Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Cyanoanilinium bromide

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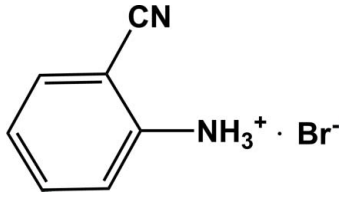
Received 18 August 2009; accepted 1 September 2009

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.025; wR factor = 0.050; data-to-parameter ratio = 19.1.

In the cation of the title compound, $C_7H_7N_2^+\cdot Br^-$, the nitrile group and the benzene ring are almost coplanar (r.m.s. deviation = 0.0043 Å). In the crystal, the cations and anions are connected by intermolecular N—H···Br hydrogen bonds, forming a two-dimensional network parallel to (010).

Related literature

For nitrile derivatives, see: Fu *et al.* (2008); Wang *et al.* (2002). Nitrile derivatives used in the construction of novel metal-organic frameworks. For applications of metal-organic coordination compounds, see: Fu *et al.* (2007); Chen *et al.* (2000); Fu & Xiong (2008); Xiong *et al.* (1999); Xie *et al.* (2003); Zhang *et al.* (2001).



Experimental

Crystal data

$C_7H_7N_2^+\cdot Br^-$
M_r = 199.06
Monoclinic, *Cc*
a = 5.7844 (12) Å
b = 15.896 (3) Å
c = 8.4882 (17) Å
β = 92.72 (3)°
V = 779.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.19 mm^{-1}
T = 298 K
0.40 × 0.05 × 0.05 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.65, T_{max} = 0.77
3848 measured reflections
1773 independent reflections
1581 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.050
S = 0.87
1773 reflections
93 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}
Absolute structure: Flack (1983), 872 Friedels pairs
Flack parameter: 0.004 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Br1	0.89	2.36	3.234 (3)	168
N1—H1B···Br1^{i}	0.89	2.47	3.355 (3)	173
N1—H1C···Br1^{ii}	0.89	2.42	3.286 (3)	164

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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*.

This work was supported by the Outstanding Doctoral Dissertation Fund from Southeast University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2593).

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supporting information

Acta Cryst. (2009). E**65**, o2407 [doi:10.1107/S1600536809035223]

2-Cyanoanilinium bromide

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S1. Comment

The construction of metal-organic coordination compounds has attracted much attention owing to potential functions, such as permittivity, fluorescence, magnetism and optical properties (Fu *et al.*, 2007; Chen *et al.*, 2000; Fu & Xiong (2008); Xie *et al.*, 2003; Zhang *et al.*, 2001; Xiong *et al.*, 1999). Nitrile derivatives are a class of excellent ligands for the construction of novel metal-organic frameworks (Wang *et al.*, 2002; Fu *et al.*, 2008). We report here the crystal structure of the title compound.

In the 2-cyanoanilinium cation (Fig.1), the nitrile group and the benzene ring are almost coplanar. The nitrile group C7≡N2 bond length of 1.142 (4) Å is within the normal range.

In the crystal structure, all the amine group H atoms are involved in N—H···Br hydrogen bonds (Table 1) with Br^- anions. These hydrogen bonds along with N—H···Br hydrogen bonds link the ionic units into a two-dimensional network (Fig. 2) parallel to the (0 1 0) plane.

S2. Experimental

The commercial 2-aminobenzonitrile (3 mmol, 0.55 g) and HBr (0.5 ml) were dissolved in ethanol (20 ml). Colourless needle-shaped crystals of the title compound suitable for X-ray analysis were obtained by slow evaporation at room temperature.

S3. Refinement

All H atoms attached to C and N atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å, N—H = 0.89 Å and U_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.5U_{eq}(N). A rotating-group model was used for the -NH_3 group.

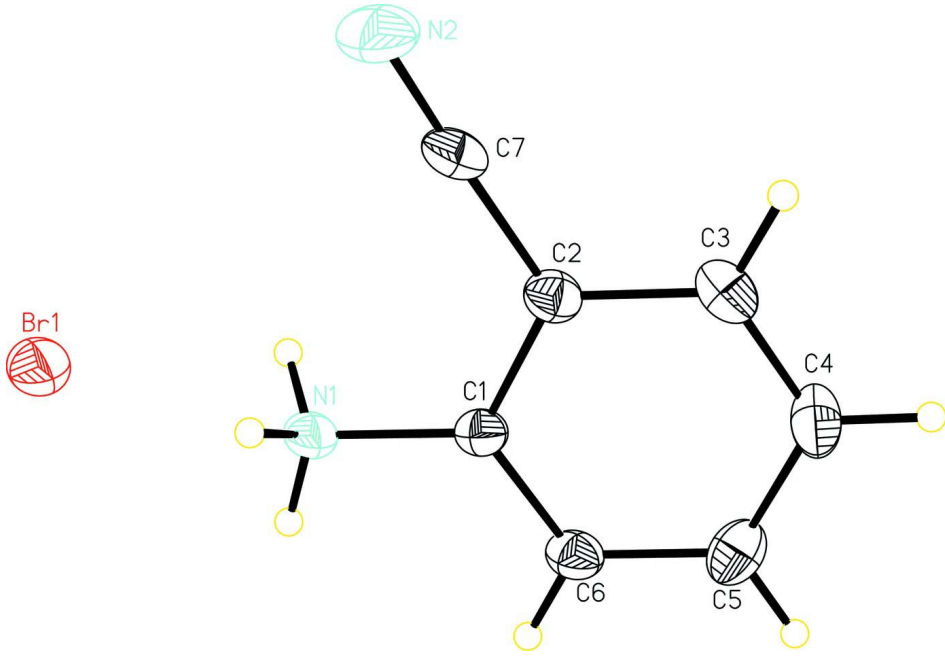

Figure 1

The structure of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

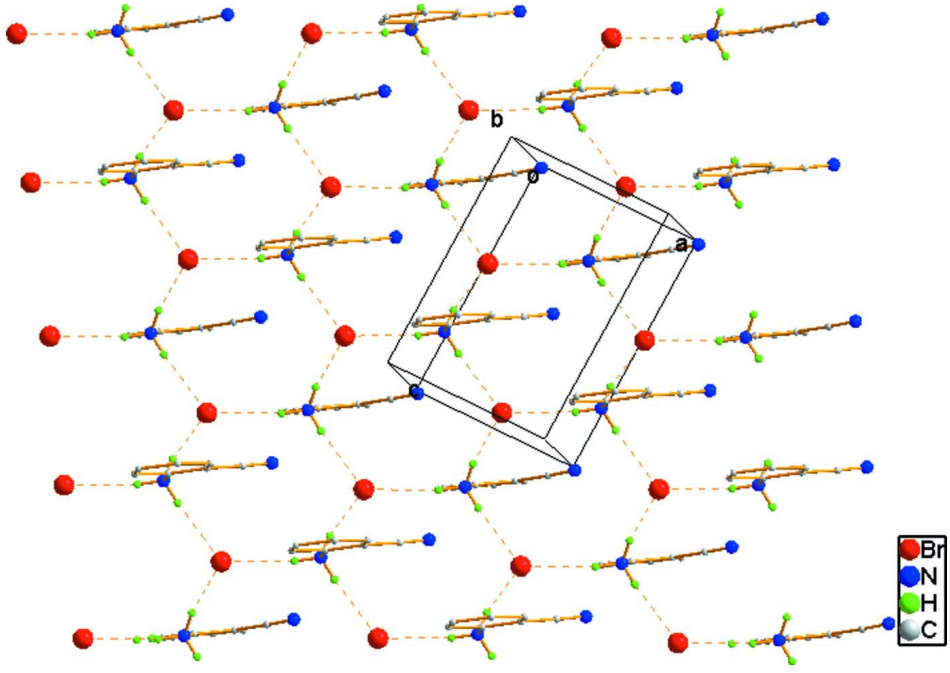

Figure 2

The crystal packing of the title compound, viewed along the *b* axis showing the N—H···Br hydrogen bonding (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity.

2-Cyanoanilinium bromide

Crystal data

$C_7H_7N_2^+ \cdot Br^-$
$M_r = 199.06$
Monoclinic, *Cc*
Hall symbol: C -2yc
$a = 5.7844$ (12) Å
$b = 15.896$ (3) Å
$c = 8.4882$ (17) Å
$\beta = 92.72$ (3)°
$V = 779.6$ (3) Å^3
$Z = 4$
$F(000) = 392$
$D_x = 1.696$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1581 reflections
$\theta = 2.6$–27.5°
$\mu = 5.19$ mm^{-1}
$T = 298$ K
Needle, colourless
0.40 × 0.05 × 0.05 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
CCD profile fitting scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.65$, $T_{max} = 0.77$
3848 measured reflections
1773 independent reflections
1581 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.6°$
$h = -7 \rightarrow 7$
$k = -20 \rightarrow 20$
$l = -10 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.050$
$S = 0.87$
1773 reflections
93 parameters
2 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
$w = 1/[\sigma^2(F_o^2) + (0.0143P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}
Extinction correction: *SHELXTL* (Version 5.1; Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0206 (8)
Absolute structure: Flack (1983), 872 Friedels pairs
Absolute structure parameter: 0.004 (13)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2$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}
Br1	0.05750 (10)	0.208462 (17)	0.44566 (9)	0.04064 (12)

N1	0.0515 (5)	0.32177 (17)	0.7619 (3)	0.0347 (6)
H1A	0.0332	0.2950	0.6701	0.052*
H1B	−0.0713	0.3127	0.8188	0.052*
H1C	0.1780	0.3027	0.8140	0.052*
C6	−0.0799 (6)	0.4675 (3)	0.7945 (5)	0.0372 (10)
H6	−0.2028	0.4473	0.8503	0.045*
C3	0.2867 (8)	0.5276 (3)	0.6309 (5)	0.0451 (11)
H3	0.4102	0.5483	0.5762	0.054*
C1	0.0755 (6)	0.4115 (2)	0.7337 (5)	0.0309 (9)
C4	0.1322 (8)	0.5822 (3)	0.6917 (5)	0.0500 (12)
H4	0.1516	0.6399	0.6788	0.060*
C7	0.4233 (6)	0.3856 (2)	0.5783 (4)	0.0410 (8)
N2	0.5521 (6)	0.3440 (2)	0.5163 (4)	0.0618 (10)
C2	0.2611 (6)	0.4411 (3)	0.6501 (4)	0.0346 (9)
C5	−0.0547 (7)	0.5521 (3)	0.7733 (5)	0.0474 (12)
H5	−0.1613	0.5894	0.8130	0.057*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.03349 (17)	0.04202 (18)	0.04729 (19)	−0.0034 (2)	0.01111 (12)	−0.0112 (3)
N1	0.0284 (14)	0.0369 (15)	0.0396 (16)	−0.0027 (12)	0.0104 (12)	−0.0036 (13)
C6	0.031 (2)	0.043 (2)	0.038 (2)	−0.0023 (18)	0.0075 (17)	−0.0038 (18)
C3	0.044 (3)	0.046 (3)	0.046 (3)	−0.012 (2)	0.007 (2)	0.003 (2)
C1	0.027 (2)	0.035 (2)	0.0309 (18)	0.0005 (15)	0.0021 (15)	−0.0028 (15)
C4	0.065 (3)	0.031 (2)	0.055 (3)	−0.004 (2)	0.008 (2)	0.003 (2)
C7	0.0303 (18)	0.049 (2)	0.044 (2)	−0.0078 (17)	0.0101 (16)	0.0045 (18)
N2	0.049 (2)	0.070 (2)	0.069 (2)	0.0068 (19)	0.031 (2)	0.0025 (18)
C2	0.032 (2)	0.039 (2)	0.032 (2)	−0.0017 (17)	0.0039 (17)	0.0032 (16)
C5	0.056 (3)	0.041 (2)	0.045 (3)	0.012 (2)	0.006 (2)	−0.007 (2)

Geometric parameters (Å, º)

N1—C1	1.455 (5)	C3—C2	1.393 (6)
N1—H1A	0.8900	C3—H3	0.9300
N1—H1B	0.8900	C1—C2	1.396 (5)
N1—H1C	0.8900	C4—C5	1.396 (6)
C6—C5	1.366 (6)	C4—H4	0.9300
C6—C1	1.382 (5)	C7—N2	1.142 (4)
C6—H6	0.9300	C7—C2	1.444 (6)
C3—C4	1.365 (6)	C5—H5	0.9300
C1—N1—H1A	109.5	C6—C1—N1	120.1 (3)
C1—N1—H1B	109.5	C2—C1—N1	119.7 (3)
H1A—N1—H1B	109.5	C3—C4—C5	120.4 (4)
C1—N1—H1C	109.5	C3—C4—H4	119.8
H1A—N1—H1C	109.5	C5—C4—H4	119.8
H1B—N1—H1C	109.5	N2—C7—C2	177.0 (4)

C5—C6—C1	120.6 (4)	C3—C2—C1	118.7 (4)
C5—C6—H6	119.7	C3—C2—C7	118.6 (4)
C1—C6—H6	119.7	C1—C2—C7	122.6 (4)
C4—C3—C2	120.5 (4)	C6—C5—C4	119.5 (4)
C4—C3—H3	119.7	C6—C5—H5	120.2
C2—C3—H3	119.7	C4—C5—H5	120.2
C6—C1—C2	120.2 (4)		
C5—C6—C1—C2	0.2 (6)	N1—C1—C2—C3	−177.0 (4)
C5—C6—C1—N1	177.8 (4)	C6—C1—C2—C7	−177.4 (4)
C2—C3—C4—C5	−0.4 (7)	N1—C1—C2—C7	5.0 (6)
C4—C3—C2—C1	−0.5 (6)	C1—C6—C5—C4	−1.1 (7)
C4—C3—C2—C7	177.6 (4)	C3—C4—C5—C6	1.2 (7)
C6—C1—C2—C3	0.6 (6)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Br1	0.89	2.36	3.234 (3)	168
N1—H1*B*···Br1^{i}	0.89	2.47	3.355 (3)	173
N1—H1*C*···Br1^{ii}	0.89	2.42	3.286 (3)	164

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