

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

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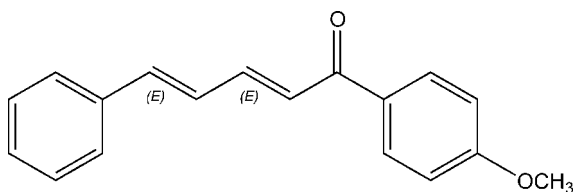
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.062; wR factor = 0.143; data-to-parameter ratio = 14.5.

The title compound, $\text{C}_{18}\text{H}_{16}\text{O}_2$, 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

$\text{C}_{18}\text{H}_{16}\text{O}_2$
 $M_r = 264.32$
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) Å³
 $Z = 4$
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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.114$

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
 $\Delta\rho_{\text{max}} = 0.11$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.14$ 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: PR2008).

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supplementary materials

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

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Comment

The title compound, (I), is an optically active molecule. The present-day demand is for large, high quality ferroelectric and 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 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 the 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 C₁₈H₁₆O₂: 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

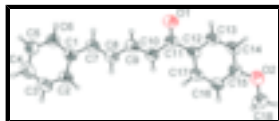


Fig. 1. The molecular structure of (I). Thermal ellipsoids at the 50% probability level.

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

Crystal data

$C_{18}H_{16}O_2$	$F_{000} = 560$
$M_r = 264.32$	$D_x = 1.229 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 29.017 (7) \text{ \AA}$	Cell parameters from 23 reflections
$b = 5.8088 (14) \text{ \AA}$	$\theta = 7.9\text{--}16.8^\circ$
$c = 8.4868 (10) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$\beta = 93.308 (16)^\circ$	$T = 298 \text{ K}$
$V = 1428.1 (5) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.35 \times 0.30 \times 0.28 \text{ mm}$

Data collection

Nonius KappaCCD area-detector diffractometer	$R_{\text{int}} = 0.114$
Radiation source: fine-focus sealed tube	$\theta_{\text{max}} = 25.5^\circ$
ω scans	$\theta_{\text{min}} = 4.5^\circ$
Absorption correction: none	$h = -35 \rightarrow 35$
13388 measured reflections	$k = -6 \rightarrow 6$
2633 independent reflections	$l = -10 \rightarrow 10$
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
$R[F^2 > 2\sigma(F^2)] = 0.062$	$w = 1/[\sigma^2(F_o^2) + (0.0295P)^2 + 0.4375P]$
$wR(F^2) = 0.143$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.12$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2633 reflections	$\Delta\rho_{\text{max}} = 0.11 \text{ e \AA}^{-3}$
181 parameters	$\Delta\rho_{\text{min}} = -0.14 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\sigma(F^2)$ 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	$U_{\text{iso}}^*/U_{\text{eq}}$
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*

supplementary materials

Atomic displacement parameters (\AA^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 (\AA , $^\circ$)

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

