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

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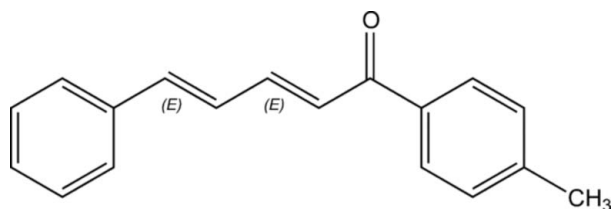
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.068; wR factor = 0.162; data-to-parameter ratio = 14.3.

The title compound, $\text{C}_{18}\text{H}_{16}\text{O}$, 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: Fichou *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

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

Data collection

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

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.068$	172 parameters
$wR(F^2) = 0.162$	H-atom parameters constrained
$S = 1.12$	$\Delta\rho_{\text{max}} = 0.23$ e Å ⁻³
2465 reflections	$\Delta\rho_{\text{min}} = -0.14$ 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).

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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.* **E62**, 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.* **E62**, 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.* **E63**, o61–o62.

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

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Comment

The title compound, **(I)**, C₁₈H₁₆O, 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 inhomogeneities. 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 C₁₈H₁₆O: 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 $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ or $1.5 U_{\text{eq}}(\text{C})$ 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

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

Data collection

Bruker-Nonius KappaCCD diffractometer	$R_{\text{int}} = 0.083$
Radiation source: fine-focus sealed tube	$\theta_{\text{max}} = 25.0^\circ$
φ and ω scans	$\theta_{\text{min}} = 4.5^\circ$
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	$w = 1/[\sigma^2(F_o^2) + (0.0454P)^2 + 0.599P]$
$R[F^2 > 2\sigma(F^2)] = 0.068$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.162$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.12$	$\Delta\rho_{\text{max}} = 0.23 \text{ e \AA}^{-3}$
2465 reflections	$\Delta\rho_{\text{min}} = -0.14 \text{ e \AA}^{-3}$
172 parameters	Extinction correction: none
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 $F^2 > 2\sigma(F^2)$ 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 (\AA^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 (\AA^2)

U^{11} U^{22} U^{33} U^{12} U^{13} U^{23}

supplementary materials

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

