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2,3-Dibromo-3-(5-bromo-2-methoxyphenyl)-1-(2,4-dichlorophenyl)propan-1-one

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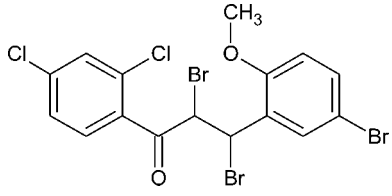
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; R factor = 0.037; wR factor = 0.099; data-to-parameter ratio = 14.9.

In the title molecule, $C_{16}H_{11}Br_3Cl_2O_2$, the chain Br atoms are in *trans* positions [Br—C—C—Br torsion angle is 179.0 (2)°]. The two benzene rings make a dihedral angle of 39.54 (15)°. The crystal packing is determined by van der Waals forces; some weak π–π interactions between the benzene rings of neighbouring molecules are also possible [the distance between their centroids is 3.753 (5) Å]. Intermolecular C—H···Br interactions are also present.

Related literature

For related structures, see: Yathirajan *et al.* (2007*a*,*b*); Butcher *et al.* (2006*a*,*b*,*c*); Harrison *et al.* (2005). Various biological activities of chalcones were reported *e.g.* by Nielsen *et al.* (1998); Rojas *et al.* (2002) and Liu *et al.* (2003). For non-linear optical (NLO) properties of chalcone derivatives, see, for example, Indira *et al.* (2002) and Sarojini *et al.* (2006).



Experimental

Crystal data

$C_{16}H_{11}Br_3Cl_2O_2$
M_r = 545.88
Monoclinic, $P2_1/c$
a = 15.9189 (8) Å
b = 7.3729 (3) Å
c = 15.4895 (7) Å
β = 98.125 (4)°
V = 1799.73 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 7.03 mm^{-1}
T = 295 (1) K
0.4 × 0.2 × 0.1 mm

Data collection

Kuma KM-4-CCD diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.12, T_{max} = 0.495
17972 measured reflections
3104 independent reflections
2223 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.099
S = 1.20
3104 reflections
209 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C32—H32···Br33^{i}	0.93	3.10	3.814 (5)	135
C361—H36A···Br3^{ii}	0.96	3.03	3.839 (7)	143
C361—H36B···Br2^{iii}	0.96	3.00	3.881 (6)	153

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, y-1, z$; (iii) $x, -y-\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1989); software used to prepare material for publication: *SHELXL97*.

ANM thanks the University of Mysore for offering research facilities.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2319).

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supplementary materials

Acta Cryst. (2007). E**63**, o4362 [**doi:10.1107/S1600536807050842**]

2,3-Dibromo-3-(5-bromo-2-methoxyphenyl)-1-(2,4-dichlorophenyl)propan-1-one

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Comment

For a structurally simple group of compounds, chalcones display an impressive array of biological activities, among which antimalarial (Liu *et al.*, 2003), antiprotozoal (Nielsen *et al.*, 1998), nitric oxide inhibition (Rojas *et al.*, 2002) and anti-cancer activities have been reported in the literature. Among several organic compounds reported for non-linear optical (NLO) properties, chalcone derivatives are notable materials for their excellent blue light transmittance and good crystallizability (Indira *et al.*, 2002; Sarojini *et al.*, 2006). They provide a necessary configuration to show NLO properties, with two planar rings connected through a conjugated double bond. The substitution of a bromo group on either of the phenyl rings greatly influences the non-centrosymmetric crystal packing. The bromo group can obviously improve the molecular first-order hyperpolarizabilities and can effectively reduce dipole - dipole interactions between the molecules. Chalcone derivatives usually have a lower melting temperature, which can be a drawback when we use these crystals in optical instruments, but chalcone dibromides usually have higher melting points and are thermally stable. A new chalcone dibromide (**1**), $C_{16}H_{12}Br_2Cl_2O_2$, was prepared by the bromination of the chalcone, (2*E*)-1-(2,4-Dichlorophenyl)-3-(2-methoxyphenyl)prop-2-en-1-one. During the bromination process the excess bromine reacted with the dibromide to form 2,3-dibromo-3-(5-bromo-2-methoxyphenyl)-1-(2,4-dichlorophenyl) propan-1-one (**1**). Due to the space group symmetry, the racemic mixture is present in the crystal structure.

The conformation of **1** (Fig. 1) can be described by the torsion angles between two approximately planar benzene rings with maximum deviations from mean planes of 0.009 (3) Å and 0.019 (3) Å for the rings C11 - C16 (A) and C31 - C36 (B), respectively, and the central C1—C2—C3 bridge (C). The values of these angles: A/B 39.54 (15)°, A/C 56.8 (3)°, and B/C 44.4 (3)° show that the rings are twisted in opposite sense with respect to the central bridge. The bromine Br2 and Br3 atoms are in mutual *trans* position, the torsion angle Br2—C2—C3—Br3 is 179.0 (2)°. The C—Br distances for C(sp^3) and C(sp^2) carbon atoms are significantly different: 2.007 (5)Å and 2.018 (5)Å for the former and 1.898 (5)Å for the latter.

In the crystal structure, besides the van der Waals forces (Fig. 2) there are also some C···C short contacts between neighbouring benzene rings: C14···C14(*1 − x,-y,1 − z*) of 3.429 (3)Å and C34···C36(*-x,-y,-z*) of 3.349 (3) Å. Only in the latter case, however, there is an overlap between the rings with the short distance of 3.753 (5) Å between their centroids, thus only in this case some π-π interaction is possible. Additionally, some directional weak C—H···Br interactions (Table 1) can be important. Short contact Cl12···Br2(*x,1 + y,z*) of 3.590 (5) Å is observed within the chains of molecules along [010] direction.

Experimental

(2E)-1-(2,4-Dichlorophenyl)-3-(2-methoxyphenyl)prop-2-en-1-one (3.07 g, 0.01 mol) was treated with bromine in acetic acid (30%) until the orange colour of the solution persisted. After stirring for half an hour, the content was poured on to crushed ice. The resulting solid mass was collected by filtration. The compound was dried and recrystallized from ethanol. Crystals suitable for structure determination were obtained from ethyl acetate by slow evaporation (yield 70%; m.p. 385–388 K). Analysis for $C_{16}H_{11}Br_3Cl_2O_2$ found (calculated): C: 35.12 (35.20), H: 1.99% (2.03%).

Refinement

The hydrogen atoms were placed in the idealized positions (C—H 0.93–0.98 Å) and refined using a riding model approximation, with U_{iso}(H)=1.2 or 1.3 U_{eq}(C).

Figures

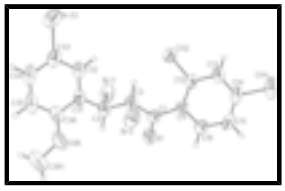

Fig. 1. The molecular structure of **1** showing the atomic numbering and displacement ellipsoids drawn at the 50% probability level.

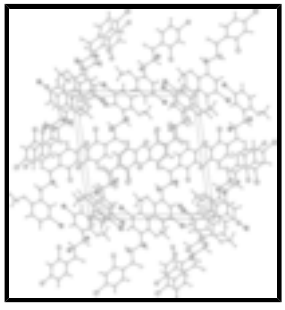

Fig. 2. A portion of the crystal packing as seen approximately along direction [010].

2,3-Dibromo-3-(5-bromo-2-methoxyphenyl)-1-(2,4-dichlorophenyl)propan-1-one

Crystal data

$C_{16}H_{11}Br_3Cl_2O_2$	F_{000} = 1048
M_r = 545.88	D_x = 2.015 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 7661 reflections
a = 15.9189 (8) Å	θ = 4–24º
b = 7.3729 (3) Å	μ = 7.03 mm^{-1}
c = 15.4895 (7) Å	T = 295 (1) K
β = 98.125 (4)º	Plate, colourless
V = 1799.73 (14) Å^3	0.4 × 0.2 × 0.1 mm
Z = 4	

Data collection

Kuma KM-4-CCD four-circle diffractometer	3104 independent reflections
Radiation source: fine-focus sealed tube	2223 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
Detector resolution: 8.1929 pixels mm^{-1}	θ_{max} = 25.0º
T = 295(1) K	θ_{min} = 2.6º

ω scans

Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2006)

T_{min} = 0.12, T_{max} = 0.495

17972 measured reflections

h = −18→18

k = −8→8

l = −18→18

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.037

$wR(F^2)$ = 0.099

S = 1.20

3104 reflections

209 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 0.70 e Å^{-3}

$\Delta\rho_{min}$ = −0.62 e Å^{-3}

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}
C1	0.3657 (3)	0.0862 (6)	0.2091 (3)	0.0477 (11)
O1	0.3990 (2)	0.0840 (5)	0.1434 (2)	0.0666 (10)
C11	0.4172 (3)	0.1263 (6)	0.2947 (3)	0.0414 (10)
C12	0.3936 (3)	0.2306 (6)	0.3619 (3)	0.0432 (11)
Cl12	0.29453 (8)	0.33676 (17)	0.35285 (9)	0.0624 (4)
C13	0.4480 (3)	0.2662 (6)	0.4375 (3)	0.0492 (11)
H13	0.4311	0.3387	0.4811	0.059*
C14	0.5279 (3)	0.1913 (6)	0.4466 (3)	0.0524 (12)
Cl14	0.59819 (10)	0.2366 (2)	0.54041 (10)	0.0784 (5)
C15	0.5540 (3)	0.0844 (7)	0.3831 (3)	0.0589 (13)
H15	0.6080	0.0335	0.3908	0.071*
C16	0.4987 (3)	0.0538 (7)	0.3077 (3)	0.0547 (12)
H16	0.5164	−0.0176	0.2642	0.066*

C2	0.2743 (3)	0.0217 (6)	0.2043 (3)	0.0508 (12)
H2	0.2455	0.0871	0.2468	0.061*
Br2	0.28480 (3)	−0.24233 (7)	0.23529 (4)	0.06278 (19)
C3	0.2234 (3)	0.0314 (7)	0.1163 (3)	0.0578 (13)
H3	0.2552	−0.0256	0.0737	0.069*
Br3	0.21543 (4)	0.30078 (7)	0.09355 (4)	0.0685 (2)
C31	0.1356 (3)	−0.0502 (6)	0.1079 (3)	0.0506 (12)
C32	0.0821 (3)	−0.0102 (6)	0.1681 (3)	0.0510 (12)
H32	0.1003	0.0653	0.2151	0.061*
C33	0.0011 (3)	−0.0831 (6)	0.1581 (3)	0.0520 (12)
Br33	−0.07145 (3)	−0.03042 (8)	0.24203 (4)	0.0726 (2)
C34	−0.0275 (3)	−0.1906 (6)	0.0881 (4)	0.0588 (13)
H34	−0.0830	−0.2333	0.0802	0.071*
C35	0.0263 (4)	−0.2350 (6)	0.0297 (4)	0.0634 (14)
H35	0.0078	−0.3117	−0.0168	0.076*
C36	0.1081 (3)	−0.1660 (6)	0.0397 (3)	0.0557 (13)
O36	0.1652 (3)	−0.2010 (6)	−0.0165 (2)	0.0818 (12)
C361	0.1462 (4)	−0.3400 (8)	−0.0815 (4)	0.086 (2)
H36A	0.1380	−0.4535	−0.0535	0.112*
H36B	0.1925	−0.3508	−0.1147	0.112*
H36C	0.0954	−0.3084	−0.1196	0.112*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.038 (3)	0.060 (3)	0.047 (3)	−0.005 (2)	0.009 (2)	−0.005 (2)
O1	0.046 (2)	0.105 (3)	0.049 (2)	−0.0172 (19)	0.0083 (18)	−0.0083 (19)
C11	0.034 (2)	0.047 (2)	0.043 (3)	−0.0069 (19)	0.003 (2)	−0.001 (2)
C12	0.035 (2)	0.048 (2)	0.044 (3)	−0.0035 (19)	−0.002 (2)	0.008 (2)
Cl12	0.0471 (7)	0.0673 (8)	0.0685 (9)	0.0130 (6)	−0.0066 (6)	−0.0155 (6)
C13	0.049 (3)	0.049 (2)	0.047 (3)	−0.004 (2)	−0.003 (2)	−0.002 (2)
C14	0.041 (3)	0.052 (3)	0.057 (3)	−0.012 (2)	−0.016 (2)	0.012 (2)
Cl14	0.0676 (9)	0.0796 (9)	0.0751 (11)	−0.0176 (7)	−0.0345 (8)	0.0084 (7)
C15	0.028 (3)	0.073 (3)	0.072 (4)	0.003 (2)	−0.004 (3)	0.006 (3)
C16	0.039 (3)	0.069 (3)	0.057 (3)	−0.003 (2)	0.009 (3)	−0.005 (2)
C2	0.039 (3)	0.060 (3)	0.051 (3)	−0.008 (2)	0.001 (2)	−0.006 (2)
Br2	0.0519 (3)	0.0546 (3)	0.0794 (4)	−0.0009 (2)	0.0010 (3)	0.0113 (2)
C3	0.047 (3)	0.064 (3)	0.059 (3)	−0.015 (2)	−0.003 (3)	−0.012 (2)
Br3	0.0631 (4)	0.0594 (3)	0.0772 (4)	−0.0182 (2)	−0.0099 (3)	0.0201 (3)
C31	0.041 (3)	0.056 (3)	0.052 (3)	−0.013 (2)	−0.006 (2)	−0.007 (2)
C32	0.042 (3)	0.055 (3)	0.052 (3)	−0.011 (2)	−0.009 (2)	−0.004 (2)
C33	0.042 (3)	0.044 (2)	0.066 (3)	−0.006 (2)	−0.006 (2)	0.008 (2)
Br33	0.0480 (3)	0.0734 (4)	0.0972 (5)	−0.0069 (3)	0.0132 (3)	0.0007 (3)
C34	0.044 (3)	0.051 (3)	0.073 (4)	−0.013 (2)	−0.020 (3)	0.008 (3)
C35	0.067 (4)	0.052 (3)	0.061 (4)	−0.018 (3)	−0.024 (3)	0.001 (2)
C36	0.061 (3)	0.054 (3)	0.049 (3)	−0.010 (2)	−0.003 (3)	−0.007 (2)
O36	0.086 (3)	0.101 (3)	0.058 (2)	−0.029 (2)	0.008 (2)	−0.033 (2)
C361	0.122 (6)	0.071 (4)	0.063 (4)	−0.017 (4)	0.006 (4)	−0.017 (3)

Geometric parameters (Å, °)

C1—O1	1.212 (5)	C3—Br3	2.018 (5)
C1—C11	1.487 (6)	C3—H3	0.9800
C1—C2	1.523 (6)	C31—C36	1.381 (6)
C11—C12	1.387 (6)	C31—C32	1.381 (6)
C11—C16	1.391 (6)	C32—C33	1.385 (6)
C12—C13	1.380 (6)	C32—H32	0.9300
C12—Cl12	1.749 (5)	C33—C34	1.368 (7)
C13—C14	1.377 (7)	C33—Br33	1.898 (5)
C13—H13	0.9300	C34—C35	1.370 (8)
C14—C15	1.369 (7)	C34—H34	0.9300
C14—Cl14	1.736 (5)	C35—C36	1.387 (7)
C15—C16	1.379 (7)	C35—H35	0.9300
C15—H15	0.9300	C36—O36	1.368 (6)
C16—H16	0.9300	O36—C361	1.438 (6)
C2—C3	1.485 (7)	C361—H36A	0.9600
C2—Br2	2.007 (5)	C361—H36B	0.9600
C2—H2	0.9800	C361—H36C	0.9600
C3—C31	1.510 (6)		
O1—C1—C11	120.0 (4)	C31—C3—Br3	110.0 (3)
O1—C1—C2	118.9 (4)	C2—C3—H3	109.3
C11—C1—C2	120.6 (4)	C31—C3—H3	109.3
C12—C11—C16	116.7 (4)	Br3—C3—H3	109.3
C12—C11—C1	127.2 (4)	C36—C31—C32	119.3 (4)
C16—C11—C1	116.0 (4)	C36—C31—C3	120.1 (4)
C13—C12—C11	122.6 (4)	C32—C31—C3	120.6 (4)
C13—C12—Cl12	115.6 (3)	C31—C32—C33	119.6 (4)
C11—C12—Cl12	121.7 (4)	C31—C32—H32	120.2
C14—C13—C12	118.0 (4)	C33—C32—H32	120.2
C14—C13—H13	121.0	C34—C33—C32	120.9 (5)
C12—C13—H13	121.0	C34—C33—Br33	119.7 (4)
C15—C14—C13	121.9 (4)	C32—C33—Br33	119.4 (4)
C15—C14—Cl14	119.1 (4)	C33—C34—C35	119.5 (5)
C13—C14—Cl14	119.0 (4)	C33—C34—H34	120.2
C14—C15—C16	118.7 (4)	C35—C34—H34	120.2
C14—C15—H15	120.7	C34—C35—C36	120.2 (5)
C16—C15—H15	120.7	C34—C35—H35	119.9
C15—C16—C11	122.1 (4)	C36—C35—H35	119.9
C15—C16—H16	119.0	O36—C36—C31	115.8 (4)
C11—C16—H16	119.0	O36—C36—C35	123.9 (5)
C3—C2—C1	115.0 (4)	C31—C36—C35	120.3 (5)
C3—C2—Br2	106.4 (3)	C36—O36—C361	119.1 (4)
C1—C2—Br2	104.1 (3)	O36—C361—H36A	109.5
C3—C2—H2	110.3	O36—C361—H36B	109.5
C1—C2—H2	110.3	H36A—C361—H36B	109.5
Br2—C2—H2	110.3	O36—C361—H36C	109.5
C2—C3—C31	115.9 (4)	H36A—C361—H36C	109.5

C2—C3—Br3	102.7 (3)	H36B—C361—H36C	109.5
O1—C1—C11—C12	140.4 (5)	Br2—C2—C3—C31	59.0 (5)
C2—C1—C11—C12	−48.3 (6)	C1—C2—C3—Br3	−66.3 (4)
O1—C1—C11—C16	−38.1 (6)	Br2—C2—C3—Br3	178.98 (19)
C2—C1—C11—C16	133.2 (4)	C2—C3—C31—C36	−132.5 (5)
C16—C11—C12—C13	1.6 (6)	Br3—C3—C31—C36	111.5 (4)
C1—C11—C12—C13	−177.0 (4)	C2—C3—C31—C32	47.4 (6)
C16—C11—C12—Cl12	177.7 (3)	Br3—C3—C31—C32	−68.5 (5)
C1—C11—C12—Cl12	−0.8 (6)	C36—C31—C32—C33	−1.5 (7)
C11—C12—C13—C14	−1.4 (6)	C3—C31—C32—C33	178.5 (4)
Cl12—C12—C13—C14	−177.7 (3)	C31—C32—C33—C34	−1.7 (7)
C12—C13—C14—C15	0.0 (7)	C31—C32—C33—Br33	179.1 (3)
C12—C13—C14—Cl14	179.1 (3)	C32—C33—C34—C35	3.7 (7)
C13—C14—C15—C16	1.0 (7)	Br33—C33—C34—C35	−177.1 (4)
Cl14—C14—C15—C16	−178.0 (4)	C33—C34—C35—C36	−2.4 (7)
C14—C15—C16—C11	−0.7 (7)	C32—C31—C36—O36	−179.1 (4)
C12—C11—C16—C15	−0.5 (7)	C3—C31—C36—O36	0.8 (7)
C1—C11—C16—C15	178.2 (4)	C32—C31—C36—C35	2.8 (7)
O1—C1—C2—C3	−23.5 (6)	C3—C31—C36—C35	−177.2 (5)
C11—C1—C2—C3	165.1 (4)	C34—C35—C36—O36	−178.8 (5)
O1—C1—C2—Br2	92.6 (5)	C34—C35—C36—C31	−0.9 (8)
C11—C1—C2—Br2	−78.8 (4)	C31—C36—O36—C361	171.0 (5)
C1—C2—C3—C31	173.7 (4)	C35—C36—O36—C361	−11.0 (8)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C32—H32···Br33^{i}	0.93	3.10	3.814 (5)	135
C361—H36A···Br3^{ii}	0.96	3.03	3.839 (7)	143
C361—H36B···Br2^{iii}	0.96	3.00	3.881 (6)	153

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

Fig. 1

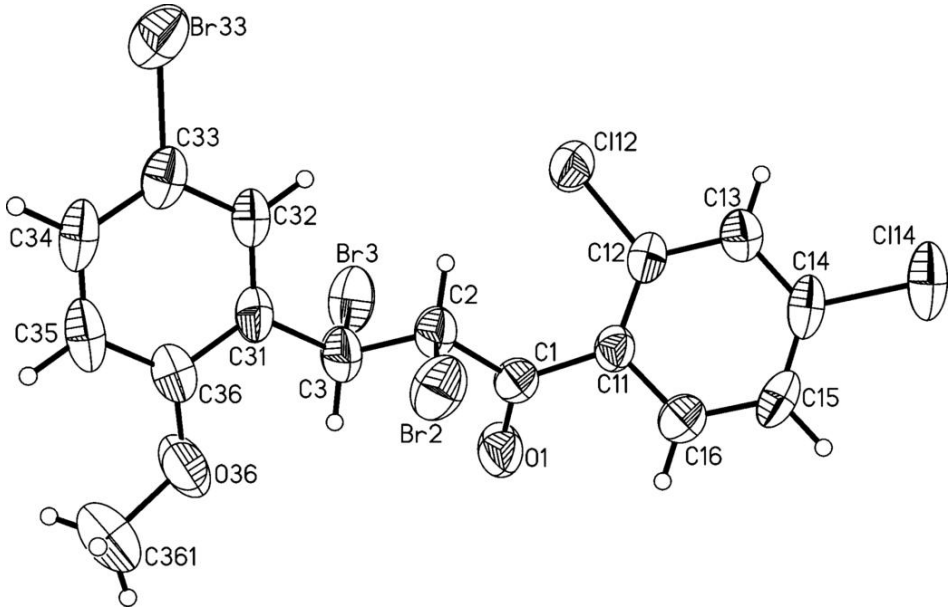
Br33
C33
C32
C34
C35
C31
C36
O36
C361
Br3
C3
C2
Br2
C1
O1
Cl12
C12
C13
C14
Cl14
C11
C15
C16

Fig. 2