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Key indicators

Single-crystal X-ray study
 $T = 297$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.058
 wR factor = 0.204
Data-to-parameter ratio = 37.3

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

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

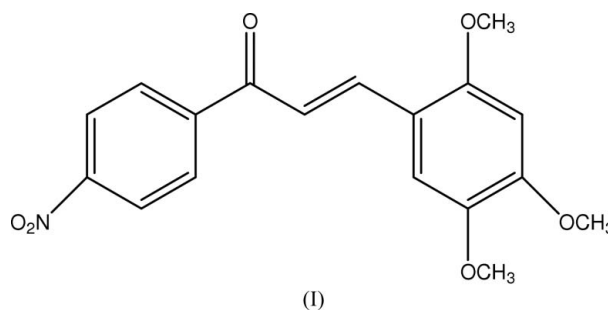
In the title compound, $\text{C}_{18}\text{H}_{17}\text{NO}_6$, the dihedral angle between the benzene rings is $43.45(5)^\circ$. There are two intramolecular hydrogen bonds in the molecule and the structure is stabilized by intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds.

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Comment

Nonlinear optical (NLO) materials capable of generating the second harmonic frequency play an important role in the domain of optoelectronics and photonics. NLO crystals with high conversion efficiencies for second harmonic generation (SHG) and that are transparent in the visible and ultraviolet ranges are required for numerous device applications (Chemla & Zyss, 1987). Within the past decade much progress has been made in the development of these organic NLO materials having large nonlinear optical coefficients. Advantages of using organic molecules as NLO materials stem from the fact that they can be designed to optimize the desired NLO property. At the molecular level, compounds likely to exhibit large values of molecular hyperpolarizability, β , must have polarizable electrons (*e.g.* π electrons) spread over a large distance. It has been shown that extended π systems with terminal donor–acceptor substituents exhibit large β values (Oudar & Chemla, 1977; Oudar, 1977). In these categories, chalcone derivatives are a class of organic compounds with excellent NLO properties (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), much better than those observed in inorganic crystals. We report here the synthesis and crystal structure of the title compound, (I) (Fig. 1). Crystals of (I) do not exhibit second-order nonlinear optical properties as they crystallize in a centrosymmetric space group.



All bond lengths and angles in (I) have normal values (Allen *et al.*, 1987) and are comparable to those in related structures (Patil *et al.*, 2006*a,b*). The dihedral angle between the benzene rings is $43.45(5)^\circ$. The least-squares plane through the enone group makes dihedral angles of $35.35(5)^\circ$ and $8.67(5)^\circ$ with the C1–C6 and C10–C15 benzene rings,

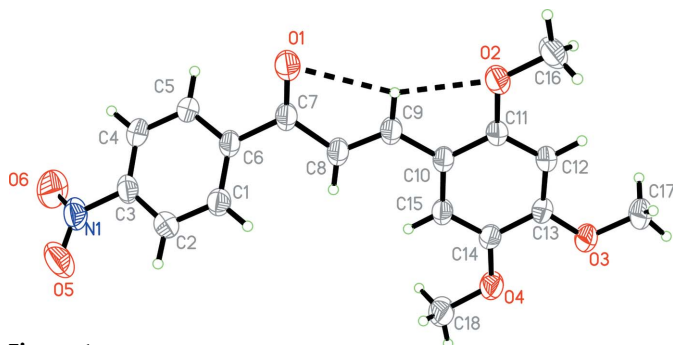


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Hydrogen bonds are drawn as dashed lines.

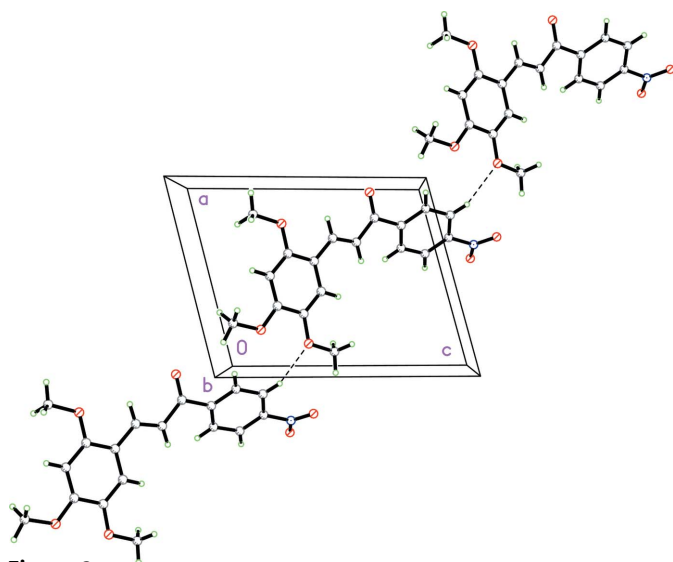


Figure 2
The crystal packing of (I), viewed down the *b* axis. Hydrogen bonds are drawn as dashed lines.

respectively. The three methoxy groups attached at atoms C11, C13 and C14 are almost coplanar with the C10–C15 benzene ring, with C16–O2–C11–C10, C17–O3–C13–C14 and C18–O4–C14–C13 torsion angles of 171.64 (12), –178.88 (11) and –179.76 (11)°, respectively. The nitro group is twisted slightly away from the plane of benzene ring with the torsion angle O5–N1–C3–C4 = –161.57 (13)°.

Intramolecular C9–H9A···O1 and C9–H9A···O2 interactions are observed in the molecular structure of (I); both interactions generate an *S*(5) ring motif (Bernstein *et al.*, 1995). The molecules form chains along the [101] direction through intermolecular C4–H4ⁱ···O4 hydrogen bonds (Table 1 and Fig. 2).

Experimental

The chalcone derivative (I) was prepared by the condensation of 2,4,5-trimethoxybenzaldehyde (0.01 mol) with 4-nitroacetophenone (0.01 mol) in ethanol (60 ml) in the presence of NaOH (2 ml, 30%). After stirring for 2 h, the contents of the flask were poured into ice-cold water (250 ml) and left to stand for 12 h. The resulting crude solid was collected by filtration, dried and purified by repeated

recrystallization from acetone. The purity of the compound was confirmed by thin-layer chromatography. Crystals suitable for single-crystal X-ray diffraction experiments were grown over a period of 12 d by the slow evaporation technique at room temperature, using acetone as the solvent.

Crystal data

C₁₈H₁₇NO₆
M_r = 343.33
 Triclinic, *P* $\bar{1}$
a = 8.5874 (2) Å
b = 9.1624 (2) Å
c = 10.9048 (2) Å
 α = 95.508 (1)°
 β = 104.062 (1)°
 γ = 97.357 (1)°

V = 818.20 (3) Å³
Z = 2
D_x = 1.394 Mg m^{–3}
 Mo *K*α radiation
 μ = 0.11 mm^{–1}
T = 297 (2) K
 Block, red
 0.41 × 0.36 × 0.35 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2005)
T_{min} = 0.873, *T_{max}* = 0.964

30783 measured reflections
 8548 independent reflections
 5213 reflections with *I* > 2σ(*I*)
R_{int} = 0.027
 θ_{\max} = 37.5°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.059
wR (*F*²) = 0.204
S = 1.03
 8548 reflections
 229 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.102P)^2 + 0.0898P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.28 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.38 \text{ e } \text{Å}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C4–H4A···O4 ⁱ	0.93	2.51	3.3773 (14)	155
C9–H9A···O1	0.93	2.54	2.8522 (15)	100
C9–H9A···O2	0.93	2.37	2.7335 (15)	103

Symmetry code: (i) *x* + 1, *y*, *z* + 1.

H atoms were placed in calculated positions with C–H distances in the range 0.93–0.96 Å. The *U*_{iso}(H) values were constrained to be 1.5*U*_{eq} of the carrier atom for methyl H atoms and 1.2*U*_{eq} for the remaining H atoms.

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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