

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

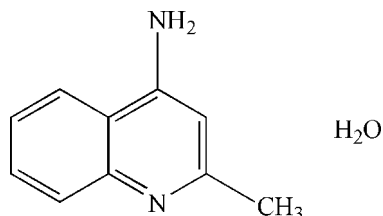
4-Amino-2-methylquinoline
monohydrateXi-Shi Tai,^{a*} Jun Xu,^b Yi-Min Feng^a and Zu-Pei Liang^a^aDepartment of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China, and ^bWeifang Institute of Supervision and Inspection of Product Quality, Weifang 261031, People's Republic of China

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Received 1 May 2008; accepted 3 May 2008

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.033; wR factor = 0.094; data-to-parameter ratio = 7.4.The crystal structure of the title compound, $\text{C}_{10}\text{H}_{10}\text{N}_2 \cdot \text{H}_2\text{O}$, is stabilized by intermolecular $\text{O}-\text{H} \cdots \text{N}$, $\text{N}-\text{H} \cdots \text{O}$ and $\text{N}-\text{H} \cdots \text{N}$ 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

 $\text{C}_{10}\text{H}_{10}\text{N}_2 \cdot \text{H}_2\text{O}$ $M_r = 176.22$ Orthorhombic, $Pna2_1$ $a = 4.7432$ (8) Å $b = 13.9070$ (13) Å $c = 14.5129$ (16) Å $V = 957.3$ (2) Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 0.08$ mm⁻¹ $T = 298$ (2) K $0.43 \times 0.35 \times 0.32$ 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 $I > 2\sigma(I)$ $R_{\text{int}} = 0.029$

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

 $\Delta\rho_{\text{max}} = 0.10$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.11$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H} \cdots A$ | $D-\text{H}$ | $\text{H} \cdots A$ | $D \cdots A$ | $D-\text{H} \cdots A$ |
|--|--------------|---------------------|--------------|-----------------------|
| $\text{O1}-\text{H1} \cdots \text{O1}^{\text{i}}$ | 0.85 | 1.94 | 2.791 (3) | 174 |
| $\text{O1}-\text{H2} \cdots \text{N1}^{\text{ii}}$ | 0.85 | 1.96 | 2.805 (3) | 171 |
| $\text{N2}-\text{H2A} \cdots \text{O1}^{\text{iii}}$ | 0.86 | 2.10 | 2.947 (4) | 168 |
| $\text{N2}-\text{H2B} \cdots \text{N2}^{\text{iv}}$ | 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).

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supplementary materials

Acta Cryst. (2008). E64, 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 \cdots N, N—H \cdots O and N—H \cdots 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 $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{carrier})$.

Figures

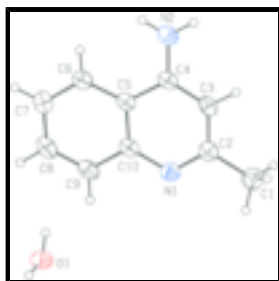


Fig. 1. The molecular structure of (I) showing 30% displacement ellipsoids.

4-Amino-2-methylquinoline monohydrate

Crystal data

$\text{C}_{10}\text{H}_{10}\text{N}_2 \cdot \text{H}_2\text{O}_1$

$M_r = 176.22$

Orthorhombic, $Pna2_1$

$F_{000} = 376$

$D_x = 1.223 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

supplementary materials

Hall symbol: P 2c -2n
 $a = 4.7432$ (8) Å
 $b = 13.9070$ (13) Å
 $c = 14.5129$ (16) Å
 $V = 957.3$ (2) Å³
 $Z = 4$

Cell parameters from 1365 reflections
 $\theta = 2.8$ – 23.5°
 $\mu = 0.08$ mm⁻¹
 $T = 298$ (2) K
Block, colourless
 $0.43 \times 0.35 \times 0.32$ mm

Data collection

Bruker SMART CCD area-detector
diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
 $T = 298$ (2) K
 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
 $\theta_{\max} = 25.0^\circ$
 $\theta_{\min} = 2.0^\circ$
 $h = -5 \rightarrow 5$
 $k = -16 \rightarrow 15$
 $l = -14 \rightarrow 17$

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
Extinction correction: none

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|--------------|--------------|----------------------------------|
| 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 (\AA^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) |

supplementary materials

Geometric parameters (\AA , $^\circ$)

| | | | |
|--------------|------------|--------------|------------|
| 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, °)

| <i>D</i> —H··· <i>A</i> | <i>D</i> —H | H··· <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> —H··· <i>A</i> |
|----------------------------|-------------|---------------|-----------------------|-------------------------|
| 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

