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3-Cyanoanilinium chloride

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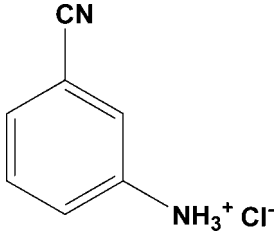
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.053; wR factor = 0.157; data-to-parameter ratio = 17.8.

In the title salt, $C_7H_7N_2^+\cdot Cl^-$, all non-H atoms of the cation are essentially coplanar (r.m.s. deviation = 0.005 Å). In the crystal structure, the organic cations and chloride ions are linked to form a two-dimensional network parallel to the (001) plane by N—H···Cl hydrogen bonds.

Related literature

For the use of amine derivatives in coordination chemistry, see: Manzur *et al.* (2007); Ismayilov *et al.* (2007); Austria *et al.* (2007).



Experimental

Crystal data

$C_7H_7N_2^+\cdot Cl^-$
M_r = 154.60
Triclinic, $P\overline{1}$
a = 4.663 (3) Å
b = 6.074 (5) Å
c = 13.212 (9) Å
α = 93.37 (5)°
β = 96.201 (19)°
γ = 96.22 (4)°
V = 368.9 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.43 mm^{-1}
T = 298 (2) K
0.25 × 0.18 × 0.18 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.901, T_{max} = 0.917
2486 measured reflections
1618 independent reflections
1342 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.157
S = 1.07
1618 reflections
91 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H9A···Cl1^{i}	0.89	2.61	3.111 (3)	116
N2—H9A···Cl1^{ii}	0.89	2.65	3.178 (3)	119
N2—H9C···Cl1^{iii}	0.89	2.73	3.278 (3)	121
N2—H9B···Cl1	0.89	2.76	3.338 (3)	124

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $x, y+1, z$; (iii) $-x+1, -y+1, -z$.

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

This work was supported by a Start-up Grant from Southeast University to Professor Ren-Gen Xiong.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2624).

References

Austria, C., Zhang, J. & Valle, H. (2007). *Inorg. Chem.* **46**, 6283–6290.
Ismayilov, R. H., Wang, W. Z. & Lee, G. H. (2007). *Dalton Trans.* pp. 2898–2907.
Manzur, J., Vega, A. & Garcia, A. M. (2007). *Eur. J. Inorg. Chem.* **35**, 5500–5510.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
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supporting information

Acta Cryst. (2008). E**64**, o1462 [doi:10.1107/S1600536808020485]

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S1. Comment

In the past five years, we have focused on the chemistry of amine derivatives because of their multiple coordination modes as ligands to metal ions and for the construction of novel metal-organic frameworks (Manzur *et al.* 2007; Ismayilov *et al.* 2007; Austria *et al.* 2007). We report here the crystal structure of the title compound, 3-cyano-benzenaminium monochloride.

In the title compound (Fig.1), the N2 atom of the amine group is protonated. The nitrile group is coplanar with the benzene ring. Bond lengths and angles lie within normal ranges.

In the crystal structure the organic cation and Cl^- ions are linked to form a two-dimensional network parallel to the (0 0 1) plane (Fig.2) by N—H···Cl hydrogen bonds (Table 1).

S2. Experimental

3-Cyanobenzenaminium monochloride (3 mmol) was dissolved in ethanol (20 ml). The solution was allowed to evaporate to obtain colourless block-shaped crystals of the title compound.

S3. Refinement

All H atoms were fixed geometrically [C-H = 0.93 Å and N-H = 0.89 Å] and treated as riding, with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(N).

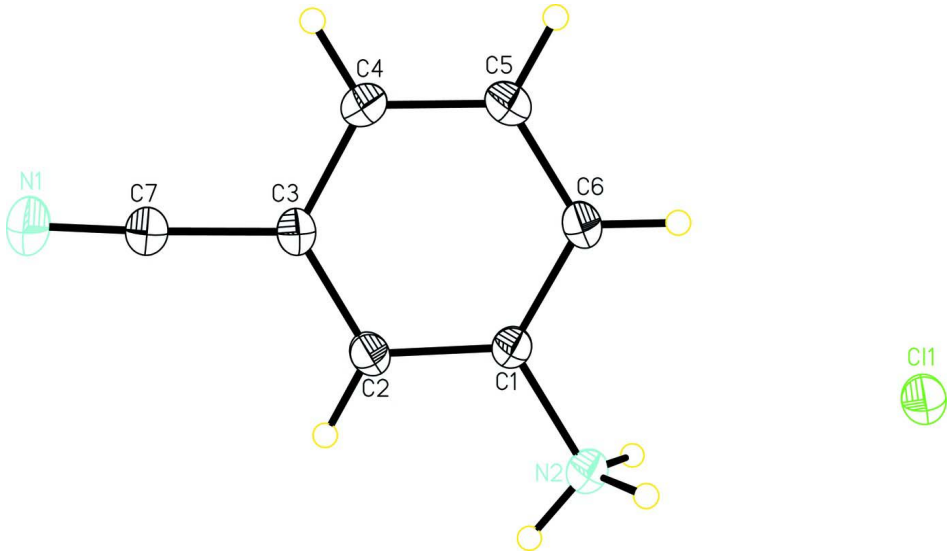

Figure 1

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

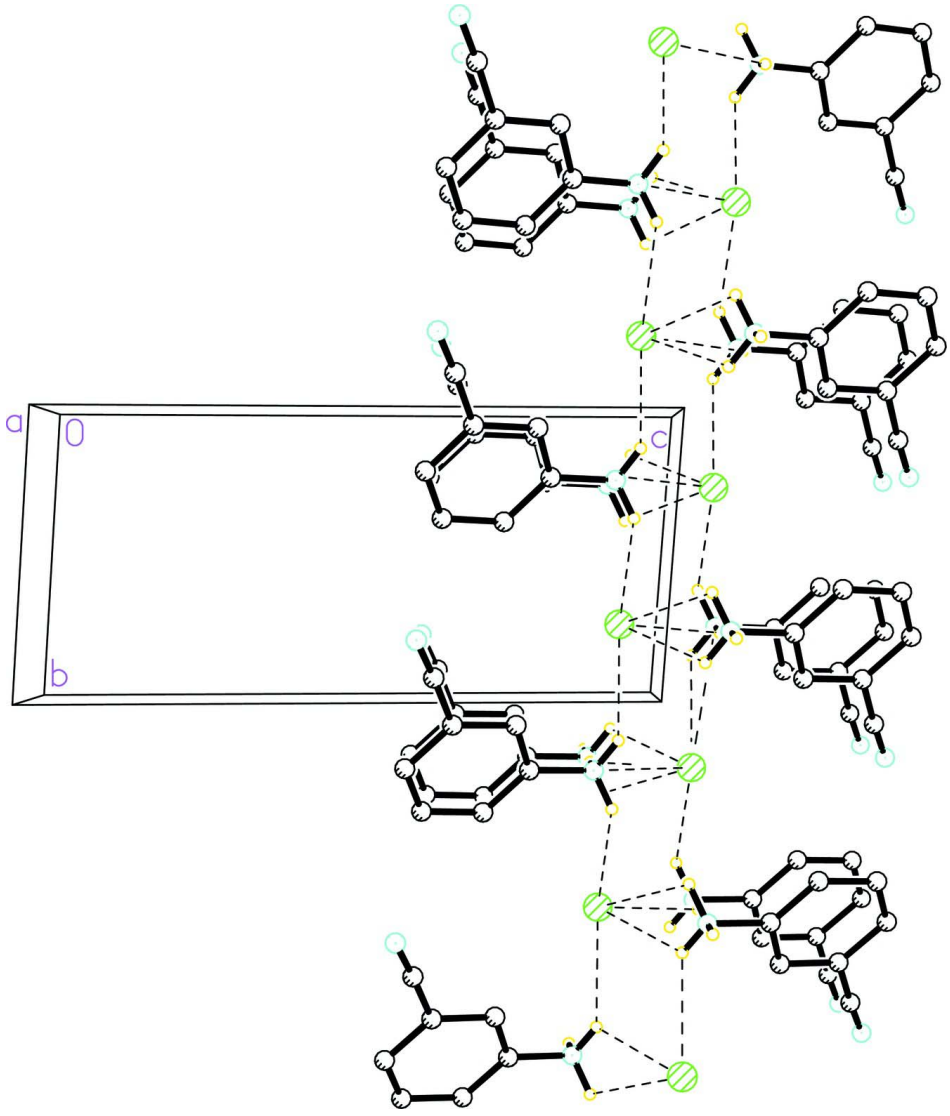

Figure 2

Part of the crystal packing of the title compound viewed along the *a* axis. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

3-Cyanoanilinium chloride

Crystal data

$C_7H_7N_2^+\cdot Cl^-$
$M_r = 154.60$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 4.663\ (3)$ Å
$b = 6.074\ (5)$ Å
$c = 13.212\ (9)$ Å
$\alpha = 93.37\ (5)°$
$\beta = 96.201\ (19)°$
$\gamma = 96.22\ (4)°$
$V = 368.9\ (5)$ Å^3
$Z = 2$
$F(000) = 160$
$D_x = 1.392$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1678 reflections
$\theta = 2.3–24.4°$
$\mu = 0.44$ mm^{-1}
$T = 298$ K
Block, colourless
0.25 × 0.18 × 0.18 mm

Data collection

Rigaku Mercury2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 13.6612 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.901, T_{max} = 0.917
2486 measured reflections
1618 independent reflections
1342 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −6→6
k = −7→5
l = −16→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.157
S = 1.07
1618 reflections
91 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
$w = 1/[\sigma^2(F_o^2) + (0.0787P)^2 + 0.2472P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.38158 (16)	0.25924 (11)	0.07001 (5)	0.0414 (3)
C1	0.0572 (5)	0.7649 (4)	0.19904 (18)	0.0302 (5)
N2	0.1472 (5)	0.7573 (4)	0.09653 (16)	0.0377 (6)
H9A	0.0747	0.8643	0.0622	0.057*
H9B	0.0816	0.6259	0.0641	0.057*
H9C	0.3402	0.7770	0.1008	0.057*
C3	−0.1968 (5)	0.9320 (4)	0.3237 (2)	0.0329 (6)
C7	−0.3747 (6)	1.0962 (5)	0.3564 (2)	0.0391 (6)
C6	0.1466 (6)	0.6149 (5)	0.2669 (2)	0.0374 (6)
H6A	0.2625	0.5081	0.2475	0.045*
N1	−0.5144 (6)	1.2233 (5)	0.3856 (2)	0.0545 (7)
C4	−0.1099 (6)	0.7815 (5)	0.3928 (2)	0.0395 (6)
H4A	−0.1675	0.7865	0.4580	0.047*
C2	−0.1148 (5)	0.9263 (4)	0.2256 (2)	0.0322 (6)
H2A	−0.1732	1.0271	0.1794	0.039*
C5	0.0624 (7)	0.6251 (5)	0.3633 (2)	0.0443 (7)

H5A	0.1229	0.5248	0.4094	0.053*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0519 (5)	0.0373 (4)	0.0395 (4)	0.0155 (3)	0.0126 (3)	0.0062 (3)
C1	0.0334 (12)	0.0304 (13)	0.0285 (12)	0.0073 (10)	0.0074 (10)	0.0027 (9)
N2	0.0446 (13)	0.0398 (13)	0.0324 (12)	0.0139 (10)	0.0107 (10)	0.0040 (9)
C3	0.0308 (12)	0.0338 (14)	0.0360 (13)	0.0102 (10)	0.0063 (10)	0.0020 (10)
C7	0.0404 (14)	0.0421 (16)	0.0380 (14)	0.0140 (12)	0.0093 (12)	0.0045 (11)
C6	0.0442 (15)	0.0333 (14)	0.0388 (14)	0.0165 (11)	0.0094 (11)	0.0065 (11)
N1	0.0597 (17)	0.0551 (17)	0.0558 (17)	0.0274 (14)	0.0191 (14)	0.0036 (13)
C4	0.0491 (16)	0.0429 (16)	0.0307 (13)	0.0136 (12)	0.0130 (12)	0.0063 (11)
C2	0.0325 (13)	0.0316 (13)	0.0346 (13)	0.0099 (10)	0.0048 (10)	0.0062 (10)
C5	0.0577 (18)	0.0420 (17)	0.0398 (15)	0.0216 (13)	0.0132 (13)	0.0154 (12)

Geometric parameters (Å, º)

C1—C6	1.380 (4)	C3—C7	1.440 (4)
C1—C2	1.385 (3)	C7—N1	1.139 (4)
C1—N2	1.460 (3)	C6—C5	1.374 (4)
N2—H9A	0.89	C6—H6A	0.93
N2—H9B	0.89	C4—C5	1.374 (4)
N2—H9C	0.89	C4—H4A	0.93
C3—C4	1.390 (4)	C2—H2A	0.93
C3—C2	1.391 (4)	C5—H5A	0.93
C6—C1—C2	121.9 (2)	C5—C6—C1	119.2 (2)
C6—C1—N2	119.8 (2)	C5—C6—H6A	120.4
C2—C1—N2	118.3 (2)	C1—C6—H6A	120.4
C1—N2—H9A	109.5	C5—C4—C3	119.1 (2)
C1—N2—H9B	109.5	C5—C4—H4A	120.4
H9A—N2—H9B	109.5	C3—C4—H4A	120.4
C1—N2—H9C	109.5	C1—C2—C3	117.5 (2)
H9A—N2—H9C	109.5	C1—C2—H2A	121.2
H9B—N2—H9C	109.5	C3—C2—H2A	121.2
C4—C3—C2	121.3 (2)	C6—C5—C4	121.0 (2)
C4—C3—C7	118.2 (2)	C6—C5—H5A	119.5
C2—C3—C7	120.4 (2)	C4—C5—H5A	119.5
N1—C7—C3	177.6 (3)		
C2—C1—C6—C5	0.2 (4)	N2—C1—C2—C3	−179.6 (2)
N2—C1—C6—C5	179.4 (3)	C4—C3—C2—C1	0.0 (4)
C2—C3—C4—C5	0.5 (4)	C7—C3—C2—C1	179.8 (2)
C7—C3—C4—C5	−179.3 (3)	C1—C6—C5—C4	0.3 (5)
C6—C1—C2—C3	−0.3 (4)	C3—C4—C5—C6	−0.6 (5)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H9*A*···Cl1^{i}	0.89	2.61	3.111 (3)	116
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Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) *x*, *y*+1, *z*; (iii) −*x*+1, −*y*+1, −*z*.