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Naphthalen-1-ylmethanol

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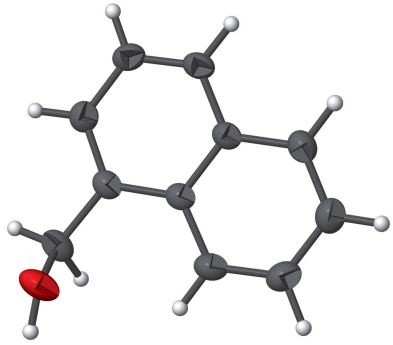
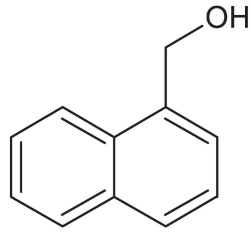
Structural data: full structural data are available from iucrdata.iucr.org

Apart from the OH group, the molecule of the title compound, $C_{11}H_{10}O$, is almost planar with all carbon atoms located within 0.03 Å of their mean plane. In the crystal, the molecules are linked by O—H···O hydrogen bonds, generating infinite chains running parallel to the [100] direction.

3D view



Chemical scheme



Structure description

The title compound, $C_{11}H_{10}O$, was first prepared by reduction of the corresponding naphthylamide (West, 1920) and by Grignard reaction involving formaldehyde (Ziegler, 1921). It is available commercially.

The title compound (Fig. 1) exhibits standard bond lengths and angles. Apart from the OH group, the molecule is almost planar: all carbon atoms are located within 0.03 Å of their mean plane and all aromatic hydrogen atoms are also within 0.04 Å of the same plane. Atom O1 is displaced from the mean plane of the other non-hydrogen atoms (r.m.s. deviation = 0.029 Å) by −1.260 (1) Å.

In the crystal, the 1-naphthalenemethanol molecules are linked by O1—H1···O1^{i} hydrogen bonds (Table 1, Fig. 2), generating infinite *C*(2) chains propagating parallel to the [100] direction: adjacent molecules in a chain are related by *a*-glide symmetry. Similar chains were observed in 1-naphthaleneethanol (Garozzo & Nazarenko, 2016). Additional C—H···C(ar) contacts involving the H4 hydrogen atom and C5 and C4 carbon atoms of another chain help to assemble the chains into a weakly bound layer lying parallel to the (010) plane (Fig. 2). These layers are held together by van der Waals forces, forming a molecular crystal.

Difference electron density maps (Fig. 3) show visible positive density at all covalent bonds and at the lone pair area of the oxygen atom. This effect comes from the limitations of the independent atom model; it results, among other shortcomings, in inflated *R* values and uncertainties of bonding parameters. Application of the Hirshfeld atom refinement

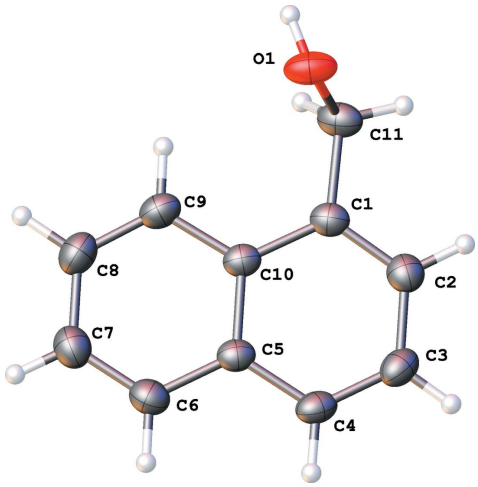


Figure 1
The molecular structure of the title compound with 50% displacement elipsoids.

with *HARt* (Fugel *et al.*, 2018) to the same dataset yields a lower $R(F)$ of 0.036 and significantly lower uncertainties for the bond lengths and angles.

Synthesis and crystallization

The title compound is commercially available from Aldrich. Recrystallization from ethanol solution yields needle-like crystals, which were used in the current study.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2

Acknowledgements

Financial support from the State University of New York for acquisition and maintenance of the X-ray diffractometer is gratefully acknowledged.

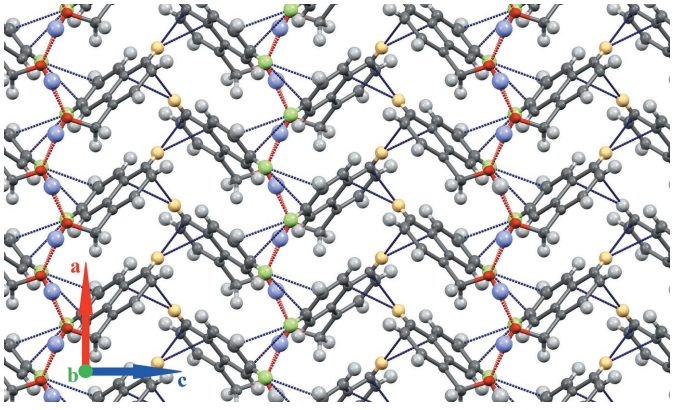


Figure 2
Packing of 1-naphthalenemethanol molecules viewed along the [010] vector. Hydrogen bonds are red, contacts shorter than sum of van der Waals radii are blue. Highlighted hydrogen atoms: H1 (pale blue), H4 (yellow), H8 (green).

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O1^{i}	0.90 (2)	1.87 (2)	2.7504 (8)	166 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{11}H_{10}O$
M_r	158.19
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	173
a, b, c (Å)	4.9306 (1), 15.7882 (5), 21.0651 (6)
V (Å^3)	1639.82 (8)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.08
Crystal size (mm)	0.58 × 0.12 × 0.1
Data collection	
Diffractometer	Bruker PHOTON-100 CMOS
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.797, 0.862
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38547, 2860, 2146
R_{int}	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.747
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.144, 1.04
No. of reflections	2860
No. of parameters	149
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.14

Computer programs: *APEX2* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2020).

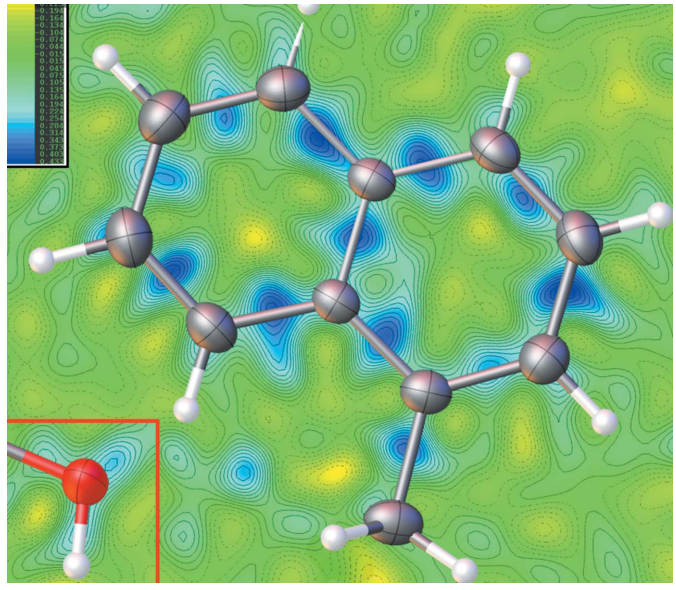


Figure 3
Difference map in the plane of the naphthalene ring system (left lower corner: lone pair area of hydroxyl group).

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full crystallographic data

IUCrData (2020). **5**, x201646 [https://doi.org/10.1107/S2414314620016466]

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Crystal data

$C_{11}H_{10}O$
M_r = 158.19
Orthorhombic, *Pbca*
a = 4.9306 (1) Å
b = 15.7882 (5) Å
c = 21.0651 (6) Å
V = 1639.82 (8) Å^3
Z = 8
F(000) = 672
D_x = 1.282 Mg m^{-3}
Melting point: 333 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9897 reflections
θ = 3.2–32.0°
μ = 0.08 mm^{-1}
T = 173 K
Needle, colourless
0.58 × 0.12 × 0.1 mm

Data collection

Bruker PHOTON-100 CMOS diffractometer
Radiation source: sealedtube
Graphite monochromator
Detector resolution: 10.8 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.797, T_{max} = 0.862
38547 measured reflections
2860 independent reflections
2146 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 32.1°, θ_{min} = 3.2°
h = −7→7
k = −23→23
l = −31→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.144
S = 1.03
2860 reflections
149 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0706P)^2 + 0.4678P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.64002 (18)	0.45528 (6)	0.27894 (4)	0.0398 (2)
H1	0.788 (5)	0.4551 (11)	0.2541 (10)	0.068 (5)*
C1	0.5128 (2)	0.39728 (7)	0.38094 (5)	0.0288 (2)
C2	0.3861 (2)	0.43905 (7)	0.42978 (5)	0.0330 (2)
H2	0.441 (3)	0.4976 (9)	0.4386 (7)	0.041 (4)*
C3	0.1852 (3)	0.39961 (8)	0.46739 (6)	0.0352 (3)
H3	0.102 (3)	0.4281 (10)	0.5013 (8)	0.045 (4)*
C4	0.1114 (2)	0.31785 (7)	0.45523 (5)	0.0325 (2)
H4	−0.027 (3)	0.2898 (9)	0.4812 (7)	0.042 (4)*
C5	0.2393 (2)	0.27146 (7)	0.40600 (5)	0.0276 (2)
C6	0.1723 (3)	0.18527 (7)	0.39480 (6)	0.0344 (3)
H6	0.027 (3)	0.1588 (9)	0.4205 (7)	0.044 (4)*
C7	0.3045 (3)	0.13985 (8)	0.34904 (6)	0.0388 (3)
H7	0.259 (4)	0.0829 (11)	0.3412 (8)	0.050 (4)*
C8	0.5083 (3)	0.17819 (8)	0.31230 (6)	0.0390 (3)
H8	0.607 (3)	0.1454 (10)	0.2784 (8)	0.050 (4)*
C9	0.5750 (2)	0.26132 (8)	0.32101 (5)	0.0336 (3)
H9	0.714 (3)	0.2873 (10)	0.2953 (7)	0.046 (4)*
C10	0.4438 (2)	0.31084 (7)	0.36840 (5)	0.0268 (2)
C11	0.7284 (2)	0.44171 (8)	0.34298 (6)	0.0349 (3)
H11A	0.777 (3)	0.4958 (10)	0.3634 (7)	0.041 (4)*
H11B	0.902 (3)	0.4052 (9)	0.3427 (7)	0.039 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0254 (4)	0.0620 (6)	0.0319 (4)	−0.0028 (4)	−0.0007 (3)	0.0145 (4)
C1	0.0253 (5)	0.0341 (5)	0.0268 (5)	−0.0015 (4)	−0.0036 (4)	0.0049 (4)
C2	0.0366 (6)	0.0322 (5)	0.0302 (5)	0.0010 (4)	−0.0043 (4)	0.0021 (4)
C3	0.0399 (6)	0.0387 (6)	0.0270 (5)	0.0087 (5)	0.0027 (4)	0.0012 (4)
C4	0.0319 (5)	0.0382 (6)	0.0274 (5)	0.0040 (4)	0.0043 (4)	0.0070 (4)
C5	0.0258 (5)	0.0323 (5)	0.0248 (5)	0.0015 (4)	−0.0012 (4)	0.0056 (4)
C6	0.0354 (6)	0.0333 (5)	0.0343 (6)	−0.0024 (4)	−0.0009 (4)	0.0059 (4)
C7	0.0451 (7)	0.0328 (6)	0.0384 (6)	−0.0006 (5)	−0.0041 (5)	−0.0004 (5)
C8	0.0408 (6)	0.0422 (6)	0.0339 (6)	0.0070 (5)	0.0014 (5)	−0.0049 (5)
C9	0.0285 (5)	0.0433 (6)	0.0290 (5)	0.0017 (4)	0.0020 (4)	0.0011 (4)
C10	0.0231 (4)	0.0330 (5)	0.0242 (4)	0.0014 (4)	−0.0023 (3)	0.0039 (4)
C11	0.0285 (5)	0.0441 (6)	0.0320 (5)	−0.0072 (5)	−0.0046 (4)	0.0072 (5)

Geometric parameters (Å, º)

O1—H1	0.90 (2)	C5—C10	1.4252 (14)
O1—C11	1.4338 (14)	C6—H6	0.989 (17)
C1—C2	1.3724 (16)	C6—C7	1.3669 (18)
C1—C10	1.4310 (15)	C7—H7	0.940 (17)

C1—C11	1.5039 (16)	C7—C8	1.4054 (19)
C2—H2	0.980 (15)	C8—H8	1.006 (17)
C2—C3	1.4131 (17)	C8—C9	1.3653 (18)
C3—H3	0.939 (16)	C9—H9	0.965 (16)
C3—C4	1.3654 (17)	C9—C10	1.4232 (16)
C4—H4	0.981 (15)	C11—H11A	0.986 (16)
C4—C5	1.4174 (15)	C11—H11B	1.032 (16)
C5—C6	1.4201 (16)		

C11—O1—H1	107.5 (14)	C6—C7—H7	120.8 (11)
C2—C1—C10	119.25 (10)	C6—C7—C8	120.22 (11)
C2—C1—C11	119.75 (10)	C8—C7—H7	119.0 (11)
C10—C1—C11	120.97 (10)	C7—C8—H8	121.0 (9)
C1—C2—H2	118.0 (9)	C9—C8—C7	120.80 (11)
C1—C2—C3	121.85 (11)	C9—C8—H8	118.2 (9)
C3—C2—H2	120.1 (9)	C8—C9—H9	120.3 (9)
C2—C3—H3	121.5 (10)	C8—C9—C10	120.87 (11)
C4—C3—C2	119.88 (11)	C10—C9—H9	118.8 (10)
C4—C3—H3	118.6 (10)	C5—C10—C1	118.78 (10)
C3—C4—H4	120.5 (9)	C9—C10—C1	123.06 (10)
C3—C4—C5	120.48 (11)	C9—C10—C5	118.14 (10)
C5—C4—H4	119.0 (9)	O1—C11—C1	110.79 (9)
C4—C5—C6	120.88 (10)	O1—C11—H11A	110.7 (9)
C4—C5—C10	119.74 (10)	O1—C11—H11B	109.3 (8)
C6—C5—C10	119.36 (10)	C1—C11—H11A	110.1 (9)
C5—C6—H6	118.8 (9)	C1—C11—H11B	109.2 (9)
C7—C6—C5	120.60 (11)	H11A—C11—H11B	106.5 (13)
C7—C6—H6	120.6 (9)		

C1—C2—C3—C4	−0.39 (18)	C6—C5—C10—C9	−0.45 (15)
C2—C1—C10—C5	1.81 (15)	C6—C7—C8—C9	−0.9 (2)
C2—C1—C10—C9	−176.55 (10)	C7—C8—C9—C10	1.34 (19)
C2—C1—C11—O1	−113.15 (12)	C8—C9—C10—C1	177.73 (11)
C2—C3—C4—C5	1.44 (17)	C8—C9—C10—C5	−0.64 (17)
C3—C4—C5—C6	177.24 (11)	C10—C1—C2—C3	−1.25 (17)
C3—C4—C5—C10	−0.83 (16)	C10—C1—C11—O1	69.09 (14)
C4—C5—C6—C7	−177.20 (11)	C10—C5—C6—C7	0.88 (17)
C4—C5—C10—C1	−0.80 (15)	C11—C1—C2—C3	−179.05 (10)
C4—C5—C10—C9	177.65 (10)	C11—C1—C10—C5	179.58 (9)
C5—C6—C7—C8	−0.22 (19)	C11—C1—C10—C9	1.22 (16)
C6—C5—C10—C1	−178.90 (10)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O1^{i}	0.90 (2)	1.87 (2)	2.7504 (8)	166 (2)

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