)	−0.004 (3)	0.012 (3)	0.017 (3)
C4	0.054 (4)	0.076 (5)	0.051 (4)	0.006 (4)	0.020 (3)	0.008 (4)
C5	0.073 (6)	0.084 (6)	0.045 (4)	−0.004 (5)	0.008 (4)	−0.011 (4)
C6	0.054 (5)	0.080 (6)	0.047 (3)	−0.007 (4)	0.004 (3)	0.002 (4)
C7	0.046 (4)	0.059 (4)	0.038 (3)	0.007 (3)	0.003 (3)	0.007 (3)
C8	0.048 (4)	0.083 (5)	0.038 (3)	0.004 (4)	0.006 (3)	0.003 (3)
C9	0.051 (4)	0.071 (5)	0.043 (3)	−0.002 (3)	0.001 (3)	−0.006 (3)
C10	0.041 (3)	0.057 (4)	0.047 (3)	0.007 (3)	0.016 (3)	0.000 (3)
C11	0.066 (4)	0.044 (4)	0.046 (3)	0.002 (3)	0.009 (3)	−0.011 (3)
C12	0.046 (4)	0.079 (6)	0.058 (4)	0.001 (4)	0.000 (3)	−0.011 (4)
C13	0.052 (4)	0.058 (4)	0.049 (3)	−0.003 (3)	0.014 (3)	−0.002 (3)
C14	0.060 (4)	0.048 (4)	0.038 (3)	0.011 (3)	0.006 (3)	0.007 (3)
C15	0.082 (6)	0.062 (5)	0.045 (4)	−0.002 (4)	0.015 (4)	0.000 (3)
C16	0.042 (3)	0.052 (4)	0.045 (3)	0.005 (3)	0.005 (3)	−0.003 (3)
C17	0.046 (4)	0.062 (5)	0.045 (3)	0.003 (3)	0.017 (3)	−0.003 (3)
C18	0.065 (5)	0.066 (5)	0.059 (4)	−0.005 (4)	0.025 (4)	−0.005 (4)

Geometric parameters (Å, °)

Cl1—C2	1.741 (8)	C9—C10	1.509 (10)
Cl2—C4	1.743 (8)	C9—H9A	0.9300
Cl3—C13	1.825 (8)	C10—C17	1.396 (11)
Cl4—C16	1.834 (7)	C10—C11	1.402 (11)
O1—C7	1.221 (9)	C11—C13	1.386 (10)
O2—C14	1.369 (7)	C11—C12	1.511 (11)
O2—C15	1.445 (10)	C12—H12A	0.9600
C1—C6	1.367 (11)	C12—H12B	0.9600
C1—C2	1.426 (11)	C12—H12C	0.9600
C1—C7	1.503 (10)	C13—C14	1.432 (11)
C2—C3	1.342 (10)	C14—C16	1.367 (11)
C3—C4	1.400 (12)	C15—H15A	0.9600
C3—H3A	0.9300	C15—H15B	0.9600
C4—C5	1.363 (13)	C15—H15C	0.9600
C5—C6	1.364 (12)	C16—C17	1.402 (10)
C5—H5A	0.9300	C17—C18	1.508 (11)
C6—H6A	0.9300	C18—H18A	0.9600
C7—C8	1.468 (9)	C18—H18B	0.9600
C8—C9	1.272 (11)	C18—H18C	0.9600
C8—H8A	0.9300		
C14—O2—C15	114.2 (6)	C13—C11—C12	119.1 (7)
C6—C1—C2	116.5 (7)	C10—C11—C12	120.9 (7)
C6—C1—C7	119.2 (7)	C11—C12—H12A	109.5
C2—C1—C7	124.0 (6)	C11—C12—H12B	109.5
C3—C2—C1	121.6 (7)	H12A—C12—H12B	109.5
C3—C2—Cl1	119.0 (6)	C11—C12—H12C	109.5
C1—C2—Cl1	119.3 (5)	H12A—C12—H12C	109.5
C2—C3—C4	118.6 (7)	H12B—C12—H12C	109.5

C2—C3—H3A	120.7	C11—C13—C14	119.2 (7)
C4—C3—H3A	120.7	C11—C13—Cl3	122.3 (6)
C5—C4—C3	121.2 (7)	C14—C13—Cl3	118.4 (5)
C5—C4—Cl2	120.4 (7)	C16—C14—O2	122.2 (7)
C3—C4—Cl2	118.3 (6)	C16—C14—C13	119.3 (6)
C4—C5—C6	118.6 (8)	O2—C14—C13	118.5 (7)
C4—C5—H5A	120.7	O2—C15—H15A	109.5
C6—C5—H5A	120.7	O2—C15—H15B	109.5
C5—C6—C1	123.1 (8)	H15A—C15—H15B	109.5
C5—C6—H6A	118.5	O2—C15—H15C	109.5
C1—C6—H6A	118.5	H15A—C15—H15C	109.5
O1—C7—C8	121.2 (7)	H15B—C15—H15C	109.5
O1—C7—C1	120.0 (6)	C14—C16—C17	122.5 (6)
C8—C7—C1	118.6 (6)	C14—C16—Cl4	115.8 (5)
C9—C8—C7	124.4 (7)	C17—C16—Cl4	121.7 (6)
C9—C8—H8A	117.8	C10—C17—C16	117.7 (6)
C7—C8—H8A	117.8	C10—C17—C18	122.7 (6)
C8—C9—C10	129.2 (7)	C16—C17—C18	119.4 (7)
C8—C9—H9A	115.4	C17—C18—H18A	109.5
C10—C9—H9A	115.4	C17—C18—H18B	109.5
C17—C10—C11	121.4 (6)	H18A—C18—H18B	109.5
C17—C10—C9	120.8 (6)	C17—C18—H18C	109.5
C11—C10—C9	117.7 (7)	H18A—C18—H18C	109.5
C13—C11—C10	119.9 (7)	H18B—C18—H18C	109.5
C6—C1—C2—C3	2.0 (11)	C17—C10—C11—C12	176.8 (7)
C7—C1—C2—C3	175.8 (7)	C9—C10—C11—C12	0.2 (11)
C6—C1—C2—Cl1	−174.9 (6)	C10—C11—C13—C14	−0.2 (11)
C7—C1—C2—Cl1	−1.1 (9)	C12—C11—C13—C14	−177.7 (7)
C1—C2—C3—C4	3.3 (11)	C10—C11—C13—Cl3	−176.9 (6)
Cl1—C2—C3—C4	−179.8 (6)	C12—C11—C13—Cl3	5.6 (11)
C2—C3—C4—C5	−6.0 (12)	C15—O2—C14—C16	−90.7 (9)
C2—C3—C4—Cl2	177.4 (6)	C15—O2—C14—C13	91.6 (9)
C3—C4—C5—C6	3.2 (13)	C11—C13—C14—C16	0.4 (11)
Cl2—C4—C5—C6	179.8 (7)	Cl3—C13—C14—C16	177.2 (6)
C4—C5—C6—C1	2.4 (14)	C11—C13—C14—O2	178.2 (7)
C2—C1—C6—C5	−5.0 (12)	Cl3—C13—C14—O2	−5.0 (10)
C7—C1—C6—C5	−179.1 (8)	O2—C14—C16—C17	−177.4 (7)
C6—C1—C7—O1	45.5 (11)	C13—C14—C16—C17	0.3 (11)
C2—C1—C7—O1	−128.2 (9)	O2—C14—C16—Cl4	0.5 (9)
C6—C1—C7—C8	−129.2 (8)	C13—C14—C16—Cl4	178.2 (6)
C2—C1—C7—C8	57.1 (10)	C11—C10—C17—C16	1.3 (11)
O1—C7—C8—C9	2.3 (14)	C9—C10—C17—C16	177.8 (7)
C1—C7—C8—C9	176.9 (8)	C11—C10—C17—C18	176.7 (7)
C7—C8—C9—C10	−178.3 (8)	C9—C10—C17—C18	−6.8 (12)
C8—C9—C10—C17	−51.5 (13)	C14—C16—C17—C10	−1.2 (11)
C8—C9—C10—C11	125.1 (10)	Cl4—C16—C17—C10	−178.9 (5)
C17—C10—C11—C13	−0.7 (11)	C14—C16—C17—C18	−176.7 (7)
C9—C10—C11—C13	−177.2 (7)	Cl4—C16—C17—C18	5.5 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3A···O1^{i}	0.93	2.55	3.471 (11)	170

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1

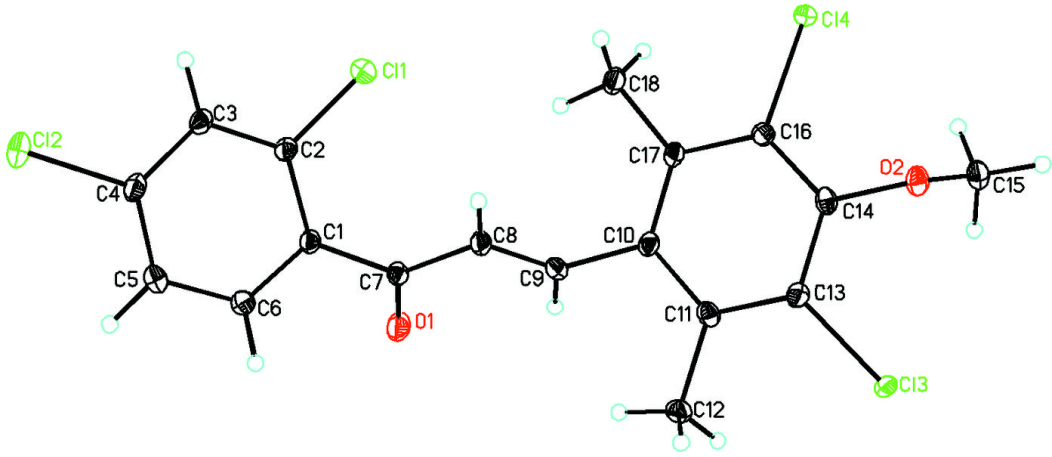
Cl4
Cl1
C18
C3
C16
Cl2
C2
C17
D2
C15
C4
C14
C1
C8
C10
C5
C7
C9
C13
C6
O1
C11
Cl3
C12

Fig. 2

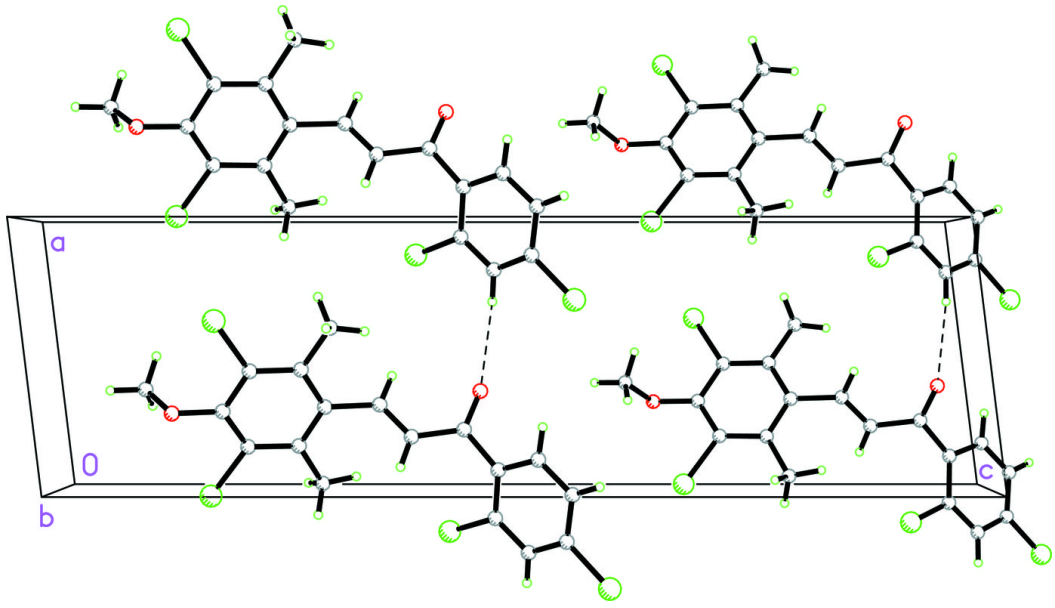

Fig. 3

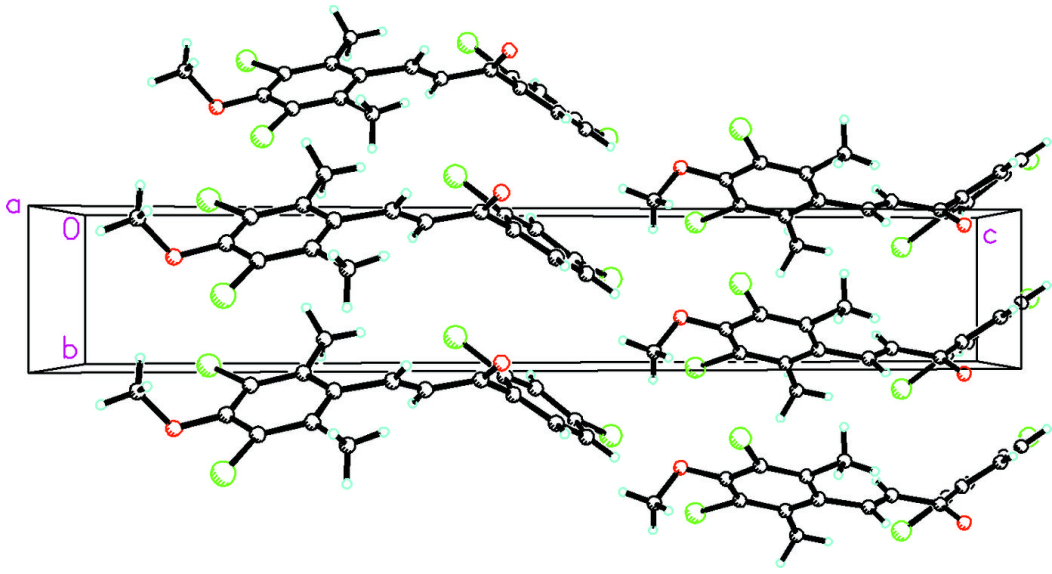

Fig. 4