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7-Amino-1,8-naphthyridin-2(1*H*)-one monohydrate

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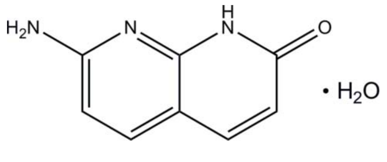
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.004 Å; R factor = 0.063; wR factor = 0.171; data-to-parameter ratio = 12.1.

In the crystal structure of the title compound, $C_8H_7N_3O\cdot H_2O$, adjacent organic molecules are linked together into a tape along the *a* axis through N—H···N and N—H···O hydrogen bonds. On the other hand, water molecules are linked together to form a chain along the *b* axis through O—H···O hydrogen bonds. The water chains and the organic molecular tapes are further connected by intermolecular O—H···O hydrogen bonds, forming a three-dimensional network. In addition, a π–π stacking interaction between the 1,8-naphthyridine ring systems with an interplanar separation of 3.246 (1) Å and a centroid–centroid distance of 3.825 (2) Å is observed.

Related literature

For applications of 1,8-naphthyridine and its derivatives in coordination chemistry, see: Oskui *et al.* (1999); Nakatani *et al.* (2003); Fang *et al.* (2004); Sinha *et al.* (2009); Fu *et al.* (2009, 2010). For related structures of 1,8-naphthyridine derivatives, see: Goswami *et al.* (2007). For the synthesis of the title compound, see: Newcome *et al.* (1981).



Experimental

Crystal data

$C_8H_7N_3O\cdot H_2O$
M_r = 179.18
Monoclinic, $P2_1/c$
a = 9.5413 (9) Å
b = 17.1560 (16) Å
c = 4.9954 (4) Å
β = 95.19 (2)°
V = 814.34 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 113 K
0.22 × 0.20 × 0.02 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.977, $T_{\max}$ = 0.998
6502 measured reflections
1432 independent reflections
906 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.085

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.171
S = 1.00
1432 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.30 e Å^{-3}
$\Delta\rho_{\min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1$^{\rm i}$	0.86	2.00	2.853 (3)	175
N1—H1B···O1$^{\rm ii}$	0.86	2.28	2.989 (3)	140
N3—H1···N2$^{\rm i}$	0.86	2.18	3.040 (3)	178
O2—H2A···O2$^{\rm iii}$	0.85	1.93	2.7758 (18)	179
O2—H2B···O1	0.85	1.97	2.823 (3)	178

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2766).

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supporting information

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7-Amino-1,8-naphthyridin-2(1*H*)-one monohydrate

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S1. Comment

The 1,8-naphthyridine and its derivatives have attracted considerable attention as an polydentate nitrogen-donor ligand, since these ligands are linked to metals with several coordination modes such as monodentate and chelating bidentate fashion with short metal-metal bonds (Oskui *et al.*, 1999). In addition, the metal 1,8-naphthyridine complexes can exhibit biocompatibility, interesting catalytic and fluorescence properties (Nakatani *et al.*, 2003; Fang *et al.*, 2004; Sinha *et al.*, 2009). Previously, we have concentrated our investigation on the chemistry of 1,8-naphthyridine derivatives and related metal coordination compounds (Fu *et al.*, 2009, 2010). Herein, we report herein the crystal structure of the title compound. Although the synthesis of the compound 7-amino-1,8-naphthyridin-2(1*H*)-one has been reported (Newcome *et al.*, 1981), no crystallographic study has been reported on this ligand until now.

The asymmetric unit of the title compound contains a crystallographically independent molecules and one water molecule (Fig. 1), in which the bond lengths and angles are generally within normal ranges in accordance with the corresponding values reported (Goswami *et al.*, 2007). The organic molecule is nearly planar with an r.m.s. deviation of 0.0146 Å. In the crystal structure, adjacent organic molecules are joined together into a one-dimensional tape propagating in the *a* axis direction (Fig. 2) through N—H···N and N—H···O hydrogen bonds (Table 1). Neighboring water molecules joined together to form a one-dimensional water chain extending along the *b* axis (Fig. 3) through OW—H···OW hydrogen bonds. These one-dimensional water chains are further connected to the adjacent one-dimensional tape motifs, forming a three-dimensional network (Fig. 3) by intermolecular OW—H···O hydrogen bonds (Table 1). In addition, a π–π stacking interaction between 1,8-naphthyridine rings may further stabilize the structure; the interplanar distance and the centrioid-centrioid distance are 3.246 (1) and 3.825 (2) Å, respectively.

S2. Experimental

The 7-amino-1,8-naphthyridin-2(1*H*)-one was synthesized according to the literature method (Newcome *et al.*, 1981). The colorless crystals of the title compound suitable for X-ray diffraction were obtained by vapor diffusion of diethyl ether into the solution of the product 7-amino-1,8-naphthyridin-2(1*H*)-one in CH_3CN-MeOH (*v*:*v* = 4:1).

S3. Refinement

All H atoms were placed in idealized positions (O—H = 0.85 Å, N—H = 0.86 Å and C—H = 0.95 Å) and refined as riding atoms with $U_{iso}(H) = 1.2U_{eq}(C, N)$ and $U_{iso}(H) = 1.5U_{eq}(O)$.

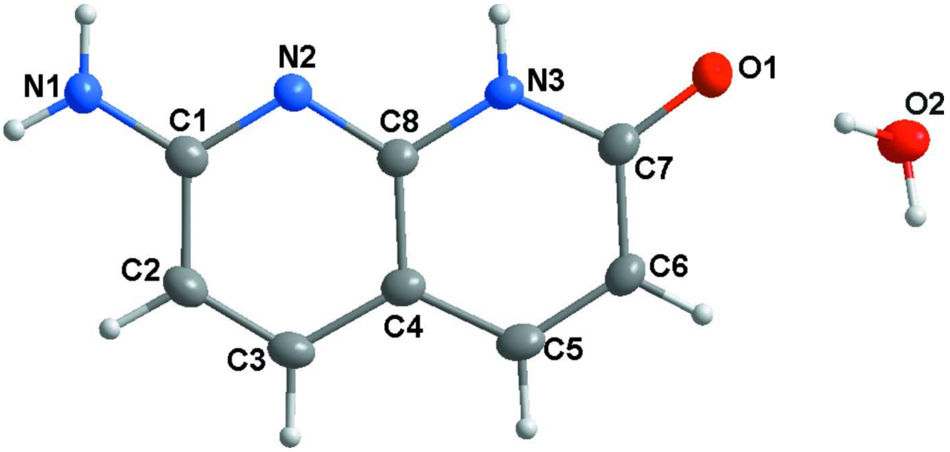

Figure 1

The asymmetric unit of the title compound, with displacement ellipsoids drawn at the 30% probability level.

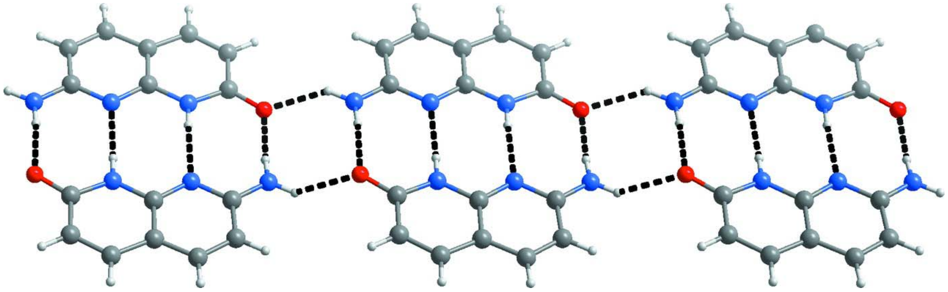

Figure 2

The tape structure of the organic molecules propagating in the *a* axis direction through N—H···N and N—H···O hydrogen bonds.

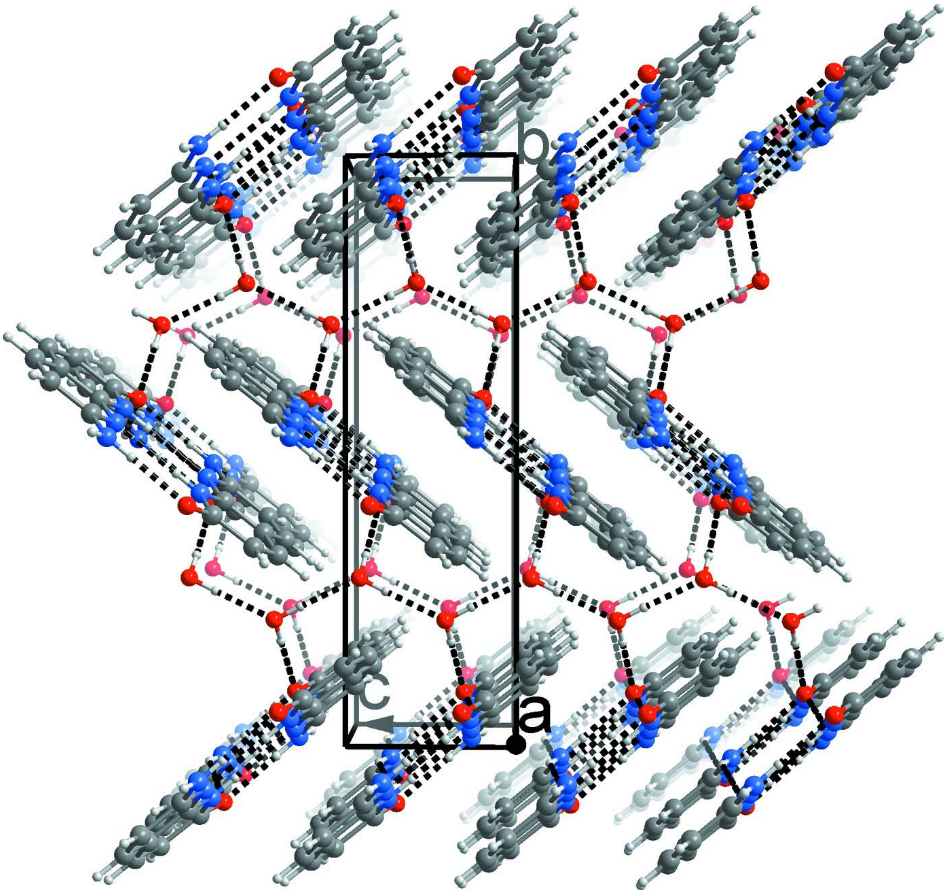

Figure 3

The three-dimensional packing of the title compound viewed along the *a* axis, showing the hydrogen bonds with dashed lines.

7-Amino-1,8-naphthyridin-2(1*H*)-one monohydrate

Crystal data

$C_8H_7N_3O \cdot H_2O$
$M_r = 179.18$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.5413$ (9) Å
$b = 17.1560$ (16) Å
$c = 4.9954$ (4) Å
$\beta = 95.19$ (2)°
$V = 814.34$ (13) Å^3
$Z = 4$
$F(000) = 376$
$D_x = 1.461$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2181 reflections
$\theta = 2.1$–27.8°
$\mu = 0.11$ mm^{-1}
$T = 113$ K
Prism, colorless
0.22 × 0.20 × 0.02 mm

Data collection

Bruker APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 14.63 pixels mm^{-1}
ω scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.977$, $T_{\max} = 0.998$
6502 measured reflections
1432 independent reflections
906 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.085$
$\theta_{\max} = 25.0°$, $\theta_{\min} = 2.1°$
$h = -11 \rightarrow 11$
$k = -20 \rightarrow 20$
$l = -5 \rightarrow 5$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.171$
$S = 1.00$
1432 reflections
118 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0752P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.30$ e Å^{-3}
$\Delta\rho_{\min} = -0.28$ 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}
O1	0.1654 (2)	0.58746 (12)	0.1928 (4)	0.0401 (6)
O2	−0.0186 (2)	0.71471 (12)	0.0843 (4)	0.0461 (7)
H2A	−0.0189	0.7369	0.2365	0.055*
H2B	0.0386	0.6772	0.1179	0.055*
N1	0.8793 (2)	0.52074 (14)	0.2402 (5)	0.0381 (7)
H1A	0.8606	0.4889	0.1089	0.046*
H1B	0.9651	0.5281	0.3036	0.046*
N2	0.6422 (2)	0.54442 (13)	0.2362 (4)	0.0286 (6)
N3	0.4034 (2)	0.56892 (13)	0.2314 (4)	0.0290 (6)
H1	0.3930	0.5370	0.0984	0.035*
C1	0.7755 (3)	0.55862 (17)	0.3454 (6)	0.0333 (7)
C2	0.8036 (3)	0.61017 (18)	0.5674 (6)	0.0364 (8)
H2	0.8978	0.6187	0.6399	0.044*
C3	0.6969 (3)	0.64711 (17)	0.6756 (6)	0.0348 (8)
H3	0.7160	0.6817	0.8229	0.042*
C4	0.5572 (3)	0.63391 (17)	0.5685 (6)	0.0322 (7)
C5	0.4358 (3)	0.66882 (16)	0.6616 (6)	0.0363 (8)
H5	0.4467	0.7030	0.8116	0.044*
C6	0.3041 (3)	0.65478 (17)	0.5423 (6)	0.0344 (8)
H6	0.2250	0.6792	0.6093	0.041*
C7	0.2846 (3)	0.60331 (16)	0.3161 (6)	0.0335 (8)
C8	0.5372 (3)	0.58251 (15)	0.3459 (6)	0.0285 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0361 (12)	0.0370 (14)	0.0470 (14)	0.0041 (9)	0.0037 (10)	0.0006 (10)
O2	0.0615 (15)	0.0333 (13)	0.0421 (14)	0.0105 (11)	−0.0025 (12)	0.0020 (10)
N1	0.0301 (13)	0.0420 (17)	0.0423 (18)	−0.0001 (11)	0.0036 (12)	−0.0050 (13)
N2	0.0308 (13)	0.0253 (13)	0.0296 (15)	−0.0033 (10)	0.0024 (11)	0.0030 (11)
N3	0.0345 (13)	0.0261 (13)	0.0265 (15)	0.0028 (10)	0.0032 (11)	−0.0016 (10)
C1	0.0382 (17)	0.0269 (17)	0.0348 (19)	−0.0047 (14)	0.0025 (14)	0.0073 (14)
C2	0.0387 (17)	0.0306 (18)	0.039 (2)	−0.0079 (13)	−0.0035 (15)	0.0043 (14)
C3	0.0460 (18)	0.0258 (17)	0.0317 (19)	−0.0060 (14)	−0.0013 (15)	0.0006 (13)
C4	0.0431 (17)	0.0230 (16)	0.0305 (19)	0.0002 (13)	0.0042 (14)	0.0037 (13)
C5	0.053 (2)	0.0227 (16)	0.0334 (19)	0.0011 (14)	0.0050 (15)	−0.0003 (14)
C6	0.0389 (17)	0.0268 (17)	0.0385 (19)	0.0054 (13)	0.0099 (15)	0.0023 (14)
C7	0.0392 (17)	0.0243 (16)	0.0377 (19)	0.0039 (13)	0.0066 (15)	0.0055 (14)
C8	0.0364 (16)	0.0192 (15)	0.0300 (18)	−0.0014 (12)	0.0037 (14)	0.0056 (13)

Geometric parameters (Å, º)

O1—C7	1.273 (3)	C1—C2	1.425 (4)
O2—H2A	0.8500	C2—C3	1.353 (4)
O2—H2B	0.8500	C2—H2	0.9500
N1—C1	1.332 (4)	C3—C4	1.409 (4)
N1—H1A	0.8600	C3—H3	0.9500
N1—H1B	0.8600	C4—C8	1.418 (4)
N2—C8	1.353 (3)	C4—C5	1.419 (4)
N2—C1	1.360 (3)	C5—C6	1.363 (4)
N3—C8	1.370 (3)	C5—H5	0.9500
N3—C7	1.378 (3)	C6—C7	1.433 (4)
N3—H1	0.8600	C6—H6	0.9500
H2A—O2—H2B	102.5	C4—C3—H3	120.2
C1—N1—H1A	120.0	C3—C4—C8	116.9 (3)
C1—N1—H1B	120.0	C3—C4—C5	125.4 (3)
H1A—N1—H1B	120.0	C8—C4—C5	117.6 (3)
C8—N2—C1	116.8 (3)	C6—C5—C4	122.0 (3)
C8—N3—C7	124.0 (3)	C6—C5—H5	119.0
C8—N3—H1	118.0	C4—C5—H5	119.0
C7—N3—H1	118.0	C5—C6—C7	120.2 (3)
N1—C1—N2	117.2 (3)	C5—C6—H6	119.9
N1—C1—C2	121.1 (3)	C7—C6—H6	119.9
N2—C1—C2	121.7 (3)	O1—C7—N3	118.9 (3)
C3—C2—C1	120.5 (3)	O1—C7—C6	124.0 (3)
C3—C2—H2	119.8	N3—C7—C6	117.1 (3)
C1—C2—H2	119.8	N2—C8—N3	116.4 (3)
C2—C3—C4	119.5 (3)	N2—C8—C4	124.5 (3)
C2—C3—H3	120.2	N3—C8—C4	119.2 (3)

C8—N2—C1—N1	179.3 (3)	C8—N3—C7—C6	−1.6 (4)
C8—N2—C1—C2	1.0 (4)	C5—C6—C7—O1	−179.6 (3)
N1—C1—C2—C3	−178.7 (3)	C5—C6—C7—N3	0.9 (4)
N2—C1—C2—C3	−0.4 (4)	C1—N2—C8—N3	178.8 (2)
C1—C2—C3—C4	0.4 (5)	C1—N2—C8—C4	−1.7 (4)
C2—C3—C4—C8	−1.0 (4)	C7—N3—C8—N2	−179.4 (2)
C2—C3—C4—C5	−179.8 (3)	C7—N3—C8—C4	1.1 (4)
C3—C4—C5—C6	178.1 (3)	C3—C4—C8—N2	1.7 (4)
C8—C4—C5—C6	−0.7 (4)	C5—C4—C8—N2	−179.4 (3)
C4—C5—C6—C7	0.1 (4)	C3—C4—C8—N3	−178.8 (2)
C8—N3—C7—O1	179.0 (2)	C5—C4—C8—N3	0.1 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.86	2.00	2.853 (3)	175
N1—H1*B*···O1^{ii}	0.86	2.28	2.989 (3)	140
N3—H1···N2^{i}	0.86	2.18	3.040 (3)	178
O2—H2*A*···O2^{iii}	0.85	1.93	2.7758 (18)	179
O2—H2*B*···O1	0.85	1.97	2.823 (3)	178

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