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6-Amino-2-naphthoic acid monohydrate

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The crystal structure of the title compound, $C_{11}H_9NO_2\cdot H_2O$, consists of 6-amino-2-naphthoic acid molecules, associated in dimers by O—H···O hydrogen bonds, and water molecules. The water molecules are hydrogen-bonded into chains which associate with the acid dimers, forming a three-dimensional framework.

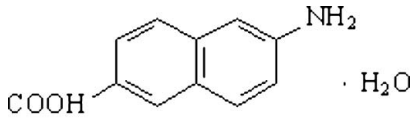
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
Disorder in solvent or counterion
R factor = 0.051
wR factor = 0.141
Data-to-parameter ratio = 11.8

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

Comment

As a precursor in the synthesis of complicated compounds for fluorescent DNA probes (Okamoto *et al.*, 2005), or as an ionizable organic compound in sorption to estuarine sediment (Burgos & Pisutpaisal, 2006), 6-amino-2-naphthoic acid has recently been investigated.



(I)

The title compound, (I), is illustrated in Fig. 1. The carboxylic acid H atom is bonded to O1, giving a slightly longer C—O distance for the hydroxyl group [C1—O1 = 1.295 (2) Å] compared to the carbonyl group [C1═O2 = 1.256 (2) Å]. The carboxyl group C1/O1/O2 is not coplanar with the naphthalene ring system C2–C11, the dihedral angle being 22.9 (2)°.

In the crystal structure, two symmetry-related 6-amino-2-naphthoic acid molecules are link head-to-head through C═O···H—O hydrogen bonds, giving a classical centrosymmetric dimer based on a motif with graph set $R_2^2(8)$. In addition, water molecules are hydrogen bonded to form chains, which associate with the acid dimers, giving a three-dimensional framework. The hydrogen-bond parameters are listed in Table 1.

Experimental

Crystals of (I) were obtained by the recrystallization from H_2O/EtOH (1:1) of 6-amino-2-naphthoic acid (purchased from ACROS).

Crystal data

$C_{11}H_9NO_2\cdot H_2O$
M_r = 205.21
Orthorhombic, *Pbcn*
a = 22.582 (5) Å
b = 12.222 (2) Å
c = 6.9793 (14) Å
V = 1926.4 (7) Å^3
Z = 8
D_x = 1.415 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100 (2) K
Block, colourless
0.22 × 0.20 × 0.20 mm

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Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.966, T_{max} = 0.980
9442 measured reflections
1837 independent reflections
1372 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 25.7°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.141
S = 1.05
1837 reflections
156 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0904P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.95 (3)	1.67 (3)	2.611 (2)	173 (3)
N1—H1A···O2^{ii}	0.85 (3)	2.57 (3)	3.310 (3)	146 (2)
N1—H1B···O1W	0.85 (2)	2.23 (3)	3.077 (3)	177 (2)
O1W—H1W···N1^{iii}	0.875 (18)	2.21 (2)	3.062 (3)	165 (3)
O1W—H2$A W$···O1W^{iv}	0.87 (2)	2.01 (3)	2.813 (4)	153 (6)
O1W—H2$B W$···O1W^{v}	0.91 (2)	2.17 (5)	2.870 (4)	133 (5)

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

H atoms bonded to C atoms were positioned geometrically and refined as riding on their carrier C atoms, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C). Amino H atoms were located in a difference map and refined freely, with U_{iso}(H) = 1.2U_{eq}(N). Carboxyl H atom H1 was located in a difference map and refined isotropically. Water H atoms were located in a difference map and refined with an O—H distance restraint of 0.85 (2) Å and U_{iso}(H) = 1.5U_{eq}(O). Water H atoms are clearly disordered over three general positions. One H-atom site, H1W, is fully occupied, while the other is disordered equally over two positions, H2AW and H2BW; these were refined with site occupation factors fixed at 0.5.

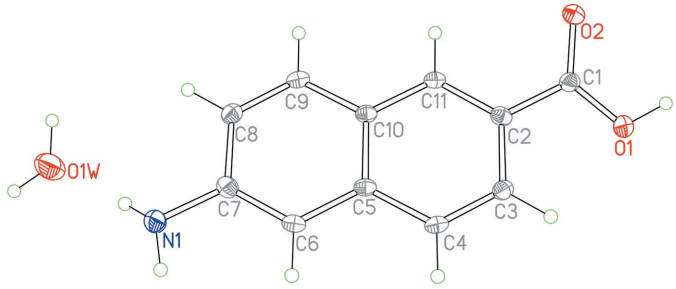

Figure 1
The molecular structure of (I), showing displacement ellipsoids drawn at the 30% probability level. A single position for the disordered water molecule is shown.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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