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3-(3,5-Difluorophenyl)-1-phenylprop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.056
wR factor = 0.122
Data-to-parameter ratio = 13.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The crystal structure of the title compound, $C_{15}H_{10}F_2O$, shows that the stereochemistry around the C=C double bond in the C=C—CO unit is *trans*.

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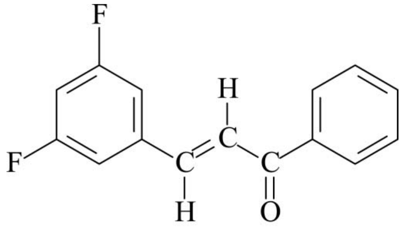
Comment

1,3-Diaryl-2-propen-1-ones, chalcones, are of great pharmacological importance, for example as antileishmaniasis (Boeck *et al.*, 2006), anticancer (Iwata *et al.*, 1995) and antimalaria (Li *et al.*, 1995) agents. In addition, chalcones are important precursors of flavones, flavonones and flavonoids, having anti-inflammatory, antihepatotoxic, anti-ulcer and antioxidant properties (Raj Narayana *et al.*, 2001). In this communication, we report the structure of the title compound, (I).



(I)

The molecular structure and numbering scheme of (I) are shown in Fig. 1. The central –CH=CH—C(=O)– link is planar, and the angle between the planes of the two terminal aromatic rings is 8.2 (1)°.

Bond lengths and angles are in the ranges reported for analogous structures (Yang *et al.*, 2006). The distances involving the C atoms in the –CH=CH—C(=O)– link are 1.320 (3) Å for C2=C3, 1.469 (3) Å for C1—C2 and 1.225 (3) Å for C1=O1.

In the crystal structure, molecules of (I) are arranged in antiparallel pairs along [010], resulting from π–π interactions between the C=C double bonds in the C=C—CO units (Fig. 2). The $\mathrm{C2{=}C3\cdots C2^{i}{=}C3^{i}}$ separation is 3.86 (5) Å, with a $\mathrm{C{=}C\cdots C}$ angle of 93.02 (2)° [symmetry code: (i) $1 - x, 1 - y, 1 - z$]. Non-classical $\mathrm{C12—H12\cdots O1^{ii}}$ hydrogen bonds link the molecules into pairs along [100] [symmetry code: (ii) $2 - x, 1 - y, 1 - z$].

Experimental

An aqueous solution of potassium hydroxide (20%, 10 ml) was added to a solution of ethanol–water (3:2 v/v, 10 ml) containing 3,5-difluorobenzaldehyde (0.7475 g, 0.005 mol). Acetophenone (0.600 g, 0.005 mol) was added in small fractions to the ethanol–water solution. The reaction mixture was stirred at low temperature (278 K) for 24 h.

Finally, the reaction yielded a white solid. The final mixture was neutralized with hydrochloric acid (10%). The product was recrystallized three times from ethanol. Colourless block crystals of (I) were obtained by slow evaporation of an ethanol solution at room temperature (yield 1.02 g, 80%; m.p. 382 K).

Crystal data

$C_{15}H_{10}F_2O$
$M_r = 244.24$
Triclinic, $P\bar{1}$
$a = 6.0359\ (12)$ Å
$b = 7.5002\ (15)$ Å
$c = 13.637\ (3)$ Å
$\alpha = 92.80\ (3)^\circ$
$\beta = 96.10\ (3)^\circ$
$\gamma = 99.82\ (3)^\circ$
$V = 603.5\ (2)$ Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 293\ (2)$ K
0.30 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: none
5771 measured reflections
2222 independent reflections
910 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.079$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.122$
$S = 0.94$
2222 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\rm max} = 0.11$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.15$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O1$^{\rm i}$	0.98 (2)	2.56 (2)	3.400 (4)	143 (2)

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

Atom H12 bonded to C12 was located in a difference map and refined with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The other H atoms were positioned geometrically, with C—H = 0.93 Å, and refined as riding, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). The phenyl groups were refined as rigid groups.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *PHICHI* (Duisenberg *et al.*, 2000); data reduction: *DIRAX* (Duisenberg, 1992); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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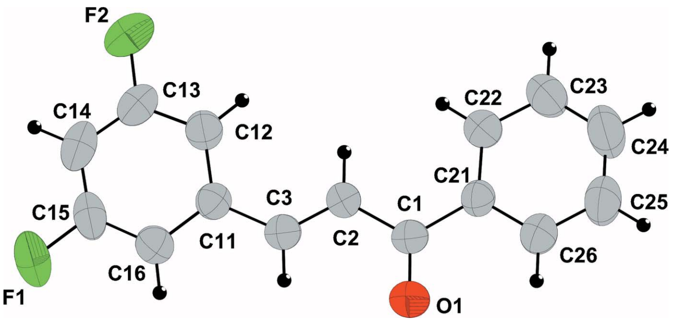

Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

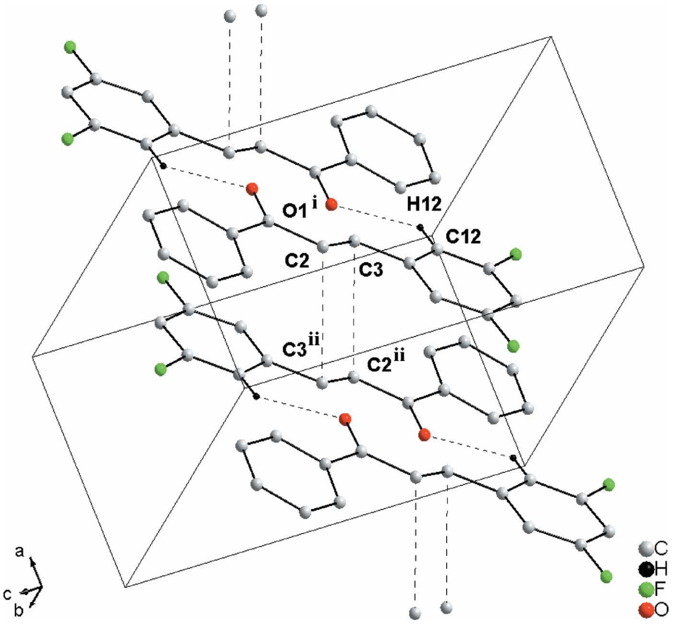

Figure 2
A view of the interactions C═C···C2═C3$^{\rm i}$ and C12—H12···O1$^{\rm ii}$. H atoms not involved in hydrogen bonds have been omitted. [Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $2 - x, 1 - y, 1 - z$.]

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