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2-Cyanoanilinium nitrate

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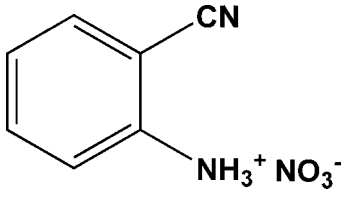
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.063; wR factor = 0.167; data-to-parameter ratio = 12.9.

In the title compound, $C_7H_7N_2^+\cdot NO_3^-$, all atoms of the cation, with the exception of two H atoms of the NH_3 group, lie on a mirror plane, while the anion lies across this plane with the N and one O atom on the mirror plane. In the crystal structure, the organic cations and NO_3^- anions are linked by N—H···N and N—H···O hydrogen bonds, forming a two-dimensional network parallel to (100).

Related literature

For the use of amino derivatives in coordination chemisty, see: Manzur *et al.* (2007); Ismayilov *et al.* (2007); Austria *et al.* (2007); Wen *et al.* (2008).



Experimental

Crystal data

$C_7H_7N_2^+\cdot NO_3^-$
M_r = 181.16
Orthorhombic, *Pnma*
a = 16.373 (3) Å
b = 6.5627 (13) Å
c = 7.9948 (16) Å
V = 859.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 298 (2) K
0.25 × 0.25 × 0.15 mm

Data collection

Rigaku Mercury2 diffractometer
Absorption correction: multi-scan (*CrystalClear*, Rigaku, 2005)
T_{min} = 0.927, T_{max} = 0.983
8381 measured reflections
1072 independent reflections
797 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.167
S = 1.12
1072 reflections
83 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.95 (3)	1.86 (3)	2.805 (2)	177 (2)
N1—H1A···N3^{i}	0.95 (3)	2.56 (3)	3.4523 (13)	156 (2)
N1—H1A···O2^{i}	0.95 (3)	2.61 (3)	3.2898 (7)	129 (2)
N1—H1B···O1^{ii}	0.94 (5)	2.13 (4)	2.979 (3)	150 (1)
N1—H1B···O1^{iii}	0.94 (5)	2.13 (4)	2.979 (3)	150 (1)
N1—H1B···N3^{ii}	0.94 (5)	2.49 (5)	3.427 (4)	180 (3)

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

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: CI2636).

References

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supplementary materials

Acta Cryst. (2008). E**64**, o1620 [**doi:10.1107/S1600536808023313**]

2-Cyanoanilinium nitrate

L.-J. Cui and X.-C. Wen

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; Wen 2008). We report here the crystal structure of the title compound, 2-cyanobenzenaminium nitrate.

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

In the crystal structure, the organic cation and NO_3^- anions are linked to form a two-dimensional network parallel to the (1 0 0) by N—H···N and N—H···O hydrogen bonds (Table 1, Fig.2).

Experimental

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

Refinement

C-bound H atoms were fixed geometrically (C-H = 0.93 Å) and treated as riding with U_{iso}(H) = 1.2U_{eq}(C). N-bound H atoms were located in a difference Fourier map and refined freely.

Figures

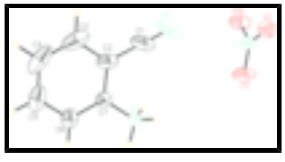

Fig. 1. A view of the title compound with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

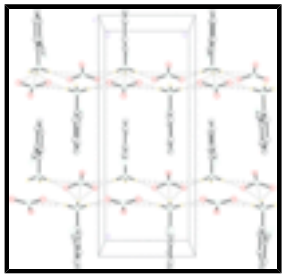

Fig. 2. Part of the crystal packing of the title compound viewed along the *c* axis. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

2-Cyanoanilinium nitrate

Crystal data

$C_7H_7N_2^+ \cdot NO_3^-$	$F_{000} = 376$
$M_r = 181.16$	$D_x = 1.401$ Mg m^{-3}
Orthorhombic, *Pnma*	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ac 2n	Cell parameters from 1592 reflections
$a = 16.373$ (3) Å	$\theta = 2.5$–27.4°
$b = 6.5627$ (13) Å	$\mu = 0.11$ mm^{-1}
$c = 7.9948$ (16) Å	$T = 298$ (2) K
$V = 859.0$ (3) Å^3	Block, colourless
$Z = 4$	0.25 × 0.25 × 0.15 mm

Data collection

Rigaku Mercury2 diffractometer	1072 independent reflections
Radiation source: fine-focus sealed tube	797 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.041$
Detector resolution: 13.6612 pixels mm^{-1}	$\theta_{max} = 27.5^\circ$
$T = 298(2)$ K	$\theta_{min} = 2.5^\circ$
ω scans	$h = -20 \rightarrow 21$
Absorption correction: multi-scan (CrystalClear, Rigaku, 2005)	$k = -8 \rightarrow 8$
$T_{min} = 0.927$, $T_{max} = 0.983$	$l = -10 \rightarrow 10$
8381 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.063$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.167$	$w = 1/[\sigma^2(F_o^2) + (0.0725P)^2 + 0.211P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.12$	$(\Delta/\sigma)_{max} = 0.001$
1072 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
83 parameters	$\Delta\rho_{min} = -0.18$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}
O1	0.76566 (11)	0.0885 (3)	0.9282 (2)	0.0793 (6)
O2	0.82708 (18)	0.2500	0.7321 (3)	0.0951 (9)
N3	0.78679 (15)	0.2500	0.8601 (3)	0.0603 (7)
N1	0.68710 (15)	0.2500	0.2370 (3)	0.0571 (7)
N2	0.6141 (4)	0.2500	0.6492 (5)	0.1409 (19)
C1	0.5859 (3)	0.2500	0.5202 (5)	0.0962 (14)
C2	0.5501 (2)	0.2500	0.3564 (4)	0.0714 (9)
C3	0.4664 (3)	0.2500	0.3345 (9)	0.1171 (18)
H3	0.4319	0.2500	0.4269	0.141*
C4	0.4342 (2)	0.2500	0.1752 (11)	0.125 (2)
H4	0.3779	0.2500	0.1609	0.150*
C5	0.4835 (3)	0.2500	0.0394 (7)	0.0980 (14)
H5	0.4609	0.2500	−0.0673	0.118*
C6	0.5668 (2)	0.2500	0.0584 (4)	0.0690 (9)
H6	0.6008	0.2500	−0.0347	0.083*
C7	0.59927 (17)	0.2500	0.2164 (3)	0.0516 (7)
H1A	0.7034 (16)	0.132 (5)	0.298 (3)	0.083 (8)*
H1B	0.714 (3)	0.2500	0.134 (6)	0.104 (14)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0975 (13)	0.0642 (11)	0.0763 (11)	0.0153 (9)	0.0278 (9)	0.0156 (8)
O2	0.0991 (19)	0.097 (2)	0.0893 (17)	0.000	0.0552 (15)	0.000
N3	0.0525 (14)	0.0693 (17)	0.0592 (14)	0.000	0.0098 (12)	0.000
N1	0.0533 (15)	0.0752 (18)	0.0426 (13)	0.000	0.0006 (11)	0.000
N2	0.205 (5)	0.161 (4)	0.057 (2)	0.000	0.034 (3)	0.000
C1	0.126 (4)	0.105 (3)	0.057 (2)	0.000	0.039 (2)	0.000
C2	0.074 (2)	0.068 (2)	0.072 (2)	0.000	0.0283 (18)	0.000
C3	0.067 (3)	0.125 (4)	0.159 (5)	0.000	0.047 (3)	0.000
C4	0.045 (2)	0.113 (4)	0.219 (7)	0.000	−0.008 (3)	0.000
C5	0.072 (3)	0.085 (3)	0.137 (4)	0.000	−0.040 (3)	0.000

C6	0.064 (2)	0.074 (2)	0.069 (2)	0.000	−0.0116 (16)	0.000
C7	0.0504 (15)	0.0517 (15)	0.0527 (16)	0.000	0.0010 (12)	0.000

Geometric parameters (Å, °)

O1—N3	1.241 (2)	C2—C7	1.378 (4)
O2—N3	1.218 (3)	C3—C4	1.378 (8)
N3—O1^{i}	1.241 (2)	C3—H3	0.93
N1—C7	1.448 (4)	C4—C5	1.353 (8)
N1—H1A	0.95 (3)	C4—H4	0.93
N1—H1B	0.94 (5)	C5—C6	1.371 (5)
N2—C1	1.130 (6)	C5—H5	0.93
C1—C2	1.434 (6)	C6—C7	1.371 (4)
C2—C3	1.382 (6)	C6—H6	0.93
O2—N3—O1^{i}	121.32 (12)	C5—C4—C3	120.9 (4)
O2—N3—O1	121.32 (12)	C5—C4—H4	119.5
O1^{i}—N3—O1	117.4 (2)	C3—C4—H4	119.5
C7—N1—H1A	109.7 (16)	C4—C5—C6	120.2 (5)
C7—N1—H1B	112 (3)	C4—C5—H5	119.9
H1A—N1—H1B	109 (2)	C6—C5—H5	119.9
N2—C1—C2	179.9 (5)	C7—C6—C5	119.2 (4)
C3—C2—C7	118.5 (4)	C7—C6—H6	120.4
C3—C2—C1	121.4 (4)	C5—C6—H6	120.4
C7—C2—C1	120.2 (3)	C6—C7—C2	121.4 (3)
C2—C3—C4	119.7 (4)	C6—C7—N1	119.4 (3)
C2—C3—H3	120.1	C2—C7—N1	119.2 (3)
C4—C3—H3	120.1		
C7—C2—C3—C4	0.0	C5—C6—C7—N1	180.0
C1—C2—C3—C4	180.0	C3—C2—C7—C6	0.0
C2—C3—C4—C5	0.0	C1—C2—C7—C6	180.0
C3—C4—C5—C6	0.0	C3—C2—C7—N1	180.0
C4—C5—C6—C7	0.0	C1—C2—C7—N1	0.0
C5—C6—C7—C2	0.0		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O1^{ii}	0.95 (3)	1.86 (3)	2.805 (2)	177 (2)
N1—H1A···N3^{ii}	0.95 (3)	2.56 (3)	3.4523 (13)	156 (2)
N1—H1A···O2^{ii}	0.95 (3)	2.61 (3)	3.2898 (7)	129 (2)
N1—H1B···O1^{iii}	0.94 (5)	2.13 (4)	2.979 (3)	150 (1)
N1—H1B···O1^{iv}	0.94 (5)	2.13 (4)	2.979 (3)	150 (1)
N1—H1B···N3^{iii}	0.94 (5)	2.49 (5)	3.427 (4)	180 (3)

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

Fig. 1

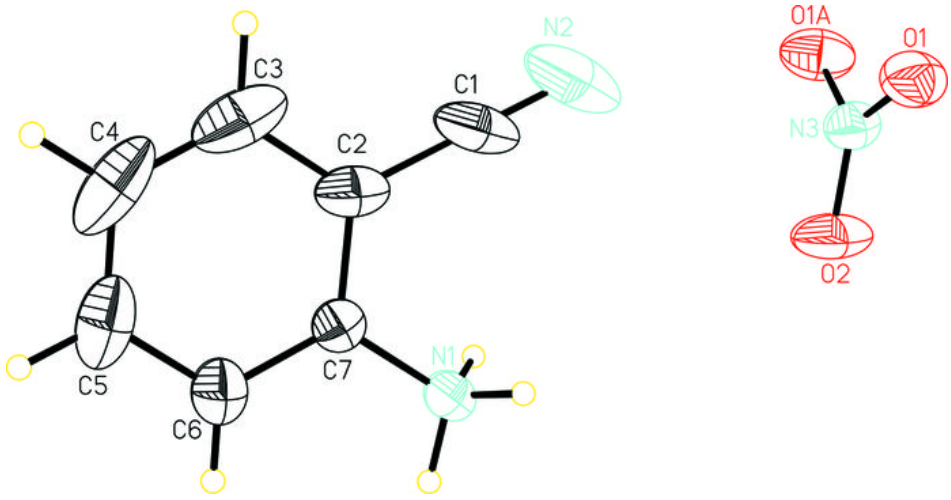

Fig. 2