

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

2,3-Dibromo-1-(2,4-dichloro-5-fluorophenyl)-3-phenylpropan-1-one

 Hoong-Kun Fun,^{a*} Samuel Robinson Jebas,^{a‡}
 Ibrahim Abdul Razak,^a M. S. Karthikeyan,^b P. S. Patil^c and
 S. M. Dharmaprakash^c
^aX-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, ^bSyngene International Pvt Limited, Plot No. 2 & 3 C, Unit-II, Bommasandra Industrial Area, Bangalore 560 099, India, and ^cDepartment of Studies in Physics, Mangalore University, Mangalagangothri, Mangalore 574 199, India

Correspondence e-mail: hkfun@usm.my

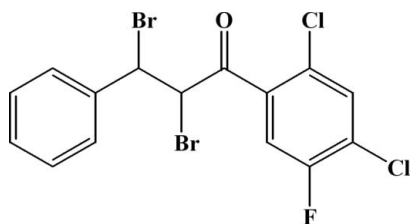
Received 23 April 2008; accepted 5 May 2008

 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; disorder in main residue; R factor = 0.041; wR factor = 0.090; data-to-parameter ratio = 25.8.

In the title compound, $\text{C}_{15}\text{H}_9\text{Br}_2\text{Cl}_2\text{FO}$, the dihedral angle between the two aromatic rings is $6.0(1)^\circ$. The dibromoethane fragment of the propan-1-one unit is disordered over two positions, with occupancies of *ca* 0.83 and 0.17. The crystal structure is stabilized by intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, $\text{C}-\text{H}\cdots\pi$ interactions, and $\text{Br}\cdots\text{Cl}$ [3.505(2) and 3.576(6) Å] and $\text{Cl}\cdots\text{F}$ [3.176(2) Å] short contacts.

Related literature

For related literature, see: Agrinskaya *et al.* (1999); Patil *et al.* (2006); John Kiran *et al.* (2007). For bond-length data, see: Allen *et al.* (1987). For the preparation, see: Shivarama Holla *et al.* (2006).



Experimental

Crystal data

 $\text{C}_{15}\text{H}_9\text{Br}_2\text{Cl}_2\text{FO}$
 $M_r = 454.94$

 Orthorhombic, *Pbca*
 $a = 7.1232(1)$ Å

 $b = 10.0757(2)$ Å

 $c = 43.0262(7)$ Å

 $V = 3088.04(9)$ Å³
 $Z = 8$
[‡] Permanent address: Department of Physics, Karunya University, Karunya Nagar, Coimbatore 641 114, India.

 Mo $K\alpha$ radiation
 $\mu = 5.60$ mm⁻¹
 $T = 100(2)$ K
 $0.40 \times 0.24 \times 0.14$ mm

Data collection

 Bruker SMART APEXII CCD
 area-detector diffractometer
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2005)
 $T_{\min} = 0.211$, $T_{\max} = 0.508$
 (expected range = 0.190–0.457)

 26343 measured reflections
 5857 independent reflections
 3681 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.056$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.089$
 $S = 0.98$
 5857 reflections
 227 parameters

 60 restraints
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.77$ e Å⁻³
 $\Delta\rho_{\min} = -0.76$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> — <i>H</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D</i> — <i>H</i> ⋯ <i>A</i>
C5—H5⋯O1 ⁱ	0.95	2.45	3.392(4)	170
C8—H8⋯O1 ⁱ	1.00	2.35	3.336(4)	169
C11—H11⋯O1 ⁱ	0.95	2.29	3.229(3)	170
C3—H3⋯Cg1 ⁱⁱ	0.95	2.96	3.652(3)	131

 Symmetry codes: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, z$; (ii) $x - \frac{3}{2}, y - \frac{1}{2}, -z - \frac{1}{2}$. Cg1 is the centroid of the C1–C6 benzene ring.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

HKF and SRJ thank the Malaysian Government and Universiti Sains Malaysia for the Science Fund grant No. 305/PFIZIK/613312. HKF and IAR also thank the Malaysian Government and Universiti Sains Malaysia for the FRGS grant No. 203/PFIZIK/671064. SRJ thanks the Universiti Sains Malaysia for a post-doctoral research fellowship. This work was also supported by the Department of Science and Technology (DST), Government of India, grant No. SR/S2/LOP-17/2006.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2588).

References

- Agrinskaya, N. V., Lukoshkin, V. A., Kudryavtsev, V. V., Nosova, G. I., Solovskaya, N. A. & Yakimanski, A. V. (1999). *Phys. Solid State*, **41**, 1914–1917.
- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–S19.
- Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- John Kiran, A., Mithun, A., Shivarama Holla, B., Shashikala, H. D., Umesh, G. & Chandrasekharan, K. (2007). *Opt. Commun.* **269**, 235–240.
- Patil, P. S., Dharmaprakash, S. M., Fun, H.-K. & Karthikeyan, M. S. (2006). *J. Cryst. Growth*, **297**, 111–116.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Shivarama Holla, B., Sooryanarayana Rao, B., Sarojini, B. K., Akberali, P. M. & Suchetha Kumari, N. (2006). *Eur. J. Med. Chem.* **41**, 657–663.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

supplementary materials

Acta Cryst. (2008). E64, o1039 [doi:10.1107/S1600536808013238]

2,3-Dibromo-1-(2,4-dichloro-5-fluorophenyl)-3-phenylpropan-1-one

H.-K. Fun, S. R. Jebas, I. A. Razak, M. S. Karthikeyan, P. S. Patil and S. M. Dharmaparakash

Comment

Derivatives of chalcone exhibit nonlinear optical (NLO) properties (Agrinskaya *et al.*, 1999; Patil *et al.*, 2006; John Kiran *et al.*, 2007). We report here the crystal structure of the title compound (Fig 1), which crystallizes in a centrosymmetric space group and this precludes the presence of second-order NLO properties.

Bond lengths and angles in the title molecule have normal values (Allen *et al.*, 1987). The dihedral angle between the benzene rings is $6.0 (1)^\circ$. The dibromoethane fragment of the propan-1-one unit is disordered over two positions.

The crystal packing is (Fig.2) stabilized by intermolecular C—H \cdots O and weak C—H \cdots π interactions involving the C1–C6 benzene ring (centroid Cg1). In addition, Br2 \cdots Cl2(-1+x,y,z) [3.505 (2) Å], Br1A \cdots Cl2(-1+x,y,z) [3.576 (6) Å] and Cl1 \cdots F1(1-x,1-y,-z) [3.176 (2) Å] short contacts are observed in the crystal structure.

Experimental

1-(2,4-Dichloro-5-fluorophenyl)-3-phenylprop-2-en-1-one (1 mmol) was prepared by a literature procedure (Shivarama Holla *et al.*, 2006). To a solution of 1-(2,4-dichloro-5-fluorophenyl)-3-phenylprop-2-en-1-one (1 mmol) in chloroform (25 ml), bromine (1 mmol) was added slowly with stirring. After the completion of addition the reaction mixture was stirred for 24 h. Excess chloroform was distilled off and crude solid was filtered and dried. The precipitated compound was recrystallized from acetone.

Refinement

The dibromoethane linkage is disordered over two positions with refined occupancies of 0.834 (6):0.166 (6). The C-Br distances were restrained to be equal, and C_{sp}²-C_{sp}³ and C_{sp}³-C_{sp}³ distances involving the disordered atoms were restrained to 1.50 (1) and 1.54 (1) Å, respectively. The U^{ij} components of disordered atoms were restrained to approximate isotropic behaviour. H atoms were positioned geometrically [C—H = 0.95 or 1.00 Å] and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

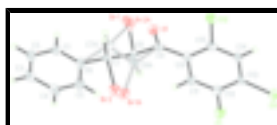


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme. Only the major disorder component is shown.

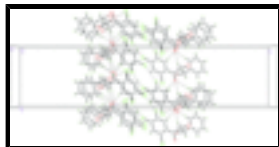


Fig. 2. The crystal packing of the title compound, viewed along the a axis. Short intra- and intermolecular contacts and hydrogen bonds are shown as dashed lines. Only the major disorder component is shown.

2,3-Dibromo-1-(2,4-dichloro-5-fluorophenyl)-3-phenylpropan-1-one

Crystal data

$C_{15}H_9Br_2Cl_2FO$	$F_{000} = 1760$
$M_r = 454.94$	$D_x = 1.957 \text{ Mg m}^{-3}$
Orthorhombic, $Pbca$	Mo $K\alpha$ radiation
Hall symbol: $-P\ 2ac\ 2ab$	$\lambda = 0.71073 \text{ \AA}$
$a = 7.1232 (1) \text{ \AA}$	Cell parameters from 4782 reflections
$b = 10.0757 (2) \text{ \AA}$	$\theta = 2.8\text{--}28.1^\circ$
$c = 43.0262 (7) \text{ \AA}$	$\mu = 5.60 \text{ mm}^{-1}$
$V = 3088.04 (9) \text{ \AA}^3$	$T = 100 (2) \text{ K}$
$Z = 8$	Block, colourless
	$0.40 \times 0.24 \times 0.14 \text{ mm}$

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	5857 independent reflections
Radiation source: fine-focus sealed tube	3681 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.056$
$T = 100(2) \text{ K}$	$\theta_{\text{max}} = 33.2^\circ$
φ and ω scans	$\theta_{\text{min}} = 1.0^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$h = -10 \rightarrow 8$
$T_{\text{min}} = 0.211$, $T_{\text{max}} = 0.508$	$k = -15 \rightarrow 15$
26343 measured reflections	$l = -52 \rightarrow 66$

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
$wR(F^2) = 0.089$	$w = 1/[\sigma^2(F_o^2) + (0.0309P)^2 + 2.3603P]$
$S = 0.99$	where $P = (F_o^2 + 2F_c^2)/3$
5857 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
227 parameters	$\Delta\rho_{\text{max}} = 0.77 \text{ e \AA}^{-3}$
60 restraints	$\Delta\rho_{\text{min}} = -0.76 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The data was collected with the Oxford Cryosystem Cobra low-temperature attachment.

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Cl1	0.58123 (10)	0.31692 (7)	-0.003788 (15)	0.02739 (16)	
Cl2	0.62659 (10)	-0.10513 (7)	0.070833 (16)	0.02701 (16)	
F1	0.3512 (3)	0.42768 (15)	0.04559 (4)	0.0314 (4)	
O1	0.3888 (3)	-0.05963 (18)	0.12256 (4)	0.0211 (4)	
C1	0.0038 (4)	0.0604 (3)	0.21381 (6)	0.0229 (6)	
H1	0.0475	-0.0286	0.2151	0.028*	
C2	-0.0915 (4)	0.1152 (3)	0.23859 (6)	0.0243 (6)	
H2	-0.1147	0.0635	0.2567	0.029*	
C3	-0.1533 (4)	0.2449 (3)	0.23723 (7)	0.0273 (6)	
H3	-0.2197	0.2822	0.2543	0.033*	
C4	-0.1181 (4)	0.3209 (3)	0.21087 (7)	0.0260 (6)	
H4	-0.1581	0.4107	0.2100	0.031*	
C5	-0.0250 (5)	0.2651 (3)	0.18597 (7)	0.0290 (7)	
H5	-0.0025	0.3166	0.1679	0.035*	
C6	0.0365 (4)	0.1337 (3)	0.18715 (6)	0.0265 (6)	
C9	0.3635 (4)	0.0567 (3)	0.11688 (6)	0.0189 (5)	
C10	0.4255 (4)	0.1189 (2)	0.08738 (6)	0.0176 (5)	
C11	0.3646 (4)	0.2472 (3)	0.07982 (6)	0.0222 (6)	
H11	0.2883	0.2949	0.0941	0.027*	
C12	0.4138 (4)	0.3047 (3)	0.05211 (6)	0.0216 (6)	
C13	0.5258 (4)	0.2405 (3)	0.03074 (6)	0.0196 (5)	
C14	0.5896 (4)	0.1134 (3)	0.03752 (6)	0.0203 (5)	
H14	0.6673	0.0677	0.0231	0.024*	
C15	0.5397 (4)	0.0535 (2)	0.06529 (6)	0.0185 (5)	
Br1	0.4779 (3)	0.1813 (3)	0.17334 (5)	0.0279 (4)	0.834 (6)
Br2	-0.06956 (14)	0.02708 (17)	0.12693 (3)	0.0296 (2)	0.834 (6)
C7	0.1226 (5)	0.0653 (3)	0.15969 (7)	0.0194 (8)	0.834 (6)
H7	0.1772	-0.0209	0.1668	0.023*	0.834 (6)
C8	0.2737 (5)	0.1420 (4)	0.14272 (7)	0.0190 (8)	0.834 (6)
H8	0.2216	0.2261	0.1339	0.023*	0.834 (6)
Br1A	-0.0440 (7)	0.0638 (6)	0.11951 (14)	0.0265 (8)	0.166 (6)

supplementary materials

Br2A	0.4743 (16)	0.1862 (16)	0.1704 (2)	0.0222 (16)	0.166 (6)
C7A	0.2193 (14)	0.0999 (16)	0.1700 (3)	0.028 (5)	0.166 (6)
H7A	0.2405	0.0025	0.1728	0.033*	0.166 (6)
C8A	0.2088 (11)	0.1248 (14)	0.1348 (3)	0.015 (4)	0.166 (6)
H8A	0.2190	0.2225	0.1311	0.018*	0.166 (6)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0264 (4)	0.0359 (4)	0.0198 (3)	0.0014 (3)	0.0055 (3)	0.0042 (3)
C12	0.0290 (4)	0.0221 (3)	0.0300 (3)	0.0083 (3)	0.0061 (3)	-0.0018 (3)
F1	0.0442 (11)	0.0200 (8)	0.0302 (9)	0.0078 (8)	0.0112 (8)	0.0069 (7)
O1	0.0246 (11)	0.0173 (9)	0.0214 (9)	0.0019 (8)	-0.0011 (8)	-0.0018 (7)
C1	0.0237 (15)	0.0222 (13)	0.0229 (13)	-0.0004 (12)	0.0020 (11)	0.0000 (10)
C2	0.0224 (15)	0.0293 (15)	0.0212 (13)	-0.0056 (12)	0.0026 (11)	0.0010 (11)
C3	0.0224 (16)	0.0323 (16)	0.0271 (15)	-0.0049 (13)	0.0061 (12)	-0.0067 (12)
C4	0.0217 (15)	0.0226 (14)	0.0338 (15)	0.0022 (12)	0.0043 (12)	-0.0038 (12)
C5	0.0381 (19)	0.0219 (14)	0.0270 (15)	0.0049 (13)	0.0102 (13)	0.0045 (11)
C6	0.0322 (18)	0.0248 (14)	0.0226 (13)	0.0052 (13)	0.0082 (12)	0.0013 (11)
C9	0.0190 (14)	0.0173 (12)	0.0203 (13)	-0.0010 (11)	0.0019 (10)	-0.0016 (10)
C10	0.0183 (13)	0.0148 (12)	0.0198 (12)	-0.0012 (10)	0.0021 (10)	-0.0022 (9)
C11	0.0250 (15)	0.0176 (13)	0.0239 (13)	0.0009 (12)	0.0051 (11)	-0.0021 (10)
C12	0.0237 (14)	0.0165 (12)	0.0245 (13)	-0.0004 (11)	0.0011 (11)	0.0019 (10)
C13	0.0182 (14)	0.0249 (14)	0.0158 (12)	-0.0051 (11)	0.0010 (10)	-0.0012 (10)
C14	0.0171 (13)	0.0245 (14)	0.0192 (12)	0.0008 (11)	0.0025 (10)	-0.0054 (10)
C15	0.0144 (13)	0.0165 (12)	0.0244 (13)	-0.0008 (10)	-0.0013 (10)	-0.0034 (10)
Br1	0.0181 (5)	0.0296 (5)	0.0359 (9)	-0.0023 (4)	-0.0012 (5)	-0.0105 (7)
Br2	0.0212 (3)	0.0379 (5)	0.0296 (4)	-0.0013 (3)	-0.0041 (3)	-0.0111 (3)
C7	0.0208 (18)	0.0182 (15)	0.0191 (15)	0.0007 (13)	-0.0027 (13)	-0.0016 (12)
C8	0.022 (2)	0.0175 (16)	0.0173 (17)	-0.0011 (15)	-0.0004 (15)	-0.0024 (12)
Br1A	0.0242 (14)	0.0302 (17)	0.0252 (16)	-0.0071 (12)	-0.0074 (11)	0.0019 (12)
Br2A	0.030 (3)	0.031 (3)	0.0061 (13)	-0.008 (2)	0.0041 (14)	-0.0099 (13)
C7A	0.027 (8)	0.021 (7)	0.035 (8)	-0.010 (6)	-0.010 (6)	0.006 (6)
C8A	0.015 (7)	0.014 (7)	0.016 (7)	-0.005 (6)	-0.007 (5)	0.003 (5)

Geometric parameters (\AA , $^\circ$)

C11—C13	1.719 (3)	C9—C8	1.544 (4)
C12—C15	1.731 (3)	C10—C11	1.402 (4)
F1—C12	1.346 (3)	C10—C15	1.414 (4)
O1—C9	1.211 (3)	C11—C12	1.371 (4)
C1—C2	1.380 (4)	C11—H11	0.95
C1—C6	1.384 (4)	C12—C13	1.379 (4)
C1—H1	0.95	C13—C14	1.390 (4)
C2—C3	1.380 (4)	C14—C15	1.385 (4)
C2—H2	0.95	C14—H14	0.95
C3—C4	1.391 (4)	Br1—C8	2.002 (4)
C3—H3	0.95	Br2—C7	2.002 (3)
C4—C5	1.380 (4)	C7—C8	1.513 (4)

C4—H4	0.95	C7—H7	1.00
C5—C6	1.395 (4)	C8—H8	1.00
C5—H5	0.95	Br1A—C8A	2.013 (8)
C6—C7	1.499 (4)	Br2A—C7A	2.014 (8)
C6—C7A	1.536 (9)	C7A—C8A	1.535 (9)
C9—C10	1.483 (4)	C7A—H7A	1.00
C9—C8A	1.509 (9)	C8A—H8A	1.00
C2—C1—C6	120.6 (3)	C12—C13—C14	118.8 (2)
C2—C1—H1	119.7	C12—C13—Cl1	119.9 (2)
C6—C1—H1	119.7	C14—C13—Cl1	121.3 (2)
C1—C2—C3	120.2 (3)	C15—C14—C13	119.9 (2)
C1—C2—H2	119.9	C15—C14—H14	120.0
C3—C2—H2	119.9	C13—C14—H14	120.0
C2—C3—C4	119.9 (3)	C14—C15—C10	121.6 (2)
C2—C3—H3	120.1	C14—C15—Cl2	115.5 (2)
C4—C3—H3	120.1	C10—C15—Cl2	122.9 (2)
C5—C4—C3	119.7 (3)	C6—C7—C8	115.9 (3)
C5—C4—H4	120.2	C6—C7—Br2	111.3 (2)
C3—C4—H4	120.2	C8—C7—Br2	104.2 (2)
C4—C5—C6	120.6 (3)	C6—C7—H7	108.4
C4—C5—H5	119.7	C8—C7—H7	108.4
C6—C5—H5	119.7	Br2—C7—H7	108.4
C1—C6—C5	118.9 (3)	C7—C8—C9	110.9 (3)
C1—C6—C7	118.5 (3)	C7—C8—Br1	107.5 (2)
C5—C6—C7	122.4 (3)	C9—C8—Br1	106.5 (2)
C1—C6—C7A	115.1 (6)	C7—C8—H8	110.6
C5—C6—C7A	117.3 (6)	C9—C8—H8	110.6
O1—C9—C10	122.5 (2)	Br1—C8—H8	110.6
O1—C9—C8A	116.5 (6)	C8A—C7A—C6	113.4 (8)
C10—C9—C8A	117.6 (6)	C8A—C7A—Br2A	89.1 (7)
O1—C9—C8	117.1 (2)	C6—C7A—Br2A	131.6 (9)
C10—C9—C8	120.3 (2)	C8A—C7A—H7A	106.7
C11—C10—C15	116.9 (2)	C6—C7A—H7A	106.7
C11—C10—C9	119.7 (2)	Br2A—C7A—H7A	106.7
C15—C10—C9	123.4 (2)	C9—C8A—C7A	113.2 (8)
C12—C11—C10	120.8 (2)	C9—C8A—Br1A	110.3 (6)
C12—C11—H11	119.6	C7A—C8A—Br1A	108.4 (8)
C10—C11—H11	119.6	C9—C8A—H8A	108.3
F1—C12—C11	119.0 (2)	C7A—C8A—H8A	108.3
F1—C12—C13	119.0 (2)	Br1A—C8A—H8A	108.3
C11—C12—C13	122.0 (2)		
C6—C1—C2—C3	-0.9 (4)	C1—C6—C7—C8	-137.6 (3)
C1—C2—C3—C4	-0.5 (4)	C5—C6—C7—C8	47.5 (4)
C2—C3—C4—C5	1.3 (4)	C7A—C6—C7—C8	-44.3 (10)
C3—C4—C5—C6	-0.9 (5)	C1—C6—C7—Br2	103.6 (3)
C2—C1—C6—C5	1.4 (5)	C5—C6—C7—Br2	-71.2 (4)
C2—C1—C6—C7	-173.7 (3)	C7A—C6—C7—Br2	-163.1 (11)
C2—C1—C6—C7A	148.2 (6)	C6—C7—C8—C9	174.9 (3)

supplementary materials

C4—C5—C6—C1	-0.5 (5)	Br2—C7—C8—C9	-62.5 (3)
C4—C5—C6—C7	174.4 (3)	C6—C7—C8—Br1	58.9 (3)
C4—C5—C6—C7A	-146.6 (6)	Br2—C7—C8—Br1	-178.49 (17)
O1—C9—C10—C11	169.1 (3)	O1—C9—C8—C7	-38.7 (4)
C8A—C9—C10—C11	10.9 (5)	C10—C9—C8—C7	145.0 (3)
C8—C9—C10—C11	-14.8 (4)	C8A—C9—C8—C7	55.5 (16)
O1—C9—C10—C15	-8.5 (4)	O1—C9—C8—Br1	77.9 (3)
C8A—C9—C10—C15	-166.7 (4)	C10—C9—C8—Br1	-98.3 (3)
C8—C9—C10—C15	167.6 (3)	C8A—C9—C8—Br1	172.1 (18)
C15—C10—C11—C12	0.4 (4)	C1—C6—C7A—C8A	151.0 (9)
C9—C10—C11—C12	-177.3 (3)	C5—C6—C7A—C8A	-61.6 (12)
C10—C11—C12—F1	179.5 (2)	C7—C6—C7A—C8A	46.7 (9)
C10—C11—C12—C13	-0.7 (4)	C1—C6—C7A—Br2A	-97.9 (12)
F1—C12—C13—C14	-179.8 (2)	C5—C6—C7A—Br2A	49.5 (13)
C11—C12—C13—C14	0.3 (4)	C7—C6—C7A—Br2A	157.8 (19)
F1—C12—C13—C11	-0.7 (4)	O1—C9—C8A—C7A	49.1 (10)
C11—C12—C13—C11	179.4 (2)	C10—C9—C8A—C7A	-151.4 (8)
C12—C13—C14—C15	0.3 (4)	C8—C9—C8A—C7A	-48.3 (12)
C11—C13—C14—C15	-178.8 (2)	O1—C9—C8A—Br1A	-72.6 (8)
C13—C14—C15—C10	-0.5 (4)	C10—C9—C8A—Br1A	86.9 (8)
C13—C14—C15—C12	179.5 (2)	C8—C9—C8A—Br1A	-170 (2)
C11—C10—C15—C14	0.2 (4)	C6—C7A—C8A—C9	-163.6 (8)
C9—C10—C15—C14	177.8 (3)	Br2A—C7A—C8A—C9	60.7 (10)
C11—C10—C15—C12	-179.9 (2)	C6—C7A—C8A—Br1A	-40.8 (13)
C9—C10—C15—C12	-2.2 (4)	Br2A—C7A—C8A—Br1A	-176.6 (8)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C5—H5 \cdots O1 ⁱ	0.95	2.45	3.392 (4)	170
C8—H8 \cdots O1 ⁱ	1.00	2.35	3.336 (4)	169
C11—H11 \cdots O1 ⁱ	0.95	2.29	3.229 (3)	170
C3—H3 \cdots Cg1 ⁱⁱ	0.95	2.96	3.652 (3)	131

Symmetry codes: (i) $-x+1/2, y+1/2, z$; (ii) $x-3/2, y, -z-1/2$.

Fig. 1

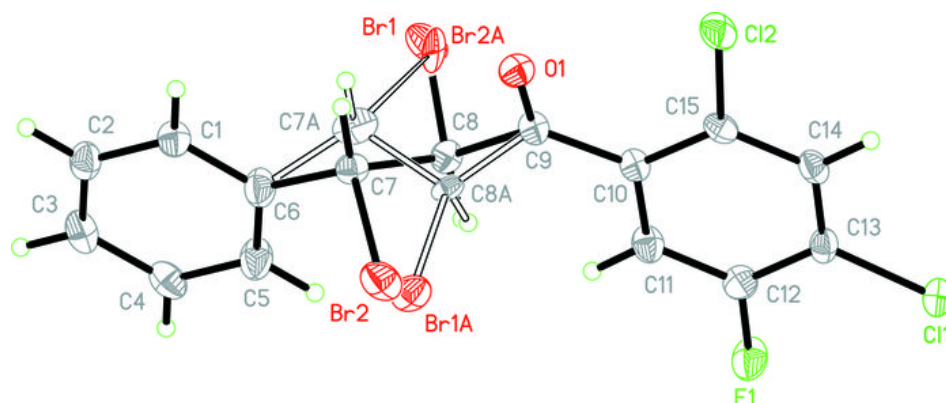


Fig. 2

