Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 1-(4-Methoxyphenyl)-5-phenylpenta-2,4-dien-1-one

**Andreas Fischer,[a]* H. S. Yathirajan,[b] B. K. Sarojini,[c] S. Bindya[b] and B. Narayana[d]**

[a]Inorganic Chemistry, School of Chemical Science and Engineering, Royal Institute of Technology (KTH), 100 44 Stockholm, Sweden, [b]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, [c]Department of Chemistry, P. A. College of Engineering, Nadupadavu, Mangalore 574 153, India, and [d]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, India
Correspondence e-mail: afischer@kth.se

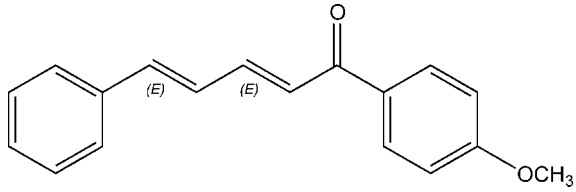
Received 28 March 2007; accepted 9 July 2007

Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.062; $wR$ factor = 0.143; data-to-parameter ratio = 14.5.

The title compound, $C_{18}H_{16}O_2$, was prepared using literature procedures and crystallized from an acetone–toluene solution (50:50 *v*/*v*). The dihedral angle between the two aromatic rings is 9.28 (8) Å. The crystal packing is stabilized by van der Waals forces.

## Related literature

For related literature, see: Butcher *et al.* (2006); Cho *et al.* (1996); Fichou *et al.* (1988); Furniss *et al.* (1989); Goto *et al.* (1991); Harrison *et al.* (2006); Indira *et al.* (2002); Sarojini *et al.* (2006); Tam *et al.* (1989); Uchida *et al.* (1998); Yathirajan *et al.* (2007).




## Experimental

### Crystal data

$C_{18}H_{16}O_2$
$M_r$ = 264.32
Monoclinic, $P2_1/c$
$a$ = 29.017 (7) Å
$b$ = 5.8088 (14) Å
$c$ = 8.4868 (10) Å
$\beta$ = 93.308 (16)°
$V$ = 1428.1 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 298 K
0.35 × 0.30 × 0.28 mm

### Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: none
13388 measured reflections
2633 independent reflections
1558 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.114

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.143
$S$ = 1.12
2633 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.11 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2007).

BKS thanks the AICTE, Government of India, for financial assistance through the Career Award for Young Teachers Scheme. SB thanks the University of Mysore for research facilities. The Swedish Research Council (VR) is acknowledged for providing funding for the single-crystal diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PR2008).

## References

Brandenburg, K. (2006). *DIAMOND*. Release 3.1d. Crystal Impact GbR, Bonn, Germany.
Butcher, R. J., Yathirajan, H. S., Sarojini, B. K., Narayana, B. & Vijaya Raj, K. K. (2006). *Acta Cryst.* E**62**, o1973–o1975.
Cho, B. R., Je, J. T., Kim, H. S., Jean, S. J., Song, O. K. & Wang, C. H. (1996). *Bull. Korean Chem. Soc.* **17**, 693–695.
Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.
Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.
Fichou, D., Watanabe, T., Takeda, T., Miyata, S., Goto, Y. & Nakayama, M. (1988). *Jpn. J. Appl. Phys.* **27**, 429–430.
Furniss, B. S., Hannaford, A. J., Smith, P. W. G. & Tatchell, A. R. (1989). Editors. *Vogel's Textbook of Practical Organic Chemistry*, 5th ed. London: Longman Group UK Ltd.
Goto, Y., Hayashi, A., Kimura, Y. & Nakayama, M. (1991). *J. Cryst. Growth*, **108**, 688–698.
Harrison, W. T. A., Sarojini, B. K., Vijaya Raj, K. K., Yathirajan, H. S. & Narayana, B. (2006). *Acta Cryst.* E**62**, o1522–o1523.
Indira, J., Karat, P. P. & Sarojini, B. K. (2002). *J. Cryst. Growth*, **242**, 209–214.
Nonius (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.
Sarojini, B. K., Narayana, B., Ashalatha, B. V., Indira, J. & Lobo, K. J. (2006). *J. Cryst. Growth*, **295**, 54–59.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tam, W., Guerin, B., Calabrese, J. C. & Stevenson, S. H. (1989). *Chem. Phys. Lett.* **154**, 93–96.
Uchida, T., Kozawa, K., Sakai, T., Aoki, M., Yoguchi, H., Abduryim, A. & Watanabe, Y. (1998). *Mol. Cryst. Liq. Cryst.* **315**, 135–140.
Westrip (2007). *publCIF*. In preparation.
Yathirajan, H. S., Bindya, S., Mithun, A., Narayana, B. & Bolte, M. (2007). *Acta Cryst.* E**63**, o61–o62.

  doi:10.1107/S1600536807033491 

# supplementary materials

*Acta Cryst.* (2007). E**63**, o3540 [ **doi:10.1107/S1600536807033491** ]

# 1-(4-Methoxyphenyl)-5-phenylpenta-2,4-dien-1-one

**A. Fischer, H. S. Yathirajan, B. K. Sarojini, S. Bindya and B. Narayana**

## Comment

The title compound, (I), is a optically active molecule. The present-day demand is for large, high quality ferroelectric and 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 nonlinear optical (NLO) crystals. The NLO effect in organic molecules originates from a strong donor–acceptor intermolecular interaction, a delocalized π-electron system, and also the ability to crystallize in noncentrosymmetric space groups. 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 hyperpolarizability is strongly influenced not only by the electronic effect but also by the steric effect of the substituent (Cho *et al.*, 1996). Among several organic compounds reported for NLO properties, chalcone derivatives are notable materials for their excellent blue light transmittance and good crystallizability. They provide a necessary configuration to show an NLO property 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, Sarojini *et al.*, 2006). The crystal structures of 1,5-bis(4-chlorophenyl)penta-1,4-dien-3-one (Butcher *et al.*, 2006), 5-phenyl-1-(2-thienyl)penta-2,4-dien-1-one (Yathirajan *et al*., 2007), and 1,5-bis(4-methoxyphenyl)penta-1,4-dien-3-one (Harrison *et al.*, 2006) have been reported. This paper reports crystal structure of the title compound. Fig 1 shows the molecular structure. The geometry of the molecule is unexceptional. The dihedral angle between the two phenyl groups is 9.28 (9)\%. The crystal packing is stabilized by van der Waals forces.

## Experimental

The title compound is synthesized according to the method reported in the literature (Furniss *et al.*, 1989) with a yield of 75–80%. The compound was purified by recrystallization from ethanol. The crystal grew by slow evaporation from an acetone:toluene solution (50:50). Analysis for $C_{18}H_{16}O_2$: Found (Calculated): C: 81.50 (81.79); H: 6.01(6.10).

## Refinement

H atoms were placed at calculated positions and refined using a riding model on the respective carrier atoms.

## Figures

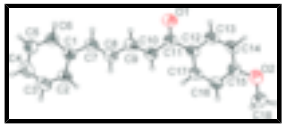


Fig. 1. The molecular structure of (I). Thermal ellipsoids at the 50% probability level.

### 1-(4-Methoxyphenyl)-5-phenylpenta-2,4-dien-1-one

*Crystal data*

| | |
|---|---|
| $C_{18}H_{16}O_2$ | $F_{000}$ = 560 |
| $M_r$ = 264.32 | $D_x$ = 1.229 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 23 reflections |
| $a$ = 29.017 (7) Å | θ = 7.9–16.8º |
| $b$ = 5.8088 (14) Å | μ = 0.08 mm$^{-1}$ |
| $c$ = 8.4868 (10) Å | $T$ = 298 K |
| β = 93.308 (16)º | Block, colourless |
| $V$ = 1428.1 (5) Å$^3$ | 0.35 × 0.30 × 0.28 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Nonius KappaCCD area-detector diffractometer | $R_{int}$ = 0.114 |
| Radiation source: fine-focus sealed tube | $\theta_{max}$ = 25.5º |
| ω scans | $\theta_{min}$ = 4.5º |
| Absorption correction: none | $h$ = −35→35 |
| 13388 measured reflections | $k$ = −6→6 |
| 2633 independent reflections | $l$ = −10→10 |
| 1558 reflections with $I > 2\sigma(I)$ | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.062 | $w = 1/[\sigma^2(F_o^2) + (0.0295P)^2 + 0.4375P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.143 | $(\Delta/\sigma)_{max} < 0.001$ |
| $S$ = 1.12 | $\Delta\rho_{max}$ = 0.11 e Å$^{-3}$ |
| 2633 reflections | $\Delta\rho_{min}$ = −0.14 e Å$^{-3}$ |
| 181 parameters | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*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 $F^2 > 2\text{sigma}(F^2)$ 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 | 0.38172 (9) | 0.0845 (4) | −0.2302 (3) | 0.0578 (6) |
| C2 | 0.36674 (9) | −0.1304 (4) | −0.2890 (3) | 0.0646 (7) |
| C3 | 0.39574 (11) | −0.2695 (5) | −0.3692 (3) | 0.0749 (8) |
| C4 | 0.43995 (12) | −0.2026 (5) | −0.3913 (3) | 0.0838 (9) |
| C5 | 0.45590 (10) | 0.0061 (5) | −0.3321 (3) | 0.0819 (8) |
| C6 | 0.42687 (10) | 0.1465 (5) | −0.2519 (3) | 0.0712 (7) |
| C7 | 0.35161 (9) | 0.2417 (4) | −0.1507 (3) | 0.0647 (7) |
| C8 | 0.31018 (9) | 0.2028 (4) | −0.0991 (3) | 0.0642 (7) |
| C9 | 0.28328 (9) | 0.3786 (4) | −0.0280 (3) | 0.0674 (7) |
| C10 | 0.24440 (9) | 0.3508 (4) | 0.0427 (3) | 0.0684 (7) |
| C11 | 0.22146 (9) | 0.5437 (4) | 0.1185 (3) | 0.0634 (7) |
| C12 | 0.17642 (8) | 0.5074 (4) | 0.1882 (3) | 0.0570 (6) |
| C13 | 0.15943 (9) | 0.6766 (4) | 0.2867 (3) | 0.0664 (7) |
| C14 | 0.11768 (9) | 0.6524 (4) | 0.3513 (3) | 0.0688 (7) |
| C15 | 0.09115 (9) | 0.4579 (4) | 0.3199 (3) | 0.0631 (7) |
| C16 | 0.10710 (9) | 0.2878 (4) | 0.2227 (3) | 0.0697 (7) |
| C17 | 0.14966 (9) | 0.3132 (4) | 0.1591 (3) | 0.0677 (7) |
| C18 | 0.02246 (11) | 0.2487 (6) | 0.3656 (4) | 0.0971 (10) |
| O1 | 0.23951 (7) | 0.7363 (3) | 0.1259 (3) | 0.0929 (7) |
| O2 | 0.04997 (6) | 0.4496 (3) | 0.3901 (2) | 0.0784 (6) |
| H2 | 0.3369 | −0.1794 | −0.2736 | 0.078* |
| H3 | 0.3852 | −0.4108 | −0.4089 | 0.090* |
| H4 | 0.4592 | −0.2977 | −0.4462 | 0.101* |
| H5 | 0.4860 | 0.0518 | −0.3461 | 0.098* |
| H6 | 0.4379 | 0.2865 | −0.2114 | 0.085* |
| H7 | 0.3630 | 0.3902 | −0.1337 | 0.078* |
| H8 | 0.2979 | 0.0548 | −0.1094 | 0.077* |
| H9 | 0.2945 | 0.5288 | −0.0322 | 0.081* |
| H10 | 0.2311 | 0.2046 | 0.0445 | 0.082* |
| H13 | 0.1768 | 0.8086 | 0.3088 | 0.080* |
| H14 | 0.1071 | 0.7674 | 0.4168 | 0.083* |
| H16 | 0.0894 | 0.1570 | 0.2001 | 0.084* |
| H17 | 0.1605 | 0.1967 | 0.0954 | 0.081* |
| H18A | 0.0156 | 0.2276 | 0.2547 | 0.146* |
| H18B | −0.0057 | 0.2664 | 0.4184 | 0.146* |
| H18C | 0.0389 | 0.1163 | 0.4073 | 0.146* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0763 (17) | 0.0467 (15) | 0.0503 (13) | 0.0012 (13) | 0.0038 (12) | 0.0023 (12) |
| C2 | 0.0840 (18) | 0.0550 (16) | 0.0548 (14) | −0.0046 (14) | 0.0018 (13) | 0.0003 (13) |
| C3 | 0.111 (2) | 0.0544 (17) | 0.0593 (16) | −0.0032 (17) | 0.0069 (16) | −0.0036 (13) |
| C4 | 0.108 (3) | 0.072 (2) | 0.0723 (19) | 0.0150 (18) | 0.0178 (17) | −0.0006 (16) |
| C5 | 0.080 (2) | 0.076 (2) | 0.090 (2) | 0.0022 (17) | 0.0174 (16) | 0.0018 (18) |
| C6 | 0.083 (2) | 0.0578 (17) | 0.0732 (17) | −0.0076 (15) | 0.0098 (15) | −0.0011 (14) |
| C7 | 0.0801 (19) | 0.0522 (15) | 0.0618 (15) | −0.0038 (14) | 0.0041 (14) | −0.0027 (13) |
| C8 | 0.0757 (19) | 0.0502 (15) | 0.0662 (16) | −0.0014 (14) | −0.0015 (14) | −0.0042 (12) |
| C9 | 0.0787 (19) | 0.0543 (16) | 0.0687 (16) | 0.0011 (14) | −0.0009 (14) | −0.0021 (14) |
| C10 | 0.0698 (18) | 0.0538 (16) | 0.0814 (18) | −0.0005 (13) | 0.0013 (15) | −0.0091 (14) |
| C11 | 0.0692 (17) | 0.0502 (16) | 0.0696 (16) | 0.0000 (13) | −0.0063 (13) | −0.0030 (13) |
| C12 | 0.0656 (16) | 0.0454 (14) | 0.0589 (14) | 0.0050 (12) | −0.0059 (12) | −0.0014 (12) |
| C13 | 0.0731 (19) | 0.0469 (15) | 0.0782 (17) | 0.0020 (13) | −0.0045 (15) | −0.0080 (13) |
| C14 | 0.0793 (19) | 0.0512 (16) | 0.0753 (17) | 0.0108 (14) | −0.0008 (15) | −0.0112 (13) |
| C15 | 0.0666 (17) | 0.0588 (16) | 0.0634 (15) | 0.0092 (14) | −0.0017 (13) | 0.0016 (14) |
| C16 | 0.0761 (19) | 0.0540 (16) | 0.0786 (18) | −0.0076 (14) | −0.0002 (15) | −0.0122 (14) |
| C17 | 0.0776 (19) | 0.0542 (16) | 0.0711 (17) | 0.0006 (14) | 0.0037 (14) | −0.0126 (13) |
| C18 | 0.083 (2) | 0.092 (2) | 0.118 (3) | −0.0125 (19) | 0.0188 (19) | −0.008 (2) |
| O1 | 0.0942 (15) | 0.0578 (12) | 0.1283 (18) | −0.0129 (11) | 0.0214 (12) | −0.0151 (12) |
| O2 | 0.0736 (12) | 0.0743 (13) | 0.0878 (13) | 0.0044 (10) | 0.0081 (10) | −0.0039 (10) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.385 (3) | C16—C17 | 1.387 (3) |
| C1—C2 | 1.401 (3) | C18—O2 | 1.420 (3) |
| C1—C7 | 1.455 (3) | C2—H2 | 0.9300 |
| C2—C3 | 1.374 (3) | C3—H3 | 0.9300 |
| C3—C4 | 1.367 (4) | C4—H4 | 0.9300 |
| C4—C5 | 1.379 (4) | C5—H5 | 0.9300 |
| C5—C6 | 1.379 (4) | C6—H6 | 0.9300 |
| C7—C8 | 1.325 (3) | C7—H7 | 0.9300 |
| C8—C9 | 1.437 (3) | C8—H8 | 0.9300 |
| C9—C10 | 1.320 (3) | C9—H9 | 0.9300 |
| C10—C11 | 1.467 (3) | C10—H10 | 0.9300 |
| C11—O1 | 1.232 (3) | C13—H13 | 0.9300 |
| C11—C12 | 1.483 (3) | C14—H14 | 0.9300 |
| C12—C17 | 1.382 (3) | C16—H16 | 0.9300 |
| C12—C13 | 1.395 (3) | C17—H17 | 0.9300 |
| C13—C14 | 1.368 (3) | C18—H18A | 0.9600 |
| C14—C15 | 1.383 (3) | C18—H18B | 0.9600 |
| C15—O2 | 1.369 (3) | C18—H18C | 0.9600 |
| C15—C16 | 1.384 (3) | | |
| C6—C1—C2 | 117.5 (2) | C2—C3—H3 | 119.6 |
| C6—C1—C7 | 120.0 (2) | C3—C4—H4 | 120.0 |

| | | | |
|---|---|---|---|
| C2—C1—C7 | 122.7 (2) | C5—C4—H4 | 120.0 |
| C3—C2—C1 | 120.6 (3) | C6—C5—H5 | 120.2 |
| C4—C3—C2 | 120.7 (3) | C4—C5—H5 | 120.2 |
| C3—C4—C5 | 119.9 (3) | C5—C6—H6 | 119.2 |
| C6—C5—C4 | 119.5 (3) | C1—C6—H6 | 119.2 |
| C5—C6—C1 | 121.7 (3) | C8—C7—H7 | 115.5 |
| C8—C7—C1 | 129.1 (2) | C1—C7—H7 | 115.5 |
| C7—C8—C9 | 123.1 (2) | C7—C8—H8 | 118.5 |
| C10—C9—C8 | 127.3 (2) | C9—C8—H8 | 118.5 |
| C9—C10—C11 | 121.9 (2) | C10—C9—H9 | 116.4 |
| O1—C11—C10 | 120.5 (2) | C8—C9—H9 | 116.4 |
| O1—C11—C12 | 119.5 (2) | C9—C10—H10 | 119.0 |
| C10—C11—C12 | 120.1 (2) | C11—C10—H10 | 119.0 |
| C17—C12—C13 | 117.8 (2) | C14—C13—H13 | 119.3 |
| C17—C12—C11 | 123.1 (2) | C12—C13—H13 | 119.3 |
| C13—C12—C11 | 119.3 (2) | C13—C14—H14 | 119.8 |
| C14—C13—C12 | 121.4 (2) | C15—C14—H14 | 119.8 |
| C13—C14—C15 | 120.3 (2) | C15—C16—H16 | 120.2 |
| O2—C15—C16 | 124.5 (2) | C17—C16—H16 | 120.2 |
| O2—C15—C14 | 115.9 (2) | C12—C17—H17 | 119.2 |
| C16—C15—C14 | 119.5 (2) | C16—C17—H17 | 119.2 |
| C15—C16—C17 | 119.6 (2) | O2—C18—H18A | 109.5 |
| C12—C17—C16 | 121.6 (2) | O2—C18—H18B | 109.5 |
| C15—O2—C18 | 117.7 (2) | H18A—C18—H18B | 109.5 |
| C3—C2—H2 | 119.7 | O2—C18—H18C | 109.5 |
| C1—C2—H2 | 119.7 | H18A—C18—H18C | 109.5 |
| C4—C3—H3 | 119.6 | H18B—C18—H18C | 109.5 |

**Fig. 1**