

(2-Phenylethyl)ammonium chloride

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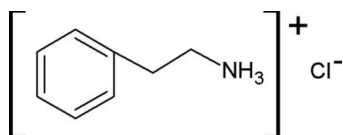
Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.027; wR factor = 0.071; data-to-parameter ratio = 13.6.

The crystal structure of the title compound, $\text{C}_8\text{H}_{12}\text{N}^+\cdot\text{Cl}^-$, determined at 100 K, is stabilized by intermolecular $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds. The benzene rings stack along the a axis, with a distance between the substituted C atom and the $para$ C atom of a neighbouring molecule at $(x + 1, y, z)$ of $3.600(3)$ Å, which suggests that $\pi-\pi$ stacking interactions also contribute to the stabilization.

Related literature

Earlier reports (Tsoucaris, 1961; Horn *et al.*, 1990) have found the same crystal structure for the title compound at room temperature. In addition, the crystal structure shows similar benzene stacks and hydrogen-bond networks as the diamine derivative of this material (Arkenbout *et al.*, 2007).

For related literature, see: Jurchescu *et al.* (2007); Le Page (1987, 1988); Spek (1988).



Experimental

Crystal data

 $\text{C}_8\text{H}_{12}\text{N}^+\cdot\text{Cl}^-$ $M_r = 157.64$ Orthorhombic, $P2_12_12_1$ $a = 4.5354(6)$ Å $b = 5.8868(8)$ Å $c = 31.991(4)$ Å $V = 854.13(19)$ Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 0.37$ mm⁻¹ $T = 100(1)$ K $0.47 \times 0.34 \times 0.16$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer

Absorption correction: multi-scan

SADABS (Bruker, 2006)

 $T_{\min} = 0.819$, $T_{\max} = 0.942$

6845 measured reflections

1884 independent reflections

1818 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.025$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.027$ $wR(F^2) = 0.071$ $S = 1.14$

1884 reflections

139 parameters

All H-atom parameters refined

 $\Delta\rho_{\text{max}} = 0.24$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.21$ e Å⁻³

Absolute structure: Flack (1983),

with 697 Friedel pairs

Flack parameter: 0.00 (7)

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N}-\text{H}9\cdots\text{Cl}^{\text{i}}$	0.95 (2)	2.32 (2)	3.2167 (13)	158 (2)
$\text{N}-\text{H}9'\cdots\text{Cl}^{\text{ii}}$	0.90 (2)	2.30 (2)	3.1696 (13)	162 (2)
$\text{N}-\text{H}9''\cdots\text{Cl}^{\text{iii}}$	0.92 (2)	2.29 (2)	3.1907 (14)	165 (2)

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

Data collection: SMART (Bruker, 2006); cell refinement: SAINT-Plus (Bruker, 2006); data reduction: SAINT-Plus; program(s) used to solve structure: DIRDIF99 (Beurskens *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: DIAMOND (Brandenburg, 2006) and PLATON (Spek, 2003); software used to prepare material for publication: PLATON.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2013).

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supplementary materials

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(2-Phenylethyl)ammonium chloride

A. H. Arkenbout, A. Meetsma and T. T. M. Palstra

Comment

There is an interest to develop organic semiconductors that will provide more versatile field effect transistors (Jurchescu *et al.*, 2007). This research is focused on making new organic materials that are easily processable and have good π - π stacking. We present here the crystal structure, at 100 K, of the title compound, (I), which is based on a benzene derivative with an ammonium group and chlorine counter ions (Fig 1.). The crystal structure is stabilized by hydrogen bonds that are formed by the ammonium group and three chlorine atoms (Fig 2.). In this way an intermolecular network is created. Besides, the benzene rings form stacks along the *a* axis. The distance between the C3...C6 ($x + 1, y, z$) is 3.600 (3) Å, which suggests that π - π stacking interactions also contribute to the stabilization of this crystal structure.

Experimental

A saturated (37%) HCl solution (5 ml, Merck) was slowly added to 2 ml of 2-Phenyl-ethylamin (Fluka, purum >99.0%), while stirring and cooling on a water bath. The resulting mixture was filtered, washed with water and dried in air. Needle like colorless crystals were obtained by recrystallization from a saturated aqueous solution *via* slow evaporation of the water at room temperature.

Refinement

All hydrogen atoms were located in a difference Fourier map and refined with isotropic displacement parameters. C—H distances were in the range of 0.91 – 1.00 (3) Å.

Figures

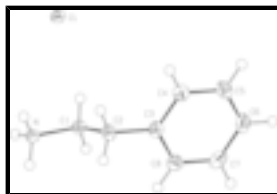


Fig. 1. Perspective (*PLATON*) drawing of the title compound. Displacement ellipsoids for non-H atoms are represented at the 50% probability level. The hydrogen atoms are shown as spheres of arbitrary radius.

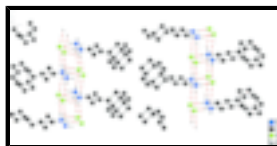


Fig. 2. Portion of the crystal packing (*DIAMOND*), showing N—H...Cl hydrogen bonds shown as red dashed lines. Colour code: Cl atoms are shown in green, N atoms in blue, C atoms in black and H atoms in grey.

(2-Phenyl)ethylammonium chloride

Crystal data

$C_8H_{12}N^+.Cl^-$

$M_r = 157.64$

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 4.5354$ (6) Å

$b = 5.8868$ (8) Å

$c = 31.991$ (4) Å

$V = 854.13$ (19) Å³

$Z = 4$

$F_{000} = 336$

The final unit cell was obtained from the xyz centroids of 4595 reflections after integration using the SAINT-Plus software package (Bruker, 2006). Reduced cell calculations did not indicate any higher metric lattice symmetry and examination of the final-atomic coordinates of the structure did not yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988).

$D_x = 1.226$ Mg m⁻³

Mo $K\alpha$ radiation

$\lambda = 0.71073$ Å

Cell parameters from 4595 reflections

$\theta = 3.2$ – 27.5°

$\mu = 0.37$ mm⁻¹

$T = 100$ (1) K

Block, colourless

$0.47 \times 0.34 \times 0.16$ mm

Data collection

Bruker Smart Apex CCD area detector diffractometer

1884 independent reflections

Radiation source: fine focus sealed Siemens Mo tube

1818 reflections with $I > 2\sigma(I)$

Monochromator: parallel mounted graphite

$R_{int} = 0.025$

Detector resolution: 66.06 pixels mm⁻¹

$\theta_{max} = 27.5^\circ$

$T = 100$ (1) K

$\theta_{min} = 3.5^\circ$

φ and ω scans

$h = -5 \rightarrow 5$

Absorption correction: multi-scan

$k = -7 \rightarrow 7$

SADABS (Bruker, 2006)

$T_{min} = 0.819$, $T_{max} = 0.942$

$l = -37 \rightarrow 41$

6845 measured reflections

Refinement

Refinement on F^2

Hydrogen site location: difference Fourier map

Least-squares matrix: full

All H-atom parameters refined

$R[F^2 > 2\sigma(F^2)] = 0.027$

$w = 1/[\sigma^2(F_o^2) + (0.0331P)^2 + 0.2312P]$

where $P = (F_o^2 + 2F_c^2)/3$

$wR(F^2) = 0.071$

$(\Delta/\sigma)_{max} < 0.001$

$S = 1.14$

$\Delta\rho_{max} = 0.24$ e Å⁻³

1884 reflections

$\Delta\rho_{min} = -0.21$ e Å⁻³

139 parameters

Extinction correction: none

Primary atom site location: heavy-atom method Absolute structure: The absolute structure of the molecule was determined by Flack's x refinement (Flack & Bernardinelli, 1999, 2000)

Secondary atom site location: structure-invariant direct methods Flack parameter: 0.00 (7)

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N	1.1098 (3)	0.0830 (2)	0.21770 (4)	0.0173 (4)
C1	0.9122 (4)	0.0687 (3)	0.18056 (5)	0.0184 (4)
C2	1.0932 (4)	0.0472 (3)	0.14066 (5)	0.0214 (5)
C3	0.8947 (4)	0.0024 (3)	0.10356 (5)	0.0204 (5)
C4	0.8476 (4)	0.1680 (3)	0.07339 (6)	0.0237 (5)
C5	0.6611 (4)	0.1269 (3)	0.03975 (6)	0.0270 (5)
C6	0.5203 (4)	-0.0815 (4)	0.03607 (6)	0.0280 (5)
C7	0.5661 (4)	-0.2473 (3)	0.06602 (6)	0.0281 (6)
C8	0.7532 (4)	-0.2063 (3)	0.09954 (6)	0.0245 (5)
Cl	0.37787 (8)	0.57866 (6)	0.21042 (1)	0.0186 (1)
H1	0.790 (5)	0.198 (4)	0.1806 (6)	0.025 (5)*
H1'	0.788 (4)	-0.067 (4)	0.1851 (6)	0.025 (5)*
H2	1.228 (5)	-0.073 (4)	0.1439 (7)	0.030 (5)*
H2'	1.216 (5)	0.186 (4)	0.1373 (7)	0.041 (6)*
H4	0.935 (5)	0.306 (4)	0.0752 (6)	0.030 (6)*
H5	0.625 (5)	0.243 (4)	0.0191 (6)	0.029 (5)*
H6	0.393 (5)	-0.110 (4)	0.0129 (7)	0.039 (6)*
H7	0.478 (5)	-0.392 (4)	0.0634 (7)	0.039 (6)*
H8	0.780 (4)	-0.320 (4)	0.1206 (7)	0.027 (5)*
H9	1.232 (5)	-0.047 (4)	0.2196 (7)	0.035 (6)*
H9'	1.224 (5)	0.207 (4)	0.2161 (7)	0.032 (6)*
H9''	0.998 (5)	0.086 (4)	0.2417 (7)	0.029 (5)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N	0.0191 (6)	0.0149 (6)	0.0180 (7)	0.0001 (7)	0.0010 (6)	-0.0006 (5)
C1	0.0177 (8)	0.0191 (7)	0.0183 (8)	0.0011 (8)	0.0005 (6)	-0.0009 (7)
C2	0.0191 (8)	0.0279 (9)	0.0172 (8)	0.0006 (8)	0.0008 (7)	-0.0002 (7)

supplementary materials

C3	0.0181 (8)	0.0259 (8)	0.0171 (8)	0.0034 (7)	0.0043 (7)	-0.0032 (6)
C4	0.0222 (9)	0.0243 (8)	0.0247 (9)	-0.0014 (7)	0.0027 (8)	0.0005 (7)
C5	0.0265 (9)	0.0339 (10)	0.0207 (8)	0.0049 (8)	0.0010 (7)	0.0024 (7)
C6	0.0250 (8)	0.0375 (10)	0.0215 (9)	0.0045 (9)	-0.0025 (7)	-0.0094 (9)
C7	0.0284 (10)	0.0247 (9)	0.0311 (10)	-0.0016 (8)	0.0040 (8)	-0.0086 (8)
C8	0.0278 (9)	0.0240 (9)	0.0217 (9)	0.0036 (8)	0.0037 (7)	-0.0006 (8)
Cl	0.0208 (2)	0.0148 (2)	0.0201 (2)	-0.0003 (2)	0.0013 (2)	0.0003 (2)

Geometric parameters (Å, °)

N—C1	1.491 (2)	C7—C8	1.389 (3)
N—H9 ⁿ	0.92 (2)	C1—H1	0.94 (2)
N—H9	0.95 (2)	C1—H1'	0.99 (2)
N—H9'	0.90 (2)	C2—H2	0.94 (2)
C1—C2	1.523 (2)	C2—H2'	1.00 (2)
C2—C3	1.513 (2)	C4—H4	0.91 (2)
C3—C8	1.392 (3)	C5—H5	0.97 (2)
C3—C4	1.388 (3)	C6—H6	0.95 (2)
C4—C5	1.390 (3)	C7—H7	0.95 (2)
C5—C6	1.388 (3)	C8—H8	0.96 (2)
C6—C7	1.383 (3)		
Cl...N ⁱ	3.1696 (13)	C8...H2 ⁱ	2.88 (2)
Cl...N ⁱⁱ	3.2167 (13)	C8...H1'	2.86 (2)
Cl...N ⁱⁱⁱ	3.2692 (14)	C8...H4 ^{xiii}	3.09 (2)
Cl...N ^{iv}	3.1907 (14)	H1...Cl	3.07 (2)
Cl...H1 ^v	2.91 (2)	H1'...Cl ^{xii}	2.91 (2)
Cl...H1	3.07 (2)	H1'...C8	2.86 (2)
Cl...H9 ⁱ	2.30 (2)	H1'...H8	2.55 (3)
Cl...H2 ⁱⁱ	3.03 (2)	H2...H9	2.43 (3)
Cl...H9 ⁱⁱ	2.32 (2)	H2...Cl ^{vi}	3.03 (2)
Cl...H9 ⁱⁱⁱ	2.95 (2)	H2...C8 ^{vii}	2.88 (2)
Cl...H9 ⁱⁱⁱ	3.06 (2)	H2'...H4	2.46 (3)
Cl...H9 ^{iv}	2.29 (2)	H2'...H9'	2.52 (3)
N...Cl ^{vi}	3.2167 (13)	H4...H2'	2.46 (3)
N...Cl ^{vii}	3.1696 (13)	H4...C8 ^v	3.09 (2)
N...Cl ^{viii}	3.1907 (14)	H5...C5 ^{xiii}	2.93 (2)
N...Cl ^{ix}	3.2692 (14)	H5...H5 ^{xiii}	2.58 (3)
C2...C8 ^{vii}	3.594 (3)	H5...H5 ^x	2.58 (3)
C3...C6 ^{vii}	3.600 (3)	H6...C7 ^{xiv}	3.05 (2)
C3...C7 ^{vii}	3.588 (3)	H6...C6 ^{xiv}	2.93 (2)
C4...C6 ^{vii}	3.590 (3)	H7...C5 ^{xii}	3.05 (2)
C6...C4 ⁱ	3.590 (3)	H8...C1	3.05 (2)
C6...C3 ⁱ	3.600 (3)	H8...H1'	2.55 (3)
C7...C3 ⁱ	3.588 (3)	H9...Cl ^{vi}	2.32 (2)

C8...C2 ⁱ	3.594 (3)	H9...H2	2.43 (3)
C1...H8	3.05 (2)	H9...Cl ^{ix}	2.95 (2)
C5...H7 ^v	3.05 (2)	H9'...Cl ^{ix}	3.06 (2)
C5...H5 ^x	2.93 (2)	H9'...H2'	2.52 (3)
C6...H6 ^{xi}	2.93 (2)	H9'...Cl ^{vii}	2.30 (2)
C7...H6 ^{xi}	3.05 (2)	H9''...Cl ^{viii}	2.29 (2)
H9'—N—H9''	111 (2)	C2—C1—H1	112.7 (12)
C1—N—H9'	110.4 (14)	C2—C1—H1'	111.3 (12)
C1—N—H9''	109.6 (14)	H1—C1—H1'	108.5 (18)
C1—N—H9	110.9 (14)	C1—C2—H2	108.7 (14)
H9—N—H9''	107 (2)	C1—C2—H2'	108.9 (13)
H9—N—H9'	109 (2)	C3—C2—H2	110.0 (14)
N—C1—C2	110.41 (14)	C3—C2—H2'	113.1 (13)
C1—C2—C3	110.57 (15)	H2—C2—H2'	105.4 (19)
C2—C3—C4	120.97 (16)	C3—C4—H4	121.2 (13)
C2—C3—C8	120.05 (15)	C5—C4—H4	118.2 (13)
C4—C3—C8	118.98 (16)	C4—C5—H5	120.7 (13)
C3—C4—C5	120.64 (16)	C6—C5—H5	119.4 (13)
C4—C5—C6	119.96 (17)	C5—C6—H6	120.0 (14)
C5—C6—C7	119.72 (17)	C7—C6—H6	120.3 (14)
C6—C7—C8	120.26 (17)	C6—C7—H7	120.8 (14)
C3—C8—C7	120.43 (17)	C8—C7—H7	118.9 (14)
N—C1—H1	107.9 (13)	C3—C8—H8	119.6 (13)
N—C1—H1'	105.7 (11)	C7—C8—H8	120.0 (13)
N—C1—C2—C3	172.74 (13)	C4—C3—C8—C7	-0.5 (3)
C1—C2—C3—C4	108.95 (19)	C3—C4—C5—C6	-0.1 (3)
C1—C2—C3—C8	-70.3 (2)	C4—C5—C6—C7	0.1 (3)
C2—C3—C4—C5	-178.94 (17)	C5—C6—C7—C8	-0.3 (3)
C8—C3—C4—C5	0.3 (3)	C6—C7—C8—C3	0.5 (3)
C2—C3—C8—C7	178.74 (17)		

Symmetry codes: (i) $x-1, y, z$; (ii) $x-1, y+1, z$; (iii) $-x+2, y+1/2, -z+1/2$; (iv) $-x+1, y+1/2, -z+1/2$; (v) $x, y+1, z$; (vi) $x+1, y-1, z$; (vii) $x+1, y, z$; (viii) $-x+1, y-1/2, -z+1/2$; (ix) $-x+2, y-1/2, -z+1/2$; (x) $x+1/2, -y+1/2, -z$; (xi) $x+1/2, -y-1/2, -z$; (xii) $x, y-1, z$; (xiii) $x-1/2, -y+1/2, -z$; (xiv) $x-1/2, -y-1/2, -z$.

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N—H9...Cl ^{vi}	0.95 (2)	2.32 (2)	3.2167 (13)	158 (2)
N—H9'...Cl ^{vii}	0.90 (2)	2.30 (2)	3.1696 (13)	162 (2)
N—H9''...Cl ^{viii}	0.92 (2)	2.29 (2)	3.1907 (14)	165 (2)

Symmetry codes: (vi) $x+1, y-1, z$; (vii) $x+1, y, z$; (viii) $-x+1, y-1/2, -z+1/2$.

Fig. 1

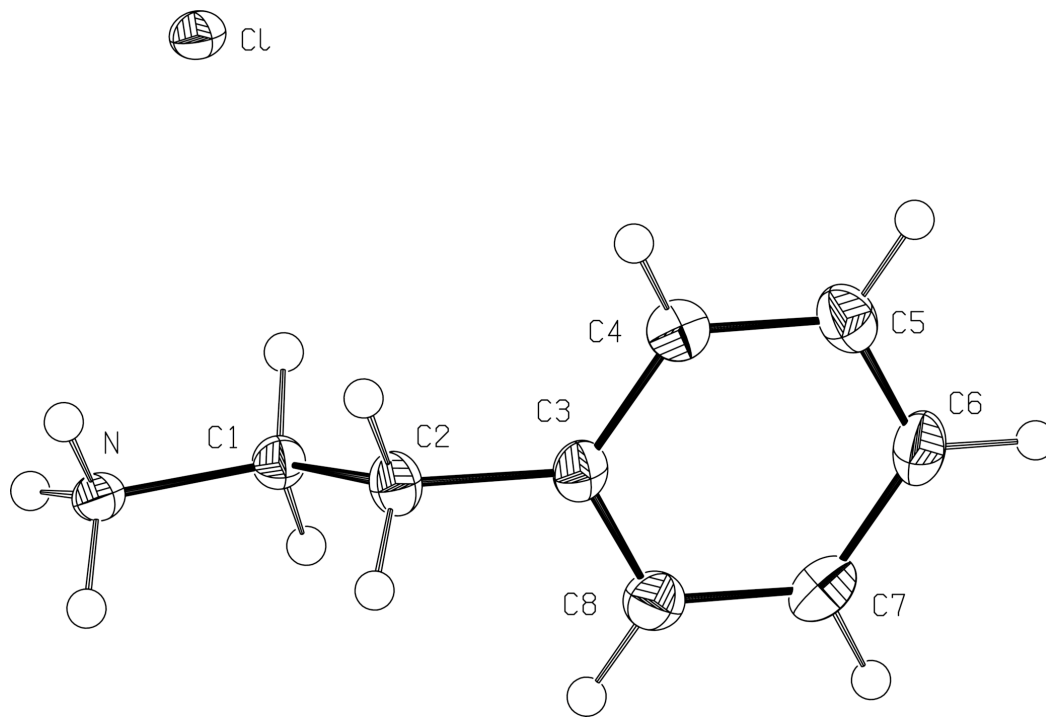


Fig. 2

