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Diisopropylammonium nitrite

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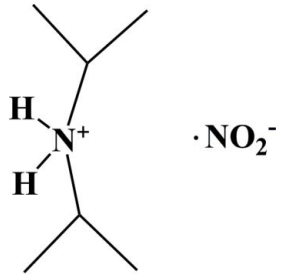
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.084; wR factor = 0.285; data-to-parameter ratio = 22.4.

In the title molecular salt, $C_6H_{16}N^+\cdot NO_2^-$, the cation forms two N—H···O hydrogen bonds to nearby nitrite anions which link the ionic units into chains propagating along the b-axis direction.

Related literature

For a related structure, see: Xu (2012). For background to molecular ferroelectric compounds, see: Fu *et al.* (2011).



Experimental

Crystal data

$C_6H_{16}N^+\cdot NO_2^-$
M_r = 148.21
Monoclinic, $P2_1/n$
a = 8.2314 (16) Å
b = 7.7466 (15) Å
c = 14.583 (3) Å
β = 94.16 (3)°
V = 927.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 298 K
0.10 × 0.03 × 0.03 mm

Data collection

Rigaku Mercury2 CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
T_{min} = 0.910, T_{max} = 1.000
9189 measured reflections
2127 independent reflections
1130 reflections with $I > 2\sigma(I)$
R_{int} = 0.075

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.084
$wR(F^2)$ = 0.285
S = 1.07
2127 reflections
95 parameters
15 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 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—H1E···O1	0.90	1.90	2.800 (3)	174
N1—H1D···O1^{i}	0.90	2.00	2.869 (3)	161

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

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: HB6657).

References

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Xu, J. (2012). *Acta Cryst.* E**68**, o894.

supplementary materials

Acta Cryst. (2012). E**68**, o986 [doi:10.1107/S1600536812008574]

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Comment

Simple organic salts containig amino cations have attracted an attention as materials which display ferroelectric-paraelectric phase transitions (Fu *et al.*, 2011). As part of our ongonig studies in this area, (Xu, 2012), various amines have been studied and a series of new materials with this organic molecules have been elaborated. Herein we present the crystal structure of the title compound, di-isopropylammonium nitrite.

The asymmetric unit of the title compound contains one di-isopropylammonium cation and one NO_2^- anion (Fig. 1). The amino N atom was protonated. The O-N-O bond angle of NO_2- anion is 116.4 (4)°. And the other geometric parameters of the title compound are in the normal range.

In the crystal structure, all the ammonium H atoms are involved in intermolecular N—H···O H-bonding interactions with both the O atoms of the NO_2^- anion (with N···O distances of 2.800 (3)Å and 2.869 (3)Å, respectively). These hydrogen bonds link the ionic units into a one-dimentional chain along the *b*-axis (Table 1 and Fig.2).

Experimental

A mixture of di-isopropylamine (0.8 mmol), HCl (0.8 mmol) and $NaNO_2$ (0.8 mmol) were dissolved in EtOH/distilled water (1:1 *v*/*v*) solvent. The solution was slowly evaporated in air affording colourless block-shaped crystals of the title compound.

Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C-H = 0.98 Å(C methine) and C-H = 0.96 Å(C methyl) with U_{iso}(H) = 1.2U_{eq}(C methine) and U_{iso}(H) = 1.5U_{eq}(C methyl). The positional parameters of the H atoms (N) were refined freely. And in the last stage of the refinement, they were constrained with N—H = 0.90Å, and U_{iso}(H)=1.2U_{eq}(N).

Computing details

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear* (Rigaku, 2005); data reduction: *CrystalClear* (Rigaku, 2005); 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* (Sheldrick, 2008).

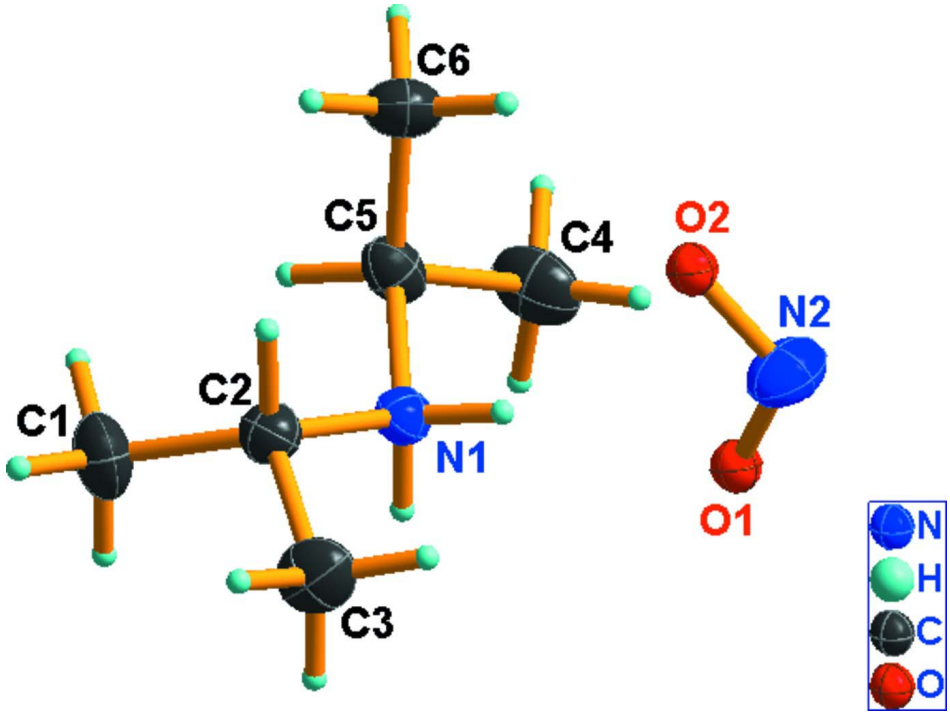

Figure 1

A view of the title compound with displacement ellipsoids drawn at the 30% probability level.

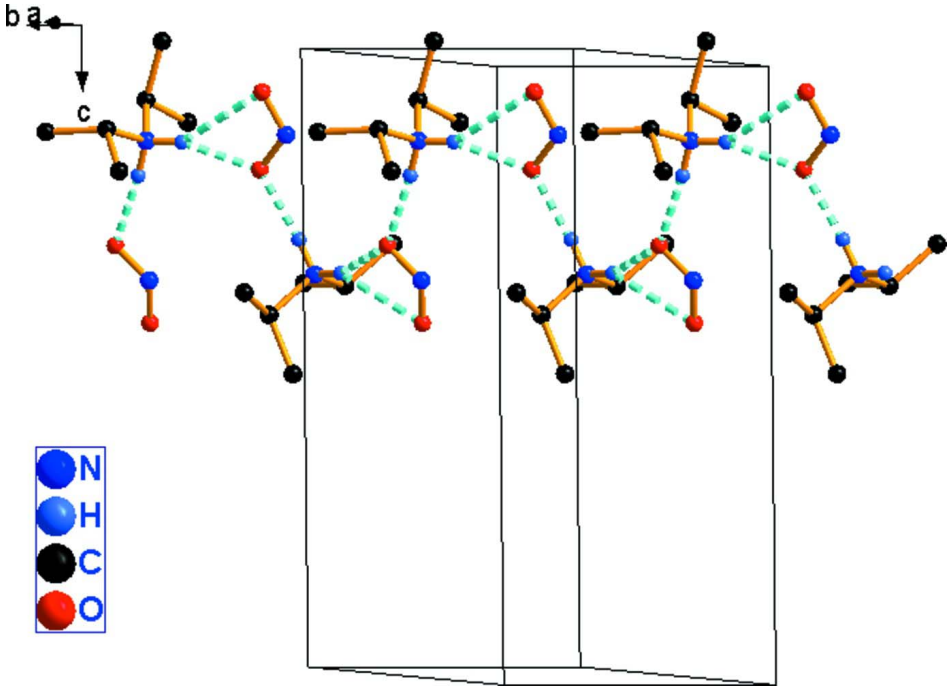

Figure 2

The crystal packing of the title compound showing the one-dimensionnal hydrogen bondings chain along the *b* axis (dashed line). H atoms not involved in hydrogen bonding (dashed line) have been omitted for clarity.

Diisopropylammonium nitrite

Crystal data

$C_6H_{16}N^+·NO_2^-$
M_r = 148.21
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 8.2314 (16) Å
b = 7.7466 (15) Å
c = 14.583 (3) Å
β = 94.16 (3)°
V = 927.5 (3) Å^3
Z = 4
$F(000)$ = 328
D_x = 1.061 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2127 reflections
θ = 3.6–27.5°
μ = 0.08 mm^{-1}
T = 298 K
Block, colourless
0.10 × 0.03 × 0.03 mm

Data collection

Rigaku Mercury2 CCD 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} = 0.910, T_{max} = 1.000
9189 measured reflections
2127 independent reflections
1130 reflections with $I > 2\sigma(I)$
R_{int} = 0.075
θ_{max} = 27.5°, θ_{min} = 3.6°
h = −10→10
k = −10→10
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.084
$wR(F^2)$ = 0.285
S = 1.07
2127 reflections
95 parameters
15 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
$w = 1/[\sigma^2(F_o^2) + (0.1379P)^2 + 0.0979P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-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	0.6713 (3)	0.1958 (3)	0.35567 (15)	0.0543 (7)
H1D	0.6950	0.0825	0.3543	0.065*
H1E	0.6890	0.2393	0.3000	0.065*
C2	0.4930 (4)	0.2132 (4)	0.3690 (2)	0.0624 (9)

H2A	0.4733	0.1702	0.4304	0.075*
O1	0.7263 (3)	0.3533 (3)	0.18791 (17)	0.0931 (9)
C5	0.7889 (4)	0.2792 (4)	0.4247 (2)	0.0686 (9)
H5A	0.7676	0.4037	0.4255	0.082*
N2	0.7438 (4)	0.2425 (4)	0.1320 (2)	0.0925 (9)
O2	0.8050 (4)	0.2847 (5)	0.0648 (2)	0.1177 (10)
C6	0.7724 (5)	0.2066 (6)	0.5196 (2)	0.0918 (12)
H6A	0.6642	0.2277	0.5376	0.138*
H6B	0.8500	0.2614	0.5626	0.138*
H6C	0.7925	0.0846	0.5192	0.138*
C3	0.3999 (4)	0.1012 (6)	0.2986 (3)	0.0909 (12)
H3A	0.4409	−0.0148	0.3032	0.136*
H3B	0.4133	0.1453	0.2381	0.136*
H3C	0.2865	0.1017	0.3099	0.136*
C4	0.9579 (5)	0.2488 (7)	0.3938 (3)	0.1037 (14)
H4A	0.9700	0.3099	0.3374	0.156*
H4B	0.9736	0.1275	0.3841	0.156*
H4C	1.0374	0.2895	0.4402	0.156*
C1	0.4425 (5)	0.3998 (5)	0.3631 (3)	0.0941 (13)
H1A	0.5025	0.4643	0.4104	0.141*
H1B	0.3280	0.4089	0.3710	0.141*
H1C	0.4646	0.4452	0.3040	0.141*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0532 (15)	0.0552 (13)	0.0547 (13)	0.0026 (10)	0.0053 (10)	0.0051 (10)
C2	0.0558 (19)	0.0711 (19)	0.0611 (17)	0.0005 (14)	0.0101 (14)	0.0032 (14)
O1	0.1178 (19)	0.0879 (17)	0.0762 (14)	0.0013 (13)	0.0258 (13)	0.0032 (11)
C5	0.063 (2)	0.0582 (17)	0.082 (2)	−0.0024 (14)	−0.0121 (16)	0.0038 (15)
N2	0.116 (2)	0.0955 (18)	0.0689 (15)	0.0076 (14)	0.0293 (14)	−0.0001 (13)
O2	0.145 (2)	0.126 (2)	0.0854 (16)	0.0130 (16)	0.0308 (15)	0.0006 (14)
C6	0.102 (3)	0.110 (3)	0.061 (2)	0.003 (2)	−0.0109 (18)	−0.005 (2)
C3	0.061 (2)	0.114 (3)	0.097 (3)	−0.0143 (19)	0.0022 (19)	−0.014 (2)
C4	0.056 (2)	0.142 (4)	0.111 (3)	−0.011 (2)	−0.003 (2)	0.025 (3)
C1	0.068 (2)	0.089 (3)	0.125 (3)	0.0240 (19)	0.006 (2)	0.003 (2)

Geometric parameters (Å, º)

N1—C5	1.492 (4)	C6—H6A	0.9600
N1—C2	1.500 (4)	C6—H6B	0.9600
N1—H1D	0.9000	C6—H6C	0.9600
N1—H1E	0.9000	C3—H3A	0.9600
C2—C1	1.505 (5)	C3—H3B	0.9600
C2—C3	1.509 (5)	C3—H3C	0.9600
C2—H2A	0.9800	C4—H4A	0.9600
O1—N2	1.200 (4)	C4—H4B	0.9600
C5—C6	1.510 (5)	C4—H4C	0.9600
C5—C4	1.512 (5)	C1—H1A	0.9600
C5—H5A	0.9800	C1—H1B	0.9600

N2—O2	1.181 (4)	C1—H1C	0.9600
C5—N1—C2	117.8 (2)	C5—C6—H6C	109.5
C5—N1—H1D	107.9	H6A—C6—H6C	109.5
C2—N1—H1D	107.9	H6B—C6—H6C	109.5
C5—N1—H1E	107.9	C2—C3—H3A	109.5
C2—N1—H1E	107.9	C2—C3—H3B	109.5
H1D—N1—H1E	107.2	H3A—C3—H3B	109.5
N1—C2—C1	110.4 (3)	C2—C3—H3C	109.5
N1—C2—C3	108.2 (2)	H3A—C3—H3C	109.5
C1—C2—C3	112.9 (3)	H3B—C3—H3C	109.5
N1—C2—H2A	108.4	C5—C4—H4A	109.5
C1—C2—H2A	108.4	C5—C4—H4B	109.5
C3—C2—H2A	108.4	H4A—C4—H4B	109.5
N1—C5—C6	111.1 (3)	C5—C4—H4C	109.5
N1—C5—C4	107.3 (3)	H4A—C4—H4C	109.5
C6—C5—C4	111.2 (3)	H4B—C4—H4C	109.5
N1—C5—H5A	109.1	C2—C1—H1A	109.5
C6—C5—H5A	109.1	C2—C1—H1B	109.5
C4—C5—H5A	109.1	H1A—C1—H1B	109.5
O2—N2—O1	116.4 (4)	C2—C1—H1C	109.5
C5—C6—H6A	109.5	H1A—C1—H1C	109.5
C5—C6—H6B	109.5	H1B—C1—H1C	109.5
H6A—C6—H6B	109.5		
C5—N1—C2—C1	63.0 (3)	C2—N1—C5—C6	60.4 (3)
C5—N1—C2—C3	−173.0 (3)	C2—N1—C5—C4	−177.8 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*E*···O1	0.90	1.90	2.800 (3)	174
N1—H1*D*···O1^{i}	0.90	2.00	2.869 (3)	161

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