Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Amino-2-methylquinoline monohydrate

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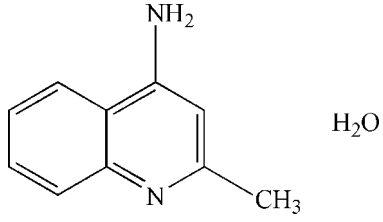
Received 1 May 2008; accepted 3 May 2008

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.033; wR factor = 0.094; data-to-parameter ratio = 7.4.

The crystal structure of the title compound, $C_{10}H_{10}N_2\cdot H_2O$, is stabilized by intermolecular O—H···N, N—H···O and N—H···N hydrogen bonds.

Related literature

For related literature, see: Tai *et al.* (2003, 2008); Tai, Yin & Feng (2007); Tai, Yin & Hao (2007); Tai, Yin *et al.* (2007); Tai & Feng (2008); Wang *et al.* (2007).



Experimental

Crystal data

$C_{10}H_{10}N_2\cdot H_2O$
M_r = 176.22
Orthorhombic, $Pna2_1$
a = 4.7432 (8) Å
b = 13.9070 (13) Å
c = 14.5129 (16) Å
V = 957.3 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 (2) K
0.43 × 0.35 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.966, T_{max} = 0.975
3925 measured reflections
882 independent reflections
716 reflections with $I > 2\sigma(I)$
R_{int} = 0.029

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.093
S = 1.04
882 reflections
119 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O1^{i}	0.85	1.94	2.791 (3)	174
O1—H2···N1^{ii}	0.85	1.96	2.805 (3)	171
N2—H2A···O1^{iii}	0.86	2.10	2.947 (4)	168
N2—H2B···N2^{iv}	0.86	2.51	3.321 (4)	158

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank the National Natural Science Foundation of China (20671073), the Natural Science Foundation of Shandong (Y2007B60), the Science and Technology Foundation of Weifang and Weifang University for research grants.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2564).

References

Bruker (2000). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tai, X. S. & Feng, Y. M. (2008). *Acta Cryst.* E**64**, o707.
Tai, X.-S., Feng, Y.-M. & Zhang, H.-X. (2008). *Acta Cryst.* E**64**, m502.
Tai, X. S., Yin, J. & Feng, Y. M. (2007). *Z. Kristallogr. New Cryst. Struct.* **222**, 398–400.
Tai, X. S., Yin, J., Feng, Y. M. & Kong, F. Y. (2007). *Chin. J. Inorg. Chem.* **23**, 1812–1814.
Tai, X.-S., Yin, J. & Hao, M.-Y. (2007). *Acta Cryst.* E**63**, m1061–m1062.
Tai, X.-S., Yin, X.-H., Tan, M.-Y. & Li, Y.-Z. (2003). *Acta Cryst.* E**59**, o681–o682.
Wang, L.-H., Yin, J. & Tai, X.-S. (2007). *Acta Cryst.* E**63**, m1664.

supplementary materials

Acta Cryst. (2008). E**64**, o1026 [**doi:10.1107/S1600536808013093**]

4-Amino-2-methylquinoline monohydrate

X.-S. Tai, J. Xu, Y.-M. Feng and Z.-P. Liang

Comment

As part of our ongoing studies of the coordination chemistry of ligands containing nitrogen (Tai *et al.*, 2003; Tai, Yin & Feng, 2007; Tai, Yin, Feng & Kong, 2007; Tai, Yin & Hao, 2007; Tai & Feng, 2008; Tai, Feng & Zhang, 2008; Wang *et al.*, 2007), we now report the structure of the title compound, (I), (Fig. 1).

In the molecule of (I), the geometrical parameters for (I) are normal. The packing is stabilized by the intermolecular O—H···N, N—H···O and N—H···N hydrogen bonds (Table 1).

Experimental

1 mmol of Ethyl benzoylacetate was added to a solution of 4-amino-2-methylquinoline (1 mmol) in 10 ml of 95% ethanol. The mixture was stirred for 2 h at refluxing temperature. Evaporating some ethanol, clear blocks of (I) were obtained after one weeks.

Refinement

The H atoms were placed geometrically (C—H = 0.93–0.96 Å, O—H = 0.852 Å, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2 or 1.5U_{eq}(carrier).

Figures

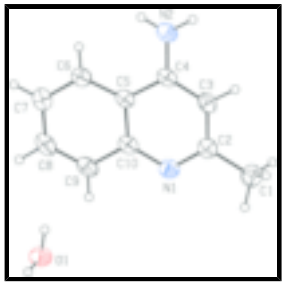


Fig. 1. The molecular structure of (I) showing 30% displacement ellipsoids.

4-Amino-2-methylquinoline monohydrate

Crystal data

$C_{10}H_{10}N_2·H_2O_1$	F_{000} = 376
M_r = 176.22	D_x = 1.223 Mg m^{-3}
Orthorhombic, *Pna*2$_1$	Mo *K*α radiation λ = 0.71073 Å

Hall symbol: P 2c -2n	Cell parameters from 1365 reflections
a = 4.7432 (8) Å	θ = 2.8–23.5º
b = 13.9070 (13) Å	μ = 0.08 mm^{-1}
c = 14.5129 (16) Å	T = 298 (2) K
V = 957.3 (2) $Å^3$	Block, colourless
Z = 4	0.43 × 0.35 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer	882 independent reflections
Radiation source: fine-focus sealed tube	716 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.029
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.0º
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -5 \rightarrow 5$
T_{min} = 0.966, T_{max} = 0.975	$k = -16 \rightarrow 15$
3925 measured reflections	$l = -14 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.032	H-atom parameters constrained
$wR(F^2)$ = 0.093	$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2 + 0.1333P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
882 reflections	$\Delta\rho_{max}$ = 0.10 e $Å^{-3}$
119 parameters	$\Delta\rho_{min}$ = −0.11 e $Å^{-3}$
1 restraint	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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	0.0728 (5)	0.56239 (17)	0.32460 (17)	0.0508 (7)
N2	0.2819 (6)	0.33360 (19)	0.49988 (18)	0.0612 (7)
H2A	0.1996	0.3288	0.5525	0.073*
H2B	0.4034	0.2911	0.4832	0.073*
O1	0.9245 (4)	0.69712 (15)	0.18915 (16)	0.0582 (6)
H1	1.0702	0.7326	0.1914	0.070*
H2	0.9510	0.6552	0.2309	0.070*
C1	−0.2458 (8)	0.6300 (2)	0.4362 (3)	0.0672 (9)
H1A	−0.2491	0.6802	0.3907	0.101*
H1B	−0.1891	0.6563	0.4945	0.101*
H1C	−0.4306	0.6024	0.4417	0.101*
C2	−0.0410 (6)	0.5538 (2)	0.4074 (2)	0.0488 (8)
C3	0.0273 (7)	0.4782 (2)	0.46651 (19)	0.0485 (7)
H3	−0.0600	0.4746	0.5238	0.058*
C4	0.2193 (6)	0.4091 (2)	0.44254 (18)	0.0452 (7)
C5	0.3470 (6)	0.4156 (2)	0.35341 (19)	0.0429 (7)
C6	0.5474 (7)	0.3508 (2)	0.3196 (2)	0.0523 (8)
H6	0.6030	0.2992	0.3562	0.063*
C7	0.6634 (8)	0.3615 (3)	0.2340 (2)	0.0608 (9)
H7	0.7952	0.3175	0.2124	0.073*
C8	0.5828 (7)	0.4388 (3)	0.1796 (3)	0.0631 (9)
H8	0.6624	0.4464	0.1215	0.076*
C9	0.3892 (7)	0.5037 (2)	0.20989 (19)	0.0568 (9)
H9	0.3382	0.5549	0.1722	0.068*
C10	0.2654 (6)	0.4944 (2)	0.29716 (19)	0.0455 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0487 (14)	0.0540 (14)	0.0498 (15)	−0.0009 (12)	−0.0061 (12)	0.0071 (12)
N2	0.0754 (19)	0.0656 (16)	0.0428 (14)	0.0058 (15)	0.0043 (13)	0.0133 (12)
O1	0.0614 (12)	0.0590 (11)	0.0544 (12)	−0.0011 (11)	−0.0117 (12)	0.0083 (10)
C1	0.062 (2)	0.066 (2)	0.074 (2)	0.0027 (18)	0.0037 (19)	−0.0011 (17)
C2	0.0423 (17)	0.0539 (17)	0.0502 (18)	−0.0078 (14)	−0.0049 (14)	−0.0016 (15)
C3	0.0465 (16)	0.0590 (18)	0.0401 (16)	−0.0100 (15)	0.0010 (13)	−0.0024 (14)
C4	0.0428 (17)	0.0520 (16)	0.0406 (15)	−0.0113 (14)	−0.0062 (13)	0.0053 (13)
C5	0.0404 (15)	0.0502 (16)	0.0381 (14)	−0.0100 (13)	−0.0040 (12)	0.0022 (11)
C6	0.0500 (17)	0.0549 (17)	0.0519 (18)	−0.0033 (14)	−0.0021 (15)	0.0059 (14)
C7	0.056 (2)	0.070 (2)	0.056 (2)	−0.0027 (16)	0.0065 (17)	−0.0026 (16)
C8	0.059 (2)	0.084 (2)	0.0464 (16)	−0.0094 (18)	0.0060 (17)	0.0093 (18)
C9	0.0569 (18)	0.069 (2)	0.0440 (19)	−0.0077 (18)	−0.0041 (14)	0.0147 (14)
C10	0.0416 (15)	0.0540 (17)	0.0408 (15)	−0.0100 (13)	−0.0067 (13)	0.0042 (13)

Geometric parameters (Å, °)

N1—C2	1.322 (4)	C3—H3	0.9300
N1—C10	1.374 (4)	C4—C5	1.431 (4)
N2—C4	1.372 (4)	C5—C6	1.399 (4)
N2—H2A	0.8600	C5—C10	1.420 (4)
N2—H2B	0.8600	C6—C7	1.367 (5)
O1—H1	0.8500	C6—H6	0.9300
O1—H2	0.8499	C7—C8	1.387 (5)
C1—C2	1.497 (5)	C7—H7	0.9300
C1—H1A	0.9600	C8—C9	1.361 (5)
C1—H1B	0.9600	C8—H8	0.9300
C1—H1C	0.9600	C9—C10	1.402 (4)
C2—C3	1.396 (4)	C9—H9	0.9300
C3—C4	1.369 (4)		
C2—N1—C10	118.2 (2)	N2—C4—C5	120.3 (3)
C4—N2—H2A	120.0	C6—C5—C10	118.7 (3)
C4—N2—H2B	120.0	C6—C5—C4	124.3 (3)
H2A—N2—H2B	120.0	C10—C5—C4	116.9 (3)
H1—O1—H2	104.5	C7—C6—C5	121.4 (3)
C2—C1—H1A	109.5	C7—C6—H6	119.3
C2—C1—H1B	109.5	C5—C6—H6	119.3
H1A—C1—H1B	109.5	C6—C7—C8	119.4 (3)
C2—C1—H1C	109.5	C6—C7—H7	120.3
H1A—C1—H1C	109.5	C8—C7—H7	120.3
H1B—C1—H1C	109.5	C9—C8—C7	121.1 (3)
N1—C2—C3	122.1 (3)	C9—C8—H8	119.4
N1—C2—C1	117.0 (3)	C7—C8—H8	119.4
C3—C2—C1	120.8 (3)	C8—C9—C10	120.8 (3)
C4—C3—C2	121.8 (3)	C8—C9—H9	119.6
C4—C3—H3	119.1	C10—C9—H9	119.6
C2—C3—H3	119.1	N1—C10—C9	118.4 (3)
C3—C4—N2	121.8 (3)	N1—C10—C5	123.1 (3)
C3—C4—C5	117.9 (3)	C9—C10—C5	118.5 (3)
C10—N1—C2—C3	−0.4 (4)	C5—C6—C7—C8	0.6 (5)
C10—N1—C2—C1	178.8 (3)	C6—C7—C8—C9	−0.4 (5)
N1—C2—C3—C4	0.9 (4)	C7—C8—C9—C10	0.1 (5)
C1—C2—C3—C4	−178.3 (3)	C2—N1—C10—C9	−179.3 (2)
C2—C3—C4—N2	−178.6 (3)	C2—N1—C10—C5	0.1 (4)
C2—C3—C4—C5	−1.0 (4)	C8—C9—C10—N1	179.5 (3)
C3—C4—C5—C6	179.6 (3)	C8—C9—C10—C5	0.1 (4)
N2—C4—C5—C6	−2.8 (4)	C6—C5—C10—N1	−179.2 (3)
C3—C4—C5—C10	0.7 (4)	C4—C5—C10—N1	−0.2 (4)
N2—C4—C5—C10	178.3 (2)	C6—C5—C10—C9	0.1 (4)
C10—C5—C6—C7	−0.5 (4)	C4—C5—C10—C9	179.1 (2)
C4—C5—C6—C7	−179.4 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O1^{i}	0.85	1.94	2.791 (3)	174
O1—H2···N1^{ii}	0.85	1.96	2.805 (3)	171
N2—H2A···O1^{iii}	0.86	2.10	2.947 (4)	168
N2—H2B···N2^{iv}	0.86	2.51	3.321 (4)	158

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

Fig. 1