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(2*E*)-1-(2,4-Dichlorophenyl)-3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one

Ray J. Butcher,[a] Jerry P. Jasinski,[b]* Anil N. Mayekar,[c] B. Narayana[d] and H. S. Yathirajan[c]

[a]Department of Chemistry, Howard University, 525 College Street NW, Washington DC 20059, USA, [b]Department of Chemistry, Keene State College, 229 Main Street, Keene, NH 03435-2001, USA, [c]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570006, India, and [d]Department of Studies in Chemistry, Mangalore University, Mangalagangotri 574199, India
Correspondence e-mail: jjasinski@keene.edu

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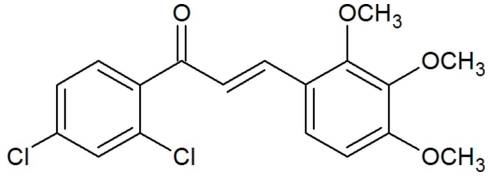
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.042; wR factor = 0.114; data-to-parameter ratio = 25.9.

In the title compound, $C_{18}H_{16}Cl_2O_4$, the mean planes of the 2,4-dichlorophenyl and 2,3,4-trimethoxyphenyl groups have a dihedral angle of 55.2 (2)°. The torsion angle connecting the ketone O atom of the prop-2-ene group to the 2,4-dichlorophenyl group is 57.3 (2)°. The crystal packing is stabilized by intermolecular C—H···O hydrogen bonding between a methoxy H atom and the ketone O atom in the prop-2-ene group, which links the molecules into chains in an alternate inverted pattern obliquely parallel to the *ac* face and diagonal along the *a* axis of the unit cell.

Related literature

For related structures, see: Teh *et al.* (2006); Sarojini *et al.* (2007); Fischer *et al.* (2007); Butcher *et al.* (2007); Yathirajan, Mayekar, Narayana *et al.* (2007*a*,*b*); Yathirajan, Mayekar, Sarojini *et al.* (2007*a*,*b*). For related literature, see: Dhar, (1981); Di Carlo *et al.* (1999); Dimmock *et al.* (1999); Goto *et al.* (1991); Opletalova & Sedivy, (1999); Indira *et al.* (2002); Lawrence *et al.* (2001); Bhat *et al.* (2005); Pandey *et al.* (2005); Sarojini *et al.* (2006); Lin *et al.* (2002).



Experimental

Crystal data

$C_{18}H_{16}Cl_2O_4$
M_r = 367.21
Monoclinic, $P2_1/n$
a = 16.5354 (7) Å
b = 4.6157 (2) Å
c = 23.1486 (11) Å
β = 102.489 (5)°
V = 1724.95 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 296 K
0.41 × 0.37 × 0.18 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.559, T_{max} = 1.000 (expected range = 0.521–0.931)
14451 measured reflections
5691 independent reflections
2371 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.114
S = 0.88
5691 reflections
220 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9*A*···O2	0.93	2.43	2.762 (2)	101
C16—H16*B*···O3	0.96	2.36	2.849 (3)	111
C18—H18*A*···O1^{i}	0.96	2.59	3.541 (3)	172

Symmetry code: (i) $x-\frac{1}{2}, -y-\frac{1}{2}, z-\frac{1}{2}$.

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: AT2394).

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supplementary materials

Acta Cryst. (2007). E**63**, o4059-o4060 [**doi:10.1107/S1600536807044303**]

(2*E*)-1-(2,4-Dichlorophenyl)-3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one

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

Comment

Chalcones are one of the major classes of natural products with widespread distribution in fruits, vegetables, spices, tea and soy based foodstuff have recently been 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), antiherpes activity, 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 has been published (Opletalova & Sedivy, 1999). Chalcones and flavonoids as anti-tuberculosis agents are also reported (Lin *et al.*, 2002). Several organic compounds reported to have NLO properties, chalcones derivatives are 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). The crystal structures of some dichloro substituted chalcones, *viz*., (2E)-1-(2,4-dichlorophenyl)-3-(quinolin-8-yl)prop-2-en-1-one, Sarojini *et al.*, (2007), (2E)-3-(biphenyl-4-yl)-1-(2,4-dichlorophenyl)prop-2-en-1-one, Fischer *et al.*, (2007); (2E)-1-(2,4-dichlorophenyl)-3-[4-(methylsulfanyl)phenyl] prop-2-en-1-one Butcher *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*a*), (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-(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 reported. A structurally very similar compound, *viz*., 1-(2,4-dichlorophenyl)-3-(2,4,5-trimethoxyphenyl)prop-2-en-1-one, which crystallizes in the triclinic space group, has also been reported (Teh *et al.*, 2006). In continuation of our work on chalcones, a new chalcone, (I), $C_{16}H_{13}FO$ has been synthesized and its crystal structure reported.

The mean planes of the 2,4-dichlorophenyl and 2,3,4-trimethoxyphenyl groups are separated by a dihedral angle of 55.2 (2)° (Fig. 1). The torsion angle connecting the ketone oxygen atom to the 2,4-dichlorophenyl group [C6–C1– C7–O1] is 57.3 (2)°. Crystal packing is stabilized by intermolecular C—H···O hydrogen bonding between a methoxy hydrogen atom and the ketone oxygen atom in the prop-2-ene group which link the molecules into chains in an alternate inverted pattern parallel to the *bc* face and diagonal along the *a* axis of the unit cell (Fig. 2).

Experimental

2,3,4-Trimethoxybenzaldehyde (1.96 g, 0.01 mol) in ethanol (50 ml) was mixed with 1-(2,4-dichlorophenyl)ethanone (1.89 g, 0.01 mol) and the mixture was treated with 10 ml of 10% KOH. The reaction mixture was then kept for constant stirring. The solid precipitate obtained was filtered, washed with ethanol and dried. Crystal growth was carried out from a 1:1

mixture of acetone and toluene by the slow evaporation technique [m.p.: 327–329 K]. Analysis found: C 58.80, H 4.34%; $C_{18}H_{16}Cl_2O_4$ requires: C 58.87, H 4.39%.

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 to 0.96 Å, and with U_{iso}(H) = 1.18–1.50U_{eq}(C).

Figures

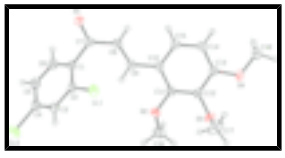

Fig. 1. Molecular structure of the title compound, showing atom labeling and 30% probability displacement ellipsoids.

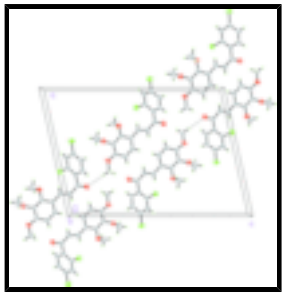

Fig. 2. Packing diagram of the title compound, viewed down the *b* axis and with 50% probability displacement ellipsoids. Dashed lines indicate intermolecular C—H···O hydrogen bonds.

(2E)-1-(2,4-Dichlorophenyl)-3-(2,3,4-trimethoxyphenyl)prop-2-en-1-one

Crystal data

$C_{18}H_{16}Cl_2O_4$	F_{000} = 760
M_r = 367.21	D_x = 1.414 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3324 reflections
a = 16.5354 (7) Å	θ = 4.6–32.5º
b = 4.6157 (2) Å	μ = 0.40 mm^{-1}
c = 23.1486 (11) Å	T = 296 K
β = 102.489 (5)º	Chunk, colourless
V = 1724.95 (13) Å^3	0.41 × 0.37 × 0.18 mm
Z = 4	

Data collection

Oxford Diffraction Gemini R CCD diffractometer	5691 independent reflections
Radiation source: fine-focus sealed tube	2371 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
Detector resolution: 10.5081 pixels mm^{-1}	θ_{max} = 32.5º

T = 296 K	θ_{min} = 4.6º
φ and ω scans	h = −24→22
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	k = −6→6
T_{min} = 0.559, T_{max} = 1.000	l = −34→32
14451 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
$R[F^2 > 2\sigma(F^2)]$ = 0.042	H-atom parameters constrained
$wR(F^2)$ = 0.114	$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.88	$(\Delta/\sigma)_{max}$ = 0.009
5691 reflections	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
220 parameters	$\Delta\rho_{min}$ = −0.42 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 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	0.65714 (3)	0.57002 (10)	0.00083 (2)	0.04970 (15)
Cl2	0.41613 (3)	−0.11621 (12)	−0.11266 (3)	0.06282 (18)
O1	0.77809 (8)	0.4482 (3)	−0.12937 (6)	0.0636 (4)
O2	0.79104 (7)	−0.0644 (2)	0.11903 (6)	0.0446 (3)
O3	0.91524 (8)	−0.1181 (3)	0.22328 (5)	0.0451 (3)
O4	1.07048 (8)	0.0060 (4)	0.22270 (6)	0.0633 (4)
C1	0.67810 (10)	0.2144 (4)	−0.08863 (7)	0.0352 (4)
C2	0.62533 (11)	0.3090 (4)	−0.05314 (7)	0.0356 (4)
C3	0.54519 (10)	0.2092 (4)	−0.06074 (8)	0.0383 (4)
H3A	0.5108	0.2750	−0.0366	0.046*
C4	0.51694 (11)	0.0103 (4)	−0.10476 (8)	0.0400 (4)
C5	0.56629 (12)	−0.0876 (4)	−0.14163 (8)	0.0444 (5)

H5A	0.5463	−0.2205	−0.1715	0.053*
C6	0.64602 (11)	0.0170 (4)	−0.13296 (8)	0.0433 (4)
H6A	0.6797	−0.0470	−0.1577	0.052*
C7	0.76435 (11)	0.3273 (4)	−0.08525 (8)	0.0422 (4)
C8	0.83050 (11)	0.2903 (5)	−0.03338 (8)	0.0499 (5)
H8A	0.8807	0.3808	−0.0336	0.060*
C9	0.82552 (11)	0.1376 (4)	0.01465 (8)	0.0404 (4)
H9A	0.7751	0.0483	0.0147	0.048*
C10	0.89131 (10)	0.0970 (4)	0.06698 (7)	0.0410 (4)
C11	0.87263 (10)	−0.0097 (4)	0.11940 (8)	0.0361 (4)
C12	0.93420 (11)	−0.0322 (4)	0.17086 (7)	0.0400 (4)
C13	1.01539 (12)	0.0394 (4)	0.17032 (8)	0.0492 (5)
C14	1.03516 (12)	0.1401 (5)	0.11867 (9)	0.0636 (6)
H14A	1.0896	0.1874	0.1179	0.076*
C15	0.97344 (12)	0.1694 (5)	0.06859 (8)	0.0600 (6)
H15A	0.9872	0.2405	0.0344	0.072*
C16	0.77199 (13)	−0.3329 (4)	0.14340 (10)	0.0583 (6)
H16A	0.7146	−0.3783	0.1285	0.087*
H16B	0.7827	−0.3178	0.1857	0.087*
H16C	0.8058	−0.4834	0.1324	0.087*
C17	0.8940 (2)	0.1146 (5)	0.25695 (10)	0.0837 (8)
H17A	0.8905	0.0460	0.2955	0.126*
H17B	0.8415	0.1932	0.2374	0.126*
H17C	0.9357	0.2625	0.2609	0.126*
C18	1.15339 (13)	0.0913 (6)	0.22577 (10)	0.0749 (8)
H18A	1.1852	0.0614	0.2652	0.112*
H18B	1.1549	0.2926	0.2157	0.112*
H18C	1.1764	−0.0223	0.1985	0.112*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0552 (3)	0.0458 (3)	0.0467 (3)	−0.0095 (2)	0.0080 (2)	−0.0104 (2)
Cl2	0.0410 (3)	0.0749 (4)	0.0710 (4)	−0.0196 (3)	0.0088 (3)	−0.0084 (3)
O1	0.0458 (8)	0.1031 (11)	0.0399 (8)	−0.0141 (8)	0.0048 (6)	0.0244 (8)
O2	0.0319 (7)	0.0504 (7)	0.0514 (8)	−0.0007 (6)	0.0089 (6)	0.0181 (6)
O3	0.0468 (8)	0.0556 (8)	0.0335 (7)	0.0021 (6)	0.0100 (6)	0.0109 (6)
O4	0.0391 (8)	0.1088 (11)	0.0364 (7)	−0.0063 (8)	−0.0041 (6)	0.0165 (8)
C1	0.0334 (9)	0.0417 (9)	0.0280 (9)	−0.0002 (8)	0.0012 (7)	0.0093 (8)
C2	0.0402 (10)	0.0358 (9)	0.0282 (9)	−0.0019 (8)	0.0014 (7)	0.0012 (7)
C3	0.0354 (10)	0.0409 (10)	0.0391 (10)	−0.0004 (8)	0.0093 (8)	0.0029 (8)
C4	0.0339 (10)	0.0436 (10)	0.0400 (10)	−0.0046 (8)	0.0020 (8)	0.0038 (8)
C5	0.0443 (11)	0.0484 (11)	0.0377 (10)	−0.0038 (9)	0.0024 (8)	−0.0057 (9)
C6	0.0408 (11)	0.0545 (11)	0.0353 (10)	−0.0001 (9)	0.0094 (8)	−0.0014 (9)
C7	0.0355 (10)	0.0575 (11)	0.0329 (10)	−0.0068 (9)	0.0063 (8)	0.0085 (9)
C8	0.0315 (10)	0.0737 (13)	0.0418 (11)	−0.0133 (9)	0.0019 (8)	0.0148 (10)
C9	0.0296 (9)	0.0520 (10)	0.0379 (10)	−0.0068 (8)	0.0035 (8)	0.0036 (9)
C10	0.0308 (9)	0.0588 (12)	0.0313 (9)	−0.0033 (8)	0.0023 (7)	0.0071 (9)

C11	0.0301 (9)	0.0411 (9)	0.0366 (9)	0.0006 (7)	0.0063 (7)	0.0063 (8)
C12	0.0378 (10)	0.0499 (10)	0.0316 (9)	0.0018 (8)	0.0058 (8)	0.0091 (8)
C13	0.0356 (10)	0.0770 (13)	0.0321 (10)	−0.0017 (10)	0.0010 (8)	0.0096 (10)
C14	0.0319 (10)	0.1145 (18)	0.0419 (11)	−0.0139 (11)	0.0028 (9)	0.0177 (12)
C15	0.0399 (11)	0.1047 (17)	0.0341 (11)	−0.0113 (11)	0.0050 (9)	0.0210 (11)
C16	0.0546 (13)	0.0536 (12)	0.0642 (14)	−0.0170 (10)	0.0074 (11)	0.0151 (11)
C17	0.130 (2)	0.0801 (17)	0.0473 (14)	0.0262 (16)	0.0334 (15)	0.0085 (12)
C18	0.0372 (12)	0.135 (2)	0.0454 (13)	−0.0092 (13)	−0.0078 (9)	0.0080 (13)

Geometric parameters (Å, °)

Cl1—C2	1.7335 (17)	C8—H8A	0.9300
Cl2—C4	1.7382 (18)	C9—C10	1.455 (2)
O1—C7	1.227 (2)	C9—H9A	0.9300
O2—C11	1.3707 (19)	C10—C15	1.391 (2)
O2—C16	1.425 (2)	C10—C11	1.405 (2)
O3—C12	1.3757 (19)	C11—C12	1.393 (2)
O3—C17	1.415 (2)	C12—C13	1.385 (2)
O4—C13	1.359 (2)	C13—C14	1.386 (3)
O4—C18	1.413 (2)	C14—C15	1.375 (2)
C1—C6	1.389 (2)	C14—H14A	0.9300
C1—C2	1.392 (2)	C15—H15A	0.9300
C1—C7	1.504 (2)	C16—H16A	0.9600
C2—C3	1.378 (2)	C16—H16B	0.9600
C3—C4	1.376 (2)	C16—H16C	0.9600
C3—H3A	0.9300	C17—H17A	0.9600
C4—C5	1.378 (3)	C17—H17B	0.9600
C5—C6	1.377 (3)	C17—H17C	0.9600
C5—H5A	0.9300	C18—H18A	0.9600
C6—H6A	0.9300	C18—H18B	0.9600
C7—C8	1.449 (2)	C18—H18C	0.9600
C8—C9	1.334 (2)		
C11—O2—C16	117.36 (14)	O2—C11—C12	121.86 (15)
C12—O3—C17	113.45 (15)	O2—C11—C10	117.34 (15)
C13—O4—C18	117.98 (15)	C12—C11—C10	120.54 (16)
C6—C1—C2	116.99 (16)	O3—C12—C13	118.87 (15)
C6—C1—C7	118.17 (16)	O3—C12—C11	120.78 (16)
C2—C1—C7	124.67 (16)	C13—C12—C11	120.32 (16)
C3—C2—C1	121.87 (16)	O4—C13—C12	115.40 (16)
C3—C2—Cl1	117.27 (14)	O4—C13—C14	124.76 (18)
C1—C2—Cl1	120.81 (13)	C12—C13—C14	119.84 (17)
C4—C3—C2	118.74 (16)	C15—C14—C13	119.31 (18)
C4—C3—H3A	120.6	C15—C14—H14A	120.3
C2—C3—H3A	120.6	C13—C14—H14A	120.3
C3—C4—C5	121.71 (16)	C14—C15—C10	122.76 (17)
C3—C4—Cl2	117.80 (14)	C14—C15—H15A	118.6
C5—C4—Cl2	120.49 (14)	C10—C15—H15A	118.6
C6—C5—C4	118.09 (17)	O2—C16—H16A	109.5
C6—C5—H5A	121.0	O2—C16—H16B	109.5

C4—C5—H5A	121.0	H16A—C16—H16B	109.5
C5—C6—C1	122.57 (17)	O2—C16—H16C	109.5
C5—C6—H6A	118.7	H16A—C16—H16C	109.5
C1—C6—H6A	118.7	H16B—C16—H16C	109.5
O1—C7—C8	120.05 (16)	O3—C17—H17A	109.5
O1—C7—C1	117.26 (15)	O3—C17—H17B	109.5
C8—C7—C1	122.67 (15)	H17A—C17—H17B	109.5
C9—C8—C7	125.54 (17)	O3—C17—H17C	109.5
C9—C8—H8A	117.2	H17A—C17—H17C	109.5
C7—C8—H8A	117.2	H17B—C17—H17C	109.5
C8—C9—C10	126.31 (16)	O4—C18—H18A	109.5
C8—C9—H9A	116.8	O4—C18—H18B	109.5
C10—C9—H9A	116.8	H18A—C18—H18B	109.5
C15—C10—C11	117.18 (16)	O4—C18—H18C	109.5
C15—C10—C9	122.78 (16)	H18A—C18—H18C	109.5
C11—C10—C9	120.00 (15)	H18B—C18—H18C	109.5
C6—C1—C2—C3	0.9 (2)	C16—O2—C11—C10	133.69 (18)
C7—C1—C2—C3	176.10 (15)	C15—C10—C11—O2	176.11 (17)
C6—C1—C2—Cl1	−176.44 (13)	C9—C10—C11—O2	−1.7 (2)
C7—C1—C2—Cl1	−1.3 (2)	C15—C10—C11—C12	1.9 (3)
C1—C2—C3—C4	0.0 (3)	C9—C10—C11—C12	−175.92 (16)
Cl1—C2—C3—C4	177.48 (13)	C17—O3—C12—C13	89.1 (2)
C2—C3—C4—C5	−0.9 (3)	C17—O3—C12—C11	−89.2 (2)
C2—C3—C4—Cl2	179.03 (13)	O2—C11—C12—O3	1.7 (3)
C3—C4—C5—C6	0.7 (3)	C10—C11—C12—O3	175.61 (16)
Cl2—C4—C5—C6	−179.19 (14)	O2—C11—C12—C13	−176.60 (17)
C4—C5—C6—C1	0.3 (3)	C10—C11—C12—C13	−2.7 (3)
C2—C1—C6—C5	−1.1 (3)	C18—O4—C13—C12	−176.4 (2)
C7—C1—C6—C5	−176.61 (16)	C18—O4—C13—C14	2.9 (3)
C6—C1—C7—O1	57.3 (2)	O3—C12—C13—O4	2.5 (3)
C2—C1—C7—O1	−117.8 (2)	C11—C12—C13—O4	−179.19 (16)
C6—C1—C7—C8	−120.8 (2)	O3—C12—C13—C14	−176.84 (18)
C2—C1—C7—C8	64.1 (3)	C11—C12—C13—C14	1.5 (3)
O1—C7—C8—C9	−172.7 (2)	O4—C13—C14—C15	−178.9 (2)
C1—C7—C8—C9	5.3 (3)	C12—C13—C14—C15	0.4 (3)
C7—C8—C9—C10	179.72 (18)	C13—C14—C15—C10	−1.2 (4)
C8—C9—C10—C15	−12.7 (3)	C11—C10—C15—C14	0.0 (3)
C8—C9—C10—C11	165.01 (19)	C9—C10—C15—C14	177.8 (2)
C16—O2—C11—C12	−52.2 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9A···O2	0.93	2.43	2.762 (2)	101
C16—H16B···O3	0.96	2.36	2.849 (3)	111
C18—H18A···O1^{i}	0.96	2.59	3.541 (3)	172

Symmetry codes: (i) *x*−1/2, −*y*−1/2, *z*−1/2.

Fig. 1

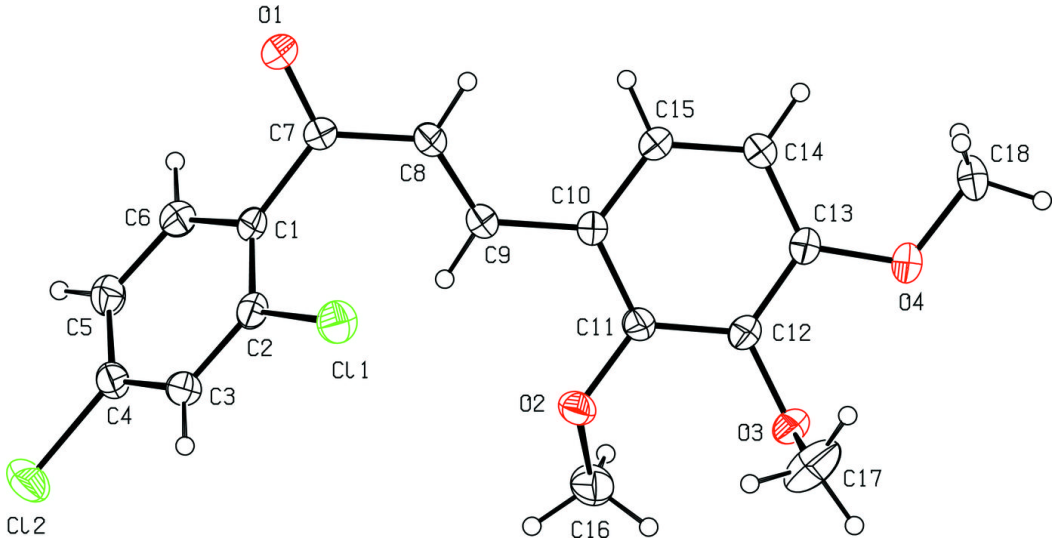
O1
C7
C8
C15
C14
C18
C6
C1
C10
C13
C9
O4
C5
C2
C11
C12
Cl1
O2
O3
C4
C3
C17
Cl2
C16

Fig. 2