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2-Cyanoanilinium tetrafluoroborate

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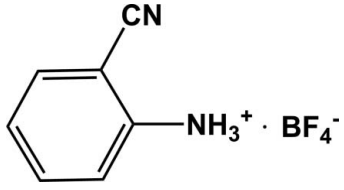
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.056; wR factor = 0.141; data-to-parameter ratio = 15.5.

In the title compound, $C_7H_7N_2^+\cdot BF_4^-$, the non-H atoms of the cation are almost coplanar (r.m.s. deviation = 0.035 Å). The cations and anions are connected by intermolecular N—H···F and N—H···N hydrogen bonds, forming a two-dimensional network parallel to $(10\bar{1})$.

Related literature

For the application 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). For general background to nitrile derivatives, see: Fu *et al.* (2008); Wang *et al.* (2002).



Experimental

Crystal data

$C_7H_7N_2^+\cdot BF_4^-$
M_r = 205.96
Monoclinic, $P2_1/n$
a = 10.971 (2) Å
b = 7.3565 (15) Å
c = 11.022 (2) Å
β = 103.11 (3)°
V = 866.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.16 mm^{-1}
T = 298 K
0.30 × 0.25 × 0.20 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.96, T_{max} = 1.00
(expected range = 0.931–0.969)
8625 measured reflections
1978 independent reflections
1417 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.141
S = 1.08
1978 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2^{i}	0.89	2.54	3.179 (3)	130
N1—H1A···F4^{ii}	0.89	2.12	2.896 (2)	146
N1—H1B···F4^{iii}	0.89	2.21	2.993 (2)	147
N1—H1C···F3	0.89	1.95	2.799 (2)	160

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, -y+1, -z+1$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2881).

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supporting information

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2-Cyanoanilinium tetrafluoroborate

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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, 2-cyanobenzenaminium tetrafluoroborate.

In the 2-cyanobenzenaminium cation (Fig.1), the nitrile group and the benzene ring are almost coplanar. The nitrile group C7≡N2 bond length of 1.150 (3) Å is within the normal range.

In the crystal structure, all the amine group H atoms are involved in N—H···F hydrogen bonds (Table 1) with F atoms of the BF_4^- anion. These hydrogen bonds along with N—H···N hydrogen bonds link the ionic units into a two-dimensional network (Fig. 2) parallel to the $(10\bar{1})$.

S2. Experimental

The commercial 2-aminobenzonitrile (3 mmol, 0.55 g) and HBF_4 (0.5 ml) were dissolved in ethanol (20 ml). Colourless block-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.

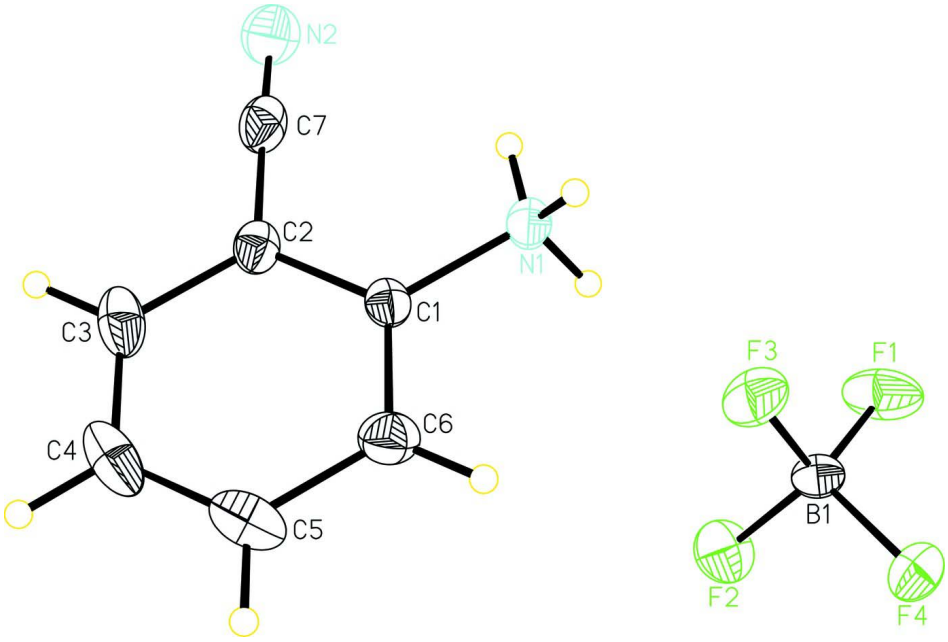

Figure 1

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

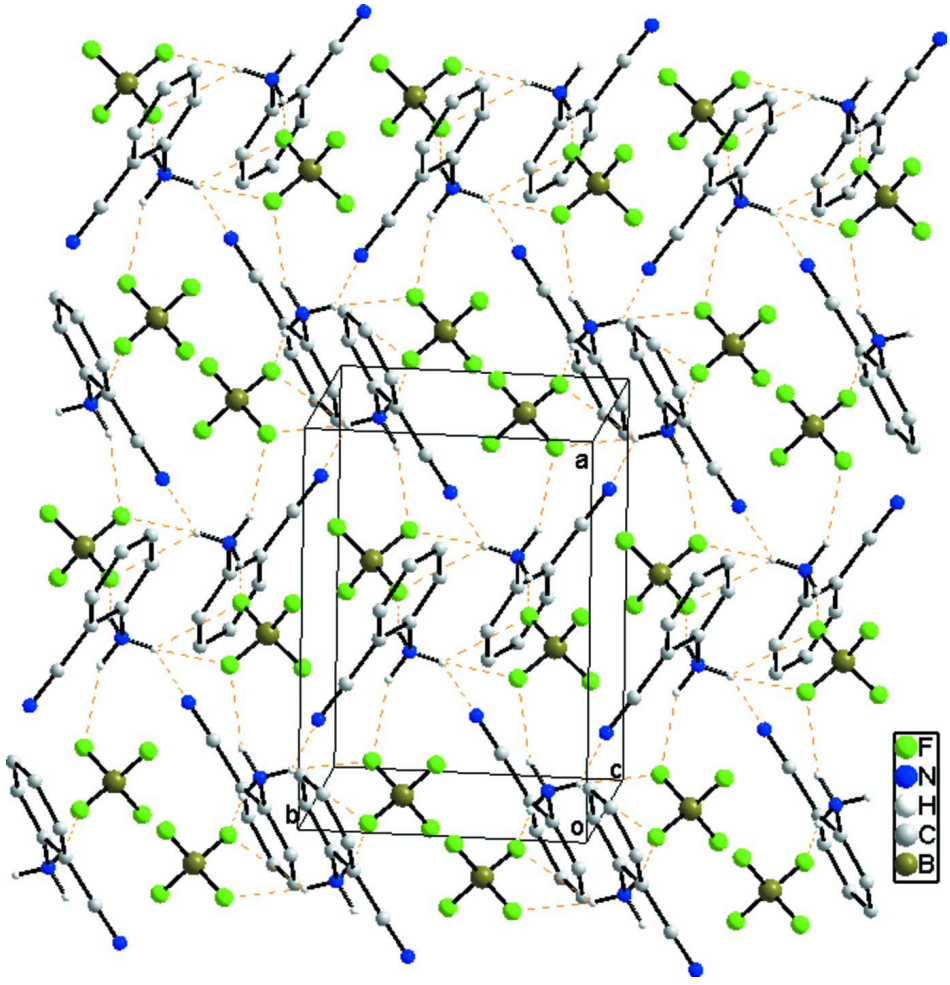

Figure 2

The crystal packing of the title compound, viewed along the *c* axis. Hydrogen bonds are shown as dashed lines. C-bound H atoms have been omitted for clarity

2-Cyanoanilinium tetrafluoroborate

Crystal data

$C_7H_7N_2^+ \cdot BF_4^-$
$M_r = 205.96$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.971\ (2)$ Å
$b = 7.3565\ (15)$ Å
$c = 11.022\ (2)$ Å
$\beta = 103.11\ (3)°$
$V = 866.4\ (3)$ Å^3
$Z = 4$

$F(000) = 416$
$D_x = 1.579$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1417 reflections
$\theta = 3.4–27.5°$
$\mu = 0.16$ mm^{-1}
$T = 298$ K
Block, colourless
0.30 × 0.25 × 0.20 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} = 0.96, T_{max} = 1.00

8625 measured reflections
1978 independent reflections
1417 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 27.5°, θ_{min} = 3.4°
h = −14→14
k = −9→9
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.141
S = 1.08
1978 reflections
128 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
$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2 + 0.4139P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 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}
F4	0.36113 (13)	0.72246 (19)	0.25229 (13)	0.0500 (4)
F3	0.48625 (14)	0.7353 (2)	0.44366 (13)	0.0575 (4)
N1	0.59296 (16)	0.6600 (3)	0.69414 (15)	0.0337 (4)
H1A	0.6182	0.5482	0.6812	0.051*
H1B	0.6589	0.7275	0.7293	0.051*
H1C	0.5548	0.7094	0.6218	0.051*
F2	0.34337 (15)	0.9602 (2)	0.37300 (16)	0.0625 (5)
C1	0.50557 (18)	0.6518 (3)	0.77689 (18)	0.0302 (5)
F1	0.51445 (14)	0.9330 (3)	0.29556 (18)	0.0737 (6)
C2	0.5337 (2)	0.7425 (3)	0.89064 (19)	0.0348 (5)
C6	0.3969 (2)	0.5547 (3)	0.7402 (2)	0.0437 (6)
H6	0.3792	0.4939	0.6643	0.052*
N2	0.7317 (2)	0.9429 (3)	0.9488 (2)	0.0586 (6)
C7	0.6444 (2)	0.8517 (3)	0.9248 (2)	0.0428 (6)
B1	0.4282 (2)	0.8402 (3)	0.3425 (2)	0.0359 (6)
C4	0.3405 (3)	0.6365 (4)	0.9311 (3)	0.0580 (8)

H4	0.2840	0.6313	0.9824	0.070*
C3	0.4507 (2)	0.7323 (3)	0.9687 (2)	0.0483 (6)
H3	0.4693	0.7897	1.0458	0.058*
C5	0.3138 (2)	0.5485 (4)	0.8180 (3)	0.0570 (7)
H5	0.2393	0.4842	0.7934	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F4	0.0566 (9)	0.0453 (8)	0.0442 (8)	−0.0023 (6)	0.0037 (7)	−0.0056 (6)
F3	0.0587 (9)	0.0613 (10)	0.0455 (8)	0.0069 (7)	−0.0029 (7)	0.0162 (7)
N1	0.0376 (10)	0.0351 (9)	0.0291 (9)	0.0028 (8)	0.0092 (7)	−0.0004 (7)
F2	0.0658 (9)	0.0467 (9)	0.0762 (11)	0.0167 (7)	0.0186 (8)	−0.0097 (8)
C1	0.0324 (10)	0.0288 (10)	0.0303 (10)	0.0072 (8)	0.0091 (8)	0.0036 (8)
F1	0.0435 (8)	0.0830 (12)	0.0922 (13)	−0.0162 (8)	0.0107 (8)	0.0342 (10)
C2	0.0420 (11)	0.0316 (11)	0.0311 (11)	0.0065 (9)	0.0091 (9)	0.0001 (9)
C6	0.0356 (12)	0.0447 (14)	0.0491 (14)	0.0034 (10)	0.0058 (10)	−0.0046 (11)
N2	0.0597 (14)	0.0587 (14)	0.0558 (14)	−0.0010 (12)	0.0095 (11)	−0.0178 (11)
C7	0.0542 (15)	0.0392 (13)	0.0347 (12)	0.0088 (12)	0.0094 (11)	−0.0075 (10)
B1	0.0324 (12)	0.0315 (12)	0.0412 (13)	0.0004 (10)	0.0030 (10)	0.0053 (11)
C4	0.0609 (17)	0.0541 (17)	0.0729 (19)	0.0135 (14)	0.0445 (15)	0.0118 (14)
C3	0.0670 (16)	0.0430 (13)	0.0422 (13)	0.0147 (12)	0.0277 (12)	0.0018 (10)
C5	0.0375 (13)	0.0529 (16)	0.085 (2)	0.0011 (12)	0.0223 (13)	0.0022 (14)

Geometric parameters (Å, º)

F4—B1	1.396 (3)	C2—C3	1.389 (3)
F3—B1	1.387 (3)	C2—C7	1.434 (3)
N1—C1	1.467 (2)	C6—C5	1.387 (4)
N1—H1A	0.89	C6—H6	0.93
N1—H1B	0.89	N2—C7	1.150 (3)
N1—H1C	0.89	C4—C5	1.376 (4)
F2—B1	1.379 (3)	C4—C3	1.379 (4)
C1—C6	1.370 (3)	C4—H4	0.93
C1—C2	1.392 (3)	C3—H3	0.93
F1—B1	1.361 (3)	C5—H5	0.93
C1—N1—H1A	109.5	F1—B1—F2	109.7 (2)
C1—N1—H1B	109.5	F1—B1—F3	110.68 (19)
H1A—N1—H1B	109.5	F2—B1—F3	111.9 (2)
C1—N1—H1C	109.5	F1—B1—F4	109.9 (2)
H1A—N1—H1C	109.5	F2—B1—F4	107.16 (18)
H1B—N1—H1C	109.5	F3—B1—F4	107.42 (19)
C6—C1—C2	121.1 (2)	C5—C4—C3	120.3 (2)
C6—C1—N1	119.06 (19)	C5—C4—H4	119.9
C2—C1—N1	119.87 (19)	C3—C4—H4	119.9
C3—C2—C1	119.3 (2)	C4—C3—C2	119.7 (2)
C3—C2—C7	120.2 (2)	C4—C3—H3	120.2

C1—C2—C7	120.42 (19)	C2—C3—H3	120.2
C1—C6—C5	119.0 (2)	C4—C5—C6	120.6 (2)
C1—C6—H6	120.5	C4—C5—H5	119.7
C5—C6—H6	120.5	C6—C5—H5	119.7
N2—C7—C2	177.7 (3)		
C6—C1—C2—C3	0.8 (3)	C5—C4—C3—C2	1.2 (4)
N1—C1—C2—C3	−179.40 (19)	C1—C2—C3—C4	−1.6 (3)
C6—C1—C2—C7	−176.6 (2)	C7—C2—C3—C4	175.8 (2)
N1—C1—C2—C7	3.2 (3)	C3—C4—C5—C6	0.0 (4)
C2—C1—C6—C5	0.4 (3)	C1—C6—C5—C4	−0.8 (4)
N1—C1—C6—C5	−179.4 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N2^{i}	0.89	2.54	3.179 (3)	130
N1—H1*A*···F4^{ii}	0.89	2.12	2.896 (2)	146
N1—H1*B*···F4^{iii}	0.89	2.21	2.993 (2)	147
N1—H1*C*···F3	0.89	1.95	2.799 (2)	160

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+3/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) *x*+1/2, −*y*+3/2, *z*+1/2.