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1-(4-Bromophenyl)-3-(2-chloro-6-fluorophenyl)prop-2-en-1-one

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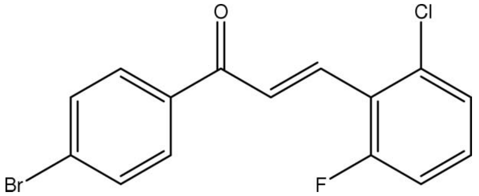
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.032; wR factor = 0.081; data-to-parameter ratio = 39.4.

In the title molecule, $C_{15}H_9BrClFO$, the dihedral angle between the two benzene rings is 22.7 (1)°. The crystal structure is stabilized by intermolecular C—H···F interactions and short Br···Cl contacts [Br···Cl = 3.579 (1) Å]. The compound can potentially exhibit second-order nonlinear optical properties as it crystallizes in a noncentrosymmetric space group.

Related literature

For bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For general background and related literature, see: Uchida *et al.* (1998); Watson *et al.* (1993); Patil, Dharmaprakash *et al.* (2006); Shettigar *et al.* (2006). For our previous work on related compounds, see: Patil, Teh, Fun, Babu *et al.* (2007); Patil, Teh, Fun, Razak *et al.* (2007).



Experimental

Crystal data

$C_{15}H_9BrClFO$
M_r = 339.58
Orthorhombic, $Pna2_1$
a = 27.8814 (4) Å
b = 3.9300 (1) Å
c = 11.9065 (2) Å
V = 1304.64 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.35 mm^{-1}
T = 100.0 (1) K
0.59 × 0.35 × 0.23 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.338, T_{max} = 0.507 (expected range = 0.308–0.462)
31202 measured reflections
6780 independent reflections
5407 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.081
S = 1.05
6780 reflections
172 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Absolute structure: Flack (1983), with 3224 Friedel pairs
Flack parameter: 0.057 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···F1^{i}	0.93	2.42	3.287 (2)	155
C8—H8A···F1	0.93	2.21	2.807 (2)	121
C9—H9A···Cl1	0.93	2.57	3.041 (2)	112
C9—H9A···O1	0.93	2.39	2.765 (3)	104

Symmetry code: (i) $-x+1, -y+3, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2409).

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supplementary materials

Acta Cryst. (2007). E**63**, o3238   [**doi:10.1107/S1600536807027365**]

1-(4-Bromophenyl)-3-(2-chloro-6-fluorophenyl)prop-2-en-1-one

P. S. Patil, M. M. Rosli, H.-K. Fun, I. A. Razak and S. M. Dharmaprakash

Comment

Chalcones with appropriate subtituents are a class of nonlinear optical materials (Patil *et al.*, 2006; Patil, Dharmaprakash *et al.*, 2007). As a part of our on-going work on the synthesis and structure determination of subtituted chalcones (Patil, Teh, Fun, Babu *et al.*, 2007, Patil, Teh, Fun, Razak *et al.*, 2007) the crystal structure of the title compound (I) was determined (Fig. 1). The title compound can potentially exhibit second-order NLO properties as it crystallizes in a non-centrosymmetric space group.

All bond lengths and angles in (I) show normal values (Allen *et al.*, 1987) and are comparable to those of a related structure (Patil, Teh, Fun, Babu *et al.*,2007; Patil, Teh, Fun, Razak *et al.*, 2007). The dihedral angle between the benzene rings is 22.7 (1)°. The least-squares plane through the enone group (O1/C7–C9) makes dihedral angles of 13.6 (1) and 9.4 (1)° with the C1–C6 and C10–C15 benzene rings, respectively.

Three intramolecular hydrogen bonds are observed in the molecular structure (Table 1). The intramolecular structure generates S(5) ring motifs for the C9—H9A···O1 and C9—H9A···Cl1 interactions and an S(6) ring motif for an C8—H8A···F1 interaction (Bernstein *et al.*, 1995). The molecules are stacked along the *b* axis and the structure is stabilized by C4—H4A···F1^{i} intermolecular interactions. Short Br1···Cl1($1 - x$, $2 - y$, $-1/2 + z$) contacts [3.579 (1) Å] also contribute to the stabilization of the crystal structure.

Experimental

The experimental procedure is comparable with that reported previously (Patil, Teh, Fun, Babu *et al.*,2007; Patil, Teh, Fun, Razak *et al.*, 2007). The actual quantities used for preparation of (I) were: 2-chloro-6-fluorobenzaldehyde (0.01 mol), 4-bromoacetophenone (0.01 mol), methanol 960 ml) and 5 ml of 10% of NaOH aqueous solution. Crystal suitable for X-ray analysis were grown by slow evaporation of an acetone solution at room temperature.

Refinement

All H atoms were refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

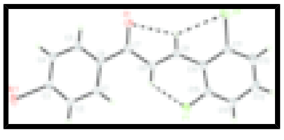

Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The dashed lines indicate a hydrogen bonds.

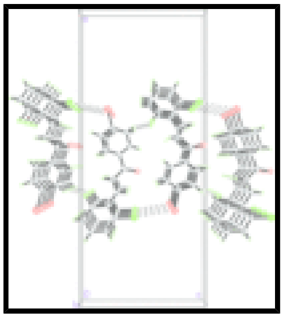

Fig. 2. The crystal packing of (I), viewed down the *b* axis. Hydrogen bonds and short contacts are shown as dashed lines.

1-(4-bromophenyl)-3-(2-chloro-6-fluorophenyl)prop-2-en-1-one

Crystal data

$C_{15}H_9BrClFO$	$F_{000} = 672$
$M_r = 339.58$	$D_x = 1.729$ Mg m^{-3}
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2c -2n	Cell parameters from 8121 reflections
$a = 27.8814$ (4) Å	$\theta = 2.3$–37.5°
$b = 3.9300$ (1) Å	$\mu = 3.35$ mm^{-1}
$c = 11.9065$ (2) Å	$T = 100.0$ (1) K
$V = 1304.64$ (4) Å^3	Block, colourless
$Z = 4$	0.59 × 0.35 × 0.23 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	6780 independent reflections
Radiation source: fine-focus sealed tube	5407 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.047$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 37.5$°
$T = 100.0(1)$ K	$\theta_{min} = 1.5$°
ω scans	$h = -47 \rightarrow 46$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$k = -6 \rightarrow 6$
$T_{min} = 0.338$, $T_{max} = 0.507$	$l = -20 \rightarrow 19$
31202 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.032$	$w = 1/[\sigma^2(F_o^2) + (0.0227P)^2 + 0.4581P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.081$	$(\Delta/\sigma)_{max} < 0.001$

$S = 1.05$	$\Delta\rho_{max} = 0.69$ e Å^{-3}
6780 reflections	$\Delta\rho_{min} = -0.30$ e Å^{-3}
172 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), with 3224 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.057 (6)
Secondary atom site location: difference Fourier map	

Special details

Experimental. The data was collected with the Oxford Cyrosystem 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 $F^2 > 2\sigma(F^2)$ 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}
Br1	0.338269 (6)	1.70184 (5)	0.72708 (2)	0.02248 (5)
Cl1	0.684369 (18)	0.41618 (14)	0.93374 (4)	0.02392 (10)
F1	0.62050 (5)	0.9222 (4)	0.57020 (10)	0.0244 (3)
O1	0.54265 (6)	1.0720 (5)	0.95820 (13)	0.0264 (3)
C1	0.47189 (7)	1.2413 (5)	0.70906 (16)	0.0180 (4)
H1A	0.4909	1.1394	0.6544	0.022*
C2	0.42735 (7)	1.3755 (5)	0.67974 (18)	0.0197 (3)
H2A	0.4163	1.3642	0.6061	0.024*
C3	0.39995 (7)	1.5256 (5)	0.76281 (17)	0.0178 (3)
C4	0.41570 (7)	1.5506 (5)	0.87334 (17)	0.0196 (4)
H4A	0.3968	1.6558	0.9275	0.024*
C5	0.45975 (7)	1.4168 (5)	0.90101 (17)	0.0190 (3)
H5A	0.4707	1.4320	0.9746	0.023*
C6	0.48825 (7)	1.2585 (5)	0.82009 (16)	0.0160 (3)
C7	0.53423 (7)	1.1020 (5)	0.85802 (16)	0.0174 (3)
C8	0.56942 (7)	0.9878 (5)	0.77217 (17)	0.0188 (3)
H8A	0.5645	1.0334	0.6964	0.023*
C9	0.60856 (7)	0.8172 (5)	0.80645 (16)	0.0168 (3)
H9A	0.6100	0.7720	0.8830	0.020*
C10	0.64912 (6)	0.6927 (5)	0.74095 (18)	0.0167 (3)
C11	0.68697 (7)	0.5114 (5)	0.79113 (17)	0.0190 (3)
C12	0.72672 (6)	0.3974 (5)	0.7325 (2)	0.0236 (3)
H12A	0.7509	0.2791	0.7694	0.028*

C13	0.73008 (8)	0.4611 (6)	0.6183 (2)	0.0259 (4)
H13A	0.7567	0.3860	0.5784	0.031*
C14	0.69366 (8)	0.6376 (6)	0.56320 (19)	0.0238 (4)
H14A	0.6954	0.6803	0.4865	0.029*
C15	0.65495 (7)	0.7471 (5)	0.62546 (19)	0.0198 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.01427 (7)	0.02028 (8)	0.03290 (9)	0.00260 (6)	−0.00130 (9)	−0.00051 (11)
Cl1	0.0223 (2)	0.0247 (2)	0.0248 (2)	0.00264 (17)	−0.00752 (18)	0.00313 (18)
F1	0.0225 (6)	0.0322 (7)	0.0186 (5)	0.0032 (5)	−0.0009 (4)	0.0036 (5)
O1	0.0253 (7)	0.0362 (9)	0.0177 (7)	0.0073 (7)	−0.0018 (5)	0.0010 (6)
C1	0.0159 (7)	0.0196 (9)	0.0186 (10)	0.0026 (5)	0.0006 (6)	−0.0008 (6)
C2	0.0165 (8)	0.0233 (10)	0.0194 (8)	0.0013 (6)	−0.0011 (6)	−0.0007 (7)
C3	0.0141 (7)	0.0163 (8)	0.0230 (8)	−0.0004 (6)	0.0002 (6)	0.0014 (6)
C4	0.0184 (8)	0.0197 (9)	0.0206 (9)	0.0012 (6)	0.0044 (6)	−0.0028 (7)
C5	0.0191 (8)	0.0205 (9)	0.0173 (8)	0.0003 (7)	0.0008 (6)	−0.0020 (6)
C6	0.0152 (7)	0.0160 (9)	0.0167 (8)	0.0003 (6)	0.0014 (6)	0.0002 (6)
C7	0.0158 (7)	0.0188 (9)	0.0175 (8)	0.0009 (6)	−0.0014 (6)	0.0003 (6)
C8	0.0166 (8)	0.0222 (9)	0.0175 (8)	0.0025 (6)	−0.0002 (6)	0.0013 (6)
C9	0.0155 (8)	0.0169 (8)	0.0181 (8)	0.0005 (6)	0.0000 (6)	0.0007 (6)
C10	0.0126 (6)	0.0164 (7)	0.0212 (10)	−0.0017 (5)	−0.0015 (6)	−0.0002 (6)
C11	0.0159 (8)	0.0160 (8)	0.0252 (9)	−0.0013 (6)	−0.0025 (6)	−0.0004 (6)
C12	0.0139 (7)	0.0184 (7)	0.0384 (10)	0.0005 (5)	−0.0014 (9)	−0.0013 (10)
C13	0.0170 (8)	0.0227 (10)	0.0380 (11)	−0.0037 (7)	0.0069 (8)	−0.0069 (8)
C14	0.0230 (9)	0.0231 (11)	0.0252 (10)	−0.0023 (7)	0.0059 (8)	−0.0040 (7)
C15	0.0176 (8)	0.0189 (10)	0.0229 (9)	−0.0012 (6)	0.0001 (6)	−0.0007 (6)

Geometric parameters (Å, °)

Br1—C3	1.9021 (19)	C7—C8	1.486 (3)
Cl1—C11	1.740 (2)	C8—C9	1.344 (3)
F1—C15	1.353 (3)	C8—H8A	0.9300
O1—C7	1.221 (2)	C9—C10	1.458 (3)
C1—C2	1.394 (3)	C9—H9A	0.9300
C1—C6	1.400 (3)	C10—C15	1.401 (3)
C1—H1A	0.9300	C10—C11	1.407 (3)
C2—C3	1.382 (3)	C11—C12	1.384 (3)
C2—H2A	0.9300	C12—C13	1.385 (4)
C3—C4	1.391 (3)	C12—H12A	0.9300
C4—C5	1.376 (3)	C13—C14	1.394 (3)
C4—H4A	0.9300	C13—H13A	0.9300
C5—C6	1.395 (3)	C14—C15	1.378 (3)
C5—H5A	0.9300	C14—H14A	0.9300
C6—C7	1.492 (3)		
C2—C1—C6	120.57 (18)	C7—C8—H8A	120.7
C2—C1—H1A	119.7	C8—C9—C10	129.38 (19)

C6—C1—H1A	119.7	C8—C9—H9A	115.3
C3—C2—C1	118.35 (19)	C10—C9—H9A	115.3
C3—C2—H2A	120.8	C15—C10—C11	114.03 (18)
C1—C2—H2A	120.8	C15—C10—C9	124.31 (18)
C2—C3—C4	122.19 (18)	C11—C10—C9	121.64 (19)
C2—C3—Br1	119.68 (15)	C12—C11—C10	123.4 (2)
C4—C3—Br1	118.12 (15)	C12—C11—Cl1	117.14 (17)
C5—C4—C3	118.77 (18)	C10—C11—Cl1	119.48 (16)
C5—C4—H4A	120.6	C11—C12—C13	119.4 (2)
C3—C4—H4A	120.6	C11—C12—H12A	120.3
C4—C5—C6	120.89 (18)	C13—C12—H12A	120.3
C4—C5—H5A	119.6	C12—C13—C14	120.18 (19)
C6—C5—H5A	119.6	C12—C13—H13A	119.9
C5—C6—C1	119.21 (18)	C14—C13—H13A	119.9
C5—C6—C7	117.66 (17)	C15—C14—C13	118.2 (2)
C1—C6—C7	123.08 (17)	C15—C14—H14A	120.9
O1—C7—C8	121.04 (18)	C13—C14—H14A	120.9
O1—C7—C6	120.04 (18)	F1—C15—C14	117.0 (2)
C8—C7—C6	118.92 (16)	F1—C15—C10	118.21 (18)
C9—C8—C7	118.54 (18)	C14—C15—C10	124.8 (2)
C9—C8—H8A	120.7		

C6—C1—C2—C3	0.1 (3)	C8—C9—C10—C15	2.9 (3)
C1—C2—C3—C4	0.9 (3)	C8—C9—C10—C11	−178.8 (2)
C1—C2—C3—Br1	−178.45 (15)	C15—C10—C11—C12	0.3 (3)
C2—C3—C4—C5	−1.0 (3)	C9—C10—C11—C12	−178.12 (18)
Br1—C3—C4—C5	178.43 (15)	C15—C10—C11—Cl1	−178.71 (15)
C3—C4—C5—C6	0.0 (3)	C9—C10—C11—Cl1	2.8 (3)
C4—C5—C6—C1	1.0 (3)	C10—C11—C12—C13	−0.2 (3)
C4—C5—C6—C7	−176.51 (19)	Cl1—C11—C12—C13	178.82 (16)
C2—C1—C6—C5	−1.0 (3)	C11—C12—C13—C14	−0.2 (3)
C2—C1—C6—C7	176.34 (19)	C12—C13—C14—C15	0.5 (3)
C5—C6—C7—O1	10.4 (3)	C13—C14—C15—F1	179.01 (19)
C1—C6—C7—O1	−167.0 (2)	C13—C14—C15—C10	−0.4 (3)
C5—C6—C7—C8	−169.02 (18)	C11—C10—C15—F1	−179.39 (18)
C1—C6—C7—C8	13.6 (3)	C9—C10—C15—F1	−1.0 (3)
O1—C7—C8—C9	7.1 (3)	C11—C10—C15—C14	0.0 (3)
C6—C7—C8—C9	−173.55 (18)	C9—C10—C15—C14	178.4 (2)
C7—C8—C9—C10	−176.82 (19)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4A···F1^{i}	0.93	2.42	3.287 (2)	155
C8—H8A···F1	0.93	2.21	2.807 (2)	121
C9—H9A···Cl1	0.93	2.57	3.041 (2)	112
C9—H9A···O1	0.93	2.39	2.765 (3)	104

Symmetry codes: (i) −*x*+1, −*y*+3, *z*+1/2.

Fig. 1

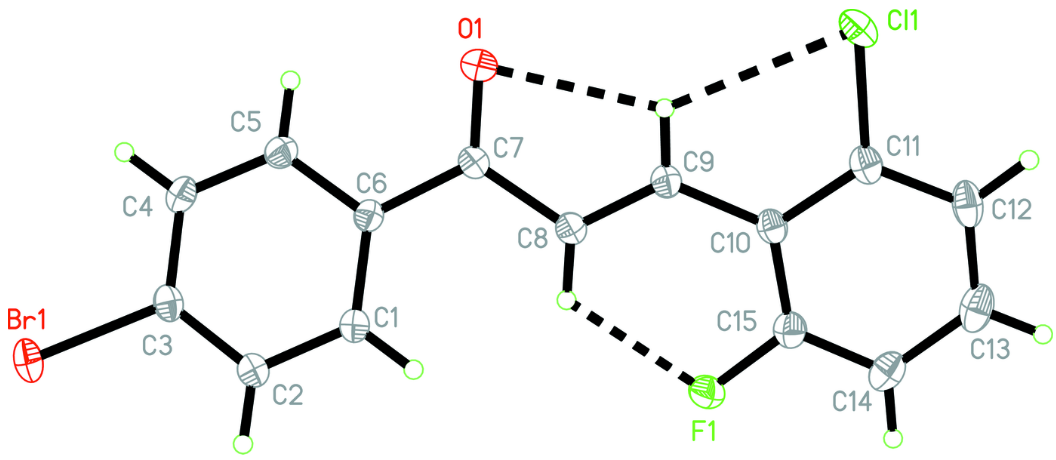

Fig. 2