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2-(4-Ethoxybenzyl)indan

Alan B. Turner and William T. A. Harrison*

Department of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, Scotland

Correspondence e-mail:
w.harrison@abdn.ac.uk

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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.

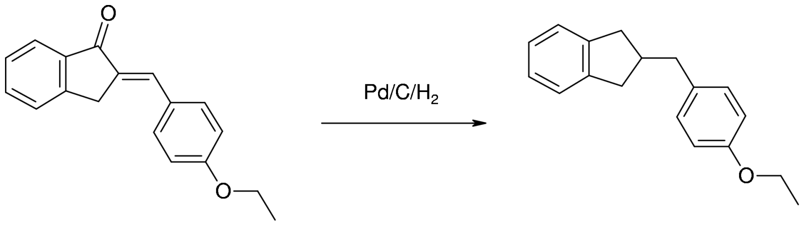
Key indicators

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.

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

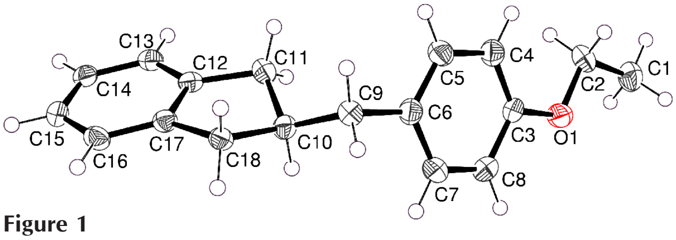


Figure 1
View of (II) (50% displacement ellipsoids and H atoms drawn as small spheres of arbitrary radius).

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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

$C_{18}H_{20}O$
$M_r = 252.34$
Monoclinic, $P2_1/c$
$a = 16.5624\ (12)$ Å
$b = 5.6290\ (3)$ Å
$c = 16.3266\ (14)$ Å
$\beta = 112.610\ (4)^\circ$
$V = 1405.14\ (17)$ Å^3
$Z = 4$

$D_x = 1.193$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3361 reflections
$\theta = 2.9$–27.5°
$\mu = 0.07$ mm^{-1}
$T = 120\ (2)$ K
Rod, colourless
0.22 × 0.06 × 0.04 mm

Data collection

Nonius KappaCCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{\min} = 0.985$, $T_{\max} = 0.997$
15379 measured reflections
2604 independent reflections

1259 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.256$
$\theta_{\max} = 25.5^\circ$
$h = -20 \rightarrow 19$
$k = -6 \rightarrow 6$
$l = -19 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.089$
$wR(F^2) = 0.211$
$S = 1.02$
2604 reflections
174 parameters
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: *SHELXL*97
Extinction coefficient: 0.023 (4)

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 $R_{\rm int}$. 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 $U_{\rm iso}(\rm H) = 1.2U_{\rm eq}(\rm C)$ or $1.5U_{\rm eq}$(methyl C) was applied as appropriate. The methyl group was allowed to rotate about the C1—C2 bond as a rigid group.

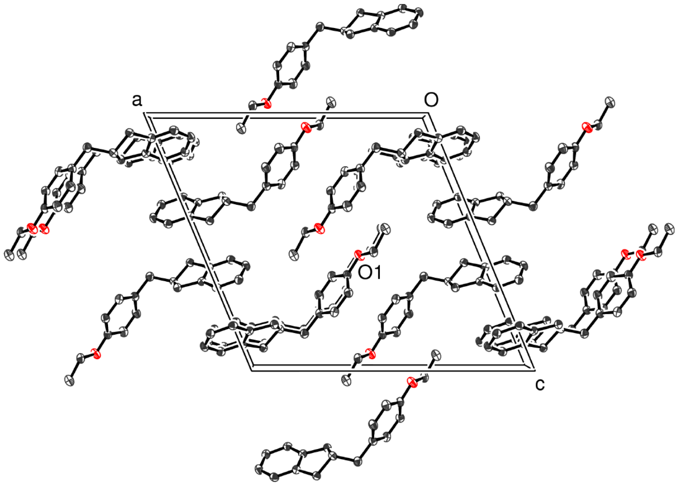

Figure 2
Unit-cell packing in (II), projected along the b axis, with all H atoms omitted for clarity.

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.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1995). *International Tables for Crystallography*, Vol. C, section 9. 5, pp. 685–706. Dordrecht: Kluwer Academic Publishers.

Bruker (1999). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.

Cromwell, W. H. & Ayer, R. P. (1960). *J. Am. Chem. Soc.* **82**, 133–141.

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.

Ganellin, C. R., Loynes, J. M., Ridley, H. F. & Spickett, R. G. W. (1967). *J. Med. Chem.* **10**, 826–833.

Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.

Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr and R. M. Sweet, pp. 307–326. New York: Academic Press.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

Watson, G. J. R., Turner, A. B. & Allen, S. (1993). *Organic Materials for Non-linear Optics* III, edited by G. J. Ashwell and D. Bloor, RSC Special Publication No. 137, pp. 112–117. London: Royal Society of Chemistry.