3-(3,4-Dimethoxyphenyl)-1-(4-fluorophenyl)-prop-2-en-1-one

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The title compound, $C_{17}H_{15}FO_3$, crystallizes in a centrosymmetric space group and thus does not show any non-linear optical activity. There are two molecules in the asymmetric unit.

Comment

Today crystals play an important role in the electronics and photonics industries, such as in the production of high efficiency 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, instrumentation engineers, materials scientists, numerical simulation specialists, physicists and crystallographers (Tareen & Kutty, 2001).
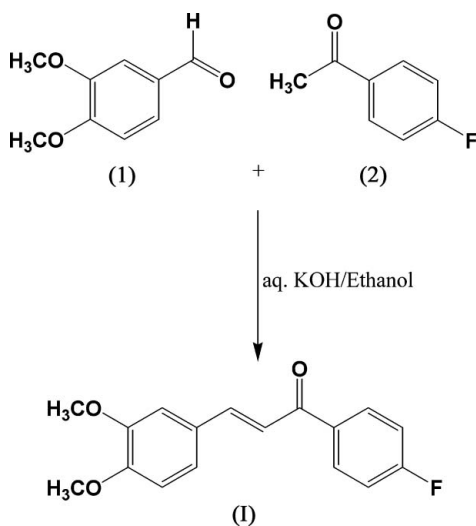
The present-day demand is for large and high quality ferroelectric or piezoelectric single crystals with minimum defects and inhomogenities. The important goal of crystal growth is the improvement of microscopic and macroscopic homogeneity, which is a necessity for any application. Different types of 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
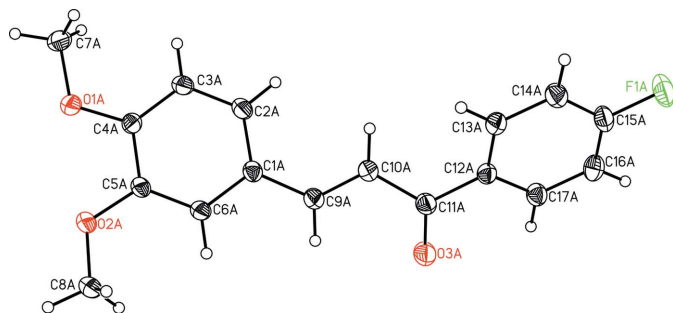
Figure 1
One of the two independent molecules of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. The other molecule is very similar.

their excellent blue light transmittance and good crystal-lizability. 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 hyperpolariz-ability, 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

$C_{17}H_{15}FO_3$	$D_x = 1.344$ Mg m^{-3}
$M_r = 286.29$	Mo $K\alpha$ radiation
Triclinic, $P\bar{1}$	Cell parameters from 2895
$a = 8.7105$ (13) Å	reflections
$b = 10.6712$ (16) Å	$\theta = 2.4$–24.5°
$c = 15.480$ (2) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 90.766$ (2)°	$T = 273$ (2) K
$\beta = 100.366$ (2)°	Block, colourless
$\gamma = 91.856$ (2)°	$0.52 \times 0.44 \times 0.23$ mm
$V = 1414.4$ (4) Å^3	
$Z = 4$	

Data collection

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

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.047$	$w = 1/[\sigma^2(F_o^2) + (0.059P)^2]$
$wR(F^2) = 0.123$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.83$	$(\Delta/\sigma)_{max} = 0.001$
6957 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
383 parameters	$\Delta\rho_{min} = -0.17$ 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 $U_{iso}(H) = 1.5U_{eq}(C)$, 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 $U_{iso}(H) = 1.2U_{eq}(C)$.

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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