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2-(4-Ethoxybenzyl)indan

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.005 Å
R factor = 0.089
wR factor = 0.211
Data-to-parameter ratio = 15.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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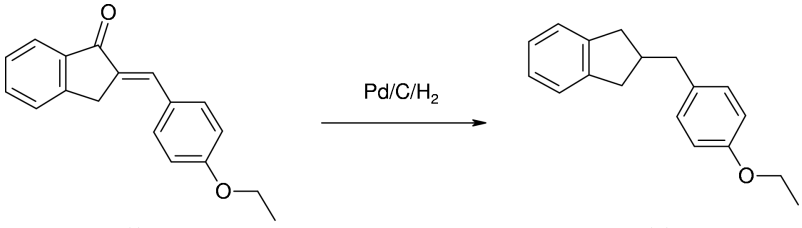
The title compound, $C_{18}H_{20}O$, arose as an unexpected hydrogenation product. All its geometrical parameters are normal and the crystal packing is controlled by van der Waals forces.

Comment

The title compound, (II), was prepared from 2-(4-ethoxybenzylidene)indan-1-one, (I), by catalytic hydrogenation over palladium/carbon. The usual product of this type of reaction is the benzylindanone (Ganellin *et al.*, 1967) or the benzylindanol (Cromwell & Ayer, 1960), but in this case there were no carbonyl or hydroxyl absorptions in the IR spectrum of (II). The ^{13}C NMR data suggested the benzylindan structure for (II), which was confirmed by the crystal structure determination described here.



(I) (II)

All the geometrical parameters for (II) (Fig. 1) lie within their expected ranges (Allen *et al.*, 1995). The five-membered ring (C10, C11, C12, C17 and C18) adopts an envelope conformation, with C10 at the flap position, displaced by 0.494 (7) Å from the least-squares plane through the other four C atoms [r.m.s. deviation = 0.006 Å and maximum = 0.007 (3) for C17]. There are no π–π interactions in (II) and the crystal packing is controlled by van der Waals forces (Fig. 2).

Experimental

A solution of 2-(4-ethoxybenzylidene)indan-1-one (0.12 g) (Watson *et al.*, 1993) in ethanol (10 ml) containing 10% Pd/C (0.04 g) was

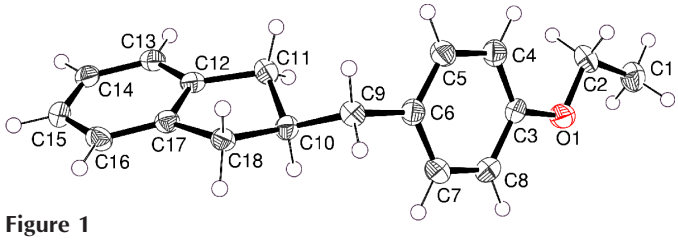


Figure 1
View of (II) (50% displacement ellipsoids and H atoms drawn as small spheres of arbitrary radius).

shaken under an atmosphere of hydrogen at 293 K for 6 h. Evaporation of the ethanol after removal of the catalyst gave (II) (0.08 g, 70%) as a colourless oil, which slowly solidified. It was recrystallized from ethyl acetate/hexane (1:4) to yield colourless crystals (m.p. 331–333 K). ^{13}C NMR (100 MHz): δ 14.9, 38.9, 40.7, 41.7, 63.4, 114.3, 124.5, 126.0, 129.7, 133.4, 143.3 and 157.2.

Crystal data

$C_{18}H_{20}O$	D_x = 1.193 Mg m^{-3}
M_r = 252.34	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3361 reflections
a = 16.5624 (12) Å	θ = 2.9–27.5°
b = 5.6290 (3) Å	μ = 0.07 mm^{-1}
c = 16.3266 (14) Å	T = 120 (2) K
β = 112.610 (4)°	Rod, colourless
V = 1405.14 (17) Å^3	0.22 × 0.06 × 0.04 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	1259 reflections with $I > 2\sigma(I)$
ω and φ scans	R_{int} = 0.256
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)	θ_{max} = 25.5°
T_{min} = 0.985, T_{max} = 0.997	$h = -20 \rightarrow 19$
15379 measured reflections	$k = -6 \rightarrow 6$
2604 independent reflections	$l = -19 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0752P)^2 + 0.112P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.089	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.211	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
S = 1.02	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
2604 reflections	Extinction correction: *SHELXL*97
174 parameters	Extinction coefficient: 0.023 (4)
H-atom parameters constrained	

Table 1
Selected torsion angles (°).

O1—C3—C4—C5	179.2 (4)	C4—C3—O1—C2	−5.5 (6)
C6—C9—C10—C18	172.3 (3)	C1—C2—O1—C3	−179.7 (4)
C6—C9—C10—C11	−67.5 (4)		

Diffraction quality was poor, as reflected in the very high merging R factor of 0.256 and the high proportion (52%) of 'unobserved' [$I < 2\sigma(I)$] reflections, even at 120 K. Merging equivalent reflections assuming only triclinic symmetry resulted in similar values for R_{int}. All H atoms were placed in calculated positions (C—H = 0.95–0.99 Å) and refined as riding on their carrier atoms. For all H atoms, the constraint U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C) was applied as appropriate. The methyl group was allowed to rotate about the C1—C2 bond as a rigid group.

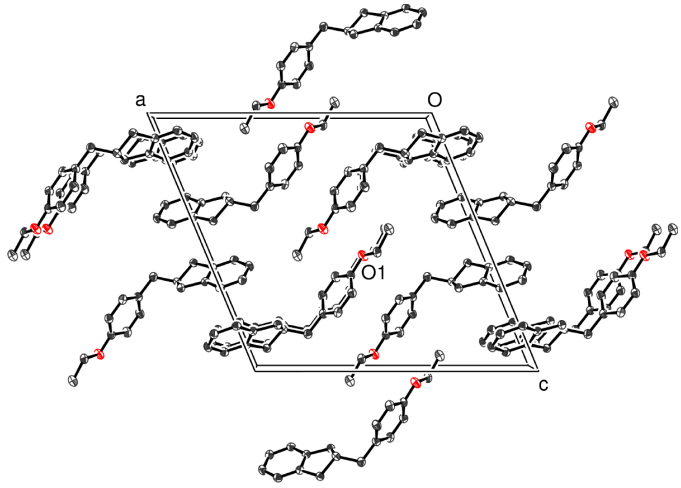


Figure 2
Unit-cell packing in (II), projected along the b axis, with all H atoms omitted for clarity.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997), *SCALEPACK* and *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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$V = 1405.14$ (17) Å^3
$Z = 4$
$F(000) = 544$
$D_x = 1.193$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3361 reflections
$\theta = 2.9$–27.5°
$\mu = 0.07$ mm^{-1}
$T = 120$ K
Rod, colourless
0.22 × 0.06 × 0.04 mm

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Radiation source: fine-focus sealed tube
Graphite monochromator
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Absorption correction: multi-scan (SADABS; Bruker, 1999)
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15379 measured reflections
2604 independent reflections
1259 reflections with $I > 2\sigma(I)$
$R_{int} = 0.256$
$\theta_{max} = 25.5°$, $\theta_{min} = 3.0°$
$h = -20 \rightarrow 19$
$k = -6 \rightarrow 6$
$l = -19 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.089$
$wR(F^2) = 0.211$
$S = 1.02$
2604 reflections
174 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0752P)^2 + 0.112P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.023 (4)

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.3190 (3)	0.0259 (8)	0.4491 (3)	0.0399 (13)
H1A	0.2825	−0.1172	0.4364	0.060*
H1B	0.3417	0.0489	0.4024	0.060*
H1C	0.2839	0.1640	0.4512	0.060*
C2	0.3947 (2)	−0.0021 (7)	0.5377 (3)	0.0338 (11)
H2A	0.3726	−0.0206	0.5857	0.041*
H2B	0.4295	−0.1445	0.5371	0.041*
C3	0.5209 (2)	0.2181 (6)	0.6295 (3)	0.0268 (10)
C4	0.5430 (2)	0.0529 (7)	0.6966 (3)	0.0295 (11)
H4	0.5063	−0.0803	0.6922	0.035*
C5	0.6207 (2)	0.0840 (7)	0.7718 (3)	0.0300 (11)
H5	0.6360	−0.0303	0.8181	0.036*
C6	0.6753 (2)	0.2753 (7)	0.7804 (3)	0.0275 (10)
C7	0.6505 (2)	0.4409 (7)	0.7118 (3)	0.0328 (12)
H7	0.6866	0.5757	0.7167	0.039*
C8	0.5749 (2)	0.4147 (7)	0.6366 (3)	0.0333 (12)
H8	0.5597	0.5291	0.5903	0.040*
C9	0.7600 (2)	0.3054 (7)	0.8602 (3)	0.0284 (11)
H9A	0.7593	0.1989	0.9082	0.034*
H9B	0.7638	0.4709	0.8819	0.034*
C10	0.8412 (2)	0.2505 (6)	0.8403 (3)	0.0259 (10)
H10	0.8375	0.3465	0.7874	0.031*
C11	0.8510 (2)	−0.0146 (6)	0.8193 (3)	0.0277 (11)
H11A	0.8307	−0.1215	0.8556	0.033*
H11B	0.8181	−0.0501	0.7557	0.033*
C12	0.9491 (2)	−0.0373 (6)	0.8442 (3)	0.0238 (10)
C13	0.9952 (2)	−0.2116 (7)	0.8208 (3)	0.0261 (10)
H13	0.9654	−0.3406	0.7840	0.031*
C14	1.0860 (2)	−0.1946 (7)	0.8520 (3)	0.0278 (11)
H14	1.1182	−0.3138	0.8365	0.033*
C15	1.1299 (2)	−0.0081 (6)	0.9051 (3)	0.0292 (11)
H15	1.1919	0.0006	0.9258	0.035*
C16	1.0835 (2)	0.1677 (6)	0.9283 (3)	0.0274 (11)
H16	1.1135	0.2980	0.9641	0.033*
C17	0.9930 (2)	0.1519 (6)	0.8990 (3)	0.0242 (10)

C18	0.9283 (2)	0.3113 (6)	0.9165 (3)	0.0244 (10)
H18A	0.9435	0.4808	0.9147	0.029*
H18B	0.9257	0.2761	0.9749	0.029*
O1	0.44753 (16)	0.2072 (5)	0.5520 (2)	0.0345 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.027 (2)	0.044 (3)	0.044 (3)	−0.0006 (19)	0.008 (2)	0.000 (2)
C2	0.025 (2)	0.039 (2)	0.037 (3)	−0.0065 (18)	0.013 (2)	−0.002 (2)
C3	0.023 (2)	0.025 (2)	0.032 (3)	0.0053 (17)	0.011 (2)	0.0022 (19)
C4	0.026 (2)	0.029 (2)	0.033 (3)	0.0004 (17)	0.011 (2)	−0.0025 (19)
C5	0.029 (2)	0.029 (2)	0.036 (3)	−0.0008 (17)	0.016 (2)	0.0003 (19)
C6	0.024 (2)	0.028 (2)	0.030 (3)	0.0016 (18)	0.0095 (19)	−0.0003 (19)
C7	0.026 (2)	0.030 (2)	0.039 (3)	−0.0053 (18)	0.009 (2)	0.001 (2)
C8	0.031 (2)	0.026 (2)	0.040 (3)	0.0046 (18)	0.012 (2)	0.0044 (19)
C9	0.026 (2)	0.028 (2)	0.032 (3)	−0.0009 (17)	0.012 (2)	0.0019 (19)
C10	0.023 (2)	0.025 (2)	0.026 (3)	−0.0005 (17)	0.0050 (18)	0.0014 (18)
C11	0.024 (2)	0.031 (2)	0.028 (3)	−0.0032 (17)	0.0099 (19)	−0.0008 (19)
C12	0.028 (2)	0.019 (2)	0.026 (2)	−0.0002 (16)	0.0120 (18)	0.0019 (17)
C13	0.030 (2)	0.023 (2)	0.024 (3)	−0.0028 (17)	0.0100 (19)	0.0018 (18)
C14	0.028 (2)	0.026 (2)	0.032 (3)	0.0037 (17)	0.014 (2)	0.0084 (19)
C15	0.022 (2)	0.030 (2)	0.034 (3)	0.0026 (18)	0.008 (2)	0.006 (2)
C16	0.028 (2)	0.024 (2)	0.028 (3)	−0.0068 (17)	0.008 (2)	−0.0029 (18)
C17	0.026 (2)	0.020 (2)	0.027 (3)	0.0006 (16)	0.0109 (19)	0.0006 (16)
C18	0.024 (2)	0.023 (2)	0.025 (3)	−0.0030 (16)	0.0082 (18)	0.0012 (17)
O1	0.0266 (15)	0.0303 (16)	0.038 (2)	−0.0045 (12)	0.0030 (14)	0.0048 (13)

Geometric parameters (Å, º)

C1—C2	1.514 (6)	C9—H9B	0.9900
C1—H1A	0.9800	C10—C18	1.538 (5)
C1—H1B	0.9800	C10—C11	1.554 (5)
C1—H1C	0.9800	C10—H10	1.0000
C2—O1	1.433 (4)	C11—C12	1.522 (5)
C2—H2A	0.9900	C11—H11A	0.9900
C2—H2B	0.9900	C11—H11B	0.9900
C3—C4	1.376 (6)	C12—C13	1.384 (5)
C3—O1	1.378 (5)	C12—C17	1.401 (5)
C3—C8	1.399 (5)	C13—C14	1.394 (5)
C4—C5	1.407 (5)	C13—H13	0.9500
C4—H4	0.9500	C14—C15	1.377 (5)
C5—C6	1.378 (5)	C14—H14	0.9500
C5—H5	0.9500	C15—C16	1.393 (5)
C6—C7	1.393 (6)	C15—H15	0.9500
C6—C9	1.512 (5)	C16—C17	1.389 (5)
C7—C8	1.384 (6)	C16—H16	0.9500
C7—H7	0.9500	C17—C18	1.508 (5)

C8—H8	0.9500	C18—H18A	0.9900
C9—C10	1.532 (5)	C18—H18B	0.9900
C9—H9A	0.9900		

C2—C1—H1A	109.5	C9—C10—C11	114.5 (3)
C2—C1—H1B	109.5	C18—C10—C11	104.3 (3)
H1A—C1—H1B	109.5	C9—C10—H10	107.8
C2—C1—H1C	109.5	C18—C10—H10	107.8
H1A—C1—H1C	109.5	C11—C10—H10	107.8
H1B—C1—H1C	109.5	C12—C11—C10	102.3 (3)
O1—C2—C1	107.4 (3)	C12—C11—H11A	111.3
O1—C2—H2A	110.2	C10—C11—H11A	111.3
C1—C2—H2A	110.2	C12—C11—H11B	111.3
O1—C2—H2B	110.2	C10—C11—H11B	111.3
C1—C2—H2B	110.2	H11A—C11—H11B	109.2
H2A—C2—H2B	108.5	C13—C12—C17	120.6 (3)
C4—C3—O1	124.9 (3)	C13—C12—C11	129.1 (3)
C4—C3—C8	120.2 (4)	C17—C12—C11	110.2 (3)
O1—C3—C8	114.9 (3)	C12—C13—C14	118.8 (4)
C3—C4—C5	119.0 (4)	C12—C13—H13	120.6
C3—C4—H4	120.5	C14—C13—H13	120.6
C5—C4—H4	120.5	C15—C14—C13	121.2 (4)
C6—C5—C4	122.0 (4)	C15—C14—H14	119.4
C6—C5—H5	119.0	C13—C14—H14	119.4
C4—C5—H5	119.0	C14—C15—C16	119.9 (4)
C5—C6—C7	117.5 (4)	C14—C15—H15	120.0
C5—C6—C9	122.0 (4)	C16—C15—H15	120.0
C7—C6—C9	120.4 (3)	C17—C16—C15	119.7 (3)
C8—C7—C6	121.9 (4)	C17—C16—H16	120.1
C8—C7—H7	119.1	C15—C16—H16	120.1
C6—C7—H7	119.1	C16—C17—C12	119.7 (4)
C7—C8—C3	119.3 (4)	C16—C17—C18	130.4 (3)
C7—C8—H8	120.3	C12—C17—C18	110.0 (3)
C3—C8—H8	120.3	C17—C18—C10	103.2 (3)
C6—C9—C10	113.2 (4)	C17—C18—H18A	111.1
C6—C9—H9A	108.9	C10—C18—H18A	111.1
C10—C9—H9A	108.9	C17—C18—H18B	111.1
C6—C9—H9B	108.9	C10—C18—H18B	111.1
C10—C9—H9B	108.9	H18A—C18—H18B	109.1
H9A—C9—H9B	107.7	C3—O1—C2	117.0 (3)
C9—C10—C18	114.2 (3)		

O1—C3—C4—C5	179.2 (4)	C17—C12—C13—C14	−0.6 (6)
C8—C3—C4—C5	−0.5 (6)	C11—C12—C13—C14	−179.9 (4)
C3—C4—C5—C6	0.2 (6)	C12—C13—C14—C15	−0.2 (6)
C4—C5—C6—C7	0.6 (6)	C13—C14—C15—C16	0.0 (6)
C4—C5—C6—C9	−178.3 (4)	C14—C15—C16—C17	1.0 (6)
C5—C6—C7—C8	−1.1 (7)	C15—C16—C17—C12	−1.8 (6)

C9—C6—C7—C8	177.9 (4)	C15—C16—C17—C18	177.9 (4)
C6—C7—C8—C3	0.8 (7)	C13—C12—C17—C16	1.6 (6)
C4—C3—C8—C7	0.0 (6)	C11—C12—C17—C16	−178.9 (4)
O1—C3—C8—C7	−179.6 (4)	C13—C12—C17—C18	−178.2 (4)
C5—C6—C9—C10	105.4 (5)	C11—C12—C17—C18	1.3 (5)
C7—C6—C9—C10	−73.5 (5)	C16—C17—C18—C10	160.0 (4)
C6—C9—C10—C18	172.3 (3)	C12—C17—C18—C10	−20.3 (4)
C6—C9—C10—C11	−67.5 (4)	C9—C10—C18—C17	156.4 (3)
C9—C10—C11—C12	−155.2 (3)	C11—C10—C18—C17	30.6 (4)
C18—C10—C11—C12	−29.6 (4)	C4—C3—O1—C2	−5.5 (6)
C10—C11—C12—C13	−162.6 (4)	C8—C3—O1—C2	174.1 (4)
C10—C11—C12—C17	18.0 (4)	C1—C2—O1—C3	−179.7 (4)