Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Redetermination of 1-naphthalenol

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.112
Data-to-parameter ratio = 16.6

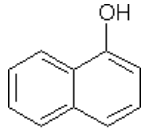
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 2 April 2004
Accepted 19 April 2004
Online 30 April 2004

In the solid state, the centrosymmetric structure of 1-naphthalenol, $C_{10}H_8O$, is stabilized by both van der Waals interactions and intermolecular O—H···O hydrogen bonds. The molecules are linked through hydrogen bonds, each of length 2.798 (1) Å, into chains which are parallel to the symmetry axis.

Comment

1-Naphthalenol, (I), is particularly important both as a synthetic precursor of the insecticide Sevin and the pesticide Dervinol (Allen *et al.*, 1997; Ortega-Algar *et al.*, 2003), and as an starting material in the synthesis of inderal, also known as Propranolol, which is an adrenergic beta blocker and widely used in the treatment of cardiovascular disorders and hypertension (Wu *et al.*, 2001; Kumamoto *et al.*, 2001). It is also well known for its use in the synthesis of *N*-phenyl-1-naphthylamine, as well as sodium 1-naphthol-4-sulfonate and hydroxy-2-naphthoic acid, which are used as a rubber antioxidant and in the manufacture of a novolac-type photoresist and dyestuff, respectively.



(I)

The first published structure determination of this compound was by Kitaijgorodskij (1945, 1949), whose analysis gave the coordinates of the centre of the naphthalene ring system and the orientation of the molecule. He suggested that there was strong bonding between the hydroxyl groups, with an O···O separation of 2.54 Å. Nearly 15 years later, the crystal structure analysis of (I), performed with the aid of X-ray photographic methods (Robinson & Hargreaves, 1964), showed that it crystallizes in the monoclinic space group $P2_1/a$, with a = 13.20, b = 4.78 and c = 13.20 Å, and β = 117.3°. Moreover, this later examination showed that both the arrangement of the molecules and the hydrogen-bond length (2.79 Å) differ significantly from those proposed by Kitaijgorodskij.

A new single-crystal study of (I), based on X-ray diffraction data obtained by the present authors, fully confirms the arrangment of molecules established by Robinson & Hargreaves. The unit cell of (I), oriented in the standard space group $P2_1/c$, contains four molecules occupying one set of general positions. These molecules are linked, *via* inter-

molecular O—H···O hydrogen bonds (Table 1), into chains running along the *b* axis.

Experimental

Crystals of 1-naphthalenol (purchased from Sigma at 99% purity) were grown from a solution in ethanol by slow evaporation of the solvent at a constant temperature of 293 K. During X-ray measurements, the crystal was held in a capillary tube to reduce its sublimation.

Crystal data

$C_{10}H_8O$
M_r = 144.16
Monoclinic, $P2_1/c$
a = 13.171 (2) Å
b = 4.798 (1) Å
c = 13.276 (3) Å
β = 117.12 (2)°
V = 746.7 (3) Å^3
Z = 4
D_x = 1.282 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 5–20°
μ = 0.08 mm^{-1}
T = 293 (2) K
Plate, white
0.52 × 0.25 × 0.07 mm

Data collection

Kuma KM-4 diffractometer
ω–2θ scans
Absorption correction: refined from ΔF (*DIFABS*; Walker & Stuart, 1983)
T_{min} = 0.974, T_{max} = 0.996
3416 measured reflections
1708 independent reflections
1197 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 27.5°
$h = -17 \rightarrow 17$
$k = -6 \rightarrow 6$
$l = -16 \rightarrow 16$
3 standard reflections
every 100 reflections
intensity decay: negligible

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.113
S = 1.02
1708 reflections
103 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0217P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O1^{i}	0.82	1.99	2.798 (1)	170

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

The positions of the H atoms were calculated and refined using *SHELXL*97 constraints (Sheldrick, 1997)

Data collection: *KM4B*8 software (Gałdecki *et al.*, 1996); cell refinement: *KM4B*8 software; data reduction: *KM4B*8 software; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1997) and *PLATON* (Spek, 2000); software used to prepare material for publication: *SHELXL*97.

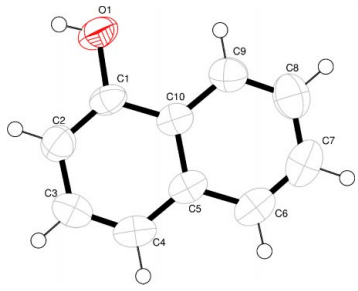


Figure 1
The molecule of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

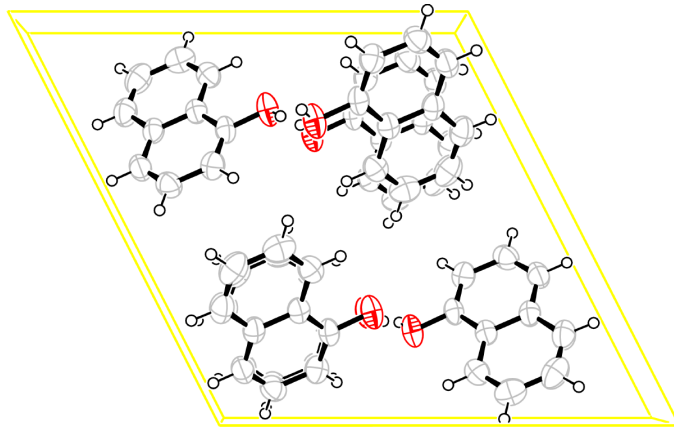


Figure 2
The unit cell contents of (I), viewed along *b*.

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