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rac-5-Methoxy-3-phenyl-2,3-dihydro-1*H*-inden-1-one

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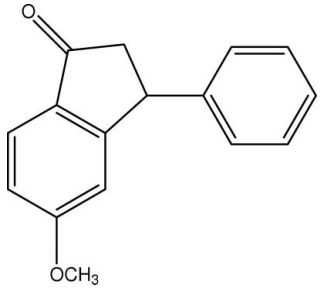
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.047; wR factor = 0.125; data-to-parameter ratio = 15.5.

In the title compound, $C_{16}H_{14}O_2$, the phenyl ring is twisted from the indan ring system with a dihedral angle of 81.53 (8)°. The crystal structure is stabilized by intermolecular C—H···O hydrogen bonds.

Related literature

For bond length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For general background and related literature, see: Wang *et al.* (2005).



Experimental

Crystal data

$C_{16}H_{14}O_2$
M_r = 238.27
Monoclinic, $P2_1/c$
a = 8.3603 (4) Å
b = 6.4935 (3) Å
c = 23.1904 (11) Å
β = 99.106 (2)°
V = 1243.09 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100.0 (1) K
0.36 × 0.19 × 0.14 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.826, T_{max} = 0.989
10552 measured reflections
2548 independent reflections
1867 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.125
S = 1.10
2548 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···O1^{i}	0.93	2.54	3.442 (2)	163
C5—H5A···O2^{ii}	0.93	2.50	3.344 (2)	151
C16—H16A···O2^{iii}	0.96	2.42	3.382 (2)	176

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y+2, -z+1$; (iii) $x+1, y-1, z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2119).

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supplementary materials

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rac-5-Methoxy-3-phenyl-2,3-dihydro-1*H*-inden-1-one

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Comment

The photochemistry of alkynes is of permanent research interest (Wang *et al.*, 2005). As part of our recent work on photoinduced reactions of aldehydes with alkynes, the title compound was obtained by the reaction of photoexcited 4-methoxybenzaldehyde with trimethylsilyphenylethyne. X-ray structure analysis of the title compound was carried out to elucidate its structure.

Since the atom C9 is chiral and the space group is centrosymmetric, the crystal is a racemate. Bond lengths and angles of the title compound are within normal ranges (Allen *et al.*, 1987). The indane ring is essentially planar with a maximum deviation of 0.053 (2)Å for atom C9. The benzene ring was twisted from the indane ring with the dihedral angle of 81.53 (8)°. The methoxy group attached at the atom C9 is almost coplanar with the indane ring with C16—O1—C3—C4 torsion angle of −179.31 (14)°.

The molecules are linked into chains approximately down the *b* axis and stabilized by three intermolecular C—H···O interactions (Table 1). These interactions form $R^2_3(8)$ hydrogen bond ring motifs (Bernstein *et al.*, 1995).

Experimental

The title compound, (I), was synthesized by photo-induced reaction between 4-methoxybenzaldehyde (0.05 *M*) and an excess amount of 1-phenyl-2-trimethyl-silylacetylene (0.15 *M*) in a benzene solution. The title compound was isolated using silica gel column chromatography. Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of the solvents from a petroleum ether-acetone solution (V:V=2:1).

Refinement

All H atoms were refined using a riding model, with C—H distances in the range 0.93–0.96 Å. The U_{iso}(H) values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H and $1.2U_{eq}$ for the remaining H atoms.

Figures

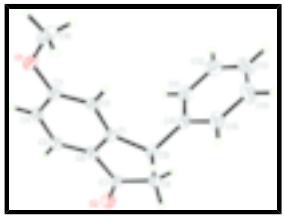

Fig. 1. The molecular structure of (I), showing the 50% probability displacement ellipsoids and the atomic numbering.

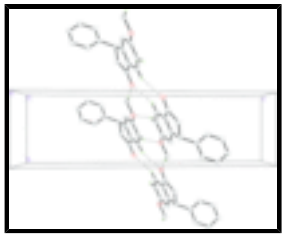

Fig. 2. The crystal packing of (I) viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

(*rac*)-5-methoxy-3-phenyl-2,3-dihydro-1*H*-inden-1-one

Crystal data

$C_{16}H_{14}O_2$	F_{000} = 504
M_r = 238.27	D_x = 1.273 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2136 reflections
a = 8.3603 (4) Å	θ = 2.5–26.5º
b = 6.4935 (3) Å	μ = 0.08 mm^{-1}
c = 23.1904 (11) Å	T = 100.0 (1) K
β = 99.106 (2)º	Block, colourless
V = 1243.09 (10) Å^3	0.36 × 0.19 × 0.14 mm
Z = 4	

Data collection

Bruker SMART APEX II CCD area-detector diffractometer	2548 independent reflections
Radiation source: fine-focus sealed tube	1867 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.047
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 26.5º
T = 100.0(1) K	θ_{min} = 1.8º
ω scans	h = −10→10
Absorption correction: multi-scan (SADABS; Bruker, 2005)	k = −7→8
T_{min} = 0.826, T_{max} = 0.989	l = −24→29
10552 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.047	H-atom parameters constrained
$wR(F^2)$ = 0.125	$w = 1/[\sigma^2(F_o^2) + (0.0518P)^2 + 0.283P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{max}$ = 0.001

2548 reflections	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
164 parameters	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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	0.38826 (13)	0.31089 (17)	0.44441 (5)	0.0249 (3)
O2	−0.23284 (14)	0.90321 (17)	0.44183 (5)	0.0278 (3)
C1	−0.04029 (19)	0.4488 (2)	0.40722 (7)	0.0190 (4)
C2	0.09832 (19)	0.3295 (2)	0.41001 (7)	0.0200 (4)
H2A	0.0945	0.1997	0.3929	0.024*
C3	0.24286 (19)	0.4095 (2)	0.43906 (7)	0.0200 (4)
C4	0.2491 (2)	0.6039 (2)	0.46562 (7)	0.0210 (4)
H4A	0.3470	0.6540	0.4852	0.025*
C5	0.1107 (2)	0.7207 (2)	0.46284 (7)	0.0209 (4)
H5A	0.1136	0.8492	0.4807	0.025*
C6	−0.03402 (19)	0.6422 (2)	0.43267 (7)	0.0190 (4)
C7	−0.1958 (2)	0.7364 (3)	0.42384 (7)	0.0207 (4)
C8	−0.3095 (2)	0.5888 (2)	0.38705 (8)	0.0244 (4)
H8A	−0.3491	0.6492	0.3492	0.029*
H8B	−0.4016	0.5574	0.4063	0.029*
C9	−0.21166 (19)	0.3908 (2)	0.37976 (7)	0.0203 (4)
H9A	−0.2500	0.2814	0.4033	0.024*
C10	−0.22593 (19)	0.3160 (3)	0.31726 (7)	0.0224 (4)
C11	−0.1548 (2)	0.4245 (3)	0.27661 (8)	0.0329 (5)
H11A	−0.0954	0.5428	0.2880	0.039*
C12	−0.1708 (3)	0.3590 (4)	0.21911 (9)	0.0444 (6)
H12A	−0.1222	0.4332	0.1923	0.053*
C13	−0.2583 (3)	0.1846 (4)	0.20172 (9)	0.0486 (6)
H13A	−0.2695	0.1413	0.1631	0.058*
C14	−0.3292 (3)	0.0744 (3)	0.24132 (9)	0.0438 (6)
H14A	−0.3887	−0.0434	0.2295	0.053*
C15	−0.3120 (2)	0.1388 (3)	0.29928 (8)	0.0313 (5)

H15A	−0.3587	0.0622	0.3261	0.038*
C16	0.3922 (2)	0.1130 (3)	0.41791 (9)	0.0361 (5)
H16A	0.4997	0.0572	0.4266	0.054*
H16B	0.3619	0.1258	0.3764	0.054*
H16C	0.3176	0.0227	0.4329	0.054*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0160 (6)	0.0255 (7)	0.0328 (7)	0.0033 (5)	0.0025 (5)	−0.0004 (5)
O2	0.0280 (7)	0.0215 (7)	0.0327 (7)	0.0061 (5)	0.0013 (5)	−0.0043 (5)
C1	0.0197 (9)	0.0205 (9)	0.0170 (8)	0.0005 (7)	0.0031 (7)	0.0023 (7)
C2	0.0199 (9)	0.0191 (9)	0.0213 (9)	0.0009 (7)	0.0041 (7)	−0.0013 (7)
C3	0.0176 (9)	0.0237 (9)	0.0191 (8)	0.0017 (7)	0.0044 (7)	0.0050 (7)
C4	0.0174 (8)	0.0250 (9)	0.0193 (8)	−0.0036 (7)	−0.0006 (7)	0.0000 (7)
C5	0.0247 (9)	0.0202 (9)	0.0178 (8)	−0.0018 (7)	0.0031 (7)	−0.0013 (7)
C6	0.0202 (9)	0.0192 (9)	0.0178 (8)	−0.0004 (7)	0.0036 (7)	0.0014 (7)
C7	0.0215 (9)	0.0214 (9)	0.0194 (8)	0.0015 (7)	0.0040 (7)	0.0018 (7)
C8	0.0207 (9)	0.0256 (10)	0.0259 (9)	0.0005 (7)	0.0009 (7)	−0.0017 (7)
C9	0.0195 (9)	0.0201 (9)	0.0207 (9)	0.0004 (7)	0.0015 (7)	0.0002 (7)
C10	0.0164 (8)	0.0265 (9)	0.0229 (9)	0.0055 (7)	−0.0010 (7)	−0.0016 (7)
C11	0.0278 (10)	0.0425 (12)	0.0267 (10)	−0.0019 (9)	−0.0003 (8)	0.0022 (9)
C12	0.0364 (12)	0.0722 (16)	0.0248 (11)	0.0109 (11)	0.0054 (9)	0.0059 (10)
C13	0.0468 (14)	0.0717 (16)	0.0238 (11)	0.0224 (12)	−0.0053 (10)	−0.0159 (11)
C14	0.0447 (13)	0.0421 (12)	0.0389 (12)	0.0059 (10)	−0.0110 (10)	−0.0177 (10)
C15	0.0311 (11)	0.0282 (10)	0.0322 (10)	0.0016 (8)	−0.0022 (8)	−0.0059 (8)
C16	0.0224 (10)	0.0236 (10)	0.0626 (14)	0.0045 (8)	0.0074 (9)	−0.0035 (9)

Geometric parameters (Å, °)

O1—C3	1.3622 (18)	C8—H8B	0.9700
O1—C16	1.427 (2)	C9—C10	1.515 (2)
O2—C7	1.2181 (19)	C9—H9A	0.9800
C1—C6	1.385 (2)	C10—C11	1.384 (2)
C1—C2	1.387 (2)	C10—C15	1.386 (2)
C1—C9	1.520 (2)	C11—C12	1.386 (3)
C2—C3	1.388 (2)	C11—H11A	0.9300
C2—H2A	0.9300	C12—C13	1.374 (3)
C3—C4	1.401 (2)	C12—H12A	0.9300
C4—C5	1.376 (2)	C13—C14	1.370 (3)
C4—H4A	0.9300	C13—H13A	0.9300
C5—C6	1.395 (2)	C14—C15	1.393 (3)
C5—H5A	0.9300	C14—H14A	0.9300
C6—C7	1.469 (2)	C15—H15A	0.9300
C7—C8	1.515 (2)	C16—H16A	0.9600
C8—C9	1.547 (2)	C16—H16B	0.9600
C8—H8A	0.9700	C16—H16C	0.9600
C3—O1—C16	117.73 (13)	C10—C9—C8	114.08 (13)

C6—C1—C2	120.77 (15)	C1—C9—C8	103.19 (13)
C6—C1—C9	111.87 (14)	C10—C9—H9A	108.4
C2—C1—C9	127.33 (14)	C1—C9—H9A	108.4
C1—C2—C3	118.06 (15)	C8—C9—H9A	108.4
C1—C2—H2A	121.0	C11—C10—C15	118.44 (16)
C3—C2—H2A	121.0	C11—C10—C9	120.72 (16)
O1—C3—C2	124.33 (14)	C15—C10—C9	120.84 (16)
O1—C3—C4	114.39 (14)	C10—C11—C12	120.84 (19)
C2—C3—C4	121.28 (15)	C10—C11—H11A	119.6
C5—C4—C3	120.22 (15)	C12—C11—H11A	119.6
C5—C4—H4A	119.9	C13—C12—C11	120.1 (2)
C3—C4—H4A	119.9	C13—C12—H12A	120.0
C4—C5—C6	118.57 (15)	C11—C12—H12A	120.0
C4—C5—H5A	120.7	C14—C13—C12	120.01 (19)
C6—C5—H5A	120.7	C14—C13—H13A	120.0
C1—C6—C5	121.08 (15)	C12—C13—H13A	120.0
C1—C6—C7	110.26 (14)	C13—C14—C15	120.0 (2)
C5—C6—C7	128.63 (15)	C13—C14—H14A	120.0
O2—C7—C6	126.94 (16)	C15—C14—H14A	120.0
O2—C7—C8	125.77 (16)	C10—C15—C14	120.59 (19)
C6—C7—C8	107.28 (13)	C10—C15—H15A	119.7
C7—C8—C9	106.95 (13)	C14—C15—H15A	119.7
C7—C8—H8A	110.3	O1—C16—H16A	109.5
C9—C8—H8A	110.3	O1—C16—H16B	109.5
C7—C8—H8B	110.3	H16A—C16—H16B	109.5
C9—C8—H8B	110.3	O1—C16—H16C	109.5
H8A—C8—H8B	108.6	H16A—C16—H16C	109.5
C10—C9—C1	113.98 (13)	H16B—C16—H16C	109.5
C6—C1—C2—C3	0.1 (2)	C6—C7—C8—C9	5.91 (18)
C9—C1—C2—C3	−177.78 (15)	C6—C1—C9—C10	129.44 (15)
C16—O1—C3—C2	0.6 (2)	C2—C1—C9—C10	−52.5 (2)
C16—O1—C3—C4	−179.31 (14)	C6—C1—C9—C8	5.19 (17)
C1—C2—C3—O1	−178.98 (14)	C2—C1—C9—C8	−176.77 (15)
C1—C2—C3—C4	0.9 (2)	C7—C8—C9—C10	−130.75 (15)
O1—C3—C4—C5	179.27 (14)	C7—C8—C9—C1	−6.57 (17)
C2—C3—C4—C5	−0.6 (2)	C1—C9—C10—C11	−47.9 (2)
C3—C4—C5—C6	−0.7 (2)	C8—C9—C10—C11	70.3 (2)
C2—C1—C6—C5	−1.4 (2)	C1—C9—C10—C15	132.82 (16)
C9—C1—C6—C5	176.78 (14)	C8—C9—C10—C15	−109.00 (18)
C2—C1—C6—C7	−179.85 (14)	C15—C10—C11—C12	0.8 (3)
C9—C1—C6—C7	−1.66 (18)	C9—C10—C11—C12	−178.50 (16)
C4—C5—C6—C1	1.7 (2)	C10—C11—C12—C13	0.1 (3)
C4—C5—C6—C7	179.80 (15)	C11—C12—C13—C14	−0.4 (3)
C1—C6—C7—O2	178.15 (16)	C12—C13—C14—C15	−0.2 (3)
C5—C6—C7—O2	−0.1 (3)	C11—C10—C15—C14	−1.4 (3)
C1—C6—C7—C8	−2.76 (18)	C9—C10—C15—C14	177.89 (16)
C5—C6—C7—C8	178.95 (16)	C13—C14—C15—C10	1.1 (3)
O2—C7—C8—C9	−174.98 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4A···O1^{i}	0.93	2.54	3.442 (2)	163
C5—H5A···O2^{ii}	0.93	2.50	3.344 (2)	151
C16—H16A···O2^{iii}	0.96	2.42	3.382 (2)	176

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

Fig. 1

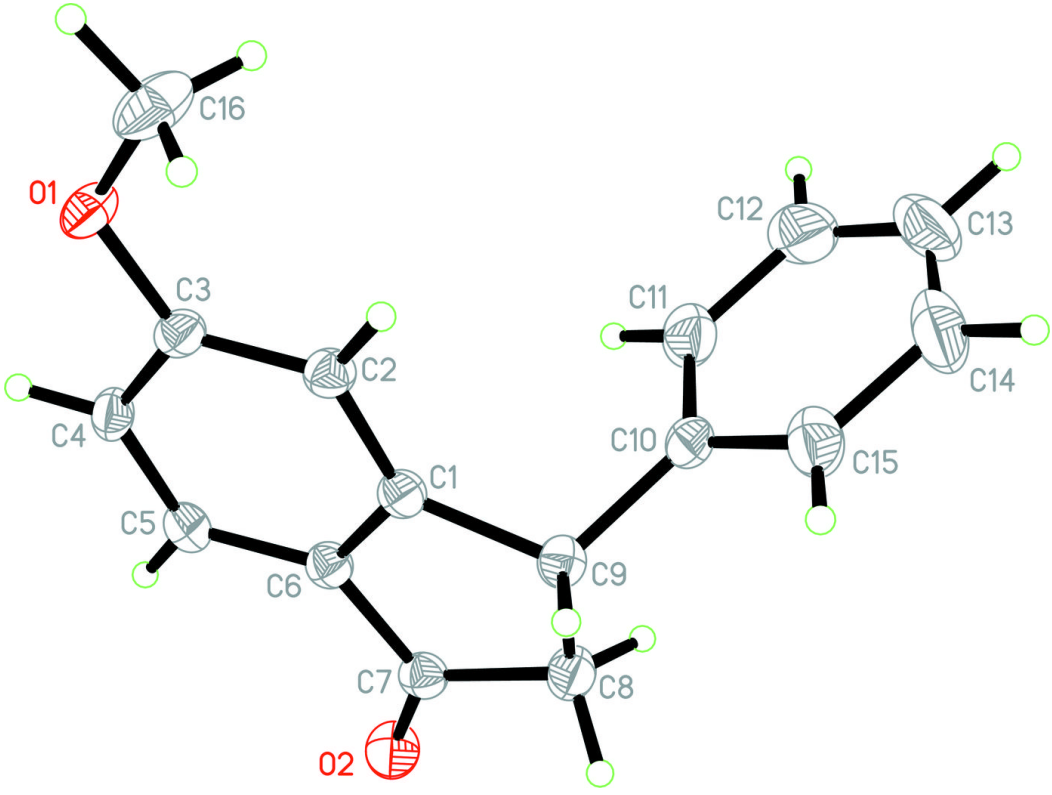

Fig. 2