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4′-Fluorochalcone

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.049
wR factor = 0.154
Data-to-parameter ratio = 16.5

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

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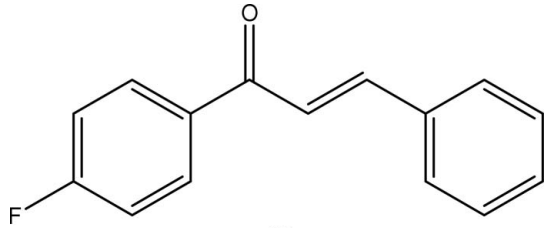
The enone fragment and the benzene rings of the title compound, $C_{15}H_{11}FO$, are each planar. The crystal packing is stabilized by weak intermolecular C—H···π interactions involving both aromatic rings; the molecules are stacked along the *b* axis.

Comment

The interest in chalcone derivatives in several disciplines stems from their biological activities, including antifungal (Boeck *et al.*, 2005) and anticoagulant properties (Shuib *et al.*, 1999), and their pharmacological activities, such as anti-protozoal (Nielsen *et al.*, 1998; Li *et al.*, 1995; Liu *et al.*, 2001), anti-inflammatory (Hsieh *et al.*, 1998), nitric oxide inhibition (Rojas *et al.*, 2002) and anticancer properties. The compounds are also used as depigmenting agents (Khatib *et al.*, 2005). Recently, it has been noted that derivatives of chalcones exhibit extremely high and fast non-linearity (Fichou *et al.*, 1988; Kitaoka *et al.*, 1990; Uchida *et al.*, 1998; Goto *et al.*, 1991; Patil *et al.*, 2006*a*,*b*; Zhang *et al.*, 1990; Zhao *et al.*, 2000). In view of these features associated with chalcones, we and others have undertaken a number of theoretical and structural studies of such compounds (Ng, Patil *et al.*, 2006; Ng, Shettigar *et al.*, 2006; Patil *et al.*, 2006*a*,*b*; Teh *et al.*, 2006; Radha Krishna *et al.*, 2005; Sathiya Moorthi *et al.*, 2005; Uchida *et al.*, 1995), and we report here the structure of the title compound, (I) (Fig. 1). Crystals of (I) do not exhibit second-order non-linear optical properties as they crystallize in a centrosymmetric space group.



(I)

The bond lengths and angles in (I) display normal values (Allen *et al.*, 1987) and agree well with those observed in related structures (Ng, Patil *et al.*, 2006; Ng, Shettigar *et al.*, 2006; Patil *et al.*, 2006*a*,*b*).

The enone group (O1/C7–C9) and the two benzene rings (C1–C6 and C10–C15) of the chalcone are each planar, with maximum deviations of 0.047 (2), 0.010 (2) and 0.006 (2) Å for atoms C7, C2 and C13, respectively.

The molecule is twisted about the C6—C7 bond, with a dihedral angle of 46.75 (5)° between the two benzene rings.

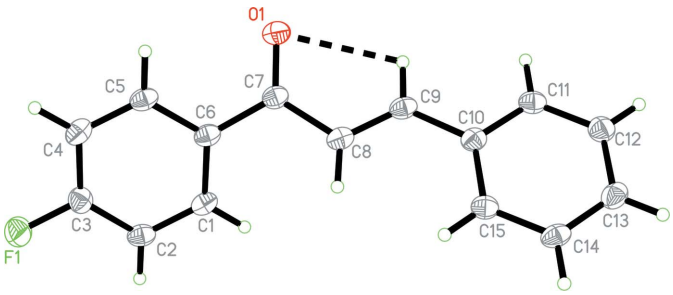


Figure 1
View of (I), showing the atomic numbering scheme and 50% probability displacement ellipsoids. The dashed line indicates a hydrogen bond.

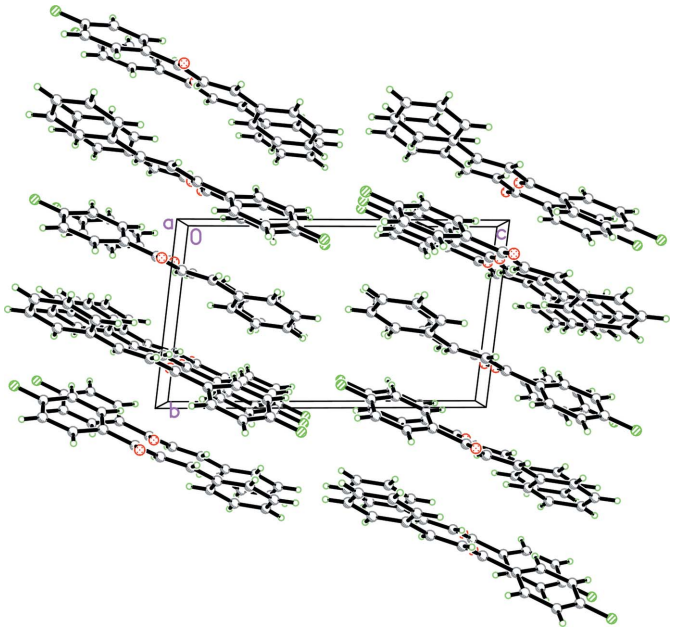


Figure 2
The crystal packing of (I), viewed down the *a* axis.

The least-squares plane through the enone fragment makes dihedral angles of 27.16 (7)° with the C1–C6 benzene ring and 20.24 (7)° with the C10–C15 benzene ring.

In the molecule, an intramolecular C9—H9*A*···O1 interaction generates an *S*(5) ring motif (Bernstein *et al.*, 1995). Aromatic rings C1–C6 (centroid *Cg*1) and C10–C15 (centroid *Cg*2) are involved in weak intermolecular C—H···π interactions (Table 1) which stabilize the crystal structure. The molecules are stacked along the *b* axis (Fig. 2).

Experimental

Benzaldehyde (0.01 mol) and 4-fluoroacetophenone (0.01 mol) were stirred in ethanol (60 ml) at room temperature. An aqueous solution of NaOH (10 ml, 30%) was added and the mixture was stirred for 4 h. The precipitate which formed was filtered, washed with water and dried. The resulting crude product was recrystallized twice from acetone. Crystals of (I) suitable for a single-crystal diffraction study were grown by slow evaporation of an acetone solution.

Crystal data

$C_{15}H_{11}FO$
M_r = 226.24
Triclinic, $P\overline{1}$
a = 5.8391 (2) Å
b = 7.4435 (3) Å
c = 13.0358 (5) Å
α = 96.592 (2)°
β = 93.947 (2)°
γ = 93.593 (2)°
V = 560.07 (4) Å^3
Z = 2
D_x = 1.342 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100.0 (1) K
Plate, yellow
0.38 × 0.30 × 0.10 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.847, T_{max} = 0.991
6883 measured reflections
2538 independent reflections
1843 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.154
S = 1.05
2538 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0877P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2*A*···*Cg*2^{i}	0.93	2.90	3.528 (2)	126
C5—H5*A*···*Cg*2^{ii}	0.93	2.84	3.442 (2)	123
C9—H9*A*···*Cg*1^{iii}	0.93	3.08	3.639 (2)	120
C14—H14*A*···*Cg*1^{iv}	0.93	2.87	3.536 (2)	129
C9—H9*A*···O1	0.93	2.48	2.814 (2)	101

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

H atoms were placed in calculated positions and constrained to ride on their carrier atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); 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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