

2-Naphthalenol

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Key indicators

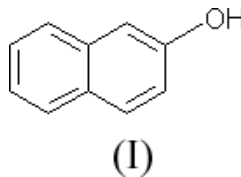
Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$
 R factor = 0.045
 wR factor = 0.093
Data-to-parameter ratio = 8.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the solid state, the non-centrosymmetric structure of the title compound, $\text{C}_{10}\text{H}_8\text{O}$, is stabilized both by van der Waals interactions and by $\text{O}-\text{H}\cdots\text{O}$ intermolecular hydrogen bonds. These hydrogen bonds link every molecule with two neighbouring non-equivalent molecules, forming chains. The asymmetric unit contains two molecules, which are related to each other by a pseudo-inversion centre.

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Comment

Because of potentially high non-linearities and a rapid response in electro-optic effects that often far surpasses those of inorganic non-linear optical (NLO) materials, some polar organic crystals which form non-centrosymmetric crystal structures are of much current interest (Babu *et al.*, 2002; Perumal *et al.*, 2002; Vijayan *et al.*, 2002; Tsunesada *et al.*, 2002; Rajendran *et al.*, 2001; Pal *et al.*, 2002). Although such properties have not been confirmed experimentally in the case of 2-naphthalenol, (I), the previous crystal structure analysis of this compound, performed with the aid of optical transforms (Watson & Hargreaves, 1958), showed that it crystallizes in the monoclinic non-centrosymmetric space group Ia , with $a = 8.185\text{ \AA}$, $b = 5.950\text{ \AA}$, $c = 36.29\text{ \AA}$ and $\beta = 119.52^\circ$. This indicates that the polar 2-naphthalenol crystals may be treated as a potential organic NLO material. The non-centrosymmetric crystal structure of this compound was, however, only partially solved by two-dimensional Fourier calculations, using X-ray photographic data. New single-crystal X-ray diffraction data obtained by us fully confirm that the structure of (I) is non-centrosymmetric, although we have used the alternative space group setting Cc , because of the smaller β angle this entails.



The unit cell of (I) contains eight molecules, occupying two non-equivalent sets of general positions. Sets of equivalent molecules stack in sheets perpendicular to the a axis, and each of these molecules is linked to two neighbouring non-equivalent molecules through $\text{O}-\text{H}\cdots\text{O}$ intermolecular hydrogen bonds (see Table 1 for details). The two molecules in the asymmetric unit are related to each other by pseudo-inversion symmetry.

A metastable modification of this compound, which is isomorphous with naphthalene, has been reported by Coppens & Hairfield (1965).

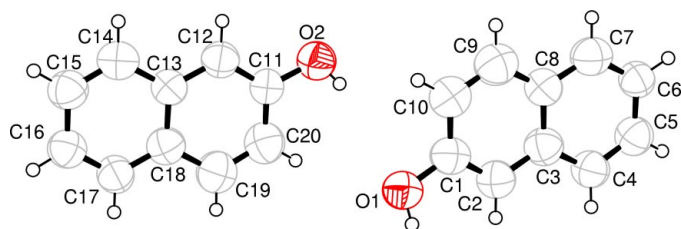


Figure 1
The asymmetric unit, with atom labels and 50% probability displacement ellipsoids.

Experimental

As a starting material we used analytically pure, commercially available 2-naphthalenol (POCH, Poland), in which five major impurities (1,1'-bi-2-naphthol, oleic acid amide, methylnaphthol, 5(12*H*)-naphthacenone and binaphthacenone) were detected and identified using gas chromatography. Analyses were performed on a Hewlett Packard 6890 GC System gas chromatograph with an FID detector (fused silica capillary column of dimensions 30 × 0.32 mm I. D.; an HP1 methyl silicone stationary phase; cool on column type injector; helium as a carrier gas). For the identification of these impurities, we also used a Hewlett Packard 5890 series II gas chromatograph equipped with MS detection, which operated under nearly the same conditions. The GC–FID analysis of a chloroform-extracted sample prepared from the commercial 2-naphthalenol has shown that its total purity is 99.49%. To remove the detected impurities, the starting material was pre-purified by twofold crystallization from anhydrous ethanol, and then two-stage zone purification was performed with the help of a multistage zone refiner (100 passages of the molten zone with a rate of 10 mm h⁻¹ in the first, and 5 mm h⁻¹ in the second stage; spectrally pure nitrogen as an inert gas). The total impurity content in the material collected from the central and upper parts of the zone-melted ingots was <0.001% by mass. Single crystals were grown from a nucleated spontaneously supercooled solution in chloroform at a constant temperature of 307 K, in an apparatus described previously by Marciniak (2002).

Crystal data

C ₁₀ H ₈ O	$D_x = 1.263 \text{ Mg m}^{-3}$
$M_r = 144.16$	Mo $K\alpha$ radiation
Monoclinic, Cc	Cell parameters from 30 reflections
$a = 32.074 (6) \text{ \AA}$	$\theta = 1.2\text{--}28.0^\circ$
$b = 5.931 (1) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 8.127 (2) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 101.18 (3)^\circ$	Needle, pale yellow
$V = 1516.7 (5) \text{ \AA}^3$	$0.40 \times 0.06 \times 0.03 \text{ mm}$
$Z = 8$	

Data collection

DARCH-1 diffractometer	$R_{\text{int}} = 0.020$
ω -2 θ scans	$\theta_{\text{max}} = 27.5^\circ$
Absorption correction: refined from ΔF (DIFABS; Walker & Stuart, 1983)	$h = -41 \rightarrow 40$
$T_{\text{min}} = 0.958$, $T_{\text{max}} = 0.998$	$k = -7 \rightarrow 7$
1875 measured reflections	$l = 0 \rightarrow 10$
1744 independent reflections	3 standard reflections
1339 reflections with $I > 2\sigma(I)$	frequency: 120 min
	intensity decay: 5%

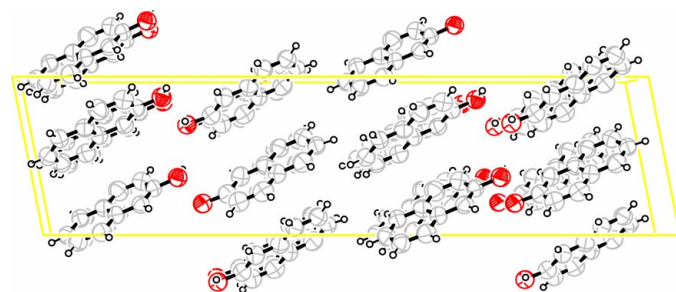


Figure 2
The crystal packing, viewed along the b axis.

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.045$	$w = 1/[\sigma^2(F_o^2) + (0.0121P)^2]$
$wR(F^2) = 0.093$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.30$	$(\Delta/\sigma)_{\text{max}} = 0.007$
1744 reflections	$\Delta\rho_{\text{max}} = 0.09 \text{ e \AA}^{-3}$
204 parameters	$\Delta\rho_{\text{min}} = -0.14 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bonding geometry (\AA , $^\circ$).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
$O1\text{---}H1\cdots O2^i$	0.82	2.14	2.764 (3)	133
$O2\text{---}H2A\cdots O1^{ii}$	0.82	2.45	2.752 (3)	103

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

H atoms were constrained with a riding model, including torsional freedom of OH groups.

Data collection: *DARCH* package (Burevestnik, 1991); cell refinement: *DARCH* package; data reduction: *DARCH* package; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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