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Naphthalene-2,7-diol

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.038
wR factor = 0.121
Data-to-parameter ratio = 8.6

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

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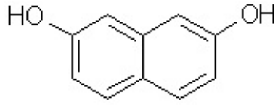
In the solid state, the structure of the title compound, $C_{10}H_8O_2$, is stabilized by both van der Waals interactions and O—H···O intermolecular hydrogen bonds with O···O distances of 2.714 (3) and 2.831 (4) Å.

Comment

Dihydroxynaphthalene derivatives are a class of intermediates important for applications in dye synthesis (Bianchi *et al.*, 1997) or as monomers in the preparation of polymers, such as polyesters (Blundell & Buckingham, 1985; Aitken *et al.*, 1992) and polynaphthooxazines (Shen & Ishida, 1996). The title compound, alternatively known as 2,7-dihydroxynaphthalene, (I), is especially important as a substrate in the Pechmann synthesis of benzochrome and benzocoumarins (Kolancilar, 2002).



(I)

To the best of our knowledge, there are reports concerning the crystal and molecular structures of only four dihydroxynaphthalene isomers, namely, 1,5-, 2,3- and 2,6-dihydroxynaphthalene (Belskii *et al.*, 1990), and 1,4-dihydroxynaphthalene (Gaultier & Hauw, 1967). In the case of the fifth isomer, (I), only the non-centrosymmetric space group $Pna2_1$ and the lattice parameters (a = 7.826, b = 17.448 and c = 5.74 Å) have been previously determined, *via* an X-ray photographic method (Ahmed, 1978). The single-crystal X-ray

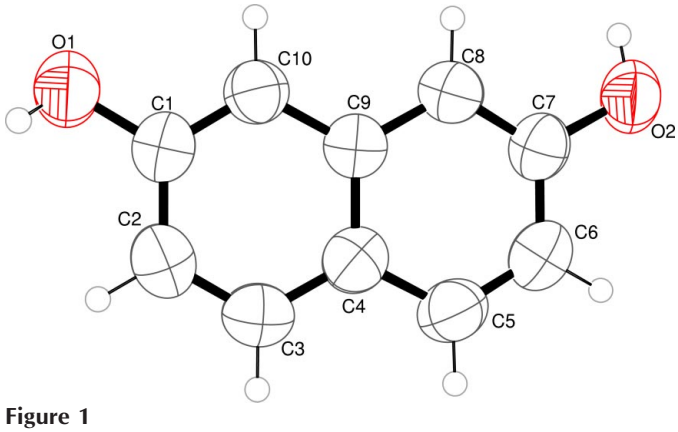


Figure 1
A view of the molecule of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

diffraction data obtained by us confirm that the title compound crystallizes in this space group.

A perspective view of the molecule of (I) is shown in Fig. 1. The molecule contains an essentially planar naphthalene ring system, with two hydroxyl groups attached to it at atoms C1 and C7. Atoms O1 and O2 are displaced from the plane of the naphthalene ring by −0.133 and −0.072 Å, respectively. For comparison, the deviations of the O atoms from this plane are 0.36 and 0.02 Å for the 1,5- and 2,6-dihydroxynaphthalene molecules, respectively. The O atoms of one of the two non-equivalent molecules of 2,3-dihydroxynaphthalene are displaced in relation to the ring plane by 0.12 and 0.09 Å; however, those belonging to the second molecule lie in the plane.

The unit cell of (I) is shown in Fig. 2. The molecules are linked together by two strong O—H···O hydrogen bonds (Table 1), which form chains running along the *a* axis. The lengths of these hydrogen bonds lie in the usual ranges and are comparable with those found for other dihydroxynaphthalene isomers (Belskii *et al.*, 1990; Gaultier & Hauw, 1967).

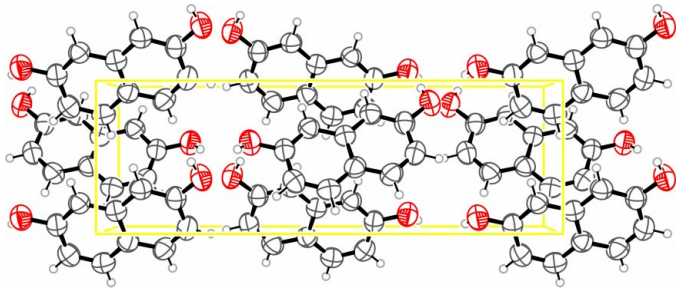


Figure 2
The unit-cell contents of (I), viewed along the *a* axis.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.82	1.95	2.714 (3)	154
O2—H2···O1^{ii}	0.82	2.11	2.831 (4)	146

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, z-\frac{1}{2}$; (ii) $-x+1, -y+1, z+\frac{1}{2}$.

Experimental

Columnar optically clear crystals of the title compound (purchased from Sigma at 99% purity) were obtained from a solution in ethanol by slow evaporation of the solvent at a constant temperature of 293 K.

Crystal data

$C_{10}H_8O_2$
M_r = 160.16
Orthorhombic, $Pna2_1$
a = 7.872 (2) Å
b = 17.463 (3) Å
c = 5.754 (2) Å
V = 791.0 (3) Å^3
Z = 4
D_x = 1.345 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20 reflections
θ = 5.2–20.0°
μ = 0.09 mm^{-1}
T = 293 (2) K
Column, colourless
0.4 × 0.06 × 0.03 mm

Data collection

Kuma KM-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: refined from ΔF (*DIFABS*; Walker & Stuart, 1983)
T_{min} = 0.986, T_{max} = 0.998
1988 measured reflections
994 independent reflections
740 reflections with $I > 2\sigma(I)$
R_{int} = 0.005
θ_{max} = 27.4°
$h = -10 \rightarrow 10$
$k = -22 \rightarrow 22$
$l = -7 \rightarrow 7$
3 standard reflections
every 50 reflections
intensity decay: 2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.121
S = 1.20
994 reflections
115 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2 + 0.0043P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.035
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.014 (4)

H atoms were placed in geometric positions, with O—H distances of 0.82 Å and C—H distances of 0.93 Å, and treated as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O). In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *KM4B8* (Gałdecki *et al.*, 1996); cell refinement: *KM4B8*; data reduction: *KM4B8*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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