organic compounds

Quinoline-2-carbonitrile

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In the title compound, $C_{10}H_6N_2$, the molecule is almost planar, with an r.m.s. deviation of 0.014 Å. The dihedral angle between the aromatic rings is 1.28 (16)°. In the crystal, molecules are stacked along the a axis by way of weak aromatic π–π stacking interactions between the benzene and pyridine rings of adjacent molecules [centroid–centroid separation = 3.7943 (19) Å].

Related literature

For the biological activity and syntheses of quinoline derivatives, see: Sasaki *et al.* (1998); Reux *et al.* (2009). For related structures, see: Fun *et al.* (2010); Loh *et al.* (2009, 2010). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986). For bond-length data, see: Allen *et al.* (1987).
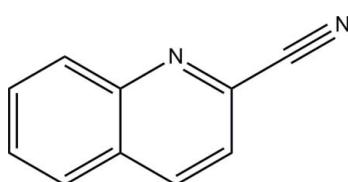
Experimental

Crystal data

$C_{10}H_6N_2$	M_r = 154.17

Orthorhombic, $P2_12_12_1$
a = 3.8497 (2) Å
b = 9.9559 (4) Å
c = 19.9639 (13) Å
V = 765.16 (7) Å^3

Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 100 K
0.36 × 0.18 × 0.03 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.971, T_{max} = 0.997

4086 measured reflections
1056 independent reflections
838 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.141
S = 1.09
1056 reflections

109 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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‡ Thomson Reuters ResearcherID: C-7581-2009.
§ Thomson Reuters ResearcherID: A-5525-2009.
¶ Thomson Reuters ResearcherID: A-3561-2009.

supporting information

Quinoline-2-carbonitrile

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S1. Comment

Heterocyclic molecules containing cyano group are useful as drug intermediates. Syntheses of the quinoline derivatives were discussed earlier (Sasaki *et al.*, 1998; Reux *et al.*, 2009). Recently, we have synthesized a number of quinoline compounds to investigate the hydrogen bonding patterns in these compounds (Loh *et al.*, 2009; 2010). Herein we report the crystal structure of quinoline-2-carbonitrile.

In the title compound, Fig. 1, the molecule is almost planar with an r.m.s. deviation of 0.014 Å. The dihedral angle between the benzene (C3–C8) and pyridine (C1–C3/N1/C8/C9) rings is 1.28 (16)°. The bond lengths (Allen *et al.*, 1987) and angles in the title compound are within normal ranges and comparable to the related structure of quinoxaline-2-carbonitrile (Fun *et al.*, 2010).

In the crystal packing, Fig. 2, the molecules are stacked along the *a* axis by way of weak aromatic π–π stacking interactions between the centroid of the benzene (*Cg*1) and the centroid of the pyridine (*Cg*2) rings of adjacent molecules [*Cg*1⋯*Cg*2 separation = 3.7943 (19) Å]. There is no significant hydrogen bond observed in this compound.

S2. Experimental

A hot methanol solution (20 ml) of quinoline-2-carbonitrile (39 mg, Aldrich) was warmed over a magnetic stirrer hotplate for a few minutes. The resulting solution was allowed to cool slowly to room temperature. Colourless plates of (I) appeared after a few days.

S3. Refinement

All H atoms were positioned geometrically with the bond length of C–H being 0.93 Å and were refined using a riding model, with U_{iso}(H) = 1.2 U_{eq}(C). In the absence of significant anomalous dispersion, 616 Friedel pairs were merged for the final refinement.

Figure 1

The molecular structure of (I) showing 50% probability displacement ellipsoids for non-H atoms.

Figure 2

The crystal structure of (I), viewed along the *a* axis.
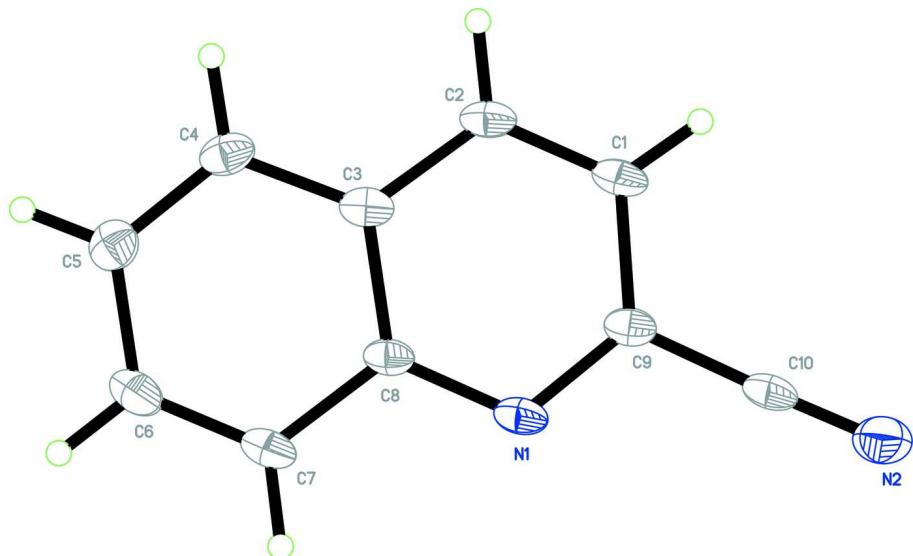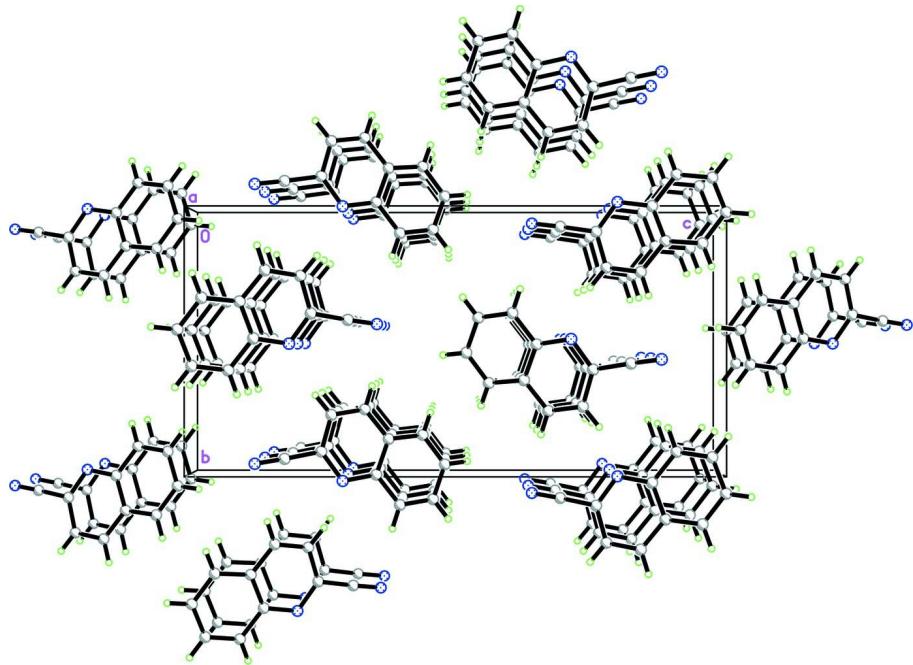
Quinoline-2-carbonitrile

Crystal data

$C_{10}H_6N_2$	$b = 9.9559\ (4)$ Å
$M_r = 154.17$	$c = 19.9639\ (13)$ Å
Orthorhombic, $P2_12_12_1$	$V = 765.16\ (7)$ Å^3
Hall symbol: P 2ac 2ab	$Z = 4$
$a = 3.8497\ (2)$ Å	$F(000) = 320$

$D_x = 1.338$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 930 reflections
$\theta = 3.7–27.4°$

$\mu = 0.08$ mm^{-1}
$T = 100$ K
Plate, colourless
$0.36 \times 0.18 \times 0.03$ mm

Data collection

Bruker SMART APEXII CCD
 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan
 (*SADABS*; Bruker, 2009)
$T_{min} = 0.971$, $T_{max} = 0.997$

4086 measured reflections
1056 independent reflections
838 reflections with $I > 2\sigma(I)$
$R_{int} = 0.059$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.7°$
$h = -4\rightarrow4$
$k = -12\rightarrow12$
$l = -25\rightarrow21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.141$
$S = 1.09$
1056 reflections
109 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
$w = 1/[\sigma^2(F_o^2) + (0.0827P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat
(Cosier & Glazer, 1986) operating at 100.0 (1) K.

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	0.7386 (8)	0.5083 (2)	0.20498 (14)	0.0185 (6)
N2	0.3930 (9)	0.4374 (2)	0.35822 (16)	0.0296 (7)
C1	0.7983 (9)	0.2683 (3)	0.22614 (16)	0.0193 (7)
H1A	0.7552	0.1964	0.2547	0.023*
C2	0.9617 (9)	0.2502 (3)	0.16647 (16)	0.0192 (7)
H2A	1.0368	0.1649	0.1541	0.023*
C3	1.0178 (9)	0.3604 (3)	0.12314 (16)	0.0174 (7)
C4	1.1815 (8)	0.3487 (3)	0.06064 (16)	0.0201 (7)
H4A	1.2662	0.2658	0.0468	0.024*
C5	1.2177 (9)	0.4589 (3)	0.01965 (18)	0.0224 (7)

H5A	1.3204	0.4498	−0.0223	0.027*
C6	1.0989 (8)	0.5855 (3)	0.04129 (17)	0.0239 (8)
H6A	1.1257	0.6595	0.0133	0.029*
C7	0.9466 (9)	0.6018 (3)	0.10188 (17)	0.0213 (7)
H7A	0.8736	0.6866	0.1154	0.026*
C8	0.8981 (8)	0.4894 (3)	0.14492 (17)	0.0162 (7)
C9	0.6962 (8)	0.4002 (3)	0.24322 (16)	0.0169 (7)
C10	0.5263 (9)	0.4229 (3)	0.30714 (17)	0.0196 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0149 (13)	0.0120 (10)	0.0284 (15)	−0.0014 (10)	−0.0013 (13)	−0.0012 (10)
N2	0.0336 (17)	0.0199 (13)	0.0353 (17)	0.0000 (12)	0.0055 (16)	−0.0013 (13)
C1	0.0146 (16)	0.0128 (12)	0.0306 (18)	0.0016 (12)	−0.0030 (15)	0.0009 (12)
C2	0.0155 (16)	0.0113 (12)	0.0307 (18)	0.0009 (12)	−0.0020 (15)	−0.0027 (12)
C3	0.0130 (15)	0.0150 (13)	0.0243 (17)	0.0006 (11)	−0.0063 (14)	−0.0028 (12)
C4	0.0134 (16)	0.0184 (14)	0.0286 (19)	0.0016 (12)	−0.0010 (15)	−0.0060 (13)
C5	0.0164 (16)	0.0251 (15)	0.0256 (17)	−0.0004 (14)	−0.0003 (15)	−0.0006 (13)
C6	0.0218 (17)	0.0167 (13)	0.0333 (19)	−0.0009 (13)	−0.0003 (16)	0.0053 (14)
C7	0.0202 (17)	0.0128 (13)	0.0311 (19)	−0.0003 (13)	−0.0039 (16)	0.0021 (12)
C8	0.0124 (15)	0.0111 (12)	0.0249 (16)	−0.0016 (11)	−0.0027 (14)	−0.0033 (12)
C9	0.0130 (14)	0.0130 (12)	0.0247 (17)	−0.0019 (12)	−0.0035 (14)	−0.0018 (11)
C10	0.0186 (17)	0.0098 (12)	0.0306 (19)	−0.0019 (12)	−0.0015 (15)	0.0008 (12)

Geometric parameters (Å, º)

N1—C9	1.329 (4)	C4—C5	1.376 (4)
N1—C8	1.360 (4)	C4—H4A	0.9300
N2—C10	1.151 (4)	C5—C6	1.409 (4)
C1—C2	1.359 (4)	C5—H5A	0.9300
C1—C9	1.413 (4)	C6—C7	1.354 (4)
C1—H1A	0.9300	C6—H6A	0.9300
C2—C3	1.414 (4)	C7—C8	1.424 (4)
C2—H2A	0.9300	C7—H7A	0.9300
C3—C4	1.402 (4)	C9—C10	1.452 (4)
C3—C8	1.432 (4)		
C9—N1—C8	116.7 (2)	C6—C5—H5A	120.1
C2—C1—C9	117.6 (3)	C7—C6—C5	121.5 (3)
C2—C1—H1A	121.2	C7—C6—H6A	119.3
C9—C1—H1A	121.2	C5—C6—H6A	119.3
C1—C2—C3	120.3 (3)	C6—C7—C8	120.1 (3)
C1—C2—H2A	119.9	C6—C7—H7A	120.0
C3—C2—H2A	119.9	C8—C7—H7A	120.0
C4—C3—C2	123.3 (2)	N1—C8—C7	118.8 (2)
C4—C3—C8	119.3 (3)	N1—C8—C3	122.5 (3)
C2—C3—C8	117.4 (3)	C7—C8—C3	118.7 (3)

C5—C4—C3	120.6 (3)	N1—C9—C1	125.4 (3)
C5—C4—H4A	119.7	N1—C9—C10	115.7 (2)
C3—C4—H4A	119.7	C1—C9—C10	118.8 (3)
C4—C5—C6	119.9 (3)	N2—C10—C9	178.2 (3)
C4—C5—H5A	120.1		
C9—C1—C2—C3	−1.4 (4)	C6—C7—C8—N1	−178.8 (3)
C1—C2—C3—C4	−179.4 (3)	C6—C7—C8—C3	0.9 (5)
C1—C2—C3—C8	0.3 (4)	C4—C3—C8—N1	−179.7 (3)
C2—C3—C4—C5	177.7 (3)	C2—C3—C8—N1	0.6 (4)
C8—C3—C4—C5	−2.0 (4)	C4—C3—C8—C7	0.6 (4)
C3—C4—C5—C6	1.9 (5)	C2—C3—C8—C7	−179.1 (3)
C4—C5—C6—C7	−0.4 (5)	C8—N1—C9—C1	−1.0 (5)
C5—C6—C7—C8	−1.0 (5)	C8—N1—C9—C10	179.8 (3)
C9—N1—C8—C7	179.4 (3)	C2—C1—C9—N1	1.8 (5)
C9—N1—C8—C3	−0.3 (4)	C2—C1—C9—C10	−179.0 (3)