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# 2-Chloro-2-phenylethylammonium chloride

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**Key indicators**

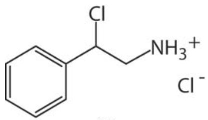
Single-crystal X-ray study
$T$ = 298 K
Mean $\sigma$(C–C) = 0.006 Å
$R$ factor = 0.039
$wR$ factor = 0.098
Data-to-parameter ratio = 16.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_8H_{11}ClN^+\cdot Cl^-$, has been obtained as an intermediate in the synthesis of 2-phenylaziridine. There are two molecules in the asymmetric unit and these are linked in the crystal structure by a network of intermolecular N—H···Cl and C—H···Cl hydrogen bonds, plus an intermolecular Cl···Cl interaction.

## Comment

A number of aziridines have been studied as substrates in ring-opening reactions under neutral conditions. In this respect, 2-phenylaziridine was of interest as it is an analogue of, and exhibits similar properties to, mexiletine (De Luca *et al.*, 2000, 2003). In this synthetic sequence, 2-chloro-2-phenylethylaminium chloride, (I), was produced as an intermediate.



(I)

The title compound crystallizes in the monoclinic centrosymmetric space group $P2_1/c$ with two molecules in the asymmetric unit (Fig. 1). The bond lengths are within the normal ranges (Allen *et al.*, 1987). There are short intermolecular hydrogen bonds (N—H···Cl and C—H···Cl) influencing the conformation of the two molecules (Taylor & Kennard, 1982). Table 1 lists selected hydrogen bonds shorter than the van der Waals distance (Bondi, 1964). There is also a short intermolecular Cl···Cl contact [Cl1···Cl4$(1 - x, \frac{1}{2} + y, \frac{3}{2} - z)$] of 3.488 (1) Å with a C12—Cl1···Cl4 angle of 176.5 (1)°.

## Experimental

The title compound was synthesized following the procedure of Galindo *et al.* (1997) and crystals suitable for X-ray analysis were obtained by dissolving the compound in ethanol, followed by addition of diethyl ether until the solution was cloudy.

*Crystal data*

| | |
|---|---|
| $C_8H_{11}ClN^+\cdot Cl^-$ | $D_x$ = 1.348 Mg m$^{-3}$ |
| $M_r$ = 192.08 | Mo $K\alpha$ radiation |
| Monoclinic, $P2_1/c$ | Cell parameters from 25 reflections |
| $a$ = 8.4813 (13) Å | $\theta$ = 12–17° |
| $b$ = 20.409 (5) Å | $\mu$ = 0.62 mm$^{-1}$ |
| $c$ = 10.939 (2) Å | $T$ = 298 (2) K |
| $\beta$ = 90.719 (13)° | Block, colourless |
| $V$ = 1893.3 (6) Å$^3$ | 0.40 × 0.20 × 0.20 mm |
| $Z$ = 8 | |

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*Data collection*

Enraf–Nonius CAD-4 diffractometer
$\omega$–$2\theta$ scans
Absorption correction: $\psi$ scan (*ABSCALC* in *OSCAIL*; McArdle & Daly, 1999; North *et al.*, 1968)
$T_{\min} = 0.789$, $T_{\max} = 0.886$
3600 measured reflections
3311 independent reflections
1320 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.031$
$\theta_{\max} = 25.0^\circ$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 24$
$l = -12 \rightarrow 12$
2 standard reflections
frequency: 120 min
intensity decay: 1%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.098$
$S = 0.87$
3311 reflections
201 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.27$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.24$ e Å$^{-3}$

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

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| N11—H11$A\cdots$Cl4$^{\rm i}$ | 0.89 | 2.24 | 3.105 (3) | 163 |
| N11—H11$B\cdots$Cl3$^{\rm ii}$ | 0.89 | 2.25 | 3.122 (3) | 168 |
| N11—H11$C\cdots$Cl3 | 0.89 | 2.46 | 3.251 (3) | 148 |
| N21—H21$A\cdots$Cl3$^{\rm i}$ | 0.89 | 2.42 | 3.173 (3) | 143 |
| N21—H21$A\cdots$Cl2$^{\rm iii}$ | 0.89 | 2.92 | 3.433 (3) | 119 |
| N21—H21$B\cdots$Cl4$^{\rm iv}$ | 0.89 | 2.22 | 3.111 (3) | 176 |
| N21—H21$C\cdots$Cl4 | 0.89 | 2.37 | 3.180 (3) | 151 |
| C21—H212$\cdots$Cl1$^{\rm i}$ | 0.97 | 2.74 | 3.560 (3) | 143 |
| C21—H212$\cdots$Cl3$^{\rm i}$ | 0.97 | 3.13 | 3.485 (3) | 104 |

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

All H atoms were positioned geometrically and refined using a riding model, fixing the aromatic C—H distances at 0.93 Å, the CH$_2$ C—H distances at 0.97 Å and the CH C—H distances at 0.98 Å, with $U_{\rm iso}$(H) = 1.3$U_{\rm eq}$(C). The NH$_3$ N—H distances were fixed at 0.89 Å, with $U_{\rm iso}$(H) = 1.4$U_{\rm eq}$(N), and the NH$_3$ groups were allowed to rotate but not to tip. The quality of the crystal was rather poor and accordingly data were only collected to $\theta_{\max} = 25.0^\circ$.

Data collection: *CAD-4-PC Software* (Enraf–Nonius, 1992); cell refinement: *CELDIM* in *CAD-4-PC Software*; data reduction: *XCAD4* (McArdle & Higgins, 1995); program(s) used to solve structure: *OSCAIL* (Version 9; McArdle, 2005) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1993); software used to prepare material for publication: *OSCAIL* (McArdle, 2005).

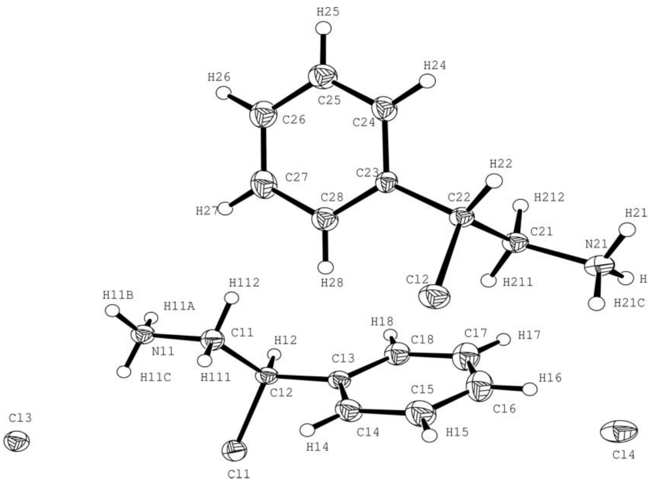

**Figure 1**
The asymmetric unit of the title compound (I) with the atomic numbering scheme. Displacement ellipsoids are drawn at the 20% probability level.

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