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(*E*)-1-(3-Bromophenyl)-3-(3-fluorophenyl)prop-2-en-1-one

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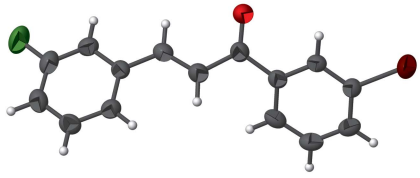
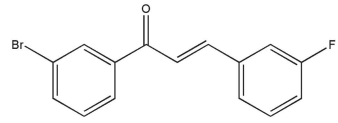
In the title compound, $C_{15}H_{10}BrFO$, the olefinic double bond adopts an *E* conformation. The molecule is non-planar as seen by the dihedral angle of 48.92 (11)° between the bromophenyl and fluorophenyl rings. The carbonyl group is twisted from the plane of the bromophenyl ring and the olefinic double bond. The *trans* conformation of the C=C double bond in the central enone group is confirmed by the C—C=C—C torsion angle of −165.7 (2)°.

3D view



Chemical scheme



Structure description

Great attention has been paid in recent years to the development of materials, including chalcone derivatives, for second and third order non-linear optical (NLO) applications such as telecommunications, optical computing, optical data storage and optical information processing (Shettigar *et al.*, 2006). Chalcones and their derivatives also demonstrate a wide range of biological activities including applications as antioxidants, antifungal, antibacterial and cardioprotective agents. In view of the broad spectrum of applications associated with chalcones and as a part of our ongoing work on such molecules (Chidan *et al.*, 2017; Harini *et al.*, 2017), we report the synthesis and crystal structure of the title compound here.

The molecule, shown in Fig. 1, is non-planar. This is evident from the dihedral angle of 48.92 (11)° between the bromophenyl and fluorophenyl rings that are bridged by the carbonyl substituent on the bromobenzene ring and olefinic double bond. This is higher

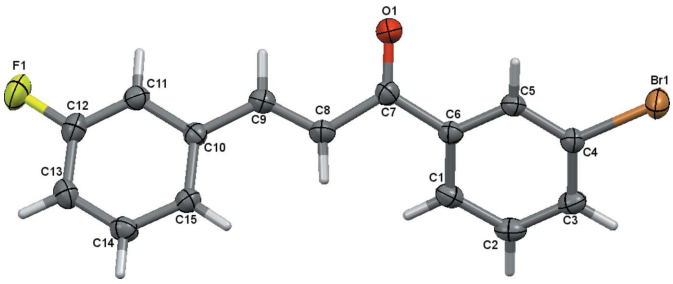


Figure 1
The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

than the value of 19.13 (15)° reported for the related chalcone derivative (*E*)-3-(2,3-dichlorophenyl)-1-(4-fluorophenyl)-prop-2-en-1-one (Naveen *et al.*, 2016). The *trans* conformation about the C7═C8 double bond in the central enone group is confirmed by a C6—C7═C8—C9 torsion angle, −165.7 (2)°. The carbonyl group at C7 is twisted from the plane of the bromophenyl ring and the olefinic double bond, as indicated by the O1—C7—C6—C5 and O1—C7—C8—C9 torsion angles of 25.4 (3) and 14.5 (4)°, respectively. No classical hydrogen bonds were found in the structure.

Synthesis and crystallization

3′-Bromoacetophenone (1.99 g, 0.01 mol) was mixed with 3-fluorobenzaldehyde (1.24 g, 0.01 mol) and dissolved in methanol (20 ml). To this solution, a catalytic amount of NaOH was added slowly, drop-by-drop, with constant stirring. The reaction mixture was stirred for 4 h. The resulting crude solid was filtered, washed several times with distilled water and finally recrystallized from methanol to give the pure chalcone. Single crystals suitable for X-ray diffraction studies were grown by the slow evaporation of the methanol solution. Yield 88%, m.p. 311–313 K.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{10}BrFO$
M_r	305.13
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	7.6032 (7), 5.9277 (6), 27.600 (3)
β (°)	93.183 (2)
V (Å^3)	1242.0 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.31
Crystal size (mm)	0.49 × 0.44 × 0.33
Data collection	
Diffractometer	Rigaku Saturn724+
Absorption correction	Multi-scan (*NUMABS*; Rigaku, 1999)
T_{min}, T_{max}	0.293, 0.408
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11350, 2983, 2228
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.662
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.034, 0.094, 1.02
No. of reflections	2983
No. of parameters	163
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.40, −0.26

Computer programs: *CrystalClear SM-Expert* (Rigaku, 2011), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

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full crystallographic data

IUCrData (2017). **2**, x170379 [https://doi.org/10.1107/S2414314617003790]

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(*E*)-1-(3-Bromophenyl)-3-(3-fluorophenyl)prop-2-en-1-one

Crystal data

$C_{15}H_{10}BrFO$
M_r = 305.13
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 7.6032 (7) Å
b = 5.9277 (6) Å
c = 27.600 (3) Å
β = 93.183 (2)°
V = 1242.0 (2) Å^3
Z = 4
$F(000)$ = 608
D_x = 1.632 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2228 reflections
θ = 1.5–28.1°
μ = 3.31 mm^{-1}
T = 100 K
Prism, green
0.49 × 0.44 × 0.33 mm

Data collection

Rigaku Saturn724+ diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 18.4 pixels mm^{-1}
profile data from ω–scans
Absorption correction: multi-scan (NUMABS; Rigaku, 1999)
T_{min} = 0.293, T_{max} = 0.408
11350 measured reflections
2983 independent reflections
2228 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 28.1°, θ_{min} = 1.5°
h = −10→9
k = −7→7
l = −33→36

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.094
S = 1.02
2983 reflections
163 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2 + 0.0964P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.69112 (4)	0.31515 (5)	0.70851 (1)	0.0627 (1)
F1	0.8178 (3)	0.7659 (3)	0.26863 (6)	0.0852 (7)
O1	0.7328 (3)	0.2879 (3)	0.51261 (6)	0.0620 (7)
C1	0.6003 (3)	0.7850 (4)	0.57483 (9)	0.0475 (7)
C2	0.5495 (3)	0.8515 (4)	0.62018 (10)	0.0515 (8)
C3	0.5749 (3)	0.7133 (4)	0.65974 (9)	0.0483 (8)
C4	0.6523 (3)	0.5051 (4)	0.65369 (8)	0.0421 (7)
C5	0.7009 (3)	0.4319 (3)	0.60926 (7)	0.0397 (6)
C6	0.6757 (3)	0.5727 (3)	0.56913 (7)	0.0401 (6)
C7	0.7279 (3)	0.4895 (4)	0.52096 (8)	0.0454 (7)
C8	0.7732 (3)	0.6600 (4)	0.48446 (9)	0.0501 (8)
C9	0.7850 (3)	0.6067 (4)	0.43836 (8)	0.0450 (7)
C10	0.8346 (3)	0.7597 (3)	0.39956 (8)	0.0388 (6)
C11	0.8041 (3)	0.6932 (4)	0.35145 (9)	0.0464 (7)
C12	0.8471 (4)	0.8349 (4)	0.31528 (9)	0.0543 (8)
C13	0.9198 (3)	1.0431 (4)	0.32362 (9)	0.0531 (8)
C14	0.9527 (3)	1.1078 (4)	0.37117 (9)	0.0496 (8)
C15	0.9101 (3)	0.9698 (4)	0.40878 (8)	0.0444 (7)
H1A	0.58430	0.88140	0.54840	0.0570*
H2A	0.49730	0.99200	0.62380	0.0620*
H3A	0.54090	0.75890	0.69010	0.0580*
H5A	0.75030	0.28960	0.60600	0.0480*
H8A	0.79380	0.80820	0.49430	0.0600*
H9A	0.75960	0.45830	0.42960	0.0540*
H11A	0.75480	0.55290	0.34410	0.0560*
H13A	0.94610	1.13760	0.29810	0.0640*
H14A	1.00470	1.24710	0.37800	0.0600*
H15A	0.93200	1.01750	0.44060	0.0530*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0882 (2)	0.0625 (2)	0.0379 (2)	0.0103 (1)	0.0080 (1)	0.0039 (1)
F1	0.1197 (15)	0.0972 (12)	0.0388 (9)	−0.0197 (11)	0.0048 (9)	−0.0105 (8)
O1	0.1000 (15)	0.0422 (10)	0.0446 (9)	−0.0032 (9)	0.0101 (9)	−0.0015 (7)
C1	0.0502 (13)	0.0354 (11)	0.0561 (14)	−0.0029 (9)	−0.0038 (11)	0.0059 (10)
C2	0.0502 (13)	0.0378 (12)	0.0666 (16)	0.0026 (9)	0.0039 (11)	−0.0067 (11)
C3	0.0496 (13)	0.0427 (12)	0.0532 (14)	−0.0005 (10)	0.0078 (11)	−0.0111 (10)
C4	0.0469 (12)	0.0404 (11)	0.0392 (11)	−0.0030 (9)	0.0046 (9)	−0.0007 (9)

C5	0.0438 (11)	0.0329 (10)	0.0425 (11)	−0.0028 (9)	0.0032 (9)	−0.0019 (9)
C6	0.0426 (11)	0.0365 (11)	0.0411 (11)	−0.0060 (9)	0.0015 (9)	−0.0003 (9)
C7	0.0536 (13)	0.0435 (12)	0.0387 (11)	−0.0074 (10)	−0.0003 (9)	0.0005 (9)
C8	0.0648 (15)	0.0413 (12)	0.0440 (12)	−0.0101 (10)	0.0027 (11)	−0.0017 (9)
C9	0.0506 (12)	0.0371 (10)	0.0474 (12)	−0.0017 (9)	0.0036 (10)	0.0004 (9)
C10	0.0387 (11)	0.0372 (10)	0.0408 (11)	0.0017 (8)	0.0057 (9)	0.0007 (8)
C11	0.0508 (13)	0.0421 (12)	0.0465 (12)	−0.0040 (9)	0.0043 (10)	−0.0073 (10)
C12	0.0595 (15)	0.0663 (16)	0.0374 (12)	0.0028 (12)	0.0052 (10)	−0.0035 (11)
C13	0.0565 (14)	0.0565 (14)	0.0471 (13)	−0.0029 (11)	0.0097 (10)	0.0089 (11)
C14	0.0492 (13)	0.0431 (12)	0.0566 (14)	−0.0088 (10)	0.0046 (11)	0.0002 (11)
C15	0.0494 (12)	0.0430 (11)	0.0408 (11)	−0.0034 (9)	0.0018 (9)	−0.0050 (9)

Geometric parameters (Å, º)

Br1—C4	1.896 (2)	C11—C12	1.358 (3)
F1—C12	1.358 (3)	C12—C13	1.367 (3)
O1—C7	1.218 (3)	C13—C14	1.377 (3)
C1—C2	1.387 (4)	C14—C15	1.374 (3)
C1—C6	1.395 (3)	C1—H1A	0.9300
C2—C3	1.370 (4)	C2—H2A	0.9300
C3—C4	1.381 (3)	C3—H3A	0.9300
C4—C5	1.371 (3)	C5—H5A	0.9300
C5—C6	1.392 (3)	C8—H8A	0.9300
C6—C7	1.492 (3)	C9—H9A	0.9300
C7—C8	1.481 (3)	C11—H11A	0.9300
C8—C9	1.319 (3)	C13—H13A	0.9300
C9—C10	1.469 (3)	C14—H14A	0.9300
C10—C11	1.392 (3)	C15—H15A	0.9300
C10—C15	1.389 (3)		
C2—C1—C6	119.7 (2)	C13—C14—C15	121.1 (2)
C1—C2—C3	121.0 (2)	C10—C15—C14	120.5 (2)
C2—C3—C4	118.7 (2)	C2—C1—H1A	120.00
Br1—C4—C3	118.86 (17)	C6—C1—H1A	120.00
Br1—C4—C5	119.22 (17)	C1—C2—H2A	120.00
C3—C4—C5	121.9 (2)	C3—C2—H2A	119.00
C4—C5—C6	119.35 (18)	C2—C3—H3A	121.00
C1—C6—C5	119.37 (19)	C4—C3—H3A	121.00
C1—C6—C7	121.99 (19)	C4—C5—H5A	120.00
C5—C6—C7	118.63 (18)	C6—C5—H5A	120.00
O1—C7—C6	120.4 (2)	C7—C8—H8A	119.00
O1—C7—C8	122.0 (2)	C9—C8—H8A	119.00
C6—C7—C8	117.64 (19)	C8—C9—H9A	117.00
C7—C8—C9	121.6 (2)	C10—C9—H9A	117.00
C8—C9—C10	126.1 (2)	C10—C11—H11A	120.00
C9—C10—C11	119.00 (19)	C12—C11—H11A	120.00
C9—C10—C15	122.7 (2)	C12—C13—H13A	121.00
C11—C10—C15	118.3 (2)	C14—C13—H13A	121.00

C10—C11—C12	119.5 (2)	C13—C14—H14A	120.00
F1—C12—C11	118.5 (2)	C15—C14—H14A	119.00
F1—C12—C13	118.4 (2)	C10—C15—H15A	120.00
C11—C12—C13	123.1 (2)	C14—C15—H15A	120.00
C12—C13—C14	117.6 (2)		

C6—C1—C2—C3	1.1 (4)	C6—C7—C8—C9	−165.7 (2)
C2—C1—C6—C5	−0.8 (3)	C7—C8—C9—C10	−177.8 (2)
C2—C1—C6—C7	178.1 (2)	C8—C9—C10—C11	−166.0 (2)
C1—C2—C3—C4	−0.1 (4)	C8—C9—C10—C15	13.6 (4)
C2—C3—C4—Br1	179.02 (18)	C9—C10—C11—C12	179.0 (2)
C2—C3—C4—C5	−1.3 (4)	C15—C10—C11—C12	−0.6 (3)
Br1—C4—C5—C6	−178.77 (17)	C9—C10—C15—C14	−179.4 (2)
C3—C4—C5—C6	1.5 (3)	C11—C10—C15—C14	0.2 (3)
C4—C5—C6—C1	−0.5 (3)	C10—C11—C12—F1	179.4 (2)
C4—C5—C6—C7	−179.5 (2)	C10—C11—C12—C13	−0.1 (4)
C1—C6—C7—O1	−153.6 (2)	F1—C12—C13—C14	−178.4 (2)
C1—C6—C7—C8	26.6 (3)	C11—C12—C13—C14	1.1 (4)
C5—C6—C7—O1	25.4 (3)	C12—C13—C14—C15	−1.5 (4)
C5—C6—C7—C8	−154.4 (2)	C13—C14—C15—C10	0.8 (4)
O1—C7—C8—C9	14.5 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···O1	0.93	2.52	2.832 (3)	100