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3-Cyanoanilinium nitrate

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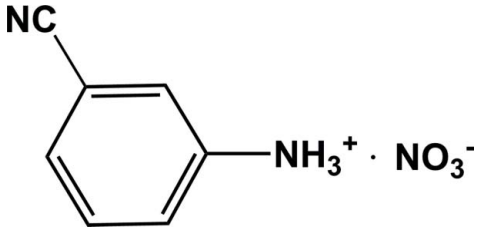
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.052; wR factor = 0.141; data-to-parameter ratio = 15.6.

In the cation of the title compound, $C_7H_7N_2^+\cdot NO_3^-$, the nitrile group and the benzene ring are almost coplanar (r.m.s. deviation = 0.006 Å). In the crystal, the ions are connected by bifurcated N—H···(O,O) hydrogen bonds, forming a two-dimensional network parallel to (001).

Related literature

For the applications of metal-organic coordination compounds, see: Fu *et al.* (2007); Chen *et al.* (2001); Fu & Xiong (2008); Xiong *et al.* (1999); Xie *et al.* (2003); Zhao *et al.* (2004). For nitrile derivatives, see: Fu *et al.* (2008); Wang *et al.* 2002.



Experimental

Crystal data

$C_7H_7N_2^+\cdot NO_3^-$
M_r = 181.16
Orthorhombic, *Pbca*
a = 10.210 (2) Å
b = 10.812 (2) Å
c = 15.398 (3) Å
V = 1699.8 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 K
0.40 × 0.25 × 0.20 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.94, T_{max} = 1.00
15905 measured reflections
1871 independent reflections
1456 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.141
S = 1.14
1871 reflections
120 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O3^{i}	0.89	2.22	3.104 (2)	173
N2—H2A···O1^{i}	0.89	2.44	3.107 (2)	133
N2—H2B···O2^{ii}	0.89	2.06	2.859 (2)	150
N2—H2B···O3^{ii}	0.89	2.25	3.049 (2)	149
N2—H2C···O2	0.89	1.85	2.738 (2)	172
N2—H2C···O1	0.89	2.56	3.090 (2)	119

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

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: CI2892).

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supporting information

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3-Cyanoanilinium nitrate

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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.*, 2001; Fu & Xiong, 2008; Xie *et al.*, 2003; Zhao *et al.*, 2004; 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, 3-cyanoanilinium nitrate.

In the 3-cyanoanilinium cation (Fig.1), the nitrile group and the benzene ring are coplanar. The nitrile group C1≡N1 bond length of 1.102 (3) Å is within the normal range.

In the crystal structure, all the amine group H atoms are involved in N—H···O hydrogen bonds (Table 1) with O atoms of the NO_3^- anion. These hydrogen bonds link the ionic units into a two-dimensional network (Fig. 2) parallel to the (001) plane.

S2. Experimental

The commercial 3-aminobenzonitrile (3 mmol, 0.55 g) and HNO_3 (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

H 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.

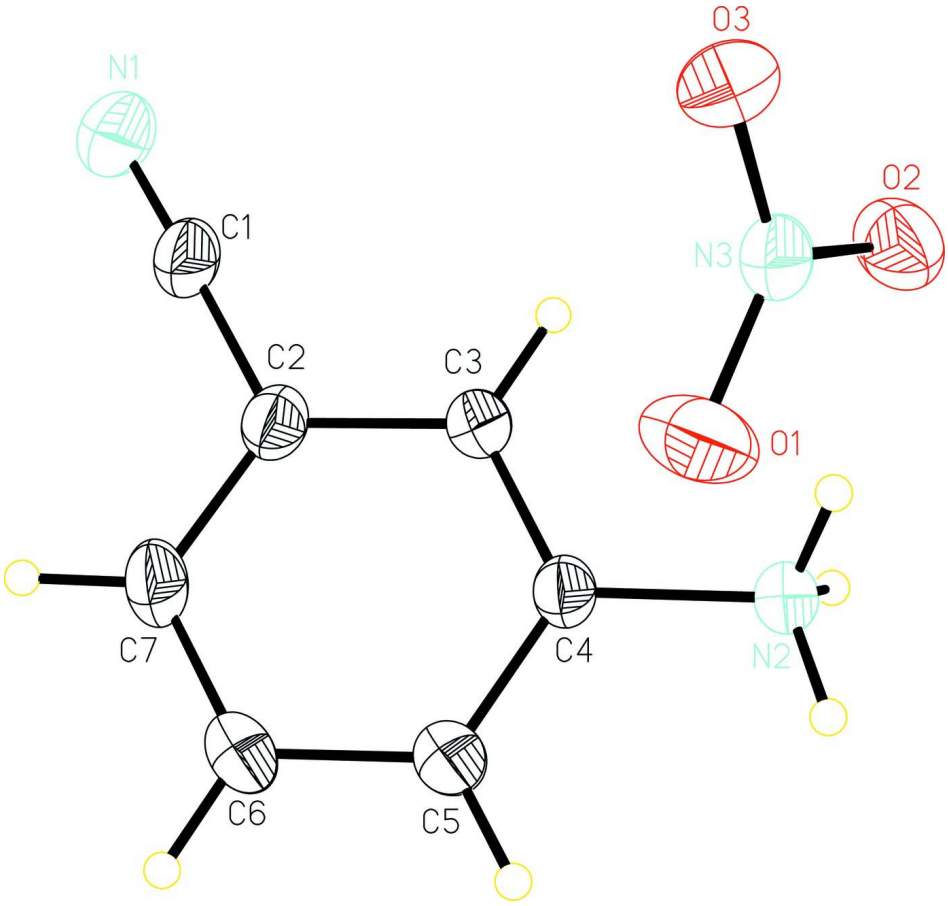

Figure 1

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

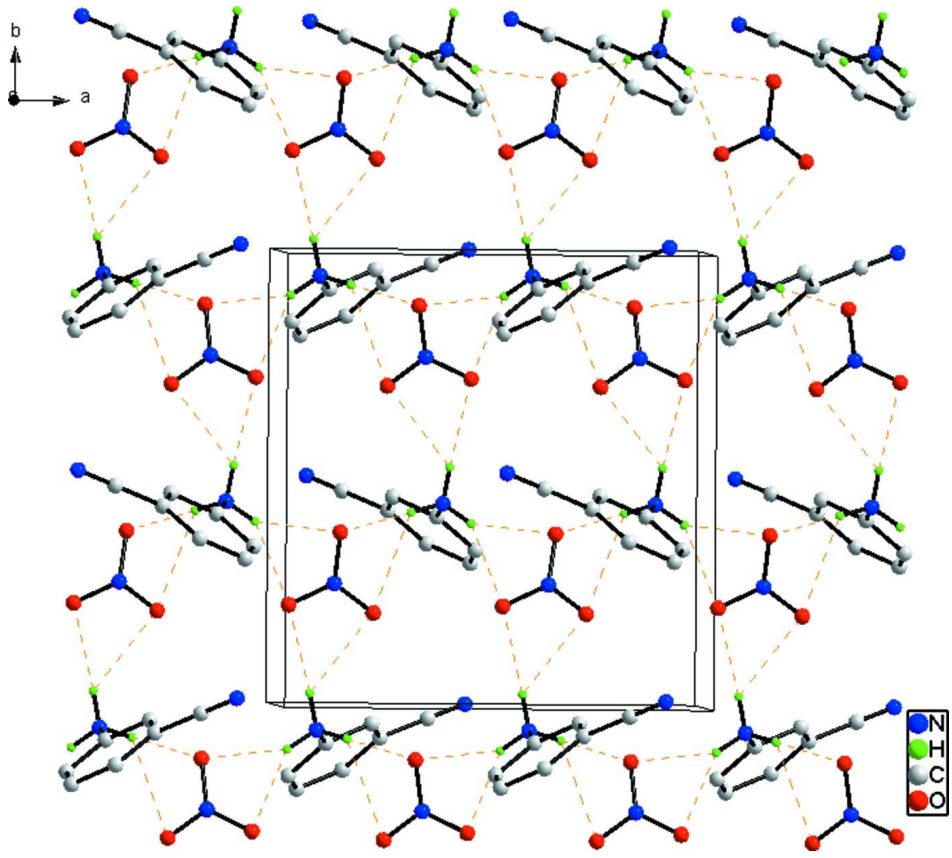

Figure 2

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

3-Cyanoanilinium nitrate

Crystal data

$C_7H_7N_2^+\cdot NO_3^-$
M_r = 181.16
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 10.210 (2) Å
b = 10.812 (2) Å
c = 15.398 (3) Å
V = 1699.8 (6) Å^3
Z = 8
F(000) = 752
D_x = 1.416 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1456 reflections
θ = 3.1–27.5°
μ = 0.11 mm^{-1}
T = 298 K
Block, colourless
0.40 × 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} = 0.94, T_{max} = 1.00
15905 measured reflections
1871 independent reflections
1456 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

θ_{max} = 27.5°, θ_{min} = 3.1°
h = −13→13
k = −13→13
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.141
S = 1.14
1871 reflections
120 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
$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.3685P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.021 (3)

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.06292 (19)	0.5067 (2)	0.39061 (13)	0.0724 (6)
N2	0.39497 (14)	0.44355 (16)	0.69503 (9)	0.0435 (4)
H2A	0.4110	0.5239	0.7016	0.065*
H2B	0.4620	0.4001	0.7158	0.065*
H2C	0.3224	0.4236	0.7238	0.065*
C1	0.1482 (2)	0.4737 (2)	0.42791 (13)	0.0526 (5)
C2	0.25733 (17)	0.43017 (19)	0.47337 (11)	0.0443 (5)
C3	0.27221 (17)	0.45958 (18)	0.56150 (11)	0.0420 (5)
H3	0.2108	0.5080	0.5904	0.050*
C4	0.37764 (16)	0.41559 (17)	0.60241 (11)	0.0382 (4)
C5	0.46585 (19)	0.34385 (19)	0.55934 (12)	0.0488 (5)
H5	0.5382	0.3131	0.5890	0.059*
C6	0.4502 (2)	0.3155 (2)	0.47200 (13)	0.0568 (6)
H6	0.5119	0.2669	0.4436	0.068*
C7	0.3461 (2)	0.3585 (2)	0.42905 (12)	0.0538 (5)
H7	0.3339	0.3403	0.3706	0.065*
O1	0.23542 (15)	0.20195 (16)	0.71257 (11)	0.0701 (5)
O2	0.16047 (13)	0.37804 (14)	0.76798 (10)	0.0594 (5)
O3	0.04000 (13)	0.21817 (14)	0.73494 (10)	0.0592 (5)
N3	0.14567 (15)	0.26571 (16)	0.73782 (10)	0.0449 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0625 (12)	0.1071 (17)	0.0476 (11)	0.0072 (12)	−0.0138 (9)	−0.0010 (11)
N2	0.0413 (8)	0.0563 (10)	0.0328 (8)	0.0053 (7)	−0.0013 (6)	−0.0047 (7)
C1	0.0517 (11)	0.0722 (14)	0.0339 (10)	−0.0038 (10)	−0.0043 (9)	−0.0017 (9)
C2	0.0432 (10)	0.0547 (12)	0.0351 (9)	−0.0056 (8)	−0.0034 (7)	0.0006 (8)
C3	0.0382 (9)	0.0536 (11)	0.0341 (9)	0.0008 (8)	0.0015 (7)	−0.0030 (8)
C4	0.0401 (9)	0.0440 (10)	0.0306 (9)	−0.0018 (8)	0.0004 (7)	−0.0021 (7)
C5	0.0473 (10)	0.0588 (12)	0.0403 (10)	0.0103 (9)	0.0008 (8)	−0.0038 (9)
C6	0.0572 (13)	0.0703 (14)	0.0429 (11)	0.0126 (11)	0.0061 (9)	−0.0134 (10)
C7	0.0612 (12)	0.0685 (14)	0.0318 (9)	−0.0020 (11)	0.0013 (9)	−0.0094 (9)
O1	0.0487 (9)	0.0727 (11)	0.0889 (12)	0.0073 (8)	0.0163 (8)	−0.0161 (9)
O2	0.0548 (9)	0.0635 (10)	0.0598 (9)	−0.0069 (7)	0.0087 (7)	−0.0173 (8)
O3	0.0395 (8)	0.0752 (10)	0.0628 (10)	−0.0077 (7)	−0.0046 (6)	−0.0065 (7)
N3	0.0440 (9)	0.0596 (11)	0.0310 (8)	−0.0007 (8)	−0.0012 (6)	0.0000 (7)

Geometric parameters (Å, º)

N1—C1	1.102 (3)	C4—C5	1.361 (3)
N2—C4	1.469 (2)	C5—C6	1.389 (3)
N2—H2A	0.89	C5—H5	0.93
N2—H2B	0.89	C6—C7	1.335 (3)
N2—H2C	0.89	C6—H6	0.93
C1—C2	1.397 (3)	C7—H7	0.93
C2—C7	1.374 (3)	O1—N3	1.211 (2)
C2—C3	1.402 (3)	O2—N3	1.309 (2)
C3—C4	1.335 (2)	O3—N3	1.196 (2)
C3—H3	0.93		
C4—N2—H2A	109.5	C3—C4—N2	118.82 (15)
C4—N2—H2B	109.5	C5—C4—N2	120.72 (16)
H2A—N2—H2B	109.5	C4—C5—C6	121.42 (18)
C4—N2—H2C	109.5	C4—C5—H5	119.3
H2A—N2—H2C	109.5	C6—C5—H5	119.3
H2B—N2—H2C	109.5	C7—C6—C5	119.66 (19)
N1—C1—C2	178.6 (2)	C7—C6—H6	120.2
C7—C2—C1	117.84 (17)	C5—C6—H6	120.2
C7—C2—C3	122.50 (17)	C6—C7—C2	118.37 (17)
C1—C2—C3	119.66 (17)	C6—C7—H7	120.8
C4—C3—C2	117.60 (17)	C2—C7—H7	120.8
C4—C3—H3	121.2	O3—N3—O1	115.22 (17)
C2—C3—H3	121.2	O3—N3—O2	121.07 (16)
C3—C4—C5	120.45 (17)	O1—N3—O2	123.69 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O3^{i}	0.89	2.22	3.104 (2)	173
N2—H2*A*···O1^{i}	0.89	2.44	3.107 (2)	133
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N2—H2*C*···O1	0.89	2.56	3.090 (2)	119

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