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1-(4-Fluorophenyl)-3-(2,4,5-trimethoxyphenyl)-prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.001 Å
R factor = 0.040
wR factor = 0.123
Data-to-parameter ratio = 25.0

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

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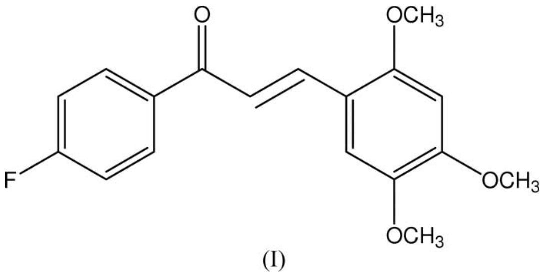
In the title compound, $C_{18}H_{17}FO_4$, the dihedral angle between the benzene rings is 12.42 (2)°. The crystal structure is stabilized by C—H$\cdots$O, C—H$\cdots\pi$ and π–π interactions.

Comment

Most chalcones with methoxy (Patil, Dharmaprakash *et al.*, 2006; Patil, Rosli, Fun, Razak, Puranik & Dharmaprakash, 2006) dimethoxy (Shettigar, Teh *et al.*, 2006; Shettigar, Patil *et al.*, 2006), trimethoxy (Patil, Ng *et al.*, 2006; Patil, Rosli, Fun, Razak & Dharmaprakash, 2006) and fluoro (Harrison *et al.*, 2006) substituents crystallize in non-centrosymmetric space groups and hence exhibit second-order (SHG) non-linear optical properties. We report here the molecular and supramolecular 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)

Bond lengths and angles in (I) have normal values (Allen *et al.*, 1987), comparable with related structures (Shettigar, Teh *et al.*, 2006; Patil, Ng *et al.*, 2006; Patil, Rosli, Fun, Razak & Dharmaprakash, 2006). The least-squares plane through the enone unit (C7–C9/O1) makes dihedral angles of 6.48 (2) and 8.53 (4)° with the C1–C6 and C10–C15 ring planes, respectively. The dihedral angle between the benzene rings is 12.42 (2)°. The methoxy groups attached at C11, C13 and C14 are almost coplanar with the C10–C15 benzene ring, with C16—O2—C11—C12, C17—O3—C13—C12 and C18—O4—C14—C15 torsion angles of 12.28 (11), −2.21 (12) and 12.27 (12)°, respectively.

Intramolecular C5—H5$A\cdots$O1, C9—H9$A\cdots$O1 and C9—H9$A\cdots$O2 interactions (Table 1) generate S(5) ring motifs (Bernstein *et al.*, 1995). The crystal structure is stabilized by intermolecular C—H$\cdots$O and C—H$\cdots\pi$ interactions (Table 1), the latter involving the C10–C15 benzene ring (*Cg* is the C10–C15 ring centroid). The crystal structure is further stabilized by $\pi\cdots\pi$ interactions, in which the centroid–centroid distance between the C1–C6 rings at (x, y, z) and ($1 - x$, $1 - y$, $1 - z$) is 3.790 (1) Å, and that between the C1–

C6 ring at (x, y, z) and the C10–C15 ring at $(1 - x, 1 - y, -z)$ is 3.702 (1) Å. The molecules are linked into chains parallel to the $[0\bar{1}1]$ direction (Fig. 2).

Experimental

4-Fluoroacetophenone (0.01 mol) in ethanol (30 ml) was mixed with 2,4,5-trimethoxybenzaldehyde (0.01 mol) in ethanol (30 ml) and the mixture was treated with an aqueous solution of sodium hydroxide (5 ml, 20%). This mixture was stirred well and left for 12 h, after which time the solid product was collected by filtration and dried. Crystals of (I) were grown from an acetone solution.

Crystal data

$C_{18}H_{17}FO_4$
$M_r = 316.32$
Triclinic, $P\bar{1}$
$a = 8.5325$ (2) Å
$b = 8.8404$ (2) Å
$c = 10.1468$ (2) Å
$\alpha = 87.048$ (1)°
$\beta = 73.313$ (1)°
$\gamma = 85.919$ (1)°

$V = 730.90$ (3) $Å^3$
$Z = 2$
$D_x = 1.437$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.11$ mm^{-1}
$T = 100.0$ (1) K
Block, yellow
0.52 × 0.52 × 0.51 mm

Data collection

Bruker SMART APEX2 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.935$, $T_{max} = 0.946$

18180 measured reflections
5266 independent reflections
4726 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 32.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.123$
$S = 1.06$
5266 reflections
211 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0739P)^2 + 0.1553P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.55$ e $Å^{-3}$
$\Delta\rho_{min} = -0.30$ e $Å^{-3}$

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C18-H18C\cdots Cg^{i}$	0.96	2.80	3.693 (1)	155
$C4-H4A\cdots O4^{ii}$	0.93	2.40	3.269 (1)	156
$C5-H5A\cdots O1$	0.93	2.43	2.751 (1)	100
$C9-H9A\cdots O1$	0.93	2.40	2.764 (1)	103
$C9-H9A\cdots O2$	0.93	2.34	2.723 (1)	104
$C18-H18B\cdots O1^{iii}$	0.96	2.46	3.379 (1)	161

Symmetry codes: (i) $-x + 1, -y + 2, -z$; (ii) $x, y - 1, z + 1$; (iii) $-x + 1, -y + 1, -z$. *Cg* is the C10–C15 ring centroid.

H atoms were positioned geometrically and treated as riding, with C—H = 0.93 or 0.96 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$ or 1.5_{eq}(methyl 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).

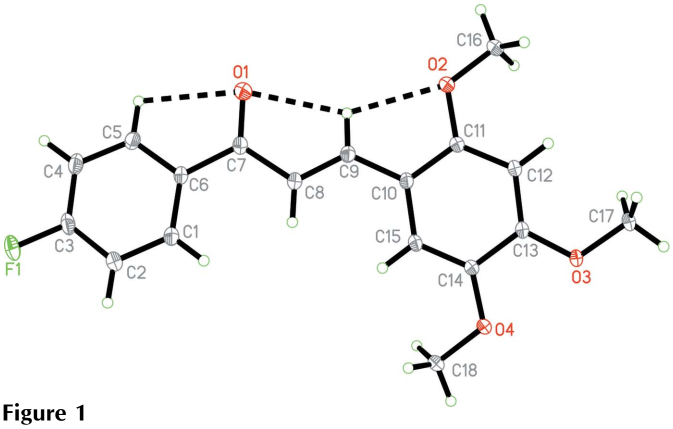


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Intramolecular hydrogen bonds are shown as dashed lines.

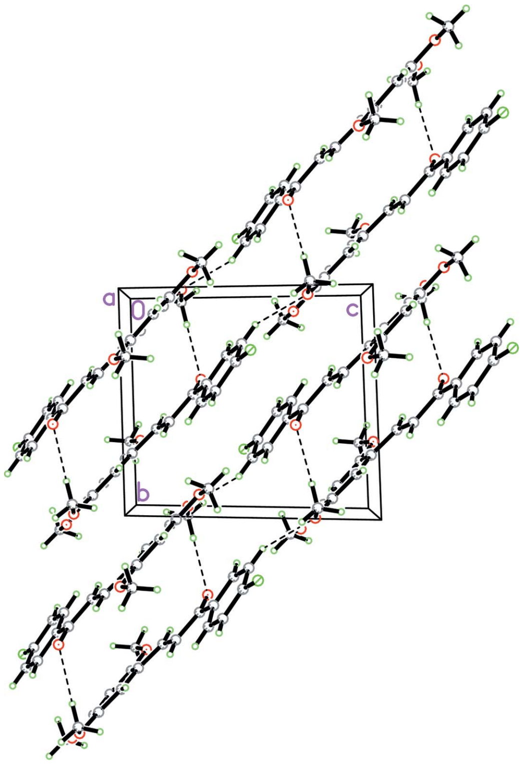


Figure 2
The crystal packing of (I), viewed down the *a* axis. Dashed lines indicate hydrogen bonds.

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