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3,4-Dimethoxychalcone

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In the title molecule, $C_{17}H_{16}O_3$, the dihedral angle between the benzene rings is 25.75 (3)°. The crystal packing is stabilized by C—H···π interactions.

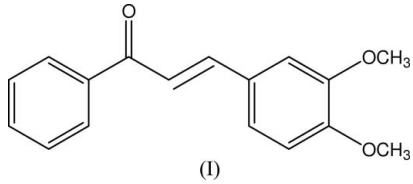
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.001 Å
R factor = 0.039
wR factor = 0.103
Data-to-parameter ratio = 23.0

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

Comment

As part of our study on non-linear optical chalcone derivatives (Patil *et al.*, 2006*a*,*b*,*c*), we report here the synthesis and crystal structure of the title compound, (I). Crystals of (I) can potentially exhibit second-order non-linear optical properties as the compound crystallizes in a non-centrosymmetric space group. A quantitative estimation has yet to be performed.



(I)

Bond lengths and angles in (I) have normal values (Allen *et al.*, 1987), comparable with related structures (Teh *et al.*, 2006; Patil *et al.*, 2006*a*,*b*,*c*). The least-squares plane through the enone group (atoms C7–C9/O1) makes dihedral angles of 26.77 (5) and 25.32 (5)° with the C1–C6 and C10–C15 benzene rings, respectively. The dihedral angle between the two benzene rings is 25.75 (3)°. The methoxy groups at C12 and C13 are almost coplanar with the C10–C15 benzene ring, with C16—O2—C12—C11 and C17—O3—C13—C14 torsion angles of −6.29 (15) and −9.36 (14)°, respectively.

An intramolecular C9—H9*A*···O1 hydrogen bond generates an *S*(5) ring motif (Bernstein *et al.*, 1995). The crystal structure is stabilized by C—H···π interactions involving the C1–C6 benzene ring (Table 1).

Experimental

Acetophenone (0.01 mol) in ethanol (25 ml) was mixed with 3,4-dimethoxybenzaldehyde (0.01 mol) in ethanol (25 ml) and the mixture was treated with an aqueous solution of sodium hydroxide (5 ml, 30%). This mixture was stirred well and left for 24 h. The resulting crude solid mass was collected by filtration and recrystallized from acetone.

Crystal data

$C_{17}H_{16}O_3$
M_r = 268.30
Orthorhombic, *Fdd*2
a = 27.7541 (4) Å
b = 34.1948 (4) Å
c = 5.6487 (1) Å
V = 5360.88 (14) Å^3
Z = 16
D_x = 1.330 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100.0 (1) K
Block, yellow
0.51 × 0.37 × 0.33 mm

Data collection

Brucker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.882, T_{max} = 0.971

41010 measured reflections
4202 independent reflections
3915 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 39.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.103
S = 1.08
4202 reflections
183 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2 + 1.2638P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···O1	0.93	2.42	2.786 (1)	103
C17—H17C···$Cg1^{i}$	0.96	2.75	3.384 (1)	124

Symmetry code: (i) $-x+1, -y, z+1$. $Cg1$ is the centroid of the C1–C6 ring.

H atoms were placed in calculated positions, with C—H = 0.93 or 0.96 Å. U_{iso} values were set equal to $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. In the absence of significant anomalous dispersion effects, Friedel pairs were merged.

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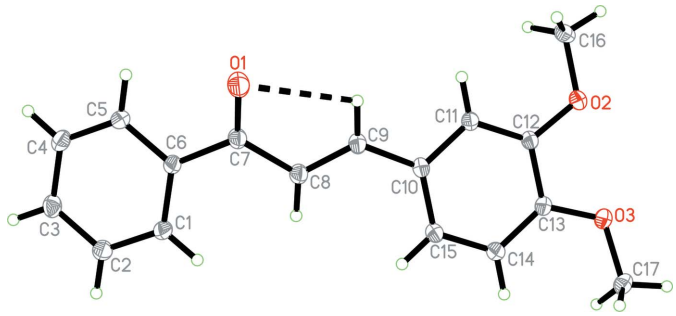

Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The intramolecular hydrogen bond is shown as a dashed line.

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