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# (2*E*,2'*E*)-3,3'-(1,4-Phenylene)bis[1-(4-fluorophenyl)-prop-2-en-1-one]

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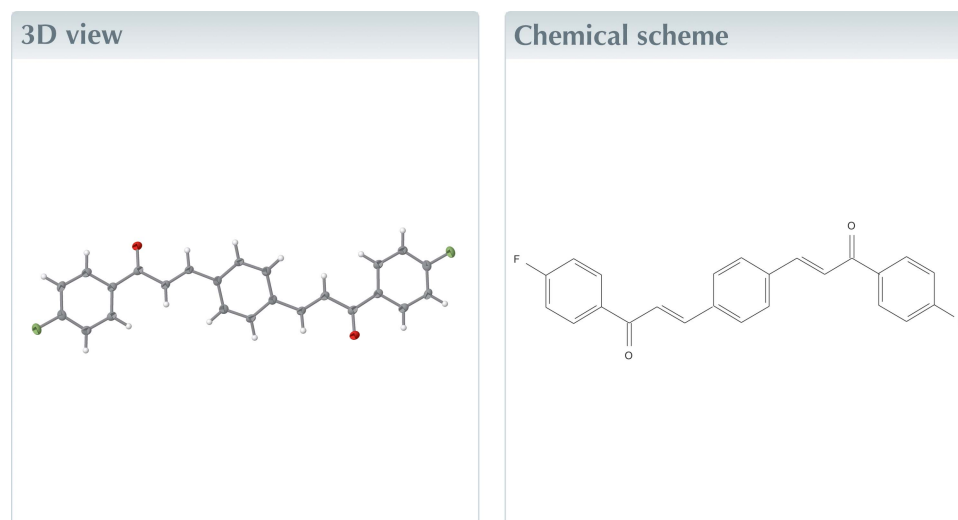
CCDC reference: 1449627

Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

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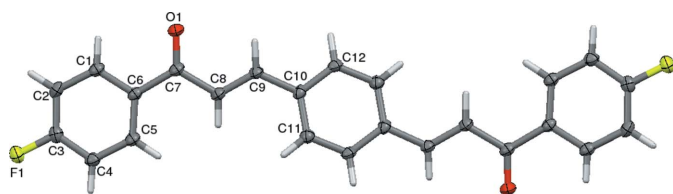
The title bis-chalcone compound, C<sub>24</sub>H<sub>16</sub>F<sub>2</sub>O<sub>2</sub>, crystallizes with one half-molecule in the asymmetric unit. The molecule lies about an inversion centre at the centroid of the central benzene ring. The olefinic double bonds adopt *E* conformations. In the crystal, C–H···O hydrogen bonds form sheets of molecules in the *ac* plane and C–H···F hydrogen bonds form zigzag chains along the *a*-axis direction. These combine to generate a three-dimensional network of molecules stacked along the *c*-axis direction.



## Structure description

Numerous studies have shown that bis-chalcones possess multiple pharmacological properties (Nowakowska, 2007). Materials with large non-linear optical (NLO) susceptibilities are of current interest in the area of harmonic generation and optical modulation. There is also considerable interest in the synthesis of new NLO materials because of their potential applications in technologies such as optical computing and optical communication (Chidan *et al.*, 2015) and because such materials play an important role in fields such as photonics and optoelectronics (Kumar *et al.* 2013). As a part of our ongoing work on such molecules (Naveen *et al.*, 2017; Rajendraprasad *et al.*, 2017), we report here the crystal structure of the title bis-chalcone derivative.

The title compound crystallizes with one half-molecule in the asymmetric unit and its structure is shown in Fig. 1. The molecule lies about an inversion centre at the centroid of



**Figure 1**

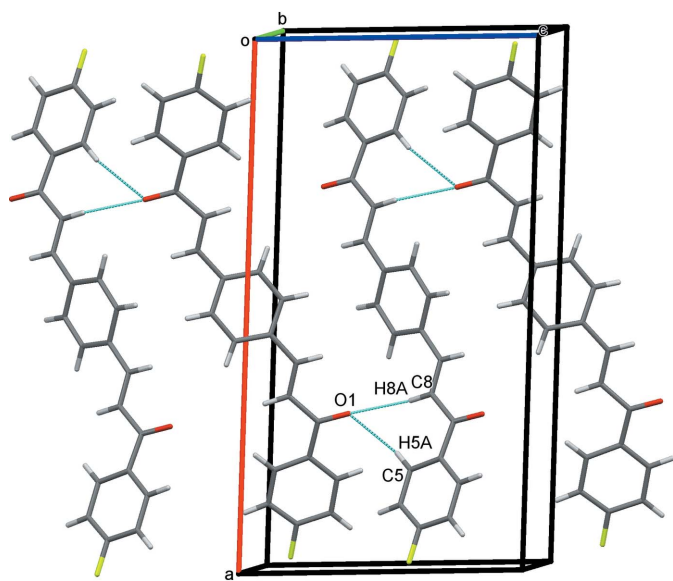
The molecular structure of the title compound, showing the atom-numbering scheme. Labelled atoms are related to unlabelled atoms by the symmetry operation  $(-x + 1, -y + 2, -z + 2)$ . Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

the central C10–C12/C10<sup>i</sup>–C12<sup>i</sup>, benzene ring [symmetry code: (i)  $-x + 1, -y + 2, -z + 2$ ]. The olefinic double bond adopts an *E* conformation. The *trans* conformation of the C=C double bond in the central enone group is confirmed by the C10–C9–C8=C7 torsion angle of  $-178.3(2)^\circ$ . This value is larger than that reported previously for the related compound (*2E,2'E*)-1,1'-(1,4-phenylene)bis(3-(3-chlorophenyl)prop-2-en-1-one) (Rajendraprasad *et al.*, 2017).

In the crystal, C5–H5A···O1 and C8–H8A···O1 hydrogen bonds link molecules into sheets in the *ac* plane, Fig. 2, while C2–H2A···F1 hydrogen bonds form zigzag chains along the *a*-axis direction (Table 1). These contacts combine to generate a three-dimensional network with molecules stacked along the *c*-axis direction, Fig. 3.

### Synthesis and crystallization

Terephthalaldehyde (1.06 g, 0.01 mol) was mixed with 4-fluoroacetophenone (2.76 g, 0.01 mol) and dissolved in methanol (30 ml). To this, 3 ml of NaOH (50%) was added. The reaction mixture was stirred for 6 h. The resulting crude solid was filtered, washed successively with distilled water and



**Figure 2**

A sheet of molecules in the *ac* plane viewed along the *b* axis, with C–H···O hydrogen bonds drawn as dashed lines.

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ ).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C2–H2A···F1 <sup>i</sup>	0.95	2.50	3.392 (3)	155
C5–H5A···O1 <sup>ii</sup>	0.95	2.59	3.515 (3)	166
C8–H8A···O1 <sup>ii</sup>	0.95	2.63	3.577 (3)	171

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

**Table 2**

Experimental details.

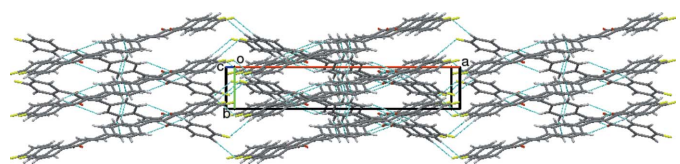
Crystal data	
Chemical formula	C <sub>24</sub> H <sub>16</sub> F <sub>2</sub> O <sub>2</sub>
<i>M<sub>r</sub></i>	374.37
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>c</i>
Temperature (K)	100
<i>a, b, c</i> ( $\text{\AA}$ )	20.405 (6), 3.8237 (11), 11.233 (3)
$\beta$ ( $^\circ$ )	93.989 (5)
<i>V</i> ( $\text{\AA}^3$ )	874.3 (4)
<i>Z</i>	2
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ ( $\text{mm}^{-1}$ )	0.10
Crystal size (mm)	0.22 × 0.15 × 0.13
Data collection	
Diffractometer	Rigaku Saturn724+
Absorption correction	Multi-scan (NUMABS; Rigaku, 1999)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.977, 0.987
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	6328, 1963, 1379
<i>R<sub>int</sub></i>	0.039
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> ( $\text{\AA}^{-1}$ )	0.647
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.069, 0.203, 1.09
No. of reflections	1963
No. of parameters	127
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ ( $\text{e \AA}^{-3}$ )	0.33, −0.37

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

finally recrystallized from methanol (90%) to give the pure bis-chalcone. Single crystals suitable for X-ray diffraction studies were grown by the slow evaporation of an acetone-methanol (1:1) solution (m.p. 402–405 K).

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.



**Figure 3**

Packing of the molecules viewed along the *c* axis, showing the zigzag arrangement of molecules and layered stacking.

### Acknowledgements

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## full crystallographic data

*IUCrData* (2017). 2, x170238 [https://doi.org/10.1107/S2414314617002383]

(2*E*,2'*E*)-3,3'-(1,4-Phenylene)bis[1-(4-fluorophenyl)prop-2-en-1-one]

C. S. Chidan Kumar, Ching Kheng Quah, S. Chandraju, N. K. Lokanath, S. Naveen and Muneer Abdoh

(2*E*,2'*E*)-3,3'-(1,4-Phenylene)bis[1-(4-fluorophenyl)prop-2-en-1-one]*Crystal data*

$C_{24}H_{16}F_2O_2$

$M_r = 374.37$

Monoclinic,  $P2_1/c$

Hall symbol: -P 2ybc

$a = 20.405$  (6) Å

$b = 3.8237$  (11) Å

$c = 11.233$  (3) Å

$\beta = 93.989$  (5)°

$V = 874.3$  (4) Å<sup>3</sup>

$Z = 2$

$F(000) = 388$

$D_x = 1.422$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 1379 reflections

$\theta = 2.0$ – $27.4$ °

$\mu = 0.10$  mm<sup>-1</sup>

$T = 100$  K

Rectangle, white

$0.22 \times 0.15 \times 0.13$  mm

*Data collection*

Rigaku Saturn724+

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 18.4 pixels mm<sup>-1</sup>

profile data from  $\omega$ -scans

Absorption correction: multi-scan

(NUMABS; Rigaku, 1999)

$T_{\min} = 0.977$ ,  $T_{\max} = 0.987$

6328 measured reflections

1963 independent reflections

1379 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 27.4$ °,  $\theta_{\min} = 2.0$ °

$h = -25$ → $26$

$k = -4$ → $4$

$l = -14$ → $14$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.069$

$wR(F^2) = 0.203$

$S = 1.09$

1963 reflections

127 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 atoms treated by a mixture of independent  
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.1169P)^2 + 0.1724P]$

where  $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.33$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.37$  e Å<sup>-3</sup>

*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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	0.02041 (7)	0.3368 (4)	0.88439 (14)	0.0309 (5)
O1	0.29100 (8)	0.6037 (5)	0.66903 (15)	0.0296 (6)
C1	0.16568 (12)	0.4078 (6)	0.7220 (2)	0.0217 (7)
C2	0.10182 (12)	0.3342 (6)	0.7470 (2)	0.0239 (8)
C3	0.08291 (11)	0.4157 (6)	0.8586 (2)	0.0223 (7)
C4	0.12399 (11)	0.5737 (6)	0.9452 (2)	0.0227 (8)
C5	0.18808 (11)	0.6453 (6)	0.9197 (2)	0.0215 (7)
C6	0.20983 (11)	0.5648 (6)	0.8074 (2)	0.0195 (7)
C7	0.27745 (12)	0.6434 (6)	0.7722 (2)	0.0218 (7)
C8	0.32763 (12)	0.7663 (6)	0.8654 (2)	0.0213 (7)
C9	0.39052 (11)	0.7978 (6)	0.8397 (2)	0.0204 (7)
C10	0.44537 (11)	0.9062 (6)	0.9229 (2)	0.0203 (7)
C11	0.43665 (12)	1.0668 (6)	1.0322 (2)	0.0219 (7)
C12	0.50979 (12)	0.8414 (6)	0.8921 (2)	0.0207 (7)
H1A	0.18000	0.35110	0.64570	0.0260*
H2A	0.07190	0.23040	0.68880	0.0290*
H4A	0.10870	0.63200	1.02070	0.0270*
H5A	0.21740	0.74970	0.97870	0.0260*
H8A	0.31510	0.82230	0.94300	0.0260*
H9A	0.40050	0.74510	0.76030	0.0250*
H11A	0.39350	1.11350	1.05480	0.0260*
H12A	0.51670	0.73270	0.81800	0.0250*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
F1	0.0202 (8)	0.0400 (9)	0.0327 (9)	-0.0027 (6)	0.0033 (6)	0.0003 (7)
O1	0.0271 (10)	0.0471 (12)	0.0147 (9)	-0.0049 (8)	0.0016 (7)	-0.0024 (8)
C1	0.0273 (13)	0.0205 (12)	0.0170 (12)	0.0007 (9)	-0.0015 (9)	0.0007 (9)
C2	0.0233 (13)	0.0247 (13)	0.0225 (13)	-0.0004 (10)	-0.0068 (9)	-0.0015 (10)
C3	0.0203 (12)	0.0194 (12)	0.0271 (14)	0.0010 (9)	0.0004 (9)	0.0044 (9)
C4	0.0243 (13)	0.0256 (14)	0.0180 (12)	0.0020 (10)	0.0008 (9)	0.0004 (9)
C5	0.0249 (13)	0.0230 (12)	0.0161 (12)	0.0004 (10)	-0.0013 (9)	0.0012 (9)
C6	0.0236 (12)	0.0180 (12)	0.0163 (12)	0.0009 (9)	-0.0020 (9)	0.0010 (8)
C7	0.0264 (13)	0.0226 (12)	0.0159 (12)	0.0002 (10)	-0.0019 (9)	0.0006 (9)
C8	0.0224 (12)	0.0253 (13)	0.0157 (12)	-0.0008 (9)	-0.0016 (9)	-0.0006 (9)

C9	0.0226 (13)	0.0241 (13)	0.0144 (12)	-0.0013 (9)	-0.0001 (9)	0.0003 (9)
C10	0.0213 (12)	0.0217 (12)	0.0175 (12)	-0.0029 (9)	-0.0017 (9)	0.0036 (9)
C11	0.0226 (12)	0.0238 (13)	0.0191 (12)	-0.0008 (9)	0.0007 (9)	0.0025 (9)
C12	0.0258 (13)	0.0227 (12)	0.0136 (12)	-0.0013 (9)	0.0009 (9)	0.0000 (9)

*Geometric parameters (Å, °)*

F1—C3	1.361 (3)	C10—C11	1.395 (3)
O1—C7	1.220 (3)	C10—C12	1.404 (3)
C1—C2	1.381 (3)	C11—C12 <sup>i</sup>	1.383 (3)
C1—C6	1.404 (3)	C1—H1A	0.9500
C2—C3	1.373 (3)	C2—H2A	0.9500
C3—C4	1.379 (3)	C4—H4A	0.9500
C4—C5	1.385 (3)	C5—H5A	0.9500
C5—C6	1.400 (3)	C8—H8A	0.9500
C6—C7	1.492 (3)	C9—H9A	0.9500
C7—C8	1.489 (3)	C11—H11A	0.9500
C8—C9	1.340 (3)	C12—H12A	0.9500
C9—C10	1.467 (3)		
C2—C1—C6	121.2 (2)	C10—C11—C12 <sup>i</sup>	120.6 (2)
C1—C2—C3	117.9 (2)	C10—C12—C11 <sup>i</sup>	121.1 (2)
F1—C3—C2	118.1 (2)	C2—C1—H1A	119.00
F1—C3—C4	118.7 (2)	C6—C1—H1A	119.00
C2—C3—C4	123.2 (2)	C1—C2—H2A	121.00
C3—C4—C5	118.5 (2)	C3—C2—H2A	121.00
C4—C5—C6	120.4 (2)	C3—C4—H4A	121.00
C1—C6—C5	118.7 (2)	C5—C4—H4A	121.00
C1—C6—C7	117.8 (2)	C4—C5—H5A	120.00
C5—C6—C7	123.5 (2)	C6—C5—H5A	120.00
O1—C7—C6	120.1 (2)	C7—C8—H8A	120.00
O1—C7—C8	121.2 (2)	C9—C8—H8A	120.00
C6—C7—C8	118.7 (2)	C8—C9—H9A	117.00
C7—C8—C9	119.9 (2)	C10—C9—H9A	117.00
C8—C9—C10	126.0 (2)	C10—C11—H11A	120.00
C9—C10—C11	123.1 (2)	C12 <sup>i</sup> —C11—H11A	120.00
C9—C10—C12	118.6 (2)	C10—C12—H12A	119.00
C11—C10—C12	118.3 (2)	C11 <sup>i</sup> —C12—H12A	119.00
C6—C1—C2—C3	-0.7 (3)	C5—C6—C7—O1	-171.6 (2)
C2—C1—C6—C5	0.3 (3)	C5—C6—C7—C8	9.1 (3)
C2—C1—C6—C7	-178.6 (2)	O1—C7—C8—C9	-7.5 (4)
C1—C2—C3—F1	-178.6 (2)	C6—C7—C8—C9	171.9 (2)
C1—C2—C3—C4	1.5 (4)	C7—C8—C9—C10	-178.3 (2)
F1—C3—C4—C5	178.3 (2)	C8—C9—C10—C11	-15.2 (4)
C2—C3—C4—C5	-1.8 (4)	C8—C9—C10—C12	163.9 (2)
C3—C4—C5—C6	1.3 (3)	C9—C10—C11—C12 <sup>i</sup>	179.0 (2)
C4—C5—C6—C1	-0.6 (3)	C12—C10—C11—C12 <sup>i</sup>	-0.1 (3)

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C4—C5—C6—C7	178.2 (2)	C9—C10—C12—C11 <sup>i</sup>	-179.1 (2)
C1—C6—C7—O1	7.2 (3)	C11—C10—C12—C11 <sup>i</sup>	0.1 (3)
C1—C6—C7—C8	-172.1 (2)	C10—C11—C12 <sup>i</sup> —C10 <sup>i</sup>	0.1 (3)

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Symmetry code: (i)  $-x+1, -y+2, -z+2$ .

*Hydrogen-bond geometry (Å, °)*

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<i>D—H</i> ⋯ <i>A</i>	<i>D—H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D—H</i> ⋯ <i>A</i>
C2—H2 <i>A</i> ⋯F1 <sup>ii</sup>	0.95	2.50	3.392 (3)	155
C5—H5 <i>A</i> ⋯O1 <sup>iii</sup>	0.95	2.59	3.515 (3)	166
C8—H8 <i>A</i> ⋯O1 <sup>iii</sup>	0.95	2.63	3.577 (3)	171

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