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1-Phenyl-3-(2,4,6-trimethoxyphenyl)-prop-2-en-1-one

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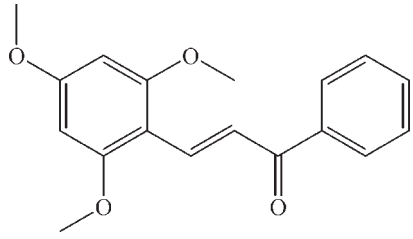
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.108; data-to-parameter ratio = 12.7.

In the title compound, $C_{18}H_{18}O_4$, the dihedral angle between the mean planes of the aromatic rings is 7.39 (6)°. The dihedral angles between the linking C—C═C—C plane and the phenyl and benzene rings are 11.27 (5) and 4.20 (5)°, respectively.

Related literature

For background to the properties and applications of chalcones, see: Satish *et al.*, (1995), Meng *et al.*, (2004), Indira *et al.*, (2002). For the synthesis, see: Migrdichian (1957).



Experimental

Crystal data

$C_{18}H_{18}O_4$ M_r = 298.32
Monoclinic, $P2_1/c$
a = 8.8921 (10) Å
b = 15.114 (3) Å
c = 11.618 (3) Å
β = 104.289 (10)°
V = 1513.1 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 K
0.12 × 0.10 × 0.05 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.989, T_{max} = 0.995
7545 measured reflections
2581 independent reflections
2037 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.108
S = 1.01
2581 reflections
203 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5119).

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supplementary materials

Acta Cryst. (2009). E**65**, o2724 [**doi:10.1107/S1600536809040227**]

1-Phenyl-3-(2,4,6-trimethoxyphenyl)prop-2-en-1-one

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Comment

In recent years, chalcones consisting of –C=C—C(O)- group have been widely researched due to their interesting properties, such as photoreaction (Satish *et al.*, 1995), biological activity (Meng *et al.*, 2004) and non-linear optical properties (Indira *et al.*, 2002). Herein, we report the synthesis and structure of the title compound.

As shown in figure 1, the C(1)—C(6) phenyl ring is taken as plane 1, another C(10)—C(15) one as plane 2 and the central C(7)—C(8)=C(9)—C(10) as plane 3, with the dihedral angles between them, A12, A13 and A23, of 7.39, 11.27 and 4.20 °, respectively, showing the two phenyl rings are rotated oppositely with respect to the central part of plane 3. The torsional angle C(7)—C(8)=C(9)—C(10) is 177.5 ° and the phenone O(1) atom deviates from plane 3 by 0.13 Å, suggesting C=O is not coplanar with this plane.

Experimental

The synthesis of the title compound was according to the related literature (Migrdichian *et al.*, (1957)). An aqueous solution of sodium hydroxide (10%, 10 ml) was added to the mixture of acetophenone (0.02 mol) and 2,4,6-trimethoxyphenylaldehyde (0.02 mol) in 95% ethanol (30 ml). The reaction mixture was stirred at room temperature for 5 h, yielding light yellow solid neutralized by hydrochloric acid (10%) and water. Colourless blocks of (I) were obtained by slow evaporation from dry ethanol. Elemental Analysis. Calc. for $C_{18}H_{18}O_4$: C 72.41, H 6.03%; Found: C 72.38, H 6.01%.

Refinement

The H atoms were placed in calculated positions (C—H = 0.93–0.96Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

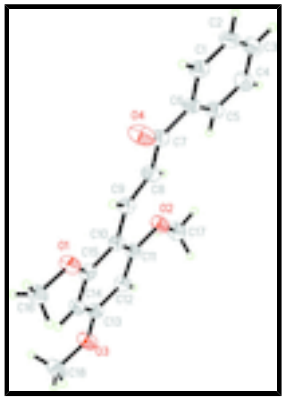


Fig. 1. A view of the structure of (I), showing 30% probability displacement ellipsoids for the non-hydrogen atoms.

1-Phenyl-3-(2,4,6-trimethoxyphenyl)prop-2-en-1-one

Crystal data

$C_{18}H_{18}O_4$	F_{000} = 632
M_r = 298.32	D_x = 1.310 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2581 reflections
a = 8.8921 (10) Å	θ = 2.4–25.0º
b = 15.114 (3) Å	μ = 0.09 mm^{-1}
c = 11.618 (3) Å	T = 293 K
β = 104.289 (10)º	Block, colourless
V = 1513.1 (5) Å^3	0.12 × 0.10 × 0.05 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	2581 independent reflections
Radiation source: fine-focus sealed tube	2037 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.037
T = 293 K	θ_{max} = 25.0º
ω scans	θ_{min} = 2.4º
Absorption correction: multi-scan (SADABS; Bruker, 2005)	h = −10→10
T_{min} = 0.989, T_{max} = 0.995	k = −17→16
7545 measured reflections	l = −13→13

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.036	$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.108	$(\Delta/\sigma)_{max} < 0.001$
S = 1.01	$\Delta\rho_{max}$ = 0.13 e Å^{-3}
2581 reflections	$\Delta\rho_{min}$ = −0.13 e Å^{-3}
203 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.329 (18)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.14370 (15)	0.24856 (10)	0.22992 (12)	0.0564 (4)
H1	−0.1511	0.2141	0.2946	0.068*
C2	−0.25419 (15)	0.31225 (11)	0.18742 (14)	0.0645 (4)
H2	−0.3356	0.3200	0.2236	0.077*
C3	−0.24594 (16)	0.36410 (11)	0.09297 (14)	0.0653 (4)
H3	−0.3202	0.4076	0.0659	0.078*
C4	−0.12883 (17)	0.35171 (10)	0.03889 (13)	0.0654 (4)
H4	−0.1228	0.3865	−0.0258	0.078*
C5	−0.01819 (15)	0.28718 (9)	0.08018 (12)	0.0550 (4)
H5	0.0607	0.2784	0.0417	0.066*
C6	−0.02275 (13)	0.23540 (9)	0.17773 (10)	0.0463 (3)
C7	0.09868 (14)	0.16867 (9)	0.23099 (11)	0.0505 (3)
C8	0.22237 (14)	0.15192 (9)	0.17349 (11)	0.0505 (4)
H8	0.2182	0.1777	0.1001	0.061*
C9	0.34224 (14)	0.10042 (8)	0.22297 (10)	0.0452 (3)
H9	0.3361	0.0743	0.2941	0.054*
C10	0.47889 (13)	0.07856 (8)	0.18512 (10)	0.0405 (3)
C11	0.51540 (14)	0.11331 (8)	0.08352 (10)	0.0431 (3)
C12	0.64572 (14)	0.08891 (8)	0.05099 (10)	0.0474 (3)
H12	0.6667	0.1122	−0.0175	0.057*
C13	0.74710 (13)	0.02941 (8)	0.11969 (11)	0.0460 (3)
C14	0.72008 (13)	−0.00523 (8)	0.22196 (10)	0.0457 (3)
H14	0.7900	−0.0443	0.2688	0.055*
C15	0.58727 (13)	0.01938 (8)	0.25291 (10)	0.0422 (3)
C16	0.65272 (16)	−0.07565 (10)	0.42236 (11)	0.0592 (4)
H16A	0.6572	−0.1275	0.3757	0.089*
H16B	0.6140	−0.0913	0.4898	0.089*
H16C	0.7548	−0.0509	0.4491	0.089*
C17	0.44269 (17)	0.21138 (9)	−0.08152 (12)	0.0616 (4)
H17A	0.5398	0.2424	−0.0602	0.092*
H17B	0.3610	0.2521	−0.1157	0.092*
H17C	0.4479	0.1661	−0.1383	0.092*
C18	0.97451 (18)	−0.05696 (11)	0.14022 (14)	0.0733 (5)

H18A	1.0180	−0.0392	0.2209	0.110*
H18B	1.0565	−0.0657	0.1009	0.110*
H18C	0.9181	−0.1112	0.1393	0.110*
O1	0.55255 (10)	−0.01251 (6)	0.35230 (8)	0.0566 (3)
O2	0.41252 (10)	0.17263 (6)	0.02034 (7)	0.0574 (3)
O3	0.87224 (10)	0.01005 (7)	0.08024 (8)	0.0639 (3)
O4	0.09522 (11)	0.13301 (8)	0.32405 (9)	0.0787 (4)

Atomic displacement parameters (Å^2)

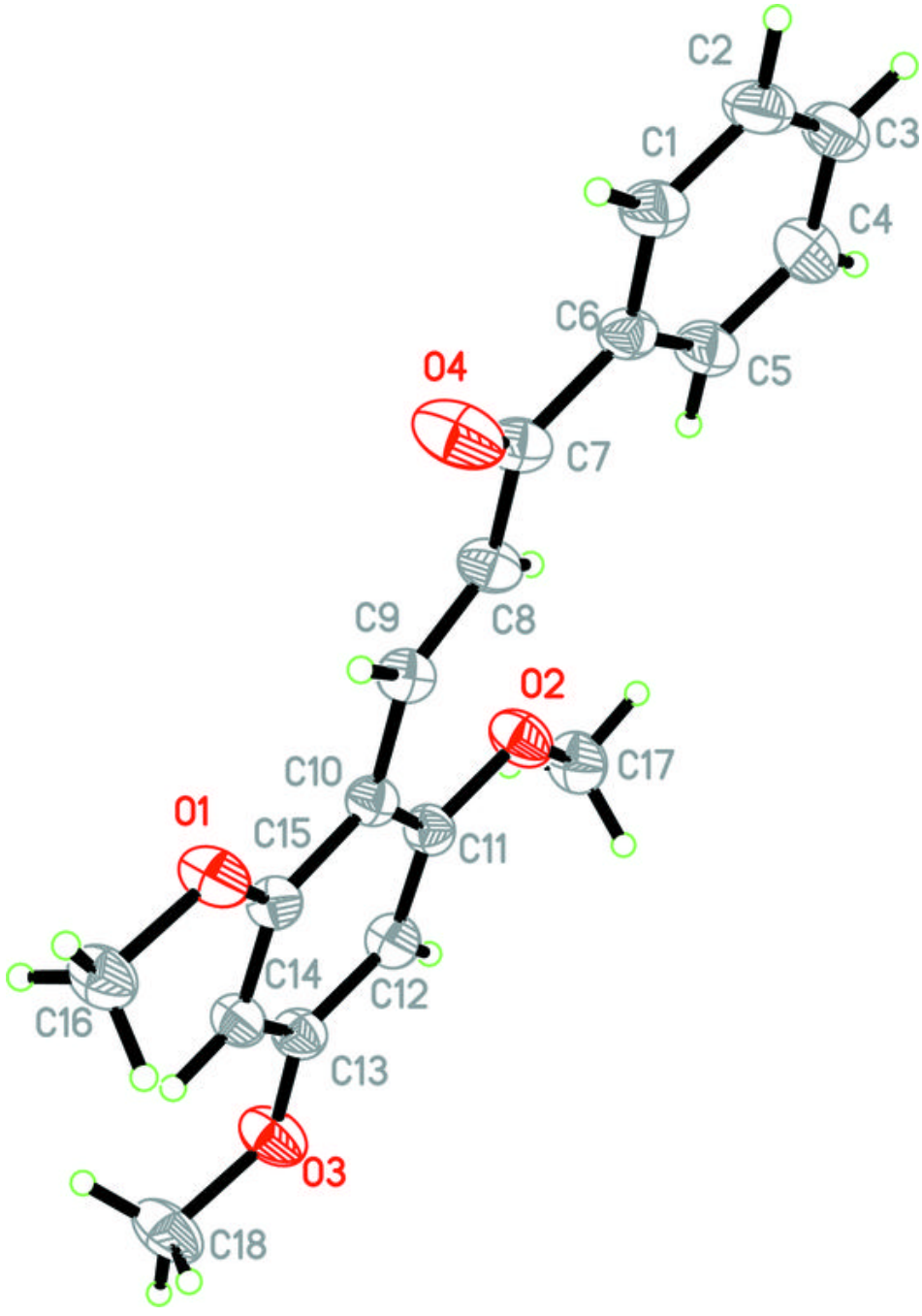
	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0473 (7)	0.0676 (9)	0.0567 (8)	−0.0009 (6)	0.0171 (6)	−0.0055 (7)
C2	0.0418 (7)	0.0773 (10)	0.0776 (10)	0.0068 (7)	0.0208 (7)	−0.0089 (8)
C3	0.0514 (8)	0.0694 (10)	0.0725 (10)	0.0144 (7)	0.0104 (7)	−0.0030 (8)
C4	0.0649 (9)	0.0683 (9)	0.0623 (9)	0.0123 (7)	0.0144 (7)	0.0046 (7)
C5	0.0487 (7)	0.0644 (9)	0.0541 (8)	0.0055 (6)	0.0166 (6)	−0.0045 (6)
C6	0.0375 (6)	0.0555 (7)	0.0446 (7)	−0.0005 (5)	0.0076 (5)	−0.0105 (6)
C7	0.0428 (7)	0.0661 (8)	0.0415 (7)	0.0028 (6)	0.0083 (5)	−0.0058 (6)
C8	0.0442 (7)	0.0645 (8)	0.0422 (7)	0.0074 (6)	0.0093 (5)	−0.0014 (6)
C9	0.0439 (7)	0.0519 (7)	0.0395 (6)	0.0012 (6)	0.0097 (5)	−0.0049 (5)
C10	0.0392 (6)	0.0437 (7)	0.0379 (6)	0.0010 (5)	0.0081 (5)	−0.0025 (5)
C11	0.0436 (7)	0.0430 (7)	0.0402 (6)	0.0021 (5)	0.0059 (5)	0.0008 (5)
C12	0.0513 (7)	0.0519 (7)	0.0413 (7)	0.0007 (6)	0.0158 (6)	0.0063 (5)
C13	0.0420 (6)	0.0506 (7)	0.0484 (7)	0.0031 (5)	0.0169 (5)	0.0025 (6)
C14	0.0428 (7)	0.0478 (7)	0.0475 (7)	0.0064 (5)	0.0131 (6)	0.0073 (5)
C15	0.0428 (7)	0.0467 (7)	0.0380 (6)	−0.0013 (5)	0.0115 (5)	0.0022 (5)
C16	0.0574 (8)	0.0705 (9)	0.0505 (8)	0.0117 (7)	0.0149 (6)	0.0197 (7)
C17	0.0695 (9)	0.0633 (9)	0.0503 (8)	0.0047 (7)	0.0117 (7)	0.0161 (6)
C18	0.0631 (9)	0.0874 (11)	0.0802 (10)	0.0323 (8)	0.0385 (8)	0.0277 (9)
O1	0.0515 (5)	0.0748 (6)	0.0479 (5)	0.0156 (5)	0.0209 (4)	0.0201 (4)
O2	0.0562 (6)	0.0661 (6)	0.0504 (5)	0.0162 (4)	0.0140 (4)	0.0177 (4)
O3	0.0564 (6)	0.0799 (7)	0.0647 (6)	0.0207 (5)	0.0328 (5)	0.0226 (5)
O4	0.0661 (7)	0.1169 (9)	0.0584 (6)	0.0289 (6)	0.0255 (5)	0.0239 (6)

Geometric parameters (Å, °)

C1—C6	1.3733 (18)	C11—C12	1.3556 (17)
C1—C2	1.3770 (19)	C12—C13	1.3797 (17)
C1—H1	0.9300	C12—H12	0.9300
C2—C3	1.365 (2)	C13—O3	1.3362 (14)
C2—H2	0.9300	C13—C14	1.3727 (17)
C3—C4	1.355 (2)	C14—C15	1.3682 (15)
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.3843 (19)	C15—O1	1.3554 (14)
C4—H4	0.9300	C16—O1	1.4172 (15)
C5—C6	1.3860 (18)	C16—H16A	0.9600
C5—H5	0.9300	C16—H16B	0.9600
C6—C7	1.4954 (18)	C16—H16C	0.9600
C7—O4	1.2153 (16)	C17—O2	1.4044 (15)

C7—C8	1.4431 (17)	C17—H17A	0.9600
C8—C9	1.3305 (17)	C17—H17B	0.9600
C8—H8	0.9300	C17—H17C	0.9600
C9—C10	1.4292 (16)	C18—O3	1.4232 (16)
C9—H9	0.9300	C18—H18A	0.9600
C10—C11	1.4014 (16)	C18—H18B	0.9600
C10—C15	1.4051 (16)	C18—H18C	0.9600
C11—O2	1.3594 (14)		
C6—C1—C2	120.67 (13)	C11—C12—C13	119.83 (11)
C6—C1—H1	119.7	C11—C12—H12	120.1
C2—C1—H1	119.7	C13—C12—H12	120.1
C3—C2—C1	120.96 (13)	O3—C13—C14	123.49 (11)
C3—C2—H2	119.5	O3—C13—C12	115.14 (11)
C1—C2—H2	119.5	C14—C13—C12	121.36 (11)
C4—C3—C2	119.55 (14)	C15—C14—C13	118.08 (11)
C4—C3—H3	120.2	C15—C14—H14	121.0
C2—C3—H3	120.2	C13—C14—H14	121.0
C3—C4—C5	119.89 (14)	O1—C15—C14	121.34 (11)
C3—C4—H4	120.1	O1—C15—C10	115.78 (10)
C5—C4—H4	120.1	C14—C15—C10	122.88 (10)
C4—C5—C6	121.29 (12)	O1—C16—H16A	109.5
C4—C5—H5	119.4	O1—C16—H16B	109.5
C6—C5—H5	119.4	H16A—C16—H16B	109.5
C1—C6—C5	117.61 (12)	O1—C16—H16C	109.5
C1—C6—C7	118.63 (12)	H16A—C16—H16C	109.5
C5—C6—C7	123.73 (11)	H16B—C16—H16C	109.5
O4—C7—C8	121.57 (12)	O2—C17—H17A	109.5
O4—C7—C6	119.54 (12)	O2—C17—H17B	109.5
C8—C7—C6	118.80 (11)	H17A—C17—H17B	109.5
C9—C8—C7	121.57 (12)	O2—C17—H17C	109.5
C9—C8—H8	119.2	H17A—C17—H17C	109.5
C7—C8—H8	119.2	H17B—C17—H17C	109.5
C8—C9—C10	130.82 (12)	O3—C18—H18A	109.5
C8—C9—H9	114.6	O3—C18—H18B	109.5
C10—C9—H9	114.6	H18A—C18—H18B	109.5
C11—C10—C15	116.18 (10)	O3—C18—H18C	109.5
C11—C10—C9	124.32 (11)	H18A—C18—H18C	109.5
C15—C10—C9	119.49 (10)	H18B—C18—H18C	109.5
O2—C11—C12	122.44 (11)	C15—O1—C16	119.06 (9)
O2—C11—C10	115.92 (10)	C11—O2—C17	119.14 (10)
C12—C11—C10	121.64 (11)	C13—O3—C18	118.25 (10)

Fig. 1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C16
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C18