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

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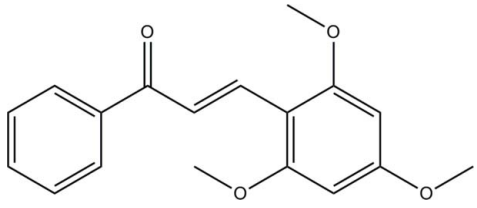
Key indicators: single-crystal X-ray study; $T$ = 273 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.039; $wR$ factor = 0.132; data-to-parameter ratio = 13.3.

In the title compound, $C_{18}H_{18}O_4$, a derivative of biologically active chalcones, the dihedral angle between the two rings is 7.43 (7)°. The molecule adopts an *E* configuration about the central olefinic bonds. In the crystal, there are no strong interactions between the molecules.

## Related literature

For related structures, see: Subbiah Pandi *et al.* (2003); Low *et al.* (2002); Yathirajan *et al.* (2006); Suwunwong *et al.* (2009); Jasinski *et al.* (2009). For background to and applications of chalcones, see: Dimmock *et al.* (1999); Sivakumar *et al.* (2009); Echeverria *et al.* (2009); Kontogiorgis *et al.* (2008); Dominguez *et al.* (2005); Nowakowska (2007).



## Experimental

### Crystal data

$C_{18}H_{18}O_4$
$M_r$ = 298.32
Monoclinic, $P2_1/c$
$a$ = 9.0052 (10) Å
$b$ = 14.9245 (17) Å
$c$ = 11.7658 (14) Å
$\beta$ = 104.315 (2)°
$V$ = 1532.2 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 273 K
0.12 × 0.10 × 0.05 mm

### Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min}$ = 0.989, $T_{max}$ = 0.996
7895 measured reflections
2701 independent reflections
2125 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.044

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.132
$S$ = 1.00
2701 reflections
203 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.16 e Å$^{-3}$

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2350).

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# supporting information

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

**Jianzhang Wu, Li Zhang, Jing Wang, Shulin Yang and Xiaokun Li**

### S1. Comment

Chalcones, which have the common skeleton of 1,3-diaryl-2-propen-1-ones, are natural products, distributed widely in fruits, vegetables etc. Natural and synthetical chalcones have wide-ranging biological properties, including antimicrobial, antifungal, antioxidant, antiangiogenic, antitumor and anti-inflammatory activities (Dimmock *et al.*, 1999; Sivakumar *et al.*, 2009; Echeverria *et al.*, 2009; Kontogiorgis *et al.*, 2008). The chalcone derivatives with trimethoxyphenyl substitution have also been reported to have a wide range of biological activities (Suwunwong *et al.*, 2009; Jasinski *et al.*, 2009; Dominguez *et al.*, 2005; Nowakowska, 2007).

The present investigation is a continuation of our broad program of work on the synthesis and structural study of chalcones and their derivatives. Investigation of these structures may be helpful in the design and synthesis of new compounds. In order to understand the geometrical features and the underlying intermolecular interactions which hold the assembly of molecules in the crystal structure, an X-ray study of the title compound was carried out.

It is approximately planar and the dihedral angle between the two rings is 7.43 (7)°. The H atoms of the central propenone group are *trans*. The average value of the bond distances [1.385 (5) Å] and exocyclic bond angles [120.7 (4)°] in the benzene and phenyl rings have normal values which agree quite well with the values reported in the literature for some analogous structures (Subbiah Pandi *et al.*, 2003; Low *et al.*, 2002; Yathirajan *et al.*, 2006).

### S2. Experimental

Acetophenone (15 mmol) was dissolved in ethanol (5 ml) and crushed KOH (15 mmol) was added. The flask was immersed in a bath of crushed ice and a solution of 2,4,6-trimethoxybenzaldehyde (15 mmol) in ethanol (5 mmol) was added. The reaction mixture was stirred at 300 K and completion of the reaction was monitored by thin-layer chromatography. Ice-cold water was added to the reaction mixture after 48 h and the yellow solid that separated was filtered off, washed with water and cold ethanol, dried and purified by column chromatography on silica gel (yield:68%). Single crystals of the title compound were grown in a $CH_2Cl_2$/$CH_3OH$ mixture (5:2 *v*/*v*) by slow evaporation (mp 436–437 K).

### S3. Refinement

The H atoms were positioned geometrically (C—H = 0.93 and 0.96 Å) and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(methyl C).

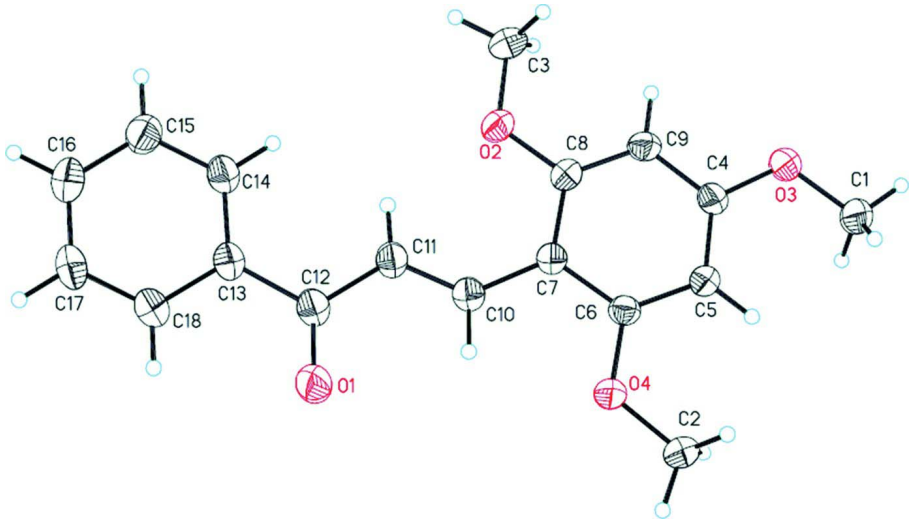


**Figure 1**

The molecular structure of the title compound, showing 30% displacement ellipsoids for the non-hydrogen atoms. Hydrogen atoms are drawn as spheres of arbitrary radius.

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

*Crystal data*

$C_{18}H_{18}O_4$
$M_r = 298.32$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.0052\ (10)$ Å
$b = 14.9245\ (17)$ Å
$c = 11.7658\ (14)$ Å
$\beta = 104.315\ (2)°$
$V = 1532.2\ (3)$ Å$^3$
$Z = 4$
$F(000) = 632$
$D_x = 1.293$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3499 reflections
$\theta = 2.7–27.9°$
$\mu = 0.09$ mm$^{-1}$
$T = 273$ K
Block, colorless
0.12 × 0.10 × 0.05 mm

*Data collection*

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.989$, $T_{max} = 0.996$
7895 measured reflections
2701 independent reflections
2125 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.3°$
$h = -10\rightarrow10$
$k = -17\rightarrow15$
$l = -13\rightarrow13$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.132$
$S = 1.00$
2701 reflections
203 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0938P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.15$ e Å$^{-3}$
$\Delta\rho_{min} = -0.16$ e Å$^{-3}$
Extinction correction: *SHELXL*, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.353 (18)

*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 | 0.9745 (2) | −0.05689 (12) | 0.14050 (16) | 0.0745 (5) |
| H1A | 1.0183 | −0.0376 | 0.2196 | 0.112* |
| H1B | 1.0548 | −0.0662 | 0.1012 | 0.112* |
| H1C | 0.9196 | −0.1119 | 0.1415 | 0.112* |
| C2 | 0.65289 (18) | −0.07567 (10) | 0.42207 (13) | 0.0599 (4) |
| H2A | 0.6579 | −0.1285 | 0.3765 | 0.090* |
| H2B | 0.6153 | −0.0913 | 0.4890 | 0.090* |
| H2C | 0.7534 | −0.0500 | 0.4479 | 0.090* |
| C3 | 0.44257 (19) | 0.21153 (10) | −0.08152 (13) | 0.0619 (4) |
| H3A | 0.5373 | 0.2441 | −0.0605 | 0.093* |
| H3B | 0.3608 | 0.2517 | −0.1166 | 0.093* |
| H3C | 0.4499 | 0.1652 | −0.1364 | 0.093* |
| C4 | 0.74716 (15) | 0.02951 (9) | 0.11985 (12) | 0.0466 (4) |
| C5 | 0.72022 (14) | −0.00525 (9) | 0.22193 (11) | 0.0462 (4) |
| H5 | 0.7898 | −0.0443 | 0.2687 | 0.055* |
| C6 | 0.58735 (14) | 0.01944 (9) | 0.25291 (11) | 0.0424 (4) |
| C7 | 0.47895 (14) | 0.07868 (8) | 0.18520 (11) | 0.0407 (4) |
| C8 | 0.51526 (15) | 0.11331 (9) | 0.08332 (11) | 0.0437 (4) |
| C9 | 0.64562 (16) | 0.08890 (9) | 0.05100 (12) | 0.0483 (4) |
| H9 | 0.6658 | 0.1122 | −0.0170 | 0.058* |
| C10 | 0.34214 (15) | 0.10052 (9) | 0.22290 (12) | 0.0456 (4) |
| H10 | 0.3369 | 0.0743 | 0.2935 | 0.055* |
| C11 | 0.22244 (15) | 0.15177 (10) | 0.17373 (12) | 0.0509 (4) |
| H11 | 0.2175 | 0.1775 | 0.1009 | 0.061* |
| C12 | 0.09861 (15) | 0.16858 (10) | 0.23113 (12) | 0.0512 (4) |
| C13 | −0.02269 (14) | 0.23528 (9) | 0.17775 (12) | 0.0469 (4) |
| C14 | −0.01819 (17) | 0.28712 (10) | 0.08031 (13) | 0.0557 (4) |
| H14 | 0.0600 | 0.2784 | 0.0426 | 0.067* |
| C15 | −0.12880 (19) | 0.35148 (11) | 0.03909 (15) | 0.0658 (5) |
| H15 | −0.1239 | 0.3863 | −0.0255 | 0.079* |
| C16 | −0.24600 (18) | 0.36410 (12) | 0.09338 (15) | 0.0665 (5) |

| | | | | |
|---|---|---|---|---|
| H16 | −0.3197 | 0.4079 | 0.0661 | 0.080* |
| C17 | −0.25405 (17) | 0.31221 (12) | 0.18758 (15) | 0.0650 (5) |
| H17 | −0.3346 | 0.3200 | 0.2232 | 0.078* |
| C18 | −0.14374 (16) | 0.24862 (11) | 0.22991 (13) | 0.0568 (4) |
| H18 | −0.1501 | 0.2141 | 0.2943 | 0.068* |
| O1 | 0.09525 (13) | 0.13297 (9) | 0.32420 (10) | 0.0788 (4) |
| O2 | 0.41260 (11) | 0.17261 (7) | 0.02032 (8) | 0.0580 (3) |
| O3 | 0.87208 (11) | 0.01000 (7) | 0.08015 (9) | 0.0645 (4) |
| O4 | 0.55259 (11) | −0.01253 (7) | 0.35229 (9) | 0.0568 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0661 (10) | 0.0857 (12) | 0.0833 (11) | 0.0327 (9) | 0.0404 (9) | 0.0290 (10) |
| C2 | 0.0601 (9) | 0.0681 (10) | 0.0523 (9) | 0.0107 (8) | 0.0156 (7) | 0.0195 (7) |
| C3 | 0.0716 (10) | 0.0603 (10) | 0.0518 (9) | 0.0047 (8) | 0.0115 (8) | 0.0158 (7) |
| C4 | 0.0438 (7) | 0.0485 (8) | 0.0512 (8) | 0.0025 (6) | 0.0186 (6) | 0.0020 (6) |
| C5 | 0.0450 (8) | 0.0464 (8) | 0.0483 (8) | 0.0063 (6) | 0.0137 (6) | 0.0071 (6) |
| C6 | 0.0441 (7) | 0.0449 (7) | 0.0390 (7) | −0.0012 (6) | 0.0119 (6) | 0.0025 (6) |
| C7 | 0.0407 (7) | 0.0426 (7) | 0.0384 (7) | 0.0006 (5) | 0.0088 (5) | −0.0029 (5) |
| C8 | 0.0455 (8) | 0.0414 (7) | 0.0421 (7) | 0.0021 (6) | 0.0067 (6) | 0.0006 (6) |
| C9 | 0.0540 (8) | 0.0510 (8) | 0.0423 (8) | 0.0014 (6) | 0.0164 (6) | 0.0065 (6) |
| C10 | 0.0455 (8) | 0.0499 (8) | 0.0409 (7) | 0.0007 (6) | 0.0097 (6) | −0.0048 (6) |
| C11 | 0.0463 (8) | 0.0626 (9) | 0.0430 (8) | 0.0072 (6) | 0.0097 (6) | −0.0019 (6) |
| C12 | 0.0445 (8) | 0.0646 (9) | 0.0433 (8) | 0.0024 (7) | 0.0086 (6) | −0.0059 (7) |
| C13 | 0.0392 (7) | 0.0536 (8) | 0.0460 (8) | −0.0003 (6) | 0.0071 (6) | −0.0107 (6) |
| C14 | 0.0504 (8) | 0.0632 (9) | 0.0559 (9) | 0.0055 (7) | 0.0174 (7) | −0.0042 (7) |
| C15 | 0.0666 (10) | 0.0660 (10) | 0.0647 (10) | 0.0118 (8) | 0.0159 (8) | 0.0051 (8) |
| C16 | 0.0532 (9) | 0.0684 (11) | 0.0751 (11) | 0.0148 (8) | 0.0107 (8) | −0.0029 (9) |
| C17 | 0.0444 (8) | 0.0741 (11) | 0.0801 (12) | 0.0072 (7) | 0.0221 (8) | −0.0086 (9) |
| C18 | 0.0496 (8) | 0.0657 (9) | 0.0580 (9) | −0.0010 (7) | 0.0188 (7) | −0.0053 (7) |
| O1 | 0.0688 (8) | 0.1132 (10) | 0.0602 (7) | 0.0294 (7) | 0.0272 (6) | 0.0240 (7) |
| O2 | 0.0577 (6) | 0.0647 (7) | 0.0522 (6) | 0.0165 (5) | 0.0150 (5) | 0.0177 (5) |
| O3 | 0.0587 (7) | 0.0769 (8) | 0.0675 (7) | 0.0206 (5) | 0.0340 (6) | 0.0224 (5) |
| O4 | 0.0533 (6) | 0.0719 (7) | 0.0500 (6) | 0.0154 (5) | 0.0216 (5) | 0.0200 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—O3 | 1.4241 (17) | C8—O2 | 1.3596 (15) |
| C1—H1A | 0.9600 | C8—C9 | 1.3697 (19) |
| C1—H1B | 0.9600 | C9—H9 | 0.9300 |
| C1—H1C | 0.9600 | C10—C11 | 1.3317 (19) |
| C2—O4 | 1.4182 (16) | C10—H10 | 0.9300 |
| C2—H2A | 0.9600 | C11—C12 | 1.4611 (19) |
| C2—H2B | 0.9600 | C11—H11 | 0.9300 |
| C2—H2C | 0.9600 | C12—O1 | 1.2244 (17) |
| C3—O2 | 1.4163 (17) | C12—C13 | 1.496 (2) |
| C3—H3A | 0.9600 | C13—C18 | 1.391 (2) |

| | | | |
|---|---|---|---|
| C3—H3B | 0.9600 | C13—C14 | 1.392 (2) |
| C3—H3C | 0.9600 | C14—C15 | 1.382 (2) |
| C4—O3 | 1.3521 (16) | C14—H14 | 0.9300 |
| C4—C9 | 1.3827 (19) | C15—C16 | 1.375 (2) |
| C4—C5 | 1.3836 (19) | C15—H15 | 0.9300 |
| C5—C6 | 1.3842 (17) | C16—C17 | 1.369 (2) |
| C5—H5 | 0.9300 | C16—H16 | 0.9300 |
| C6—O4 | 1.3688 (15) | C17—C18 | 1.375 (2) |
| C6—C7 | 1.4088 (18) | C17—H17 | 0.9300 |
| C7—C8 | 1.4158 (18) | C18—H18 | 0.9300 |
| C7—C10 | 1.4461 (18) | | |

| | | | |
|---|---|---|---|
| O3—C1—H1A | 109.5 | C8—C9—C4 | 119.73 (12) |
| O3—C1—H1B | 109.5 | C8—C9—H9 | 120.1 |
| H1A—C1—H1B | 109.5 | C4—C9—H9 | 120.1 |
| O3—C1—H1C | 109.5 | C11—C10—C7 | 130.97 (13) |
| H1A—C1—H1C | 109.5 | C11—C10—H10 | 114.5 |
| H1B—C1—H1C | 109.5 | C7—C10—H10 | 114.5 |
| O4—C2—H2A | 109.5 | C10—C11—C12 | 121.74 (13) |
| O4—C2—H2B | 109.5 | C10—C11—H11 | 119.1 |
| H2A—C2—H2B | 109.5 | C12—C11—H11 | 119.1 |
| O4—C2—H2C | 109.5 | O1—C12—C11 | 121.96 (13) |
| H2A—C2—H2C | 109.5 | O1—C12—C13 | 119.16 (13) |
| H2B—C2—H2C | 109.5 | C11—C12—C13 | 118.79 (13) |
| O2—C3—H3A | 109.5 | C18—C13—C14 | 117.99 (13) |
| O2—C3—H3B | 109.5 | C18—C13—C12 | 118.71 (13) |
| H3A—C3—H3B | 109.5 | C14—C13—C12 | 123.26 (12) |
| O2—C3—H3C | 109.5 | C15—C14—C13 | 120.66 (14) |
| H3A—C3—H3C | 109.5 | C15—C14—H14 | 119.7 |
| H3B—C3—H3C | 109.5 | C13—C14—H14 | 119.7 |
| O3—C4—C9 | 114.95 (12) | C14—C15—C16 | 120.09 (16) |
| O3—C4—C5 | 123.95 (12) | C14—C15—H15 | 120.0 |
| C9—C4—C5 | 121.09 (12) | C16—C15—H15 | 120.0 |
| C6—C5—C4 | 118.50 (12) | C15—C16—C17 | 119.95 (15) |
| C6—C5—H5 | 120.7 | C15—C16—H16 | 120.0 |
| C4—C5—H5 | 120.7 | C17—C16—H16 | 120.0 |
| O4—C6—C5 | 121.82 (11) | C16—C17—C18 | 120.38 (14) |
| O4—C6—C7 | 115.41 (11) | C16—C17—H17 | 119.8 |
| C5—C6—C7 | 122.77 (11) | C18—C17—H17 | 119.8 |
| C6—C7—C8 | 115.79 (11) | C13—C18—C17 | 120.91 (15) |
| C6—C7—C10 | 119.45 (11) | C13—C18—H18 | 119.6 |
| C8—C7—C10 | 124.75 (12) | C17—C18—H18 | 119.5 |
| O2—C8—C9 | 122.39 (12) | C8—O2—C3 | 118.82 (11) |
| O2—C8—C7 | 115.53 (11) | C4—O3—C1 | 118.07 (11) |
| C9—C8—C7 | 122.08 (12) | C6—O4—C2 | 118.61 (10) |