Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Bo Zhao,[a]* Yu-Zhi Rong[a] and Wei Huang[b]

[a]College of Chemistry and Environmental Science, Nanjing Normal University, Nanjing 210097, People's Republic of China, and [b]State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing210093, People's Republic of China
Correspondence e-mail: zhaobo@njnu.edu.cn; dr-zhaobo@hotmail.com

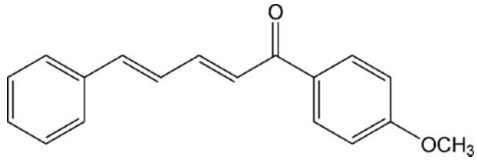
Received 5 April 2007; accepted 28 April 2007

Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.094; data-to-parameter ratio = 14.0.

In the crystal structure of the title compound, $C_{18}H_{16}O_2$, the molecules related by a c-glide plane are linked into a column running along the c axis by a weak intermolecular C—H···O hydrogen bond.

Related literature

For related literature, see: Charles & Morris (1955); Vorontsova & Kazaryan (1973); Zhao *et al.* (1999).



Experimental

Crystal data

$C_{18}H_{16}O_2$
M_r = 264.31
Monoclinic, $P2_1/c$
a = 12.004 (2) Å
b = 15.727 (2) Å
c = 8.077 (1) Å
β = 107.83 (1)°
V = 1451.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 297 (2) K
0.54 × 0.50 × 0.24 mm

Data collection

Siemens $P4$ diffractometer
Absorption correction: none
2974 measured reflections
2560 independent reflections
1439 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
3 standard reflections
every 970 reflections
intensity decay: 2.2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.094
S = 0.87
2560 reflections
183 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1^{i}	0.93	2.50	3.280 (2)	142

Symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Siemens, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors are grateful for funding from the Natural Science Foundation of Jiangsu Province Education Ministry (grant No. 05KJB430058), the High Technology Research Project of Jiangsu Province (grant No. BG-2005041) and the Natural Science Foundation of Jiangsu Science and Technology Department (grant No. BK2005118).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2156).

References

Charles, R. C. & Morris, A. D. (1955). *Org. Synth.* **2**, 167–169.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1994). *XSCANS*. Version 2.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Siemens (1995). *SHELXTL*. Version 5.0. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Vorontsova, L. G. & Kazaryan, G. S. (1973). *Zh. Strukt. Khim.* **14**, 1089–1093.
Zhao, B., Cao, Y. & Lang, J. P. (1999). *Chin. J. Struct. Chem.* **18**, 348–351.

supplementary materials

Acta Cryst. (2007). E**63**, o2971 [**doi:10.1107/S1600536807021253**]

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

B. Zhao, Y.-Z. Rong and W. Huang

Comment

The title compound, (I), was synthesized because it was expected to have a big π conjugation system which is potentially useful in the photoelectric fields and the crystal engineering. The methoxy group attached to the benzene ring deviates slightly from the molecular plane with the torsion angle of C18—O2—C15—C16 = −0.59 (2)°. The related compound, 1-phenyl-5-phenylpenta-2,4-dien-1-one (Zhao *et al.*, 1999), is more planar than its substituted derivatives (Vorontsova *et al.*, 1973) and the present compound.

In the crystal structure, the molecules stack along the *c* axis through a very week C—H···O hydrogen bond (Table 1).

Experimental

The title compound was prepared according to the literature procedure of Charles & Morris (1955). The crude product was recrystallized several times from ethanol

and the yellow single crystals were obtained by slow evaporation of a ethanol solution (m.p. 369–371 K). Analysis calculated for $C_{18}H_{16}O_2$: C 81.79, H 6.10%; found: C 81.60, H 5.99%.

Refinement

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

Figures

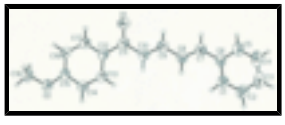


Fig. 1. The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids of non-H atoms are drawn at the 50% probability level.

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

Crystal data

$C_{18}H_{16}O_2$	F_{000} = 560
M_r = 264.31	D_x = 1.209 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 28 reflections
a = 12.004 (2) Å	θ = 2.7–15.7º

b = 15.727 (2) Å	μ = 0.08 mm^{-1}
c = 8.077 (1) Å	T = 297 (2) K
β = 107.83 (1)º	Block, yellow
V = 1451.6 (4) Å^3	0.54 × 0.50 × 0.24 mm
Z = 4	

Data collection

Siemens P4 diffractometer	R_{int} = 0.014
Radiation source: normal-focus sealed tube	θ_{max} = 25.0º
Monochromator: graphite	θ_{min} = 1.8º
T = 297(2) K	h = −14→13
ω scans	k = −18→0
Absorption correction: none	l = 0→9
2974 measured reflections	3 standard reflections
2560 independent reflections	every 970 reflections
1439 reflections with $I > 2\sigma(I)$	intensity decay: 2.2%

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.037	$w = 1/[\sigma^2(F_o^2) + (0.0495P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.094	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.87	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
2560 reflections	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
183 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0139 (15)
Secondary atom site location: difference Fourier map	

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}
O1	0.19411 (9)	0.10710 (7)	−0.09462 (16)	0.0779 (4)
O2	0.73397 (9)	0.17972 (7)	0.04888 (15)	0.0754 (4)
C1	−0.09513 (15)	0.47096 (11)	0.1517 (2)	0.0735 (5)
H1	−0.0145	0.4676	0.2027	0.088*
C2	−0.15599 (19)	0.53658 (12)	0.1957 (3)	0.0891 (6)
H2	−0.1163	0.5769	0.2765	0.107*
C3	−0.2744 (2)	0.54324 (14)	0.1218 (3)	0.0949 (7)
H3	−0.3151	0.5879	0.1521	0.114*
C4	−0.33271 (18)	0.48377 (17)	0.0028 (3)	0.0975 (7)
H4	−0.4131	0.4883	−0.0491	0.117*
C5	−0.27211 (16)	0.41723 (13)	−0.0401 (2)	0.0819 (6)
H5	−0.3126	0.3766	−0.1194	0.098*
C6	−0.15188 (14)	0.40975 (11)	0.0328 (2)	0.0616 (4)
C7	−0.09118 (14)	0.33810 (10)	−0.0168 (2)	0.0655 (5)
H7	−0.1380	0.2972	−0.0884	0.079*
C8	0.02322 (13)	0.32510 (10)	0.0292 (2)	0.0622 (4)
H8	0.0711	0.3661	0.0990	0.075*
C9	0.07948 (14)	0.25328 (11)	−0.0195 (2)	0.0619 (4)
H9	0.0322	0.2112	−0.0864	0.074*
C10	0.19482 (13)	0.24269 (11)	0.0243 (2)	0.0637 (4)
H10	0.2424	0.2839	0.0938	0.076*
C11	0.25122 (14)	0.17021 (10)	−0.0299 (2)	0.0588 (4)
C12	0.37840 (13)	0.17344 (9)	−0.00920 (19)	0.0529 (4)
C13	0.45110 (14)	0.23974 (10)	0.0734 (2)	0.0643 (5)
H13	0.4197	0.2849	0.1188	0.077*
C14	0.56818 (14)	0.23975 (11)	0.0891 (2)	0.0680 (5)
H14	0.6151	0.2847	0.1449	0.082*
C15	0.61673 (14)	0.17356 (10)	0.0229 (2)	0.0583 (4)
C16	0.54681 (15)	0.10737 (10)	−0.0613 (2)	0.0620 (4)
H16	0.5786	0.0627	−0.1075	0.074*
C17	0.42928 (14)	0.10812 (10)	−0.0762 (2)	0.0607 (4)
H17	0.3825	0.0633	−0.1331	0.073*
C18	0.79246 (15)	0.11007 (12)	0.0003 (3)	0.0913 (6)
H18A	0.7779	0.0594	0.0566	0.110*
H18B	0.8751	0.1211	0.0350	0.110*
H18C	0.7639	0.1026	−0.1235	0.110*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0749 (8)	0.0590 (8)	0.0965 (9)	−0.0060 (6)	0.0216 (7)	−0.0063 (7)
O2	0.0646 (7)	0.0727 (8)	0.0924 (9)	0.0057 (6)	0.0294 (6)	−0.0050 (7)
C1	0.0682 (11)	0.0671 (11)	0.0934 (14)	−0.0034 (10)	0.0368 (10)	−0.0038 (11)
C2	0.0998 (16)	0.0662 (13)	0.1164 (17)	−0.0003 (11)	0.0553 (14)	−0.0053 (12)

C3	0.1090 (18)	0.0872 (16)	0.1075 (18)	0.0339 (13)	0.0611 (15)	0.0227 (14)
C4	0.0766 (14)	0.137 (2)	0.0822 (15)	0.0354 (14)	0.0297 (12)	0.0191 (15)
C5	0.0672 (12)	0.1093 (16)	0.0706 (12)	0.0114 (11)	0.0234 (10)	−0.0019 (11)
C6	0.0599 (11)	0.0667 (11)	0.0634 (11)	0.0034 (9)	0.0267 (9)	0.0090 (9)
C7	0.0639 (11)	0.0676 (11)	0.0667 (11)	−0.0031 (9)	0.0223 (9)	−0.0034 (9)
C8	0.0605 (11)	0.0678 (11)	0.0618 (11)	−0.0028 (9)	0.0239 (9)	−0.0032 (9)
C9	0.0669 (11)	0.0615 (10)	0.0607 (10)	−0.0009 (9)	0.0245 (8)	0.0011 (9)
C10	0.0633 (11)	0.0670 (11)	0.0616 (11)	−0.0022 (9)	0.0203 (8)	−0.0063 (9)
C11	0.0681 (11)	0.0527 (11)	0.0548 (10)	0.0020 (9)	0.0177 (8)	0.0043 (8)
C12	0.0631 (10)	0.0467 (9)	0.0496 (9)	0.0015 (8)	0.0185 (8)	0.0031 (8)
C13	0.0675 (11)	0.0600 (11)	0.0686 (11)	0.0046 (9)	0.0254 (9)	−0.0138 (9)
C14	0.0694 (11)	0.0649 (11)	0.0699 (12)	−0.0060 (9)	0.0214 (9)	−0.0165 (9)
C15	0.0618 (11)	0.0585 (11)	0.0566 (10)	0.0074 (9)	0.0210 (8)	0.0056 (8)
C16	0.0748 (11)	0.0456 (9)	0.0694 (11)	0.0084 (8)	0.0278 (9)	0.0008 (8)
C17	0.0724 (11)	0.0460 (9)	0.0640 (11)	0.0005 (8)	0.0215 (9)	0.0007 (8)
C18	0.0735 (12)	0.0849 (14)	0.1222 (17)	0.0179 (11)	0.0398 (12)	0.0016 (12)

Geometric parameters (Å, °)

O1—C11	1.2283 (17)	C9—C10	1.3303 (19)
O2—C15	1.3613 (17)	C9—H9	0.930
O2—C18	1.4196 (19)	C10—C11	1.460 (2)
C1—C2	1.372 (2)	C10—H10	0.930
C1—C6	1.383 (2)	C11—C12	1.485 (2)
C1—H1	0.930	C12—C17	1.387 (2)
C2—C3	1.367 (3)	C12—C13	1.392 (2)
C2—H2	0.930	C13—C14	1.372 (2)
C3—C4	1.370 (3)	C13—H13	0.930
C3—H3	0.930	C14—C15	1.379 (2)
C4—C5	1.378 (3)	C14—H14	0.930
C4—H4	0.930	C15—C16	1.379 (2)
C5—C6	1.387 (2)	C16—C17	1.379 (2)
C5—H5	0.930	C16—H16	0.930
C6—C7	1.463 (2)	C17—H17	0.930
C7—C8	1.3242 (19)	C18—H18A	0.960
C7—H7	0.930	C18—H18B	0.960
C8—C9	1.432 (2)	C18—H18C	0.960
C8—H8	0.930		
C15—O2—C18	118.55 (13)	O1—C11—C10	120.58 (15)
C2—C1—C6	121.00 (18)	O1—C11—C12	119.76 (14)
C2—C1—H1	119.4	C10—C11—C12	119.65 (14)
C3—C2—C1	120.6 (2)	C17—C12—C13	117.09 (14)
C3—C2—H2	119.6	C17—C12—C11	119.41 (14)
C2—C3—C4	119.6 (2)	C13—C12—C11	123.50 (14)
C2—C3—H3	120.2	C14—C13—C12	121.25 (15)
C3—C4—C5	119.9 (2)	C14—C13—H13	119.3
C3—C4—H4	120.1	C13—C14—C15	120.44 (16)
C4—C5—C6	121.2 (2)	C13—C14—H14	119.8
C4—C5—H5	119.3	O2—C15—C14	115.23 (15)

C1—C6—C5	117.59 (16)	O2—C15—C16	125.05 (14)
C1—C6—C7	123.07 (15)	C14—C15—C16	119.72 (15)
C5—C6—C7	119.34 (16)	C15—C16—C17	119.24 (15)
C8—C7—C6	127.08 (16)	C15—C16—H16	120.4
C8—C7—H7	116.5	C16—C17—C12	122.24 (15)
C7—C8—C9	125.50 (16)	C16—C17—H17	119.0
C7—C8—H8	117.3	C15—O2—C18	118.57 (14)
C10—C9—C8	124.43 (16)	H18A—C18—H18B	109.5
C10—C9—H9	117.8	H18A—C18—H18C	109.5
C9—C10—C11	123.93 (16)	H18B—C18—H18C	109.5
C9—C10—H10	118.0		
C6—C1—C2—C3	−0.4 (3)	C10—C11—C12—C17	−173.78 (14)
C1—C2—C3—C4	0.0 (3)	O1—C11—C12—C13	−175.43 (15)
C2—C3—C4—C5	0.8 (3)	C10—C11—C12—C13	5.5 (2)
C3—C4—C5—C6	−1.2 (3)	C17—C12—C13—C14	−0.7 (2)
C2—C1—C6—C5	0.0 (2)	C11—C12—C13—C14	−179.97 (15)
C2—C1—C6—C7	−179.27 (16)	C12—C13—C14—C15	0.0 (2)
C4—C5—C6—C1	0.8 (3)	C18—O2—C15—C14	173.68 (15)
C4—C5—C6—C7	−179.90 (16)	C18—O2—C15—C16	−5.9 (2)
C1—C6—C7—C8	−6.5 (3)	C13—C14—C15—O2	−178.89 (14)
C5—C6—C7—C8	174.21 (16)	C13—C14—C15—C16	0.7 (2)
C6—C7—C8—C9	178.84 (14)	O2—C15—C16—C17	178.82 (14)
C7—C8—C9—C10	178.09 (16)	C14—C15—C16—C17	−0.7 (2)
C8—C9—C10—C11	−178.35 (14)	C15—C16—C17—C12	0.0 (2)
C9—C10—C11—O1	−13.0 (2)	C13—C12—C17—C16	0.6 (2)
C9—C10—C11—C12	166.06 (15)	C11—C12—C17—C16	179.98 (14)
O1—C11—C12—C17	5.3 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···O1^{i}	0.93	2.50	3.280 (2)	142

Symmetry codes: (i) *x*, −*y*+1/2, *z*+1/2.

Fig. 1