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N-Benzylpropan-2-aminium chloride

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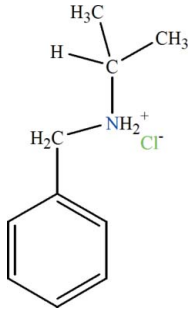
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.021; wR factor = 0.057; data-to-parameter ratio = 22.9.

In the crystal structure of title salt, $C_{10}H_{16}N^+\cdot Cl^-$, the amino H atoms are involved in intermolecular N—H···Cl hydrogen bonding, generating a zigzag chain propagating in [100].

Related literature

For related structures, see: Pourayoubi & Sabbaghi (2007); Yazdanbakhsh & Sabbaghi (2007).



Experimental

Crystal data

$C_{10}H_{16}N^+\cdot Cl^-$
M_r = 185.69
Orthorhombic, $Pna2_1$
a = 9.9666 (6) Å
b = 18.0379 (11) Å
c = 5.7307 (4) Å
V = 1030.25 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 100 K
0.50 × 0.40 × 0.30 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.818, T_{max} = 0.910
11694 measured reflections
2720 independent reflections
2662 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.057
S = 1.07
2720 reflections
119 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Absolute structure: Flack (1983), 1229 Friedel pairs
Flack parameter: −0.02 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl1	0.853 (13)	2.288 (13)	3.1296 (9)	168.8 (11)
N1—H2···Cl1^{i}	0.877 (14)	2.255 (14)	3.1257 (9)	171.9 (13)

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; 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*.

Support of this investigation by Ferdowsi University of Mashhad is gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2732).

References

Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
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supplementary materials

Acta Cryst. (2010). E**66**, o708 [**doi:10.1107/S1600536810006707**]

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M. Pourayoubi and M. Negari

Comment

In the previous works, the structure determination of $[NH_2(CH_2C_6H_5)(CH(CH_3)_2)][CCl_3C(O)NHP(O)(O)(OCH_3)]$ (Pourayoubi & Sabbaghi, 2007) and $[NH_2(CH_2C_6H_5)(CH(CH_3)_2)]$ $[CF_3C(O)NHP(O)(O)(N(CH_2C_6H_5)(CH(CH_3)_2)]$ (Yazdanbakhsh & Sabbaghi, 2007) have been investigated; we report here on the crystal structure of title compound, the chloride salt of *N*-benzyl-2-propanaminium cation (Fig. 1). Both hydrogen atoms of NH_2 groups are involved in intermolecular N—H···Cl hydrogen bonding with neighbouring Cl^- anions [N1···Cl1 = 3.1296 (9) Å, N1···Cl2 = 3.1257 (9) Å] into an extended 1-D zigzag chain (Fig. 2).

Experimental

The title compound is a by-product of the preparation of $P(O)[OC_6H_5][N(CH_2C_6H_5)(CH(CH_3)_2)]_2$ [from the reaction between $P(O)[OC_6H_5]Cl_2$ and $NH(CH_2C_6H_5)(CH(CH_3)_2)$, with 1:4 mole ratio] which is crystallized in $CH_3C(O)CH_3$.

Refinement

The H atoms of the NH2 group were located from the difference Fourier synthesis and refined isotropically, no restraints were used. Finally, the geometrical and thermal parameters obtained for these H-atoms, as well as parameters of the hydrogen bonds for these H-atoms included, were rather realistic. The H(C) atom positions were calculated and refined in isotropic approximation in riding model with the Uiso(H) parameters equal to 1.2 Ueq(Ci), for methyl groups equal to 1.5 Ueq(Cii), where U(Ci) and U(Cii) are respectively the equivalent thermal parameters of the carbon atoms to which corresponding H atoms are bonded.

Figures

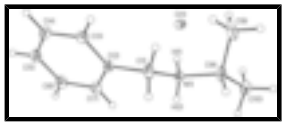

Fig. 1. The molecular structure of the title salt, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50 % probability level.

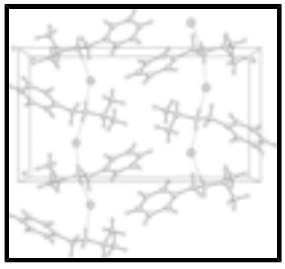

Fig. 2. Fragment of crystal packing (projection along *c* crystal axis), the hydrogen bonds are shown by dash line.

N-Benzylpropan-2-aminium chloride

Crystal data

$C_{10}H_{16}N^+ \cdot Cl^-$	$F(000) = 400$
$M_r = 185.69$	$D_x = 1.197$ Mg m^{-3}
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2c -2n	Cell parameters from 8636 reflections
$a = 9.9666$ (6) Å	$\theta = 2.3$–$34.0°$
$b = 18.0379$ (11) Å	$\mu = 0.32$ mm^{-1}
$c = 5.7307$ (4) Å	$T = 100$ K
$V = 1030.25$ (11) Å^3	Prism, colourless
$Z = 4$	0.50 × 0.40 × 0.30 mm

Data collection

Bruker APEXII CCD diffractometer	2720 independent reflections
Radiation source: fine-focus sealed tube	2662 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.023$
φ and ω scans	$\theta_{max} = 29.0°$, $\theta_{min} = 2.3°$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$h = -13 \rightarrow 13$
$T_{min} = 0.818$, $T_{max} = 0.910$	$k = -24 \rightarrow 24$
11694 measured reflections	$l = -7 \rightarrow 7$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.021$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.057$	$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2 + 0.1229P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
2720 reflections	$\Delta\rho_{max} = 0.25$ e Å^{-3}
119 parameters	$\Delta\rho_{min} = -0.15$ e Å^{-3}
1 restraint	Absolute structure: Flack (1983), 1229 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.02 (4)

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 $F^2 > \sigma(F^2)$ 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}
Cl1	0.212804 (19)	0.282008 (11)	0.24289 (5)	0.01590 (6)
N1	0.47016 (8)	0.26697 (4)	0.55218 (15)	0.01274 (15)
H1	0.3950 (14)	0.2666 (7)	0.481 (2)	0.013 (3)*
H2	0.5322 (12)	0.2517 (7)	0.455 (3)	0.014 (3)*
C1	0.47024 (10)	0.21793 (5)	0.7630 (2)	0.01667 (19)
H1A	0.4181	0.2423	0.8884	0.020*
H1B	0.5636	0.2123	0.8190	0.020*
C2	0.41198 (9)	0.14208 (5)	0.71879 (19)	0.01422 (17)
C3	0.32866 (10)	0.11207 (6)	0.88949 (19)	0.01721 (19)
H3A	0.3064	0.1405	1.0235	0.021*
C4	0.27777 (10)	0.04055 (6)	0.8647 (2)	0.0205 (2)
H4A	0.2218	0.0202	0.9826	0.025*
C5	0.30877 (11)	−0.00100 (6)	0.6679 (2)	0.0192 (2)
H5A	0.2743	−0.0498	0.6512	0.023*
C6	0.39045 (10)	0.02910 (5)	0.49499 (19)	0.0188 (2)
H6A	0.4105	0.0010	0.3591	0.023*
C7	0.44277 (10)	0.10012 (5)	0.52059 (18)	0.01675 (18)
H7A	0.4995	0.1202	0.4033	0.020*
C8	0.50162 (11)	0.34699 (5)	0.6084 (2)	0.0195 (2)
H8A	0.5825	0.3487	0.7116	0.023*
C9	0.38428 (13)	0.38228 (5)	0.7366 (2)	0.0281 (2)
H9A	0.3631	0.3530	0.8758	0.042*
H9B	0.3059	0.3837	0.6335	0.042*
H9C	0.4083	0.4329	0.7830	0.042*
C10	0.53322 (12)	0.38753 (6)	0.3829 (2)	0.0256 (2)
H10A	0.6057	0.3617	0.3007	0.038*
H10B	0.5613	0.4384	0.4184	0.038*
H10C	0.4530	0.3887	0.2840	0.038*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.01334 (10)	0.01922 (10)	0.01515 (10)	0.00008 (7)	−0.00118 (9)	0.00016 (10)
N1	0.0131 (4)	0.0111 (3)	0.0140 (4)	−0.0004 (3)	−0.0017 (3)	0.0011 (3)
C1	0.0237 (4)	0.0127 (4)	0.0136 (5)	−0.0013 (3)	−0.0044 (4)	0.0014 (3)
C2	0.0155 (4)	0.0114 (4)	0.0157 (4)	0.0011 (3)	−0.0018 (4)	0.0034 (4)
C3	0.0181 (4)	0.0173 (4)	0.0162 (4)	0.0020 (3)	0.0013 (4)	0.0012 (4)

C4	0.0197 (5)	0.0199 (5)	0.0221 (6)	−0.0024 (4)	0.0022 (4)	0.0062 (4)
C5	0.0189 (4)	0.0143 (4)	0.0243 (5)	−0.0027 (4)	−0.0041 (4)	0.0029 (3)
C6	0.0209 (4)	0.0163 (4)	0.0192 (5)	−0.0003 (4)	−0.0018 (4)	−0.0021 (4)
C7	0.0187 (4)	0.0154 (4)	0.0162 (4)	−0.0016 (3)	0.0008 (4)	0.0003 (4)
C8	0.0234 (5)	0.0113 (4)	0.0238 (5)	−0.0048 (4)	−0.0083 (4)	0.0010 (4)
C9	0.0512 (6)	0.0125 (4)	0.0205 (5)	0.0038 (4)	0.0042 (6)	−0.0007 (5)
C10	0.0241 (5)	0.0171 (5)	0.0355 (6)	−0.0021 (4)	0.0051 (5)	0.0084 (4)

Geometric parameters (Å, °)

N1—C1	1.4974 (13)	C5—H5A	0.9500
N1—C8	1.5118 (13)	C6—C7	1.3910 (14)
N1—H1	0.853 (14)	C6—H6A	0.9500
N1—H2	0.877 (14)	C7—H7A	0.9500
C1—C2	1.5076 (12)	C8—C10	1.5178 (16)
C1—H1A	0.9900	C8—C9	1.5207 (17)
C1—H1B	0.9900	C8—H8A	1.0000
C2—C3	1.3927 (14)	C9—H9A	0.9800
C2—C7	1.3990 (14)	C9—H9B	0.9800
C3—C4	1.3934 (15)	C9—H9C	0.9800
C3—H3A	0.9500	C10—H10A	0.9800
C4—C5	1.3892 (16)	C10—H10B	0.9800
C4—H4A	0.9500	C10—H10C	0.9800
C5—C6	1.3925 (15)		
C1—N1—C8	113.08 (8)	C7—C6—C5	120.21 (10)
C1—N1—H1	112.4 (9)	C7—C6—H6A	119.9
C8—N1—H1	107.0 (8)	C5—C6—H6A	119.9
C1—N1—H2	109.1 (9)	C6—C7—C2	120.11 (9)
C8—N1—H2	106.8 (8)	C6—C7—H7A	119.9
H1—N1—H2	108.2 (14)	C2—C7—H7A	119.9
N1—C1—C2	113.60 (9)	N1—C8—C10	108.76 (9)
N1—C1—H1A	108.8	N1—C8—C9	110.07 (8)
C2—C1—H1A	108.8	C10—C8—C9	111.67 (9)
N1—C1—H1B	108.8	N1—C8—H8A	108.8
C2—C1—H1B	108.8	C10—C8—H8A	108.8
H1A—C1—H1B	107.7	C9—C8—H8A	108.8
C3—C2—C7	119.39 (8)	C8—C9—H9A	109.5
C3—C2—C1	117.67 (9)	C8—C9—H9B	109.5
C7—C2—C1	122.88 (9)	H9A—C9—H9B	109.5
C2—C3—C4	120.36 (9)	C8—C9—H9C	109.5
C2—C3—H3A	119.8	H9A—C9—H9C	109.5
C4—C3—H3A	119.8	H9B—C9—H9C	109.5
C5—C4—C3	120.08 (9)	C8—C10—H10A	109.5
C5—C4—H4A	120.0	C8—C10—H10B	109.5
C3—C4—H4A	120.0	H10A—C10—H10B	109.5
C4—C5—C6	119.83 (9)	C8—C10—H10C	109.5
C4—C5—H5A	120.1	H10A—C10—H10C	109.5
C6—C5—H5A	120.1	H10B—C10—H10C	109.5
C8—N1—C1—C2	168.17 (8)	C4—C5—C6—C7	1.03 (16)

N1—C1—C2—C3	−138.75 (10)	C5—C6—C7—C2	−0.91 (15)
N1—C1—C2—C7	44.10 (12)	C3—C2—C7—C6	−0.02 (14)
C7—C2—C3—C4	0.83 (15)	C1—C2—C7—C6	177.09 (9)
C1—C2—C3—C4	−176.43 (9)	C1—N1—C8—C10	166.04 (8)
C2—C3—C4—C5	−0.71 (16)	C1—N1—C8—C9	−71.33 (11)
C3—C4—C5—C6	−0.22 (16)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···Cl1	0.853 (13)	2.288 (13)	3.1296 (9)	168.8 (11)
N1—H2···Cl1^{i}	0.877 (14)	2.255 (14)	3.1257 (9)	171.9 (13)

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

Fig. 1

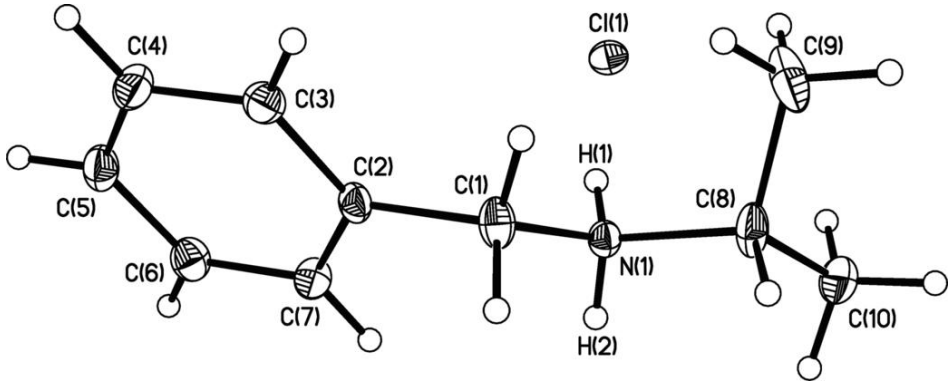

Fig. 2