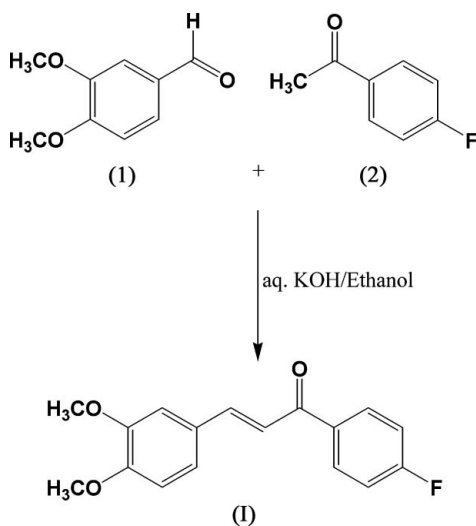


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Key indicators

Single-crystal X-ray study
 $T = 273$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.047
 wR factor = 0.123
Data-to-parameter ratio = 18.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.3-(3,4-Dimethoxyphenyl)-1-(4-fluorophenyl)-
prop-2-en-1-oneThe title compound, $\text{C}_{17}\text{H}_{15}\text{FO}_3$, crystallizes in a centrosym-
metric space group and thus does not show any non-linear
optical activity. There are two molecules in the asymmetric
unit.Received 22 March 2006
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Comment

Today crystals play an important role in the electronics and
photonics industries, such as in the production of high effi-
ciency photovoltaic cells, the fabrication of bright and long-
lasting light-emitting diodes (LED), and in liquid-crystal
displays (LCD). Crystal growth is a multidisciplinary field,
which demands the collaboration of chemical and process
engineers, electrical and mechanical engineers, instrumenta-
tion engineers, materials scientists, numerical simulation
specialists, physicists and crystallographers (Tareen & Kutty,
2001).The present-day demand is for large and high quality
ferroelectric or piezoelectric single crystals with minimum
defects and inhomogenities. The important goal of crystal
growth is the improvement of microscopic and macroscopic
homogeneity, which is a necessity for any application.
Different types of crystals being used are semiconductor
crystals, oxide crystals, alkali halide crystals and non-linear
optical (NLO) crystals. The NLO effect in organic molecules
originates from a strong donor-acceptor intermolecular
interaction and a delocalized π -electron system, and is also
due to the ability to crystallize in a non-centrosymmetric
space group. Among several organic compounds reported for NLO
properties, chalcone derivatives are important materials for

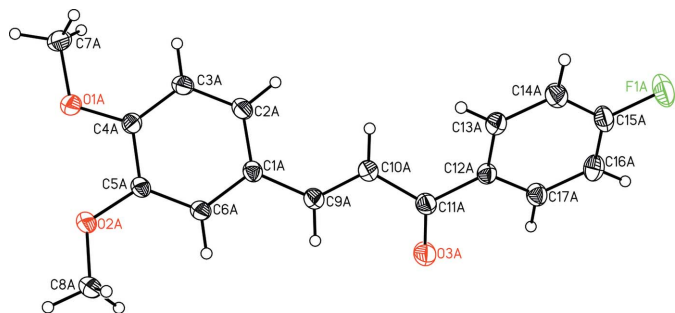


Figure 1
One of the two independent molecules of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The other molecule is very similar.

their excellent blue light transmittance and good crystallizability. They provide a necessary configuration to show NLO properties, with two planar rings connected through a conjugated double bond (Goto *et al.*, 1991; Uchida *et al.*, 1998; Tam *et al.*, 1989; Indira *et al.*, 2002). Substitution on either of the phenyl rings greatly influences non-centrosymmetric crystal packing. It is speculated that, in order to improve the activity, more bulky substituents should be introduced to increase the spontaneous polarization of non-centrosymmetric crystals (Fichou *et al.*, 1988). The molecular hyperpolarizability, β , is strongly influenced, not only by the electronic effect, but also by the steric effect of the substituent (Cho *et al.*, 1996). Crystal structures of similar compounds with a 4-hydroxy group (Ravishankar *et al.*, 2003), an 4-amino group (Selvi *et al.*, 2003) or a 3-methyl group (Sharma *et al.*, 1997) instead of a 4-fluoro group have been reported. Prompted by this and in a continuation of our quest to synthesize newer materials which can find use in the photonics industry, we have synthesized new chalcones and studied their SHG efficiency. The present work reports the crystal structure of the title compound, (I). Its metrical parameters are similar to those observed in other chalcone derivatives (Butcher, Yathirajan, Mithun *et al.*, 2006; Butcher, Yathirajan, Anilkumar *et al.*, 2006; Butcher, Yathirajan, Sarojini *et al.*, 2006).

The title molecule is inherently chiral due the fact that the two phenyl rings are mutually twisted with respect to the C9—C10—C11 backbone [dihedral twist angles of 47.81 (6) and 50.18 (5)° for molecules *A* and *B*, respectively]. However, there are two molecules of opposite hand in the asymmetric unit. This can most clearly be seen from the torsion angles C1—C9—C10—C11 and C9—C10—C11—C12 for the two moieties [−176.11 (16) and −168.98 (17)° for molecule *A*, and 177.96 (16) and 166.93 (16)°deg; for molecule *B*]. Thus, the title compound crystallizes in a centrosymmetric space group. Apart from these torsion angles, the metrical parameters of both molecules do not differ significantly.

Experimental

4-Fluoroacetophenone (1.28 g, 0.01 mol) in ethanol was mixed with veratraldehyde (1.66 g, 0.01 mol) in ethanol and the mixture was

treated with an aqueous solution of potassium hydroxide (20 ml, 5%). This mixture was stirred well and left to stand for 24 h. The resulting solid mass was collected by filtration. The compound was dried and recrystallized from ethanol. Single crystals were obtained from a solvent mixture of acetone–toluene (9:1) (yield 90%, m.p. 363–365 K). Analysis, calculated for $C_{17}H_{15}FO_3$: C 71.3, H 5.28%; found C 71.5, H 5.72%.

Crystal data

$C_{17}H_{15}FO_3$
 $M_r = 286.29$
Triclinic, $P\bar{1}$
 $a = 8.7105$ (13) Å
 $b = 10.6712$ (16) Å
 $c = 15.480$ (2) Å
 $\alpha = 90.766$ (2)°
 $\beta = 100.366$ (2)°
 $\gamma = 91.856$ (2)°
 $V = 1414.4$ (4) Å³
 $Z = 4$

$D_x = 1.344$ Mg m^{−3}
Mo $K\alpha$ radiation
Cell parameters from 2895 reflections
 $\theta = 2.4$ – 24.5 °
 $\mu = 0.10$ mm^{−1}
 $T = 273$ (2) K
Block, colourless
 $0.52 \times 0.44 \times 0.23$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
phi and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.950$, $T_{\max} = 0.977$
14595 measured reflections
6957 independent reflections
3244 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.046$
 $\theta_{\max} = 28.3$ °
 $h = -11 \rightarrow 11$
 $k = -14 \rightarrow 14$
 $l = -20 \rightarrow 20$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.123$
 $S = 0.83$
6957 reflections
383 parameters
H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.059P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.21$ e Å^{−3}
 $\Delta\rho_{\min} = -0.17$ e Å^{−3}

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry, with C—H distances of 0.98 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$, but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.95–1.00 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT-Plus (Bruker, 1999); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

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