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4-Amino-2-methylquinoline monohydrate

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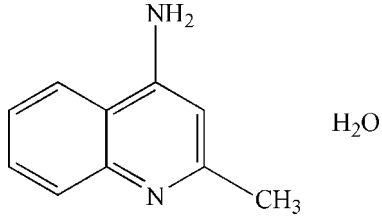
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.033; wR factor = 0.094; data-to-parameter ratio = 7.4.

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*.

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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.

supporting information

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

4-Amino-2-methylquinoline monohydrate

Xi-Shi Tai, Jun Xu, Yi-Min Feng and Zu-Pei Liang

S1. 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).

S2. 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.

S3. 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).

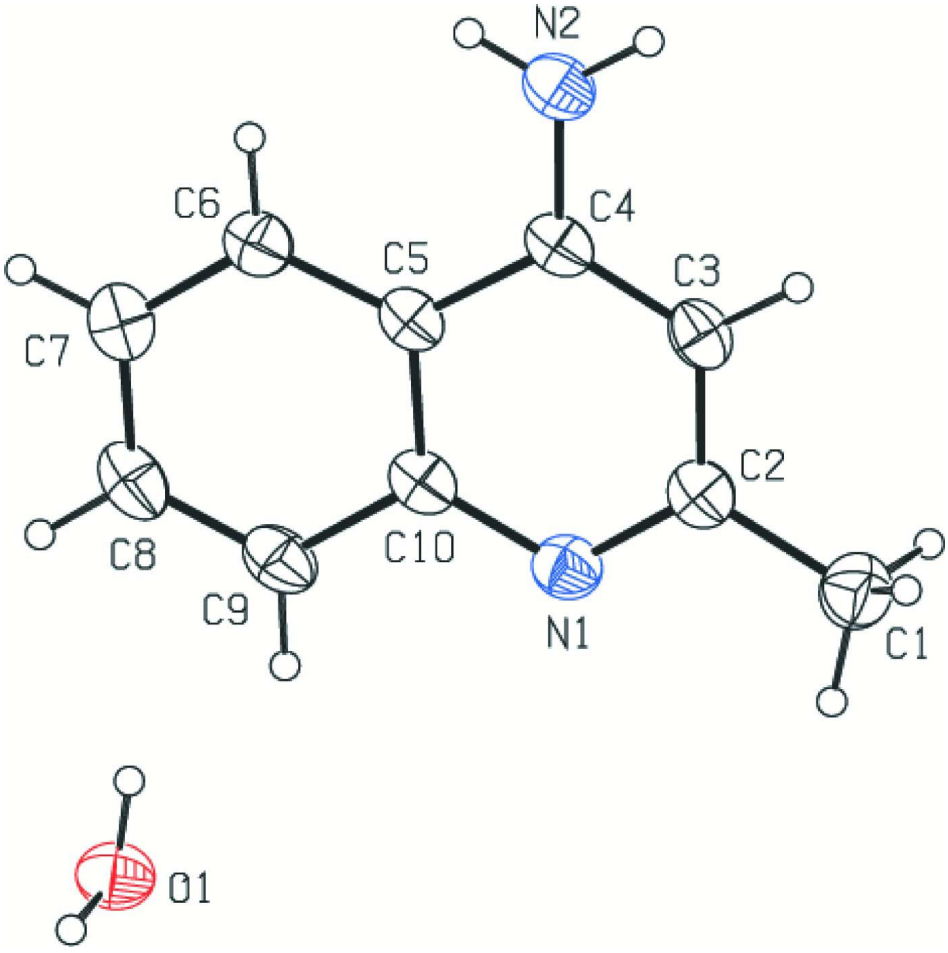

Figure 1

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

4-Amino-2-methylquinoline monohydrate

Crystal data

$C_{10}H_{10}N_2 \cdot H_2O$
$M_r = 176.22$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 4.7432\ (8)$ Å
$b = 13.9070\ (13)$ Å
$c = 14.5129\ (16)$ Å
$V = 957.3\ (2)$ Å^3
$Z = 4$
$F(000) = 376$
$D_x = 1.223$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1365 reflections
$\theta = 2.8$–$23.5°$
$\mu = 0.08$ mm^{-1}
$T = 298$ K
Block, colourless
0.43 × 0.35 × 0.32 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
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
θ_{max} = 25.0°, θ_{min} = 2.0°
h = −5→5
k = −16→15
l = −14→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.093
S = 1.05
882 reflections
119 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2 + 0.1333P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 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 (Å²)

	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 (Å²)

	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, º)

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, º)

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—H2*A*···O1^{iii}	0.86	2.10	2.947 (4)	168
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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*.