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5-Amino-1-naphthol

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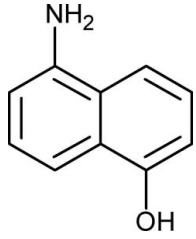
Key indicators: single-crystal X-ray study; T = 130 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.091; data-to-parameter ratio = 8.0.

In the title compound, $C_{10}H_9NO$, the amino and the hydroxy groups act both as a single donor and a single acceptor in hydrogen bonding. In the crystal, molecules are connected *via* chains of intermolecular ···N—H···O—H··· interactions, forming a two-dimensional polymeric structure resembling the hydrogen-bonded molecular assembly found in the crystal structure of naphthalene-1,5-diol. Within this layer, molecules related by a translation along the *a* axis are arranged into slipped stacks *via* π–π stacking interactions [interplanar distance = 3.450 (4) Å]. The amino N atom shows sp^3 hybridization and the two attached H atoms are located on the same side of the aromatic ring.

Related literature

For the crystal structure of 1,5-dihydroxynaphthalene, see: Belskii *et al.* (1990). For amino-hydroxy group recognition and packing motifs of aminols, see: Ermer & Eling (1994); Hanessian *et al.* (1994); Allen *et al.* (1997); Dey *et al.* (2005).



Experimental

Crystal data

$C_{10}H_9NO$
M_r = 159.18
Orthorhombic, $P2_12_12_1$
a = 4.8607 (2) Å
b = 12.3175 (6) Å
c = 13.0565 (5) Å
V = 781.71 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 130 K
0.30 × 0.15 × 0.02 mm

Data collection

Kuma KM-4-CCD κ-geometry diffractometer
Absorption correction: none
8484 measured reflections
963 independent reflections
726 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.091
S = 1.06
963 reflections
121 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O11—H11O···N12^{i}	0.94 (3)	1.83 (3)	2.749 (3)	167 (3)
N12—H12B···O11^{ii}	0.96 (3)	2.09 (3)	3.046 (3)	171 (2)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2154).

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supporting information

Acta Cryst. (2009). E**65**, o2964 [https://doi.org/10.1107/S1600536809045152]

5-Amino-1-naphthol

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S1. Comment

Amino-hydroxy group recognition has been at the focus of crystal engineering since Ermer & Eling (1994) and Hanessian *et al.* (1994) noticed the complementarity of hydroxy and amino groups as regards hydrogen-bond donors and acceptors. Shortly after it was demonstrated with simple 1,2- and 1,3-aminophenols that molecular features, such as functional groups, do not necessarily result in a single manner of the molecular arrangement, and that strong N—H···O and O—H···N hydrogen bonding is frequently unable to exclude other factors from controlling the crystal packing (Allen *et al.*, 1997; Dey *et al.* 2005). Here we report on the crystal structure of a simple aminonaphthol which, as regards the substitution pattern, can be considered as an analogue of 1,4-aminophenol.

The molecular structure of the title compound is shown in Fig. 1, and the geometrical parameters are available in the archived CIF. Whereas 1,4-aminophenol forms a tetrahedral network, *via* N—H···O and O—H···N hydrogen bonds (Ermer & Eling, 1994), in the title compound the molecules are connected *via* chains of ···N—H···O—H··· interactions to form a two-dimensional polymeric structure (Fig. 2, Table 1). The two-dimensional assembly of the molecules joined by hydrogen bonding resembles that formed by 1,5-dihydroxynaphthalene (Belskii *et al.*, 1990). One amino H-atom is not involved in hydrogen bonding and does not take part in any other specific interactions.

S2. Experimental

Single crystals of the commercially available 5-amino-1-naphthol (Aldrich) were obtained from chloroform solution by slow evaporation.

S3. Refinement

In the absence of significant anomalous scattering effects, Friedel pairs were averaged. All H-atoms were located in electron-density difference maps. The H-atoms of the OH and NH groups were freely refined: O-H = 0.94 (3) Å, N-H = 0.95 (3)- 0.96 (3) Å. The C-bound H-atoms were placed at calculated positions, with C—H = 0.93 Å, and refined as riding on their carrier C-atom, with U_{iso}(H) = 1.2U_{eq}(C). .

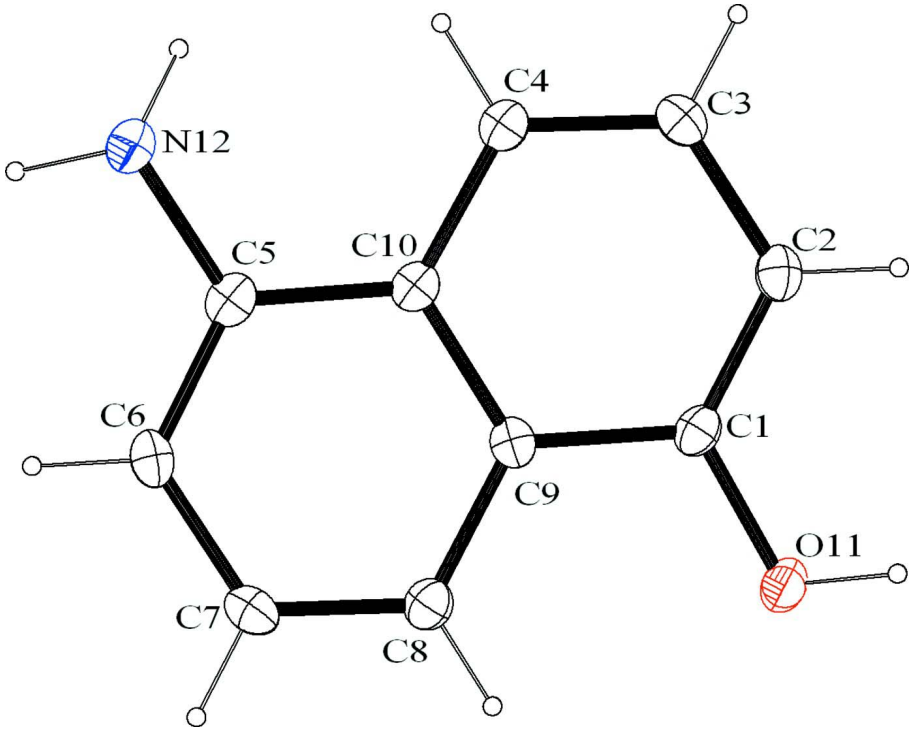

Figure 1

The molecular structure of the title compound, with displacement ellipsoids shown at the 30% probability level.

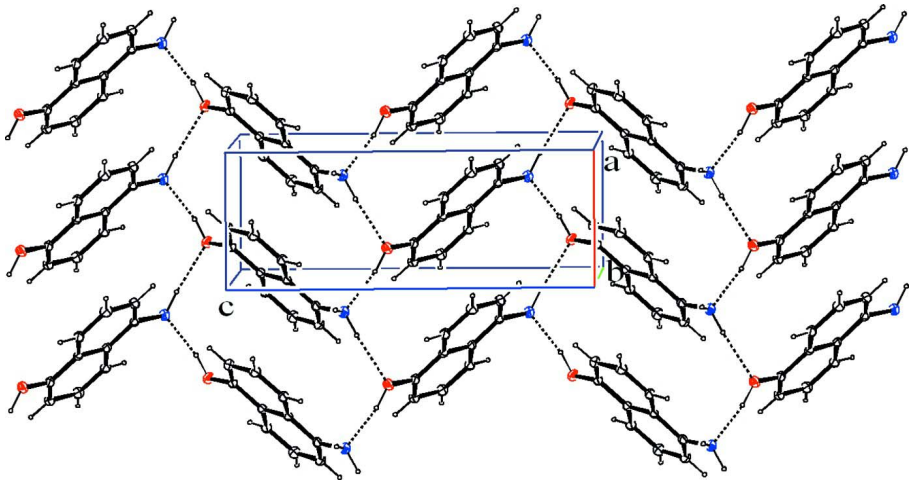

Figure 2

The crystal packing, viewed along the b-axis, of the title compound, showing the two-dimensional hydrogen-bonded assembly (hydrogen bonds are shown as dashed lines).

5-Amino-1-naphthol

Crystal data

$C_{10}H_9NO$
$M_r = 159.18$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab

$a = 4.8607\ (2)$ Å
$b = 12.3175\ (6)$ Å
$c = 13.0565\ (5)$ Å
$V = 781.71\ (6)$ Å^3

$Z = 4$
$F(000) = 336$
$D_x = 1.353$ Mg m^{-3}
Melting point: 461 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2383 reflections

$\theta = 4$–$27°$
$\mu = 0.09$ mm^{-1}
$T = 130$ K
Plate, pale pink
0.30 × 0.15 × 0.02 mm

Data collection

Kuma KM-4-CCD κ-geometry diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
8484 measured reflections
963 independent reflections

726 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 26.4°$, $\theta_{min} = 4.5°$
$h = -6 \rightarrow 5$
$k = -15 \rightarrow 15$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.091$
$S = 1.06$
963 reflections
121 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0554P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.2605 (5)	0.48405 (18)	0.50574 (15)	0.0232 (5)
C2	0.1125 (5)	0.57846 (19)	0.51109 (17)	0.0269 (6)
H2	−0.0135	0.5887	0.5638	0.032*
C3	0.1504 (5)	0.65964 (19)	0.43738 (17)	0.0268 (6)
H3	0.0466	0.7230	0.4409	0.032*
C4	0.3386 (5)	0.64703 (19)	0.35998 (17)	0.0248 (6)
H4	0.3630	0.7022	0.3122	0.030*
C5	0.6956 (5)	0.53275 (18)	0.27339 (16)	0.0239 (6)
C6	0.8417 (5)	0.43775 (19)	0.26935 (17)	0.0265 (6)
H6	0.9701	0.4269	0.2175	0.032*
C7	0.7983 (5)	0.35673 (19)	0.34304 (17)	0.0283 (6)

H7	0.9009	0.2931	0.3399	0.034*
C8	0.6085 (5)	0.36936 (19)	0.41937 (17)	0.0256 (6)
H8	0.5795	0.3141	0.4667	0.031*
C9	0.4571 (5)	0.46670 (19)	0.42580 (16)	0.0215 (5)
C10	0.4964 (5)	0.55036 (18)	0.35220 (16)	0.0215 (5)
O11	0.2370 (4)	0.40173 (13)	0.57550 (11)	0.0289 (4)
H11O	0.067 (7)	0.404 (2)	0.609 (2)	0.058 (10)*
N12	0.7265 (5)	0.61211 (18)	0.19544 (14)	0.0275 (5)
H12A	0.699 (6)	0.685 (2)	0.2155 (18)	0.044 (8)*
H12B	0.899 (6)	0.601 (2)	0.1610 (19)	0.038 (8)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0231 (12)	0.0279 (13)	0.0186 (10)	−0.0035 (12)	−0.0020 (11)	0.0014 (10)
C2	0.0250 (13)	0.0332 (14)	0.0226 (11)	−0.0002 (12)	0.0011 (11)	−0.0024 (11)
C3	0.0261 (13)	0.0255 (13)	0.0288 (12)	0.0028 (12)	−0.0008 (11)	−0.0047 (11)
C4	0.0250 (13)	0.0272 (13)	0.0223 (11)	−0.0030 (11)	−0.0017 (11)	0.0001 (10)
C5	0.0244 (14)	0.0283 (13)	0.0192 (10)	−0.0070 (11)	−0.0053 (10)	−0.0014 (10)
C6	0.0232 (13)	0.0334 (13)	0.0229 (11)	0.0006 (12)	0.0024 (10)	−0.0056 (11)
C7	0.0294 (15)	0.0244 (13)	0.0311 (12)	0.0055 (12)	−0.0022 (11)	−0.0044 (11)
C8	0.0273 (13)	0.0278 (13)	0.0216 (11)	−0.0011 (11)	−0.0013 (11)	−0.0004 (10)
C9	0.0187 (12)	0.0263 (13)	0.0194 (10)	−0.0006 (11)	−0.0030 (10)	−0.0036 (10)
C10	0.0204 (12)	0.0249 (13)	0.0191 (10)	−0.0044 (11)	−0.0044 (10)	−0.0006 (10)
O11	0.0269 (9)	0.0356 (10)	0.0243 (8)	−0.0003 (9)	0.0036 (8)	0.0061 (8)
N12	0.0271 (12)	0.0316 (13)	0.0237 (10)	−0.0025 (12)	0.0005 (10)	0.0016 (9)

Geometric parameters (Å, º)

C1—O11	1.368 (2)	C5—C10	1.430 (3)
C1—C2	1.369 (3)	C6—C7	1.402 (3)
C1—C9	1.431 (3)	C6—H6	0.9300
C2—C3	1.400 (3)	C7—C8	1.367 (3)
C2—H2	0.9300	C7—H7	0.9300
C3—C4	1.372 (3)	C8—C9	1.409 (3)
C3—H3	0.9300	C8—H8	0.9300
C4—C10	1.420 (3)	C9—C10	1.422 (3)
C4—H4	0.9300	O11—H11O	0.94 (3)
C5—C6	1.370 (3)	N12—H12A	0.95 (3)
C5—N12	1.419 (3)	N12—H12B	0.96 (3)
O11—C1—C2	123.5 (2)	C7—C6—H6	119.9
O11—C1—C9	115.5 (2)	C8—C7—C6	121.4 (2)
C2—C1—C9	120.99 (19)	C8—C7—H7	119.3
C1—C2—C3	120.2 (2)	C6—C7—H7	119.3
C1—C2—H2	119.9	C7—C8—C9	119.5 (2)
C3—C2—H2	119.9	C7—C8—H8	120.2
C4—C3—C2	120.9 (2)	C9—C8—H8	120.2

C4—C3—H3	119.6	C8—C9—C10	120.4 (2)
C2—C3—H3	119.6	C8—C9—C1	121.3 (2)
C3—C4—C10	120.5 (2)	C10—C9—C1	118.3 (2)
C3—C4—H4	119.7	C4—C10—C9	119.1 (2)
C10—C4—H4	119.7	C4—C10—C5	123.0 (2)
C6—C5—N12	120.4 (2)	C9—C10—C5	117.9 (2)
C6—C5—C10	120.6 (2)	C1—O11—H11O	111.6 (18)
N12—C5—C10	118.9 (2)	C5—N12—H12A	116.2 (15)
C5—C6—C7	120.2 (2)	C5—N12—H12B	109.1 (15)
C5—C6—H6	119.9	H12A—N12—H12B	113 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O11—H11*O*···N12^{i}	0.94 (3)	1.83 (3)	2.749 (3)	167 (3)
N12—H12*B*···O11^{ii}	0.96 (3)	2.09 (3)	3.046 (3)	171 (2)

Symmetry codes: (i) −*x*+1/2, −*y*+1, *z*+1/2; (ii) −*x*+3/2, −*y*+1, *z*−1/2.