Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(2-Chlorophenyl)-1,5-bis(4-chlorophenyl)pentane-1,5-dione

Jerry P. Jasinski,[a]* Ray J. Butcher,[b] H. S. Yathirajan,[c] B. Narayana[d] and M. T. Swamy[e]

[a]Department of Chemistry, Keene State College, 229 Main Street, Keene, NH 03435-2001, USA, [b]Department of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA, [c]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, [d]Department of Studies in Chemistry, Mangalore University, Mangalagangotri 574 199, India, and [e]Department of Chemistry, Sambhram Institute of technology, Bangalore 560 098, India
Correspondence e-mail: jjasinski@keene.edu

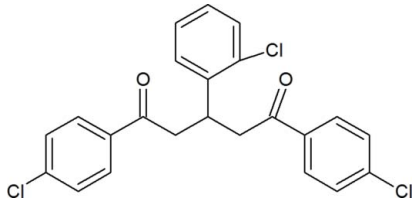
Received 11 November 2007; accepted 14 November 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.118; data-to-parameter ratio = 26.4.

In the title compound, $C_{23}H_{17}Cl_3O_2$, the dihedral angles between the 2-chlorophenyl group and the two 4-chlorophenyl groups are 88.9 (3) and 12.9 (2)°, while the angle between the mean planes of the two 4-chlorophenyl groups is 77.9 (5)°. The crystal packing is stabilized by intermolecular C—H···O interactions between an H atom from each of the two 4-chlorophenyl groups and a ketone O atom in neighboring molecules, which link the molecules into chains diagonally along the *ac* plane of the unit cell. Additional intermolecular π–π stacking interactions occur between adjacent 2-chlorophenyl rings as well as between one of the 4-chlorophenyl rings and a 2-chlorophenyl ring, the distances between the centroids of interacting rings being 3.931 (6) and 3.9915 (4) Å, respectively.

Related literature

For related structures, see: Insuasty *et al.* (2006); Teh *et al.* (2006); Huang *et al.* (2006); Qiu *et al.* (2006*a*,*b*); Butcher *et al.* (2007); Yathirajan *et al.* (2006, 2007). For related literature, see: Krohnke *et al.* (1976): Hirsch & Bailey, (1978).



Experimental

Crystal data

$C_{23}H_{17}Cl_3O_2$
M_r = 431.72
Triclinic, $P\overline{1}$
a = 7.1717 (8) Å
b = 7.7000 (15) Å
c = 18.901 (6) Å
α = 85.88 (2)°
β = 83.518 (15)°
γ = 77.656 (12)°
V = 1011.9 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.47 mm^{-1}
T = 296 K
0.45 × 0.39 × 0.28 mm

Data collection

Oxford Diffraction Gemini R CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.712, T_{max} = 0.877
14729 measured reflections
6690 independent reflections
3147 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.118
S = 0.93
6690 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7A—H7AA···O1A^{i}	0.93	2.50	3.306 (2)	145
C7B—H7BA···O1B^{ii}	0.93	2.51	3.2917 (17)	142

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$.

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*.

MTS thanks the Sambhram Institute of Technology 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: AT2485).

References

Bruker (2000). *SHELXTL*. Version 6.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Butcher, R. J., Jasinski, J. P., Yathirajan, H. S., Bindya, S. & Narayana, B. (2007). *Acta Cryst.* E**63**, o3330.
Hirsch, S. S. & Bailey, W. J. (1978). *J. Org. Chem.* **43**, 4090–4094.
Huang, X.-Q., Tan, Y.-X., Dou, J.-M., Li, D.-C. & Zhang, C.-S. (2006). *Acta Cryst.* E**62**, o5257–o5258.
Insuasty, B., Torres, H., Cobo, J., Low, J. N. & Glidewell, C. (2006). *Acta Cryst.* C**62**, o39–o41.
Krohnke, F. (1976). *Synthesis*, pp. 1–24.
Oxford Diffraction (2007). *CrysAlisPro* and *CrysAlis RED*. Versions 1.171.31.8. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Qiu, X.-Y., Liu, W.-S. & Zhu, H.-L. (2006*a*). *Acta Cryst.* E**62**, o1826–o1827.
Qiu, X.-Y., Yang, S., Liu, W.-S. & Zhu, H.-L. (2006*b*). *Acta Cryst.* E**62**, o2533–o2534.

  doi:10.1107/S1600536807059089

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Teh, J. B.-J., Patil, P. S., Fun, H.-K., Dharmaprakash, S. M., Razak, I. A. & Kalluraya, B. (2006). *Acta Cryst.* E**62**, o5024–o5026.
Yathirajan, H. S., Malte, K., Narayana, B., Sreevidya, T. V. & Bolte, M. (2007). *Acta Cryst.* E**63**, o228–o229.
Yathirajan, H. S., Sarojini, B. K., Ashalatha, B. V., Narayana, B. & Bolte, M. (2006). *Acta Cryst.* E**62**, o4554–o4555.

supplementary materials

Acta Cryst. (2007). E**63**, o4808-o4809 [**doi:10.1107/S1600536807059089**]

3-(2-Chlorophenyl)-1,5-bis(4-chlorophenyl)pentane-1,5-dione

J. P. Jasinski, R. J. Butcher, H. S. Yathirajan, B. Narayana and M. T. Swamy

Comment

1,5-Diketones are important synthetic intermediates and starting materials in the synthesis of many heterocyclic compounds (Hirsch & Bailey, 1978; Krohnke, 1976). The structures of related compounds *viz*., 1,5-bis(4-chlorophenyl)-3-(2-chloroquinolin-3-yl)pentane-1,5-dione (Insuasty *et al*. 2006), 1,5-(4-dichlorophenyl)-3-(2,5-dimethoxyphenyl)pentane-1,5-dione (Teh *et al.* 2006), 3-(2-furyl)-1,5-bis(4-methylphenyl)pentane-1,5-dione (Huang *et al.* 2006), 1,5-bis(4-chlorophenyl)-3-(4-pyridyl)pentane-1,5dione (Qiu *et al.* 2006*a*), 3-(3-chlorophenyl)-1,5-bis(4-nitrophenyl)pentane-1,5-dione (Qiu *et al.* 2006*b*), 1,5-bis (3-bromothien-2-yl) −3- (2,3,5-trichlorophenyl)pentane-1,5-dione, (Butcher *et al.* 2007), 1,5-bis(3-bromo-2-thienyl)-3-(3-nitrophenyl)pentane-1,5-dione (Yathirajan *et al.* 2006), 1,5-bis(4-bromophenyl)-3-(3-nitrophenyl)pentane-1,5-dione, (Yathirajan *et al.* 2007) have been reported. A new 1,5-dione, (I), $C_{23}H_{17}Cl_3O_2$ was synthesized and the crystal structure is reported here.

In the title compound, $C_{23}H_{17}Cl_3O_2$, the dihedral angles between the 2-chlorophenyl group and the two 4-chlorophenyl groups are 88.9 (3) and 12.9 (2)°, while the angle between the mean planes of the two 4-chlorophenyl groups is 77.9 (5)° (Fig. 1). The crystal packing is stabilized by intermolecular C–H···O interactions between a hydrogen atom from each of the two the two 4-chlorophenyl groups and its nearby ketone oxygen in neighboring molecules which link the molecules into chains diagonally and oblique along the *ac* plane of the unit cell (Fig. 2). Additional intermolecular π-π stacking interactions occur between adjacent 2-chlorophenyl rings [*Cg*3 = center of gravity of the 4-chlorolphenyl ring (C3B–C8B); *Cg*3···*Cg*3 = 3.931 (6) Å; 1 − *x*, 1 − *y*, −*z*] as well as between one of the 4-chlorophenyl rings and a 2-chlorophenyl ring [*Cg*1 = center of gravity of the 2-chlorolphenyl ring (C1–C6); *Cg*1···*Cg*3 = 3.931 (6) Å; *x*, −1 + *y*, *z*].

Experimental

4-Chloroacetophenone (1.54 g, 0.1 mol) in ethanol (30 ml) was mixed with 2-chlorobenzaldehyde (0.7 g, 0.05 mol) and the mixture was treated with an aqueous solution of sodium hydroxide (5 ml, 30%) (Fig. 3). This mixture was stirred well and left for 12 h. The resulting crude solid mass was collected by filtration, washed, dried and recrystallized from toluene (yield 85%., m.p.: 401 K). The initially formed 1-(4-methoxyphenyl)-3-(2-chlorophenyl)prop-2-en-1-one, underwent Michael addition, resulting in the formation of the novel title compound (I). Analysis found: C 63.90, H 3.94%; $C_{23}H_{17}Cl_3O_2$ requires: C 63.98, H 3.97%.

Refinement

The H atoms were placed in their calculated positions and then refined using the riding model with C—H = 0.93 to 0.98 Å, and with U_{iso}(H) = 1.19 or 1.21U_{eq}(C).

Figures

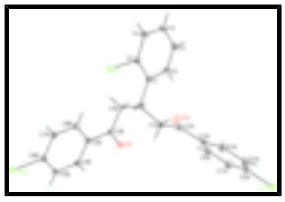


Fig. 1. Molecular structure of the title compound, showing atom labeling and 50% probability displacement ellipsoids.

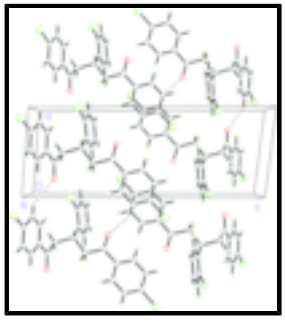


Fig. 2. Packing diagram of the title compound, viewed down the *b* axis. Dashed lines indicate intramolecular C—H···O hydrogen bonds.

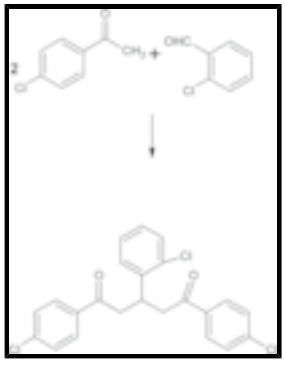


Fig. 3. Synthetic scheme for $C_{23}H_{17}Cl_3O_2$.

3-(2-Chlorophenyl)-1,5-bis(4-chlorophenyl)pentane-1,5-dione

Crystal data

$C_{23}H_{17}Cl_3O_2$	$Z = 2$
$M_r = 431.72$	$F_{000} = 444$
Triclinic, $P\overline{1}$	$D_x = 1.417$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.1717$ (8) Å	Cell parameters from 4806 reflections
$b = 7.7000$ (15) Å	$\theta = 4.5$–32.6º
$c = 18.901$ (6) Å	$\mu = 0.47$ mm^{-1}
$\alpha = 85.88$ (2)º	$T = 296$ K
$\beta = 83.518$ (15)º	Prism, pale yellow
$\gamma = 77.656$ (12)º	0.45 × 0.39 × 0.28 mm
$V = 1011.9$ (4) Å^3	

Data collection

Oxford Diffraction Gemini R CCD diffractometer	6690 independent reflections
Radiation source: fine-focus sealed tube	3147 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.024$
Detector resolution: 10.5081 pixels mm^{-1}	$\theta_{max} = 32.7^{o}$
$T = 296$ K	$\theta_{min} = 4.6^{o}$
φ and ω scans	$h = -10 \rightarrow 10$
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	$k = -11 \rightarrow 11$
$T_{min} = 0.712$, $T_{max} = 0.877$	$l = -28 \rightarrow 25$
14729 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
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.118$	$w = 1/[\sigma^2(F_o^2) + (0.0598P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.93$	$(\Delta/\sigma)_{max} = 0.001$
6690 reflections	$\Delta\rho_{max} = 0.24$ e $Å^{-3}$
253 parameters	$\Delta\rho_{min} = -0.33$ 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 $F^2 > 2$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}
Cl	0.99371 (5)	0.01789 (6)	0.20354 (3)	0.07076 (15)
Cl1A	−0.20263 (8)	0.29570 (8)	0.60074 (3)	0.09081 (19)
Cl1B	0.84843 (6)	0.85651 (6)	0.01648 (3)	0.07311 (16)
O1A	0.59359 (15)	0.16616 (18)	0.37462 (6)	0.0739 (4)

O1B	0.22035 (13)	0.35855 (15)	0.14247 (6)	0.0630 (3)
C	0.55268 (17)	0.10895 (17)	0.23407 (7)	0.0392 (3)
H0A	0.6438	0.1859	0.2371	0.047*
C1	0.65483 (18)	−0.08305 (17)	0.24669 (7)	0.0407 (3)
C2	0.85377 (19)	−0.13735 (19)	0.23327 (7)	0.0464 (3)
C3	0.9461 (2)	−0.3130 (2)	0.24106 (9)	0.0629 (4)
H3A	1.0786	−0.3451	0.2314	0.075*
C4	0.8422 (3)	−0.4397 (2)	0.26302 (10)	0.0718 (5)
H4A	0.9041	−0.5583	0.2685	0.086*
C5	0.6468 (3)	−0.3926 (2)	0.27701 (10)	0.0725 (5)
H5A	0.5758	−0.4785	0.2925	0.087*
C6	0.5560 (2)	−0.2157 (2)	0.26790 (8)	0.0572 (4)
H6A	0.4231	−0.1855	0.2765	0.069*
C1A	0.37939 (18)	0.16621 (19)	0.28840 (7)	0.0445 (3)
H1AA	0.3097	0.2827	0.2731	0.053*
H1AB	0.2945	0.0835	0.2886	0.053*
C2A	0.4284 (2)	0.17464 (19)	0.36322 (7)	0.0455 (3)
C3A	0.26998 (19)	0.19997 (18)	0.42202 (7)	0.0438 (3)
C4A	0.3106 (2)	0.2179 (2)	0.49019 (8)	0.0632 (4)
H4AA	0.4371	0.2101	0.4990	0.076*
C5A	0.1676 (3)	0.2470 (3)	0.54553 (9)	0.0712 (5)
H5AA	0.1968	0.2592	0.5914	0.085*
C6A	−0.0180 (2)	0.2578 (2)	0.53224 (8)	0.0585 (4)
C7A	−0.0643 (2)	0.2376 (2)	0.46536 (9)	0.0646 (4)
H7AA	−0.1909	0.2435	0.4571	0.078*
C8A	0.0818 (2)	0.2081 (2)	0.41048 (8)	0.0549 (4)
H8AA	0.0525	0.1936	0.3649	0.066*
C1B	0.49133 (18)	0.12994 (18)	0.15762 (7)	0.0421 (3)
H1BA	0.6040	0.0926	0.1245	0.051*
H1BB	0.4045	0.0509	0.1539	0.051*
C2B	0.39471 (18)	0.31623 (18)	0.13577 (7)	0.0423 (3)
C3B	0.51050 (18)	0.44822 (18)	0.10689 (7)	0.0394 (3)
C4B	0.41837 (19)	0.61665 (19)	0.08326 (7)	0.0446 (3)
H4BA	0.2851	0.6452	0.0864	0.054*
C5B	0.5207 (2)	0.74129 (19)	0.05538 (8)	0.0499 (4)
H5BA	0.4577	0.8529	0.0391	0.060*
C6B	0.7180 (2)	0.69894 (19)	0.05180 (7)	0.0462 (3)
C7B	0.81408 (19)	0.5351 (2)	0.07542 (8)	0.0496 (4)
H7BA	0.9473	0.5092	0.0734	0.060*
C8B	0.71080 (19)	0.40966 (19)	0.10217 (8)	0.0473 (3)
H8BA	0.7751	0.2975	0.1174	0.057*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.03547 (19)	0.0776 (3)	0.0992 (4)	−0.01499 (18)	−0.0055 (2)	0.0040 (2)
Cl1A	0.0917 (4)	0.1141 (4)	0.0619 (3)	−0.0255 (3)	0.0284 (3)	−0.0169 (3)
Cl1B	0.0674 (3)	0.0560 (3)	0.0960 (4)	−0.0229 (2)	0.0084 (2)	0.0000 (2)

O1A	0.0434 (6)	0.1231 (11)	0.0596 (7)	−0.0194 (6)	−0.0097 (5)	−0.0207 (7)
O1B	0.0355 (5)	0.0703 (7)	0.0783 (8)	−0.0073 (5)	−0.0019 (5)	0.0118 (6)
C	0.0321 (6)	0.0422 (7)	0.0430 (7)	−0.0085 (5)	−0.0022 (5)	−0.0012 (6)
C1	0.0408 (7)	0.0434 (7)	0.0380 (7)	−0.0088 (6)	−0.0050 (6)	−0.0014 (6)
C2	0.0412 (7)	0.0518 (8)	0.0449 (8)	−0.0059 (6)	−0.0061 (6)	−0.0035 (6)
C3	0.0597 (9)	0.0604 (10)	0.0619 (10)	0.0079 (8)	−0.0141 (8)	−0.0075 (8)
C4	0.0958 (14)	0.0450 (9)	0.0655 (11)	0.0078 (9)	−0.0128 (10)	−0.0028 (8)
C5	0.0992 (14)	0.0477 (10)	0.0722 (12)	−0.0243 (9)	−0.0028 (10)	0.0048 (8)
C6	0.0560 (9)	0.0520 (9)	0.0626 (10)	−0.0152 (7)	0.0024 (8)	0.0025 (7)
C1A	0.0370 (6)	0.0525 (8)	0.0426 (8)	−0.0044 (6)	−0.0054 (6)	−0.0062 (6)
C2A	0.0436 (7)	0.0503 (8)	0.0434 (8)	−0.0097 (6)	−0.0063 (6)	−0.0047 (6)
C3A	0.0489 (8)	0.0460 (8)	0.0377 (8)	−0.0106 (6)	−0.0078 (6)	−0.0028 (6)
C4A	0.0553 (9)	0.0898 (12)	0.0461 (9)	−0.0146 (9)	−0.0080 (8)	−0.0116 (8)
C5A	0.0819 (12)	0.0957 (14)	0.0375 (9)	−0.0184 (10)	−0.0064 (9)	−0.0131 (8)
C6A	0.0639 (10)	0.0621 (10)	0.0472 (9)	−0.0140 (8)	0.0086 (8)	−0.0065 (7)
C7A	0.0496 (9)	0.0892 (13)	0.0559 (10)	−0.0167 (8)	−0.0001 (8)	−0.0095 (9)
C8A	0.0502 (8)	0.0758 (11)	0.0395 (8)	−0.0145 (7)	−0.0037 (7)	−0.0059 (7)
C1B	0.0411 (7)	0.0465 (8)	0.0381 (7)	−0.0089 (6)	0.0003 (6)	−0.0046 (6)
C2B	0.0365 (7)	0.0524 (8)	0.0360 (7)	−0.0047 (6)	−0.0034 (6)	−0.0022 (6)
C3B	0.0367 (6)	0.0482 (8)	0.0317 (7)	−0.0042 (6)	−0.0047 (5)	−0.0030 (6)
C4B	0.0388 (7)	0.0464 (8)	0.0463 (8)	−0.0010 (6)	−0.0074 (6)	−0.0056 (6)
C5B	0.0518 (8)	0.0411 (8)	0.0531 (9)	0.0001 (6)	−0.0081 (7)	−0.0029 (7)
C6B	0.0498 (8)	0.0462 (8)	0.0434 (8)	−0.0130 (6)	−0.0006 (6)	−0.0042 (6)
C7B	0.0361 (7)	0.0604 (9)	0.0500 (9)	−0.0069 (6)	−0.0039 (6)	0.0025 (7)
C8B	0.0377 (7)	0.0495 (8)	0.0496 (8)	−0.0004 (6)	−0.0049 (6)	0.0066 (6)

Geometric parameters (Å, °)

Cl—C2	1.7439 (15)	C3A—C8A	1.379 (2)
Cl1A—C6A	1.7368 (16)	C4A—C5A	1.374 (2)
Cl1B—C6B	1.7380 (15)	C4A—H4AA	0.9300
O1A—C2A	1.2156 (16)	C5A—C6A	1.366 (2)
O1B—C2B	1.2173 (15)	C5A—H5AA	0.9300
C—C1	1.5183 (18)	C6A—C7A	1.370 (2)
C—C1A	1.5285 (18)	C7A—C8A	1.382 (2)
C—C1B	1.5450 (19)	C7A—H7AA	0.9300
C—H0A	0.9800	C8A—H8AA	0.9300
C1—C6	1.3759 (19)	C1B—C2B	1.5042 (19)
C1—C2	1.3976 (18)	C1B—H1BA	0.9700
C2—C3	1.379 (2)	C1B—H1BB	0.9700
C3—C4	1.364 (3)	C2B—C3B	1.4831 (19)
C3—H3A	0.9300	C3B—C4B	1.3910 (19)
C4—C5	1.370 (3)	C3B—C8B	1.3972 (18)
C4—H4A	0.9300	C4B—C5B	1.371 (2)
C5—C6	1.386 (2)	C4B—H4BA	0.9300
C5—H5A	0.9300	C5B—C6B	1.378 (2)
C6—H6A	0.9300	C5B—H5BA	0.9300
C1A—C2A	1.504 (2)	C6B—C7B	1.372 (2)
C1A—H1AA	0.9700	C7B—C8B	1.374 (2)

C1A—H1AB	0.9700	C7B—H7BA	0.9300
C2A—C3A	1.488 (2)	C8B—H8BA	0.9300
C3A—C4A	1.375 (2)		
C1—C—C1A	112.96 (11)	C6A—C5A—C4A	119.09 (15)
C1—C—C1B	107.79 (11)	C6A—C5A—H5AA	120.5
C1A—C—C1B	110.64 (10)	C4A—C5A—H5AA	120.5
C1—C—H0A	108.4	C5A—C6A—C7A	121.53 (14)
C1A—C—H0A	108.4	C5A—C6A—Cl1A	120.38 (13)
C1B—C—H0A	108.4	C7A—C6A—Cl1A	118.08 (13)
C6—C1—C2	115.99 (13)	C6A—C7A—C8A	118.44 (15)
C6—C1—C	121.92 (12)	C6A—C7A—H7AA	120.8
C2—C1—C	121.97 (12)	C8A—C7A—H7AA	120.8
C3—C2—C1	122.17 (14)	C3A—C8A—C7A	121.32 (14)
C3—C2—Cl	117.63 (12)	C3A—C8A—H8AA	119.3
C1—C2—Cl	120.19 (11)	C7A—C8A—H8AA	119.3
C4—C3—C2	119.73 (16)	C2B—C1B—C	114.25 (11)
C4—C3—H3A	120.1	C2B—C1B—H1BA	108.7
C2—C3—H3A	120.1	C—C1B—H1BA	108.7
C3—C4—C5	120.13 (16)	C2B—C1B—H1BB	108.7
C3—C4—H4A	119.9	C—C1B—H1BB	108.7
C5—C4—H4A	119.9	H1BA—C1B—H1BB	107.6
C4—C5—C6	119.39 (16)	O1B—C2B—C3B	120.07 (12)
C4—C5—H5A	120.3	O1B—C2B—C1B	119.50 (13)
C6—C5—H5A	120.3	C3B—C2B—C1B	120.43 (11)
C1—C6—C5	122.57 (15)	C4B—C3B—C8B	118.21 (13)
C1—C6—H6A	118.7	C4B—C3B—C2B	119.49 (11)
C5—C6—H6A	118.7	C8B—C3B—C2B	122.30 (12)
C2A—C1A—C	114.47 (11)	C5B—C4B—C3B	121.13 (12)
C2A—C1A—H1AA	108.6	C5B—C4B—H4BA	119.4
C—C1A—H1AA	108.6	C3B—C4B—H4BA	119.4
C2A—C1A—H1AB	108.6	C4B—C5B—C6B	119.10 (13)
C—C1A—H1AB	108.6	C4B—C5B—H5BA	120.5
H1AA—C1A—H1AB	107.6	C6B—C5B—H5BA	120.5
O1A—C2A—C3A	121.13 (13)	C7B—C6B—C5B	121.52 (13)
O1A—C2A—C1A	120.22 (13)	C7B—C6B—Cl1B	119.20 (11)
C3A—C2A—C1A	118.61 (12)	C5B—C6B—Cl1B	119.28 (11)
C4A—C3A—C8A	118.37 (13)	C6B—C7B—C8B	119.09 (13)
C4A—C3A—C2A	119.48 (13)	C6B—C7B—H7BA	120.5
C8A—C3A—C2A	122.15 (12)	C8B—C7B—H7BA	120.5
C5A—C4A—C3A	121.23 (15)	C7B—C8B—C3B	120.94 (13)
C5A—C4A—H4AA	119.4	C7B—C8B—H8BA	119.5
C3A—C4A—H4AA	119.4	C3B—C8B—H8BA	119.5
C1A—C—C1—C6	38.87 (18)	C4A—C5A—C6A—C7A	1.0 (3)
C1B—C—C1—C6	−83.68 (15)	C4A—C5A—C6A—Cl1A	−179.63 (14)
C1A—C—C1—C2	−145.14 (12)	C5A—C6A—C7A—C8A	−0.9 (3)
C1B—C—C1—C2	92.31 (14)	Cl1A—C6A—C7A—C8A	179.71 (13)
C6—C1—C2—C3	−0.3 (2)	C4A—C3A—C8A—C7A	1.4 (2)
C—C1—C2—C3	−176.50 (13)	C2A—C3A—C8A—C7A	−177.85 (15)

C6—C1—C2—Cl	178.12 (11)	C6A—C7A—C8A—C3A	−0.3 (3)
C—C1—C2—Cl	1.90 (18)	C1—C—C1B—C2B	−177.57 (10)
C1—C2—C3—C4	−0.5 (2)	C1A—C—C1B—C2B	58.46 (15)
Cl—C2—C3—C4	−178.91 (13)	C—C1B—C2B—O1B	−95.04 (15)
C2—C3—C4—C5	0.3 (3)	C—C1B—C2B—C3B	84.40 (14)
C3—C4—C5—C6	0.7 (3)	O1B—C2B—C3B—C4B	−4.2 (2)
C2—C1—C6—C5	1.3 (2)	C1B—C2B—C3B—C4B	176.39 (11)
C—C1—C6—C5	177.49 (14)	O1B—C2B—C3B—C8B	176.04 (13)
C4—C5—C6—C1	−1.5 (3)	C1B—C2B—C3B—C8B	−3.40 (19)
C1—C—C1A—C2A	67.11 (15)	C8B—C3B—C4B—C5B	0.7 (2)
C1B—C—C1A—C2A	−171.94 (11)	C2B—C3B—C4B—C5B	−179.14 (13)
C—C1A—C2A—O1A	12.0 (2)	C3B—C4B—C5B—C6B	−0.9 (2)
C—C1A—C2A—C3A	−170.18 (12)	C4B—C5B—C6B—C7B	0.1 (2)
O1A—C2A—C3A—C4A	1.4 (2)	C4B—C5B—C6B—Cl1B	179.99 (11)
C1A—C2A—C3A—C4A	−176.42 (14)	C5B—C6B—C7B—C8B	1.1 (2)
O1A—C2A—C3A—C8A	−179.32 (16)	Cl1B—C6B—C7B—C8B	−178.87 (11)
C1A—C2A—C3A—C8A	2.9 (2)	C6B—C7B—C8B—C3B	−1.3 (2)
C8A—C3A—C4A—C5A	−1.4 (3)	C4B—C3B—C8B—C7B	0.5 (2)
C2A—C3A—C4A—C5A	177.96 (16)	C2B—C3B—C8B—C7B	−179.73 (13)
C3A—C4A—C5A—C6A	0.2 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7A—H7AA···O1A^{i}	0.93	2.50	3.306 (2)	145
C7B—H7BA···O1B^{ii}	0.93	2.51	3.2917 (17)	142

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

Fig. 1

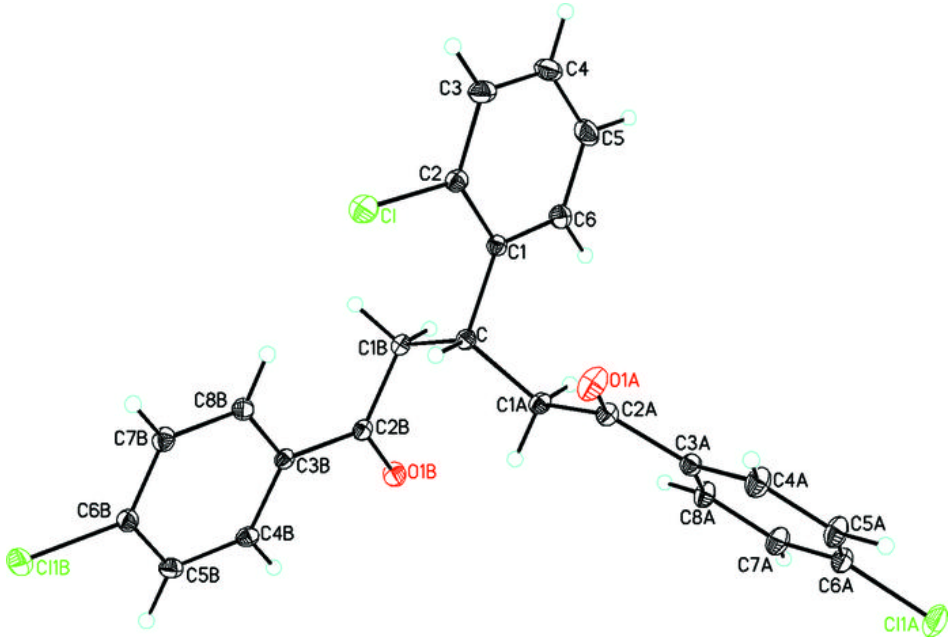

C4
C3
C5
C2
Cl
C6
C1
C1B
C
O1A
C1A
C2A
C8B
C7B
C2B
C3A
C3B
O1B
C4A
C6B
C8A
C5A
C4B
C7A
C11B
C5B
C6A
C11A

Fig. 2

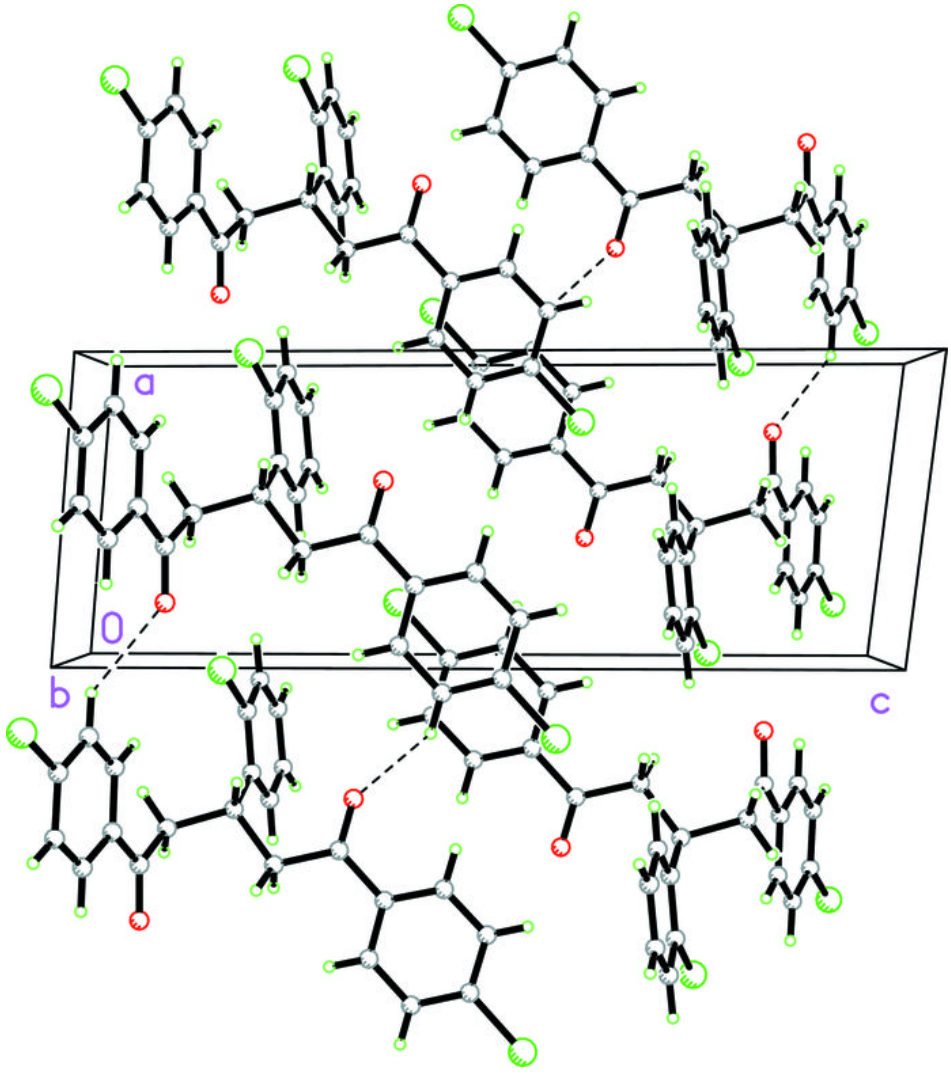


Fig. 3