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Quinolin-3-amine

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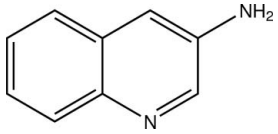
Key indicators: single-crystal X-ray study; T = 200 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.091; data-to-parameter ratio = 10.0.

In the crystal structur of the achiral title compound, $C_9H_8N_2$, N—H···N hydrogen bonds connect the molecules into zigzag chains in [100]. Weak intermolecular N–H···π interactions further consolidate the crystal packing.

Related literature

For novel applications of quinolin-3-amine and its derivatives, see: Rohmer *et al.* (2010); Kaneshiro *et al.* (2011). For the crystal structure of a rhodium coordination compound featuring the title compound as a ligand, see: Garralda *et al.* (1999). For graph-set analysis of hydrogen bonds, see: Etter *et al.* (1990); Bernstein *et al.* (1995).



Experimental

Crystal data

$C_9H_8N_2$
M_r = 144.17
Orthorhombic, $P2_12_12_1$
a = 7.6223 (3) Å
b = 7.6289 (3) Å
c = 12.6967 (4) Å
V = 738.31 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 200 K
0.55 × 0.52 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.950, T_{max} = 0.988
6898 measured reflections
1077 independent reflections
1015 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.091
S = 1.03
1077 reflections
108 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

Cg is the centroid of the C1/C5–C9 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···N1^{i}	0.90 (2)	2.22 (2)	3.0761 (17)	158.2 (18)
N2—H2A···Cg^{ii}	0.85 (2)	2.60 (2)	3.3101 (15)	142.3 (19)

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

Data collection: *APEX2* (Bruker, 2010); cell refinement: *SAINT* (Bruker, 2010); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5347).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2008). *SADABS*. Bruker Inc., Madison, Wisconsin, USA.
Bruker (2010). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, USA.
Etter, M. C., MacDonald, J. C. & Bernstein, J. (1990). *Acta Cryst.* B**46**, 256–262.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Garralda, M. A., Hernandez, R., Pinilla, E. & Rosario Torres, M. (1999). *J. Organomet. Chem.* **586**, 150–158.
Kaneshiro, K., Fukuyama, Y., Iwamoto, S., Sekiya, S. & Tanaka, K. (2011). *Anal. Chem.* **83**, 3663–3667.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Rohmer, M., Meyer, B., Mank, M., Stahl, B., Bahr, U. & Karas, M. (2010). *Anal. Chem.* **82**, 3719–3726.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

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Quinolin-3-amine

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S1. Comment

3-Aminoquinoline and its derivatives have found applications in matrix-assisted laser desorption ionization (MALDI) mass-spectrometry of oligosaccharides (Rohmer *et al.*, 2010) and glycans (Kaneshiro *et al.*, 2011). Herewith we present the crystal structure of 3-aminoquinoline, (I).

In (I) (Fig. 1), the molecule bears an amino group in *meta* position to the intracyclic nitrogen atom. Intracyclic angles in the six-membered ring containing the nitrogen atom cover a range of 117.42 (12)–125.27 (11) ° with the smallest angle found on the carbon atom bearing the amino group and the biggest angle present on the hydrogen-bearing carbon atom in *ortho* position to the intracyclic nitrogen atom. The molecule is essentially planar (r.m.s. deviation of of all fitted non-hydrogen atoms = 0.0091 Å). The least-squares planes defined by the non-hydrogen atoms of the heterocycle on the one hand and the atoms of the amino group on the other hand intersect at an angle of 11.97(2.58) °.

In the crystal, N–H···N hydrogen bonds (Table 1) are observed between the amino group and the intracyclic nitrogen atom that connect the molecules to zigzag chains along the crystallographic *a* axis (Fig. 2). In terms of graph-set analysis (Etter *et al.*, 1990; Bernstein *et al.*, 1995), the descriptor for these contacts is $C^1_1(5)$ on the unary level. In addition, a N–H···π interaction (Table 1) involving the non-heterocyclic moiety of the quinoline core as acceptor contribute to the crystal packing stability.

S2. Experimental

To a solution of 3-nitroquinoline (1 g, 0.0057 mol) in methanol (20 ml) 10% palladium on carbon (0.10 g) was added. The batch was hydrogenated at a pressure of 10 bar for 12 h. Subsequently, the reaction mixture was filtered and concentrated under reduced pressure to afford the title compound as a pale yellow solid. The solid was dissolved in absolute ethanol and allowed to stand and evaporate at room temperature overnight. The crystalline solid that developed was filtered and dried under high vacuum (yield: 0.8 g, 97.5%).

S3. Refinement

C-bound H atoms were placed in calculated positions (C—H 0.95 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2U_{eq}(C). Both amino H atoms were located on a difference Fourier map and refined freely. In the absence of strong anomalous scatterers, 737 Friedel pairs were merged before the final refinement.

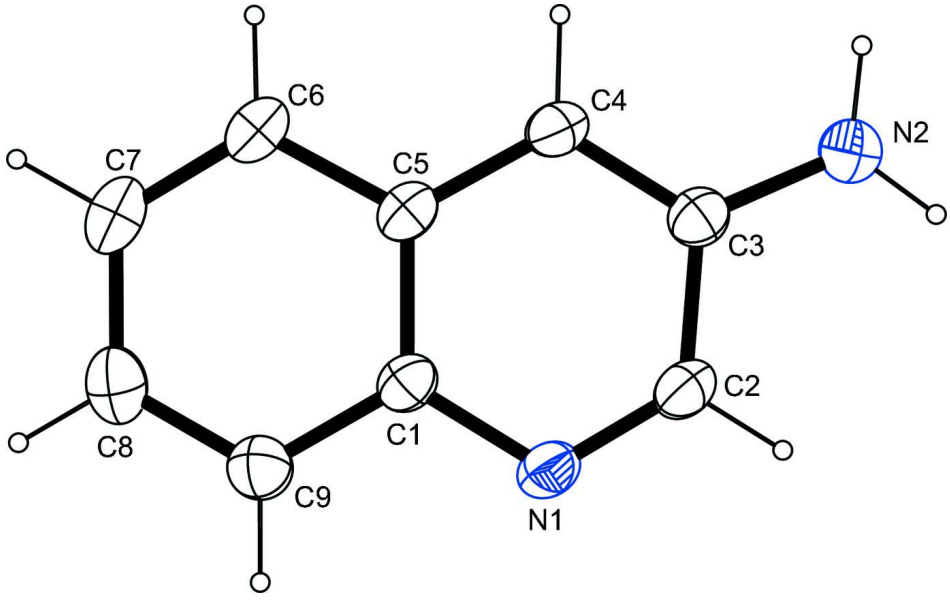

Figure 1

The molecular structure of the title compound, with atom labels and anisotropic displacement ellipsoids (drawn at the 50% probability level).

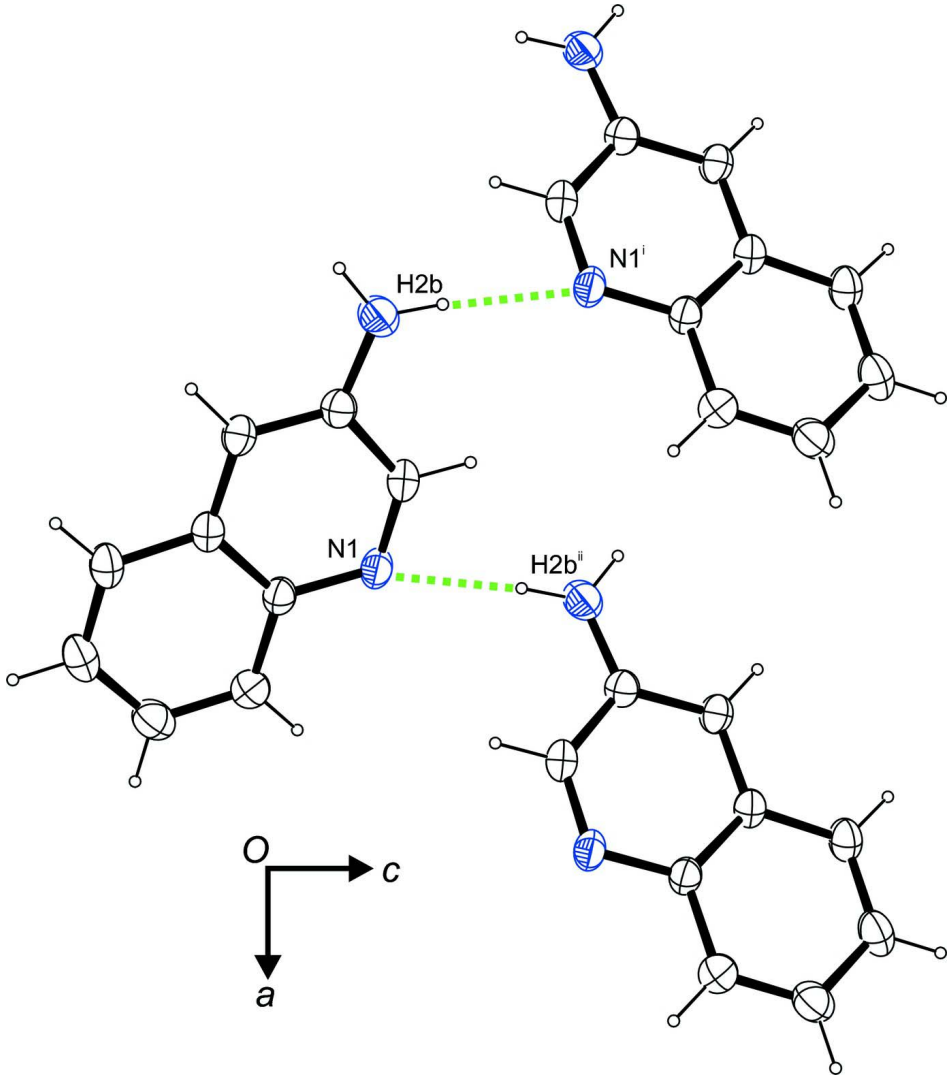

Figure 2

A portion of the crystal packing viewed along [010]. Dashed lines indicate N–H···N hydrogen bonds. Symmetry codes: (i) *x* - 1/2, -*y* + 1/2, -*z* + 1; (ii) *x* + 1/2, -*y* + 1/2, -*z* + 1.

Quinolin-3-amine

Crystal data

$C_9H_8N_2$
M_r = 144.17
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
a = 7.6223 (3) Å
b = 7.6289 (3) Å
c = 12.6967 (4) Å
V = 738.31 (5) Å^3
Z = 4
F(000) = 304

D_x = 1.297 Mg m^{-3}
Melting point = 366–368 K
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 5242 reflections
θ = 2.7–28.3°
μ = 0.08 mm^{-1}
T = 200 K
Block, colourless
0.55 × 0.52 × 0.15 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.950, T_{max} = 0.988
6898 measured reflections
1077 independent reflections
1015 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 28.3°, θ_{min} = 3.1°
h = −6→10
k = −9→10
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.091
S = 1.03
1077 reflections
108 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2 + 0.1011P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Special details

Refinement. Due to the absence of a strong anomalous scatterer, the Flack parameter is meaningless. Thus, Friedel opposites (737 pairs) have been merged and the item was removed from the CIF.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.25487 (15)	0.26319 (16)	0.38612 (8)	0.0280 (3)
N2	−0.18546 (17)	0.08305 (19)	0.39280 (11)	0.0359 (3)
H2A	−0.258 (3)	0.023 (3)	0.3568 (15)	0.056 (6)*
H2B	−0.198 (2)	0.098 (3)	0.4628 (17)	0.043 (5)*
C1	0.30327 (17)	0.23241 (17)	0.28353 (9)	0.0249 (3)
C2	0.09884 (17)	0.21121 (18)	0.41581 (9)	0.0277 (3)
H2	0.0663	0.2323	0.4869	0.033*
C3	−0.02593 (17)	0.12565 (16)	0.35016 (9)	0.0253 (3)
C4	0.02155 (18)	0.09412 (17)	0.24707 (10)	0.0265 (3)
H4	−0.0576	0.0376	0.2003	0.032*
C5	0.18933 (16)	0.14693 (17)	0.21189 (9)	0.0244 (3)
C6	0.24840 (19)	0.11883 (19)	0.10713 (10)	0.0299 (3)
H6	0.1743	0.0609	0.0580	0.036*
C7	0.4113 (2)	0.17449 (19)	0.07635 (10)	0.0344 (3)
H7	0.4488	0.1553	0.0059	0.041*
C8	0.52397 (19)	0.2599 (2)	0.14793 (11)	0.0353 (3)
H8	0.6366	0.2982	0.1256	0.042*
C9	0.47097 (17)	0.28794 (19)	0.25005 (11)	0.0313 (3)
H9	0.5474	0.3448	0.2982	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0323 (5)	0.0323 (6)	0.0193 (5)	−0.0026 (5)	−0.0030 (4)	−0.0003 (4)
N2	0.0318 (6)	0.0443 (7)	0.0316 (6)	−0.0081 (5)	0.0052 (5)	−0.0086 (6)
C1	0.0277 (6)	0.0263 (6)	0.0207 (5)	0.0017 (5)	−0.0018 (5)	0.0009 (5)
C2	0.0340 (6)	0.0299 (6)	0.0191 (5)	−0.0004 (5)	−0.0012 (5)	−0.0007 (5)
C3	0.0279 (6)	0.0238 (5)	0.0243 (6)	0.0009 (5)	−0.0004 (5)	−0.0006 (5)
C4	0.0306 (6)	0.0264 (6)	0.0226 (5)	−0.0013 (5)	−0.0021 (5)	−0.0045 (5)
C5	0.0303 (6)	0.0228 (6)	0.0202 (5)	0.0027 (5)	−0.0006 (5)	−0.0003 (5)
C6	0.0382 (7)	0.0298 (6)	0.0218 (6)	0.0032 (5)	0.0015 (5)	−0.0037 (5)
C7	0.0430 (7)	0.0348 (7)	0.0254 (5)	0.0059 (6)	0.0084 (6)	−0.0008 (5)
C8	0.0320 (6)	0.0389 (7)	0.0350 (7)	0.0010 (6)	0.0070 (6)	0.0052 (6)
C9	0.0294 (7)	0.0347 (7)	0.0298 (6)	−0.0008 (5)	−0.0009 (5)	0.0008 (6)

Geometric parameters (Å, º)

N1—C2	1.3091 (17)	C4—C5	1.4133 (18)
N1—C1	1.3740 (16)	C4—H4	0.9500
N2—C3	1.3701 (17)	C5—C6	1.4205 (17)
N2—H2A	0.85 (2)	C6—C7	1.369 (2)
N2—H2B	0.90 (2)	C6—H6	0.9500
C1—C9	1.4122 (18)	C7—C8	1.410 (2)
C1—C5	1.4167 (17)	C7—H7	0.9500
C2—C3	1.4231 (17)	C8—C9	1.375 (2)
C2—H2	0.9500	C8—H8	0.9500
C3—C4	1.3792 (17)	C9—H9	0.9500
C2—N1—C1	117.72 (11)	C4—C5—C1	118.88 (11)
C3—N2—H2A	119.4 (14)	C4—C5—C6	122.66 (12)
C3—N2—H2B	116.8 (12)	C1—C5—C6	118.45 (12)
H2A—N2—H2B	122.1 (18)	C7—C6—C5	120.52 (13)
N1—C1—C9	118.50 (12)	C7—C6—H6	119.7
N1—C1—C5	121.52 (12)	C5—C6—H6	119.7
C9—C1—C5	119.98 (11)	C6—C7—C8	120.78 (12)
N1—C2—C3	125.27 (11)	C6—C7—H7	119.6
N1—C2—H2	117.4	C8—C7—H7	119.6
C3—C2—H2	117.4	C9—C8—C7	120.04 (13)
N2—C3—C4	124.50 (12)	C9—C8—H8	120.0
N2—C3—C2	118.07 (11)	C7—C8—H8	120.0
C4—C3—C2	117.42 (12)	C8—C9—C1	120.22 (13)
C3—C4—C5	119.19 (12)	C8—C9—H9	119.9
C3—C4—H4	120.4	C1—C9—H9	119.9
C5—C4—H4	120.4		
C2—N1—C1—C9	179.86 (12)	C9—C1—C5—C4	−179.41 (11)
C2—N1—C1—C5	−0.20 (19)	N1—C1—C5—C6	−179.74 (12)
C1—N1—C2—C3	−0.3 (2)	C9—C1—C5—C6	0.20 (18)

N1—C2—C3—N2	−178.55 (13)	C4—C5—C6—C7	179.12 (12)
N1—C2—C3—C4	0.3 (2)	C1—C5—C6—C7	−0.5 (2)
N2—C3—C4—C5	178.95 (12)	C5—C6—C7—C8	0.3 (2)
C2—C3—C4—C5	0.15 (18)	C6—C7—C8—C9	0.1 (2)
C3—C4—C5—C1	−0.61 (18)	C7—C8—C9—C1	−0.4 (2)
C3—C4—C5—C6	179.80 (12)	N1—C1—C9—C8	−179.82 (13)
N1—C1—C5—C4	0.66 (18)	C5—C1—C9—C8	0.2 (2)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C1/C5–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···N1^{i}	0.90 (2)	2.22 (2)	3.0761 (17)	158.2 (18)
N2—H2*A*···*Cg*^{ii}	0.85 (2)	2.60 (2)	3.3101 (15)	142.3 (19)

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