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

# 1-(4-Methylphenyl)-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

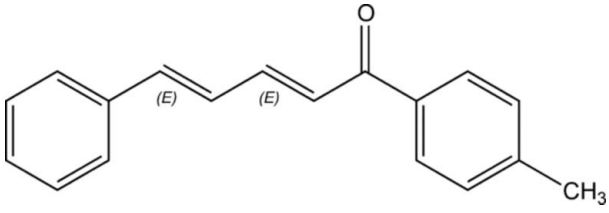
Received 28 March 2007; accepted 24 April 2007

Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.068; $wR$ factor = 0.162; data-to-parameter ratio = 14.3.

The title compound, $C_{18}H_{16}O$, features two conjugate double bonds, both in $E$ conformations. The molecule is essentially planar: the dihedral angle between the two phenyl groups is 9.4 (1)°.

## Related literature

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




## Experimental

### Crystal data

$C_{18}H_{16}O$
$M_r$ = 248.33
Monoclinic, $P2_1/c$
$a$ = 7.7215 (12) Å
$b$ = 10.6985 (12) Å
$c$ = 17.331 (3) Å
$\beta$ = 99.550 (13)°
$V$ = 1411.9 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 298 K
0.46 × 0.44 × 0.16 mm

### Data collection

Bruker-Nonius KappaCCD diffractometer
Absorption correction: none
12654 measured reflections
2465 independent reflections
1411 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.083

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.068
$wR(F^2)$ = 0.162
$S$ = 1.12
2465 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 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 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: RZ2134).

## 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). *Vogel's Textbook of Practical Organic Chemistry*, 5th ed, p. 1034. 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 B. V., 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/S1600536807020582 

# supplementary materials

*Acta Cryst.* (2007). E**63**, o2832 [ **doi:10.1107/S1600536807020582** ]

# 1-(4-Methylphenyl)-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)**, $C_{18}H_{16}O$, 1-(4-methylphenyl)-5-phenylpenta-2,4-dien-1-one is an optically active molecule. The present-day demand is for large and high quality ferroelectric, 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 non-centrosymmetric 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. The paper reports crystal structure of the title compound. Fig. 1 shows the molecular structure. The geometry is unexceptional.

## 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 is purified by recrystallization from ethanol. The crystal growth is done in acetone solvent by slow evaporation technique (m.p.333-37 K). Analysis for $C_{18}H_{16}O$: Found (Calculated): C: 87.50 (87.06%); H: 6.31 (6.49%).

## Refinement

H atoms were placed at calculated positions and refined as riding on the respective carrier atoms, with C—H = 0.93-0.96 Å and $U_{iso}(H) = 1.2\ U_{eq}(C)$ or $1.5\ U_{eq}(C)$ for methyl H atoms.

## Figures

Fig. 1. : The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

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

*Crystal data*

| | |
|---|---|
| $C_{18}H_{16}O$ | $F_{000} = 528$ |
| $M_r = 248.33$ | $D_x = 1.170$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation<br>$\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 31 reflections |
| $a = 7.7215$ (12) Å | $\theta = 5.8$–$19.2$º |
| $b = 10.6985$ (12) Å | $\mu = 0.07$ mm$^{-1}$ |
| $c = 17.331$ (3) Å | $T = 298$ K |
| $\beta = 99.550$ (13)º | Block, colourless |
| $V = 1411.9$ (4) Å$^3$ | 0.46 × 0.44 × 0.16 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker-Nonius KappaCCD diffractometer | $R_{int} = 0.083$ |
| Radiation source: fine-focus sealed tube | $\theta_{max} = 25.0$º |
| φ and ω scans | $\theta_{min} = 4.5$º |
| Absorption correction: none | $h = -9 \rightarrow 9$ |
| 12654 measured reflections | $k = -12 \rightarrow 12$ |
| 2465 independent reflections | $l = -20 \rightarrow 20$ |
| 1411 reflections with $I > 2\sigma(I)$ | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | H-atom parameters constrained |
| Least-squares matrix: full | $w = 1/[\sigma^2(F_o^2) + (0.0454P)^2 + 0.599P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)] = 0.068$ | $(\Delta/\sigma)_{max} < 0.001$ |
| $wR(F^2) = 0.162$ | $\Delta\rho_{max} = 0.23$ e Å$^{-3}$ |
| $S = 1.12$ | $\Delta\rho_{min} = -0.14$ e Å$^{-3}$ |
| 2465 reflections | Extinction correction: none |
| 172 parameters | |
| Primary atom site location: structure-invariant direct methods | |
| Secondary atom site location: difference Fourier map | |

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 | 0.8540 (4) | 0.4877 (3) | 0.58254 (18) | 0.0693 (9) |
| C2 | 0.9516 (5) | 0.4357 (3) | 0.6484 (2) | 0.0797 (10) |
| C3 | 0.9547 (5) | 0.4901 (4) | 0.7199 (2) | 0.0812 (10) |
| C4 | 0.8622 (5) | 0.5971 (4) | 0.72512 (19) | 0.0854 (11) |
| C5 | 0.7655 (4) | 0.6509 (3) | 0.65946 (17) | 0.0696 (9) |
| C6 | 0.7598 (4) | 0.5958 (3) | 0.58691 (15) | 0.0555 (7) |
| C7 | 0.6567 (4) | 0.6560 (3) | 0.51811 (17) | 0.0654 (8) |
| C8 | 0.6335 (4) | 0.6166 (3) | 0.44402 (16) | 0.0639 (8) |
| C9 | 0.5317 (4) | 0.6825 (3) | 0.38073 (17) | 0.0632 (8) |
| C10 | 0.5010 (4) | 0.6488 (3) | 0.30626 (16) | 0.0605 (8) |
| C11 | 0.3920 (4) | 0.7267 (3) | 0.24737 (17) | 0.0578 (8) |
| C12 | 0.3346 (4) | 0.6776 (3) | 0.16667 (15) | 0.0510 (7) |
| C13 | 0.3969 (4) | 0.5667 (3) | 0.13931 (16) | 0.0622 (8) |
| C14 | 0.3401 (4) | 0.5283 (3) | 0.06311 (17) | 0.0674 (9) |
| C15 | 0.2203 (4) | 0.5965 (3) | 0.01268 (16) | 0.0601 (8) |
| C16 | 0.1533 (4) | 0.7044 (3) | 0.04084 (18) | 0.0681 (9) |
| C17 | 0.2110 (4) | 0.7453 (3) | 0.11586 (18) | 0.0656 (8) |
| C18 | 0.1592 (5) | 0.5536 (4) | −0.07059 (17) | 0.0819 (11) |
| O1 | 0.3463 (3) | 0.8317 (2) | 0.26439 (12) | 0.0830 (7) |
| H1 | 0.8520 | 0.4490 | 0.5344 | 0.083* |
| H2 | 1.0158 | 0.3631 | 0.6442 | 0.096* |
| H3 | 1.0192 | 0.4543 | 0.7644 | 0.097* |
| H4 | 0.8640 | 0.6347 | 0.7736 | 0.102* |
| H5 | 0.7039 | 0.7246 | 0.6640 | 0.084* |
| H7 | 0.6010 | 0.7305 | 0.5272 | 0.078* |
| H8 | 0.6866 | 0.5420 | 0.4331 | 0.077* |
| H9 | 0.4814 | 0.7574 | 0.3931 | 0.076* |
| H10 | 0.5490 | 0.5747 | 0.2910 | 0.073* |
| H13 | 0.4771 | 0.5181 | 0.1723 | 0.075* |
| H14 | 0.3842 | 0.4544 | 0.0457 | 0.081* |
| H16 | 0.0678 | 0.7500 | 0.0085 | 0.082* |
| H17 | 0.1666 | 0.8194 | 0.1328 | 0.079* |
| H18A | 0.2329 | 0.5901 | −0.1042 | 0.123* |
| H18B | 0.0396 | 0.5795 | −0.0872 | 0.123* |
| H18C | 0.1664 | 0.4641 | −0.0731 | 0.123* |

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

| $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| C1 | 0.084 (2) | 0.069 (2) | 0.0520 (19) | 0.0019 (18) | 0.0018 (16) | −0.0047 (16) |
| C2 | 0.091 (3) | 0.072 (2) | 0.074 (2) | 0.0115 (19) | 0.0060 (19) | 0.0054 (19) |
| C3 | 0.081 (2) | 0.100 (3) | 0.057 (2) | 0.000 (2) | −0.0065 (17) | 0.014 (2) |
| C4 | 0.094 (3) | 0.113 (3) | 0.046 (2) | −0.001 (2) | 0.0017 (18) | −0.005 (2) |
| C5 | 0.070 (2) | 0.087 (2) | 0.0516 (19) | 0.0044 (18) | 0.0093 (15) | −0.0084 (17) |
| C6 | 0.0551 (17) | 0.0655 (19) | 0.0453 (17) | −0.0020 (15) | 0.0061 (13) | −0.0011 (15) |
| C7 | 0.070 (2) | 0.070 (2) | 0.0549 (19) | 0.0020 (17) | 0.0052 (15) | −0.0034 (16) |
| C8 | 0.068 (2) | 0.068 (2) | 0.0533 (19) | 0.0007 (16) | 0.0040 (15) | −0.0024 (16) |
| C9 | 0.0635 (19) | 0.068 (2) | 0.0554 (19) | −0.0002 (15) | 0.0019 (15) | 0.0007 (16) |
| C10 | 0.0664 (19) | 0.065 (2) | 0.0477 (17) | 0.0007 (16) | 0.0025 (14) | −0.0029 (15) |
| C11 | 0.0599 (18) | 0.061 (2) | 0.0532 (19) | −0.0036 (15) | 0.0103 (14) | 0.0016 (15) |
| C12 | 0.0543 (17) | 0.0542 (17) | 0.0452 (16) | −0.0035 (14) | 0.0101 (13) | 0.0066 (13) |
| C13 | 0.0660 (19) | 0.073 (2) | 0.0466 (17) | 0.0136 (16) | 0.0053 (14) | 0.0071 (15) |
| C14 | 0.082 (2) | 0.068 (2) | 0.0519 (19) | 0.0115 (17) | 0.0086 (16) | −0.0052 (16) |
| C15 | 0.0641 (19) | 0.070 (2) | 0.0457 (17) | −0.0134 (16) | 0.0091 (14) | 0.0078 (16) |
| C16 | 0.076 (2) | 0.068 (2) | 0.055 (2) | −0.0005 (17) | −0.0041 (16) | 0.0149 (16) |
| C17 | 0.075 (2) | 0.0575 (19) | 0.062 (2) | 0.0062 (16) | 0.0050 (17) | 0.0089 (15) |
| C18 | 0.087 (2) | 0.104 (3) | 0.0521 (19) | −0.018 (2) | 0.0022 (17) | 0.0051 (18) |
| O1 | 0.1052 (19) | 0.0669 (15) | 0.0716 (15) | 0.0141 (13) | −0.0017 (13) | −0.0121 (12) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.373 (4) | C15—C18 | 1.516 (4) |
| C1—C2 | 1.379 (4) | C16—C17 | 1.377 (4) |
| C2—C3 | 1.367 (4) | C1—H1 | 0.9300 |
| C3—C4 | 1.358 (5) | C2—H2 | 0.9300 |
| C4—C5 | 1.381 (4) | C3—H3 | 0.9300 |
| C5—C6 | 1.384 (4) | C4—H4 | 0.9300 |
| C6—C7 | 1.471 (4) | C5—H5 | 0.9300 |
| C7—C8 | 1.337 (4) | C7—H7 | 0.9300 |
| C8—C9 | 1.427 (4) | C8—H8 | 0.9300 |
| C9—C10 | 1.325 (4) | C9—H9 | 0.9300 |
| C10—C11 | 1.471 (4) | C10—H10 | 0.9300 |
| C11—O1 | 1.227 (3) | C13—H13 | 0.9300 |
| C11—C12 | 1.494 (4) | C14—H14 | 0.9300 |
| C12—C17 | 1.391 (4) | C16—H16 | 0.9300 |
| C12—C13 | 1.391 (4) | C17—H17 | 0.9300 |
| C13—C14 | 1.386 (4) | C18—H18A | 0.9600 |
| C14—C15 | 1.373 (4) | C18—H18B | 0.9600 |
| C15—C16 | 1.385 (4) | C18—H18C | 0.9600 |
| C6—C1—C2 | 121.0 (3) | C4—C3—H3 | 120.4 |
| C3—C2—C1 | 120.5 (3) | C2—C3—H3 | 120.4 |
| C4—C3—C2 | 119.1 (3) | C3—C4—H4 | 119.5 |
| C3—C4—C5 | 120.9 (3) | C5—C4—H4 | 119.5 |
| C4—C5—C6 | 120.4 (3) | C4—C5—H5 | 119.8 |
| C1—C6—C5 | 118.0 (3) | C6—C5—H5 | 119.8 |
| C1—C6—C7 | 123.0 (3) | C8—C7—H7 | 116.1 |
| C5—C6—C7 | 119.0 (3) | C6—C7—H7 | 116.1 |
| C8—C7—C6 | 127.8 (3) | C7—C8—H8 | 118.1 |

| | | | |
|---|---|---|---|
| C7—C8—C9 | 123.7 (3) | C9—C8—H8 | 118.1 |
| C10—C9—C8 | 127.2 (3) | C10—C9—H9 | 116.4 |
| C9—C10—C11 | 121.0 (3) | C8—C9—H9 | 116.4 |
| O1—C11—C10 | 120.3 (3) | C9—C10—H10 | 119.5 |
| O1—C11—C12 | 119.6 (3) | C11—C10—H10 | 119.5 |
| C10—C11—C12 | 120.1 (3) | C14—C13—H13 | 119.8 |
| C17—C12—C13 | 117.8 (3) | C12—C13—H13 | 119.8 |
| C17—C12—C11 | 118.6 (3) | C15—C14—H14 | 119.1 |
| C13—C12—C11 | 123.6 (3) | C13—C14—H14 | 119.1 |
| C14—C13—C12 | 120.4 (3) | C17—C16—H16 | 119.4 |
| C15—C14—C13 | 121.7 (3) | C15—C16—H16 | 119.4 |
| C14—C15—C16 | 117.9 (3) | C16—C17—H17 | 119.4 |
| C14—C15—C18 | 121.3 (3) | C12—C17—H17 | 119.4 |
| C16—C15—C18 | 120.8 (3) | C15—C18—H18A | 109.5 |
| C17—C16—C15 | 121.1 (3) | C15—C18—H18B | 109.5 |
| C16—C17—C12 | 121.1 (3) | H18A—C18—H18B | 109.5 |
| C6—C1—H1 | 119.5 | C15—C18—H18C | 109.5 |
| C2—C1—H1 | 119.5 | H18A—C18—H18C | 109.5 |
| C3—C2—H2 | 119.7 | H18B—C18—H18C | 109.5 |
| C1—C2—H2 | 119.7 | | |

**Fig. 1**