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7-(Hydroxymethyl)-1a,7b-dihydro-1*H*-cyclopropa[*a*]naphthalene

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Key indicators

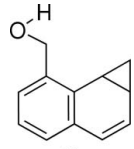
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.006 Å
R factor = 0.058
wR factor = 0.168
Data-to-parameter ratio = 13.1

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

In the title compound, $C_{12}H_{12}O$, the cyclopropane ring makes a dihedral angle of 73.1 (2)° with the naphthalene ring system.

Comment

Reduction of 1,8-naphthoic anhydride with lithium aluminium hydride has been used by a number of investigators as a source of 1,8-bis(hydroxymethyl)naphthalene (Beyler & Sarett, 1952; Bockelheide & Vick, 1956; Trost, 1967; Cason *et al.*, 1973). We attempted to react naphthalene-1,8-dicarboxylic anhydride with lithium aluminium hydride in tetrahydrofuran in one step to give 1,8-bis(hydroxymethyl)naphthalene, but instead compound (I) was obtained. We here report the crystal structure of the title compound, (I).



(I)

Bond lengths and angles in (I) are normal (Table 1). The dihedral angle between the C1–C10 and C7/C8/C11 planes is 73.1 (2)° (Fig. 1).

Experimental

Compound (I) was prepared according to the reported precedure of Popovici-Müller & Spencer (1997). Yellow single crystals suitable for X-ray diffraction were obtained by recrystallization from absolute ethanol.

Crystal data

$C_{12}H_{12}O$
M_r = 172.22
Tetragonal, $I4_1/a$
a = 20.373 (3) Å
c = 8.618 (2) Å
V = 3577.0 (11) Å^3
Z = 16
D_x = 1.279 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 22 reflections
θ = 4.4–7.6°
μ = 0.08 mm^{-1}
T = 292 (2) K
Block, yellow
0.25 × 0.25 × 0.22 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
1722 measured reflections
1601 independent reflections
628 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.2°
$h = 0 \rightarrow 24$
$k = 0 \rightarrow 24$
$l = 0 \rightarrow 10$
3 standard reflections
every 300 reflections
intensity decay: 0.2%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0786P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.058$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.168$	$\Delta\rho_{max} = 0.17$ e Å^{-3}
$S = 0.92$	$\Delta\rho_{min} = -0.16$ e Å^{-3}
1601 reflections	Extinction correction: *SHELXL97*
122 parameters	Extinction coefficient: 0.0013 (8)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O1—C12	1.413 (4)	C7—C8	1.510 (5)
C1—C9	1.392 (5)	C8—C9	1.479 (5)
C1—C12	1.478 (5)	C8—C11	1.481 (5)
C7—C11	1.494 (5)		
C11—C7—C8	59.1 (2)	C8—C11—C7	61.0 (3)
C8—C7—H7	116.8	O1—C12—C1	113.1 (3)

The H atoms were placed in calculated positions, with C—H = 0.93–0.98 Å and O—H = 0.82 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = U_{eq}(C,O)$.

Data collection: *DIFRAC* (Gabe *et al.*, 1995); cell refinement: *DIFRAC*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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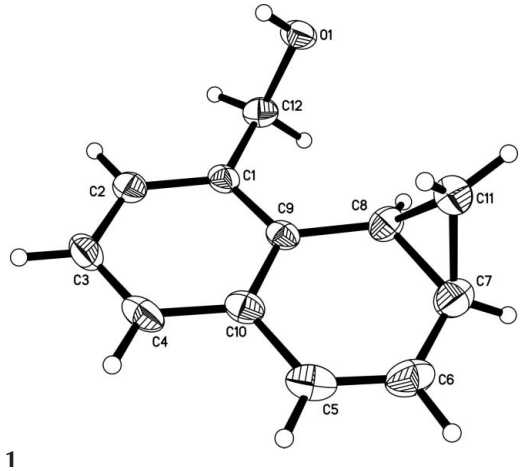

Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering.

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