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2-Methylanilinium nitrate

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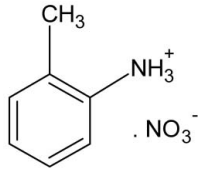
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.050; wR factor = 0.135; data-to-parameter ratio = 18.7.

The crystal structure of the title compound, $C_7H_{10}N^+\cdot NO_3^-$, consists of anion–cation layers parallel to the (100) plane, generated by N—H···O hydrogen bonds. 16 of the 22 atoms (the exceptions being two O and four H atoms) lie on a mirror plane.

Related literature

For related structures see: Benali-Cherif, Direm *et al.* (2007); Benali-Cherif, Allouche *et al.* (2007); Bendeif *et al.* (2007).



Experimental

Crystal data

$C_7H_{10}N^+\cdot NO_3^-$
M_r = 170.17
Orthorhombic, *Pnma*
a = 16.5632 (2) Å
b = 6.7242 (2) Å
c = 7.6849 (3) Å
V = 855.90 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
0.15 × 0.1 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
9040 measured reflections
1331 independent reflections
895 reflections with $I > 2\sigma(I)$
R_{int} = 0.075

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.135
S = 1.05
1331 reflections
71 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H11···N2	0.85	2.61	3.441 (2)	168
N1—H11···O3	0.85	2.23	2.9974 (17)	150
N1—H11···O3^{i}	0.85	2.23	2.9974 (17)	150
N1—H12···O3^{ii}	0.88	1.97	2.8466 (14)	176

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

Data collection: *KappaCCD Server Software* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We Dr M. Giorgi from LBS–UMR 6517, Facult\é des Sciences et Techniques de Saint Jérôme, Marseille, France, for providing diffraction facilities and le Centre Universitaire de Khenchela for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2199).

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supplementary materials

Acta Cryst. (2007). E**63**, o3287 [**doi:10.1107/S1600536807029716**]

2-Methylanilinium nitrate

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Comment

O-toluidine is used in the manufacture of rubber vulcanization accelerator, hypnotic and anesthetic pharmaceuticals, and pesticides. 2-Methylaniline is highly toxic to humans when absorbed through the skin,inhaled as vapor or swallowed, hemoglobine is changed to methemoglobinand and caused damage to the cells of the central nervous system.

The crystal structure of *o*-methylanilinium nitrate, (I), was determined as part of our investigations on the structural characteristics of organic-inorganic layered compounds and an ongoing study on D—H···A hydrogen-bonding in systems of hybrid materials including anilinium derivatives such as 4-Carboxyanilinium hydrogensulfate (Benali-Cherif, Direm *et al.*, 2007), 2-carboxyanilinium dihydrogenphosphate (Benali-Cherif, Allouche *et al.*, 2007) and guaninium phosphite and guaninium phosphate salts (Bendeif *et al.* 2007).

The asymmetric unit of (I) contains a monoprotonated *o*-methylanilinium cation and nitrate anion (Figure 1). Intra atomic bond distances and angles in the title compound shows the monprotonation of the organic entity and confirms the presence of the nitrate (NO_3^-) anion. All atoms in the asymetric unit except three are positionned on a mirror plane (x, 1/4, z).

The structure of ($C_7H_{10}N^+$. NO_3^-) is composed of cationic ($C_7H_{10}N^+$), and anionic (NO_3^-) entities which are linked by N—H···O hydrogen bonds to build up layers developping parallel to the (1 0 0) plane (Table 1, Fig. 2).

Experimental

Single crystals of the title compound are prepared by slow evaporation at room temperature of an aqueous solution of *o*-methylaniline (C_7H_9N) and nitrate acid (HNO_3) in the stoichiometric ration 1:1.

Refinement

Aromatic H atoms were located in difference Fourier syntheses and were allowed to ride on their parent C atoms with C—H = 0.93 Å and U_{iso} = 1.2U_{eq}(C). The methyle and and amonium H-atoms of the cation entity were located in difference Fourier syntheses but were not refined.

Figures

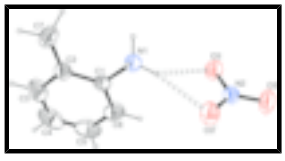

Fig. 1. Molecular view of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines. H atoms are represented as small spheres of arbitrary radii. [Symmetry code: (i) x, 1/2 − y, z]

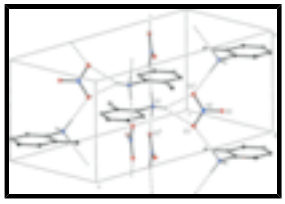

Fig. 2. Partial packing view showing the hydrogen-bonding network. H atoms not involved in H bonds have been omitted for clarity. [Symmetry code: (i) *x*, 1/2 − *y*, *z*; (ii) 1/2 − *x*, −*y*, 1/2 + *z*.]

2-Methylanilinium nitrate

Crystal data

$C_7H_{10}N^+\cdot NO_3^-$	F_{000} = 360
M_r = 170.17	D_x = 1.321 Mg m^{-3}
Orthorhombic, *Pnma*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2n	Cell parameters from 1467 reflections
a = 16.5632 (2) Å	θ = 2.9–30.0º
b = 6.7242 (2) Å	μ = 0.10 mm^{-1}
c = 7.6849 (3) Å	*T* = 293 (2) K
V = 855.90 (4) Å^3	Prism, brown
Z = 4	0.15 × 0.1 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer	895 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.075
Monochromator: graphite	θ_{max} = 30.0º
T = 293(2) K	θ_{min} = 2.9º
ω–θ scans	*h* = 0→23
Absorption correction: none	*k* = 0→9
9040 measured reflections	*l* = 0→10
1331 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.050	H-atom parameters constrained
$wR(F^2)$ = 0.135	$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 0.1577P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
1331 reflections	$\Delta\rho_{max}$ = 0.14 e Å^{-3}
71 parameters	$\Delta\rho_{min}$ = −0.16 e Å^{-3}
4 restraints	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Primary atom site location: structure-invariant direct methods

Extinction coefficient: 0.23 (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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.40546 (11)	0.2500	0.7455 (2)	0.0478 (5)
C2	0.44414 (12)	0.2500	0.9045 (2)	0.0566 (5)
C3	0.52755 (15)	0.2500	0.8999 (4)	0.0880 (8)
H3	0.5563	0.2500	1.0039	0.106*
C4	0.56892 (16)	0.2500	0.7448 (5)	0.1032 (11)
H4	0.6251	0.2500	0.7456	0.124*
C5	0.52909 (18)	0.2500	0.5908 (4)	0.0943 (9)
H5	0.5577	0.2500	0.4866	0.113*
C6	0.44633 (15)	0.2500	0.5899 (3)	0.0722 (6)
H6	0.4182	0.2500	0.4852	0.087*
C7	0.39797 (17)	0.2500	1.0725 (3)	0.0797 (7)
H71	0.4314	0.2500	1.1725	0.120*
H72	0.3651	0.1307	1.0813	0.120*
N1	0.31729 (9)	0.2500	0.74140 (19)	0.0532 (4)
H11	0.3021	0.2500	0.6356	0.080*
H12	0.2989	0.1443	0.7967	0.080*
N2	0.22458 (9)	0.2500	0.3407 (2)	0.0527 (4)
O2	0.18148 (12)	0.2500	0.2138 (2)	0.0919 (6)
O3	0.24779 (7)	0.09186 (15)	0.40892 (14)	0.0761 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0494 (10)	0.0416 (8)	0.0525 (9)	0.000	0.0035 (7)	0.000
C2	0.0555 (11)	0.0532 (10)	0.0611 (11)	0.000	−0.0069 (8)	0.000
C3	0.0553 (14)	0.0946 (19)	0.114 (2)	0.000	−0.0189 (14)	0.000
C4	0.0474 (13)	0.0858 (19)	0.176 (4)	0.000	0.0188 (18)	0.000
C5	0.085 (2)	0.0830 (18)	0.115 (2)	0.000	0.0503 (18)	0.000
C6	0.0780 (16)	0.0786 (15)	0.0599 (12)	0.000	0.0207 (10)	0.000
C7	0.0927 (17)	0.0981 (18)	0.0484 (11)	0.000	−0.0069 (11)	0.000
N1	0.0518 (9)	0.0583 (9)	0.0497 (8)	0.000	−0.0026 (7)	0.000

N2	0.0469 (8)	0.0547 (9)	0.0566 (9)	0.000	−0.0044 (7)	0.000
O2	0.0976 (13)	0.0913 (13)	0.0868 (11)	0.000	−0.0493 (10)	0.000
O3	0.0922 (9)	0.0513 (6)	0.0848 (8)	−0.0052 (5)	−0.0271 (6)	0.0099 (5)

Geometric parameters (Å, °)

C1—C6	1.374 (3)	C5—H5	0.9300
C1—C2	1.380 (2)	C6—H6	0.9300
C1—N1	1.461 (2)	C7—H71	0.9467
C2—C3	1.382 (3)	C7—H72	0.9714
C2—C7	1.501 (3)	N1—H11	0.8508
C3—C4	1.375 (4)	N1—H12	0.8826
C3—H3	0.9300	N2—O2	1.209 (2)
C4—C5	1.355 (4)	N2—O3^{i}	1.2465 (12)
C4—H4	0.9300	N2—O3	1.2465 (12)
C5—C6	1.371 (4)		
C6—C1—C2	122.80 (18)	C6—C5—H5	120.3
C6—C1—N1	118.31 (17)	C5—C6—C1	119.3 (2)
C2—C1—N1	118.89 (15)	C5—C6—H6	120.4
C1—C2—C3	116.2 (2)	C1—C6—H6	120.4
C1—C2—C7	121.70 (18)	C2—C7—H71	113.6
C3—C2—C7	122.1 (2)	C2—C7—H72	110.2
C4—C3—C2	121.3 (3)	H71—C7—H72	105.7
C4—C3—H3	119.3	C1—N1—H11	108.4
C2—C3—H3	119.3	C1—N1—H12	109.6
C5—C4—C3	121.0 (2)	H11—N1—H12	111.0
C5—C4—H4	119.5	O2—N2—O3^{i}	121.45 (8)
C3—C4—H4	119.5	O2—N2—O3	121.45 (8)
C4—C5—C6	119.4 (2)	O3^{i}—N2—O3	117.10 (15)
C4—C5—H5	120.3		

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—H11···N2	0.85	2.61	3.441 (2)	168
N1—H11···O3	0.85	2.23	2.9974 (17)	150
N1—H11···O3^{i}	0.85	2.23	2.9974 (17)	150
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Symmetry codes: (i) *x*, −*y*+1/2, *z*; (ii) −*x*+1/2, −*y*, *z*+1/2.

Fig. 1

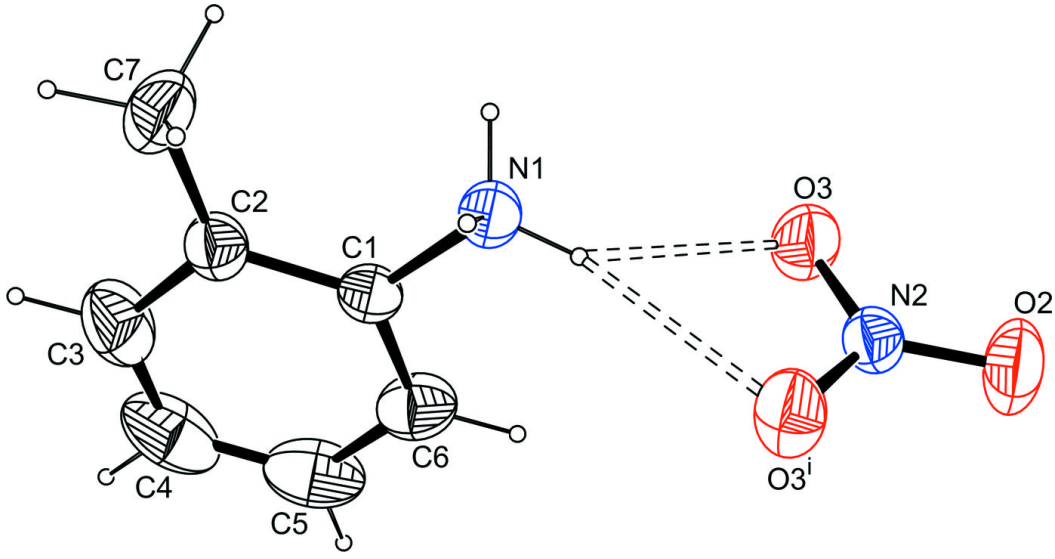

Fig. 2