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7-Acetylamino-2,4-dimethyl-1,8-naphthyridine

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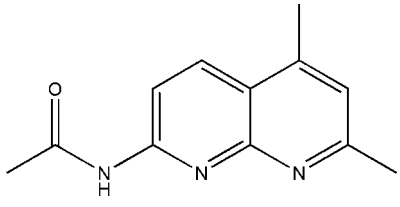
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.048; wR factor = 0.153; data-to-parameter ratio = 13.5.

The air-stable title compound, $C_{12}H_{13}N_3O$, which is of interest due to its antibacterial properties, is an almost planar molecule in which the ten atoms forming the 1,8-naphthyridine ring have an r.m.s. deviation of 0.03 Å from the least-squares plane calculated using the ten atoms. The plane of the acetylamino group is slightly inclined [11.7 (2)°] to the plane of the 1,8-naphthyridine ring.

Related literature

For related literature, see: Catalano *et al.* (2000); Chen *et al.* (2001); Ferrarini *et al.* (1997, 2000); He & Lippard (2001); Henry & Hammond (1977); Mogilaiah *et al.* (2001); Nakatani *et al.* (2000); Roma *et al.* (2000); Saito *et al.* (2001).



Experimental

Crystal data

$C_{12}H_{13}N_3O$
M_r = 215.25
Monoclinic, $P2_1/n$
a = 7.970 (8) Å
b = 7.309 (7) Å
c = 19.071 (18) Å
β = 91.883 (14)°
V = 1110.4 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.52 × 0.36 × 0.24 mm

Data collection

SMART 1K CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
T_{min} = 0.970, T_{max} = 0.980
5375 measured reflections
1959 independent reflections
1169 reflections with $I > 2\sigma(I)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.153
S = 1.02
1959 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Bergerhoff, 1996) and *XP* (Bruker, 2000); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2000).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ER2027).

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S1. Comment

The 1,8-naphthyridine compounds have been the focus of studies and practical applications as antibacterial agents (Mogilaiah *et al.*, 2001). Recent parallels in biological activity of this class of compounds have been found in the form of antibacterial (Chen *et al.*, 2001), antiinflammatory (Roma *et al.*, 2000), antihypertensive (Ferrarini *et al.*, 2000), and antiplatelet activity (Ferrarini *et al.*, 1997). In addition to medicinal applications, this class of compounds have been employed in the study of bioorganic and bioorganometallic processes (Saito *et al.*, 2001; He *et al.*, 2001; Nakatani *et al.*, 2000). The structure of the $C_{12}H_{13}N_3O$ in (I) is shown in Fig. 1 and selected bond lengths and angles are given in Table. 1. The structure of this compound is a rigid nearly planar molecule with an r.m.s. deviation of 0.03 Å for the ten atoms making up the 1,8-naphthyridine ring. The least square plane calculated from the atoms of the acetyl amino group make an dihedral angle of 11.7 (2) ° to the least square plane of the 1,8-naphthyridine ring All bond distances are essentially identical to those found in the literature (Catalano *et al.*, 2000).

S2. Experimental

2-amino-5, 7-Dimethyl-1, 8-naphthyridine (Henry *et al.*, 1977) (4.0 g, 0.10 mol) was added to a Ac_2O (15 ml) solution under an atmosphere of N_2. After the solution was stirred at reflux temperature for 1 h, excess solvent was removed and the final product was obtained following flash chromatography. Then, the compound was dissolved in CH_2Cl_2 and recrystallized by slow diffusion of aether into the CH_2Cl_2 solution. Yellow crystals suitable for X-ray diffraction were obtained.

S3. Refinement

All H atoms were placed in calculated positions. The H atoms were then constrained to an ideal geometry with C—H distances of 0.93–0.96 Å, U_{iso}(H) = 1.2U_{eq}(C) and N—H distance of 0.86 Å with U_{iso}(H) = 1.2U_{eq}(N).

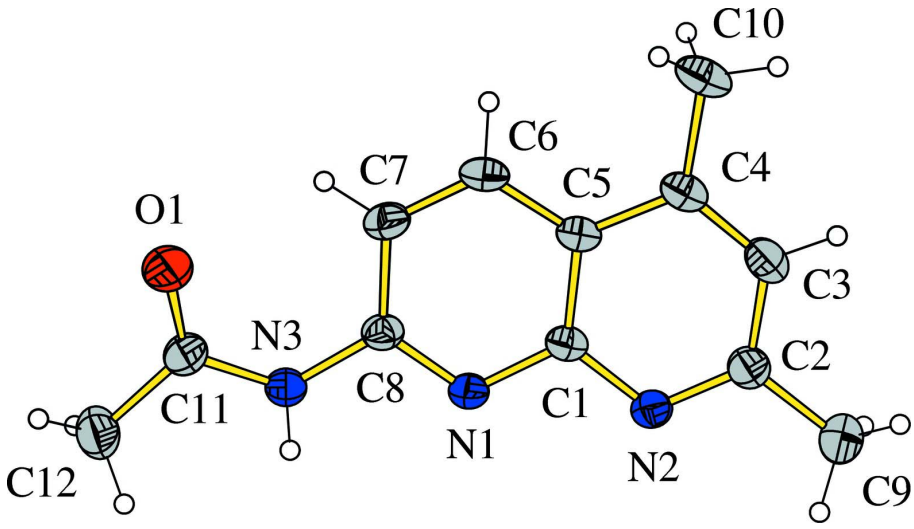

Figure 1

The molecular structure of the title compound drawn with *DIAMOND* (Bergerhoff, 1996). Displacement ellipsoids at the 30% probability level.

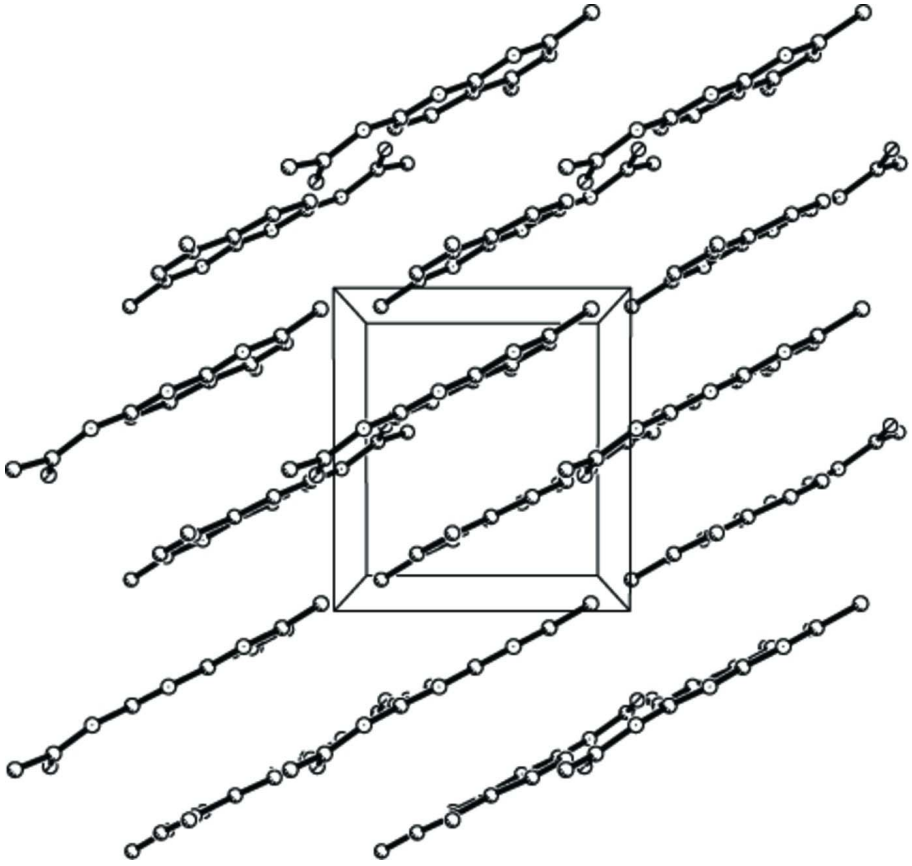

Figure 2

The packing of the title compound viewed along the *c* axis, drawn with *XP* (Bruker, 2000). H atoms have been omitted. The molecules shown are centered around *z*=0.0.

7-Acetylamino-2,4-dimethyl-1,8-naphthyridine

Crystal data

$C_{12}H_{13}N_3O$
$M_r = 215.25$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.970\ (8)$ Å
$b = 7.309\ (7)$ Å
$c = 19.071\ (18)$ Å
$\beta = 91.883\ (14)°$
$V = 1110.4\ (18)$ Å^3
$Z = 4$
$F(000) = 456.0$
$D_x = 1.288$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1274 reflections
$\theta = 2.7–25.2°$
$\mu = 0.09$ mm^{-1}
$T = 298$ K
Block, pale yellow
0.52 × 0.36 × 0.24 mm

Data collection

SMART 1K CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2002)
$T_{min} = 0.970$, $T_{max} = 0.980$
5375 measured reflections
1959 independent reflections
1169 reflections with $I > 2\sigma(I)$
$R_{int} = 0.036$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.1°$
$h = -9\rightarrow9$
$k = -8\rightarrow8$
$l = -18\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.153$
$S = 1.02$
1959 reflections
145 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
$w = 1/[\sigma^2(F_o^2) + (0.0724P)^2 + 0.2527P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ 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}
N1	0.8038 (2)	0.1591 (3)	0.16857 (10)	0.0416 (5)
N2	0.6692 (2)	−0.1164 (3)	0.15749 (10)	0.0443 (6)
N3	0.9292 (3)	0.4340 (3)	0.18935 (10)	0.0483 (6)
H3	0.8956	0.4199	0.2314	0.058*

O1	1.0871 (3)	0.6171 (3)	0.12288 (10)	0.0856 (8)
C1	0.7455 (3)	0.0253 (3)	0.12480 (11)	0.0391 (6)
C2	0.6113 (3)	−0.2514 (4)	0.11782 (13)	0.0480 (7)
C3	0.6280 (3)	−0.2537 (4)	0.04464 (14)	0.0546 (7)
H3A	0.5891	−0.3546	0.0192	0.066*
C4	0.6991 (3)	−0.1130 (4)	0.01004 (12)	0.0472 (7)
C5	0.7602 (3)	0.0348 (3)	0.05134 (12)	0.0410 (6)
C6	0.8324 (3)	0.1936 (4)	0.02437 (13)	0.0498 (7)
H6	0.8425	0.2063	−0.0238	0.060*
C7	0.8875 (3)	0.3283 (4)	0.06768 (13)	0.0519 (7)
H7	0.9331	0.4351	0.0499	0.062*
C8	0.8742 (3)	0.3032 (3)	0.14080 (12)	0.0415 (6)
C9	0.5235 (4)	−0.4030 (4)	0.15366 (15)	0.0654 (8)
H9A	0.5582	−0.4054	0.2023	0.098*
H9B	0.5514	−0.5173	0.1322	0.098*
H9C	0.4045	−0.3839	0.1496	0.098*
C10	0.7102 (4)	−0.1127 (4)	−0.06836 (13)	0.0670 (9)
H10A	0.6876	−0.2334	−0.0861	0.100*
H10B	0.8208	−0.0758	−0.0809	0.100*
H10C	0.6291	−0.0287	−0.0882	0.100*
C11	1.0292 (3)	0.5810 (4)	0.17874 (14)	0.0531 (7)
C12	1.0655 (4)	0.6957 (4)	0.24196 (16)	0.0728 (9)
H12A	1.1689	0.7605	0.2364	0.109*
H12B	1.0749	0.6188	0.2827	0.109*
H12C	0.9759	0.7818	0.2475	0.109*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0491 (12)	0.0434 (12)	0.0325 (11)	−0.0017 (10)	0.0048 (9)	0.0003 (10)
N2	0.0509 (12)	0.0426 (13)	0.0394 (12)	0.0014 (10)	0.0001 (9)	0.0032 (10)
N3	0.0605 (13)	0.0505 (14)	0.0348 (11)	−0.0094 (11)	0.0131 (10)	−0.0031 (10)
O1	0.1048 (17)	0.1011 (18)	0.0518 (13)	−0.0489 (14)	0.0190 (12)	0.0028 (12)
C1	0.0413 (13)	0.0436 (15)	0.0323 (13)	0.0071 (11)	0.0007 (10)	−0.0007 (11)
C2	0.0502 (15)	0.0443 (16)	0.0490 (16)	0.0052 (12)	−0.0052 (13)	0.0001 (13)
C3	0.0593 (17)	0.0520 (18)	0.0515 (17)	0.0047 (14)	−0.0120 (14)	−0.0105 (14)
C4	0.0478 (15)	0.0560 (17)	0.0376 (14)	0.0117 (13)	−0.0033 (11)	−0.0068 (13)
C5	0.0408 (13)	0.0503 (16)	0.0318 (13)	0.0076 (12)	0.0005 (10)	0.0005 (12)
C6	0.0562 (15)	0.0649 (18)	0.0285 (13)	0.0037 (14)	0.0053 (11)	0.0025 (13)
C7	0.0626 (17)	0.0556 (17)	0.0381 (14)	−0.0031 (14)	0.0096 (12)	0.0073 (13)
C8	0.0463 (14)	0.0448 (15)	0.0339 (13)	0.0024 (12)	0.0073 (11)	0.0011 (12)
C9	0.073 (2)	0.0542 (19)	0.069 (2)	−0.0094 (15)	−0.0014 (16)	0.0020 (15)
C10	0.078 (2)	0.085 (2)	0.0372 (15)	0.0111 (17)	−0.0053 (14)	−0.0135 (15)
C11	0.0555 (16)	0.0564 (18)	0.0479 (16)	−0.0107 (14)	0.0118 (13)	0.0033 (14)
C12	0.087 (2)	0.068 (2)	0.065 (2)	−0.0249 (18)	0.0199 (16)	−0.0170 (16)

Geometric parameters (Å, º)

N1—C8	1.313 (3)	C5—C6	1.401 (3)
N1—C1	1.357 (3)	C6—C7	1.349 (4)
N2—C2	1.318 (3)	C6—H6	0.9300
N2—C1	1.363 (3)	C7—C8	1.414 (3)
N3—C11	1.357 (3)	C7—H7	0.9300
N3—C8	1.392 (3)	C9—H9A	0.9600
N3—H3	0.8600	C9—H9B	0.9600
O1—C11	1.204 (3)	C9—H9C	0.9600
C1—C5	1.411 (3)	C10—H10A	0.9600
C2—C3	1.406 (4)	C10—H10B	0.9600
C2—C9	1.488 (4)	C10—H10C	0.9600
C3—C4	1.356 (4)	C11—C12	1.489 (4)
C3—H3A	0.9300	C12—H12A	0.9600
C4—C5	1.414 (3)	C12—H12B	0.9600
C4—C10	1.501 (4)	C12—H12C	0.9600
C8—N1—C1	118.2 (2)	C8—C7—H7	120.8
C2—N2—C1	117.4 (2)	N1—C8—N3	114.4 (2)
C11—N3—C8	128.2 (2)	N1—C8—C7	123.3 (2)
C11—N3—H3	115.9	N3—C8—C7	122.3 (2)
C8—N3—H3	115.9	C2—C9—H9A	109.5
N1—C1—N2	114.5 (2)	C2—C9—H9B	109.5
N1—C1—C5	122.5 (2)	H9A—C9—H9B	109.5
N2—C1—C5	123.0 (2)	C2—C9—H9C	109.5
N2—C2—C3	122.4 (2)	H9A—C9—H9C	109.5
N2—C2—C9	117.0 (2)	H9B—C9—H9C	109.5
C3—C2—C9	120.5 (2)	C4—C10—H10A	109.5
C4—C3—C2	121.9 (2)	C4—C10—H10B	109.5
C4—C3—H3A	119.0	H10A—C10—H10B	109.5
C2—C3—H3A	119.0	C4—C10—H10C	109.5
C3—C4—C5	116.7 (2)	H10A—C10—H10C	109.5
C3—C4—C10	121.7 (2)	H10B—C10—H10C	109.5
C5—C4—C10	121.6 (3)	O1—C11—N3	123.3 (3)
C6—C5—C1	117.0 (2)	O1—C11—C12	121.6 (3)
C6—C5—C4	124.5 (2)	N3—C11—C12	115.1 (2)
C1—C5—C4	118.5 (2)	C11—C12—H12A	109.5
C7—C6—C5	120.6 (2)	C11—C12—H12B	109.5
C7—C6—H6	119.7	H12A—C12—H12B	109.5
C5—C6—H6	119.7	C11—C12—H12C	109.5
C6—C7—C8	118.4 (2)	H12A—C12—H12C	109.5
C6—C7—H7	120.8	H12B—C12—H12C	109.5