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# 3-[4-(3-Aminopropyl)piperazin-1-yl]propan-1-aminium chloride

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The title compound, $C_{10}H_{25}N_4^+\cdot Cl^-$, contains monoprotonated amine cations and chloride anions. The cations form chains along the [101] direction *via* N—H···N bonds, while N—H···Cl hydrogen bonds link the anions and cations into a three-dimensional structure.

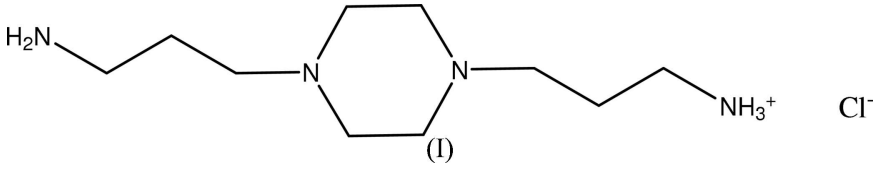
**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.002 Å
$R$ factor = 0.029
$wR$ factor = 0.033
Data-to-parameter ratio = 10.7

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

## Comment

In solvothermal synthesis, organic amines are generally used as structure-directing agents, and it is known that sometimes salts of the amines appear as unwanted side products. However, recent work on the solvothermal synthesis of phosphates (Rao *et al.*, 2000) and sulfates (Behera *et al.*, 2004) suggests that these amine salts might play a role in the formation of open-framework phases. It has also been found that the use of amine salts as sources of structure-directing agents may result in the formation of new open-framework structures.




(I)

In the title compound, $C_{10}H_{25}N_4^+\cdot Cl^-$, (I), which was the unexpected product of a solvothermal reaction, the amine 1,4-bis(3-aminopropyl)piperazine (bapp) crystallizes as a monoprotonated cation, $H^+$bapp, accompanied by a charge-balancing chloride anion (Fig. 1). As well as electrostatic forces, the anions and cations in (I) interact by means of hydrogen bonds (Table 1). The $H^+$bapp cations are connected by strong N—H···N hydrogen bonds, forming infinite chains that run along the [101] direction. The chains are cross-linked by N—H···Cl bonds arising from the terminal $-NH_2$ and $-NH_3^+$ groups to form layers parallel to the *ac* plane (Fig. 2). Further N—H···Cl hydrogen bonds link the layers into a three-dimensional structure (Fig. 3).

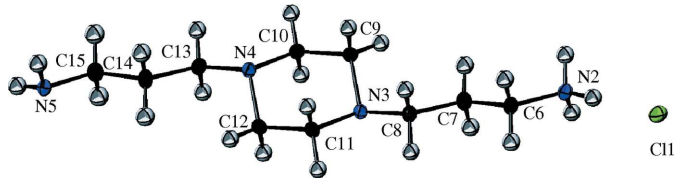



**Figure 1**
View of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for the H atoms).

## Experimental

A mixture of CuCl (2 mmol), Te (1 mmol) and 1,4-bis(3-aminopropyl)piperazine (4.2 ml) was loaded into a 23 ml Teflon-lined steel autoclave, heated for 13 days at 473 K and then cooled to room temperature over a period of 12 h. The product, consisting of hygroscopic colourless needles of (I) and a black powder, was filtered and washed with methanol and acetone.

### *Crystal data*

$C_{10}H_{25}N_4^+\cdot Cl^-$
$M_r$ = 236.79
Monoclinic, $P2_1/c$
$a$ = 10.9035 (9) Å
$b$ = 15.9679 (13) Å
$c$ = 7.8750 (6) Å
$\beta$ = 96.693 (4)°
$V$ = 1361.74 (19) Å$^3$
$Z$ = 4
$D_x$ = 1.155 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.26 mm$^{-1}$
$T$ = 293 K
Needle, colourless
0.50 × 0.10 × 0.10 mm

### *Data collection*

Bruker–Nonius APEX2 CCD area-detector diffractometer
$\omega/2\theta$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.811, $T_{max}$ = 0.974
18638 measured reflections
3967 independent reflections
2257 reflections with $I > 3.00\sigma(I)$
$R_{int}$ = 0.023
$\theta_{max}$ = 30.1°

### *Refinement*

Refinement on $F$
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.033
$S$ = 1.11
2257 reflections
211 parameters
Only H-atom coordinates refined
$W = [1 - (\delta F/6\sigma F)^2]^2/[0.491T_0(x) + 0.340T_1(x) + 0.263T_2(x)]$ where $T_i$ are Chebychev polynomials and $x = F/F_{max}$ (Watkin, 1994; Prince, 1982)
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H23···N5$^{i}$ | 0.93 (2) | 1.83 (2) | 2.7574 (18) | 175 (2) |
| N2—H21···Cl1$^{i}$ | 0.91 (2) | 2.27 (2) | 3.1761 (12) | 176 (2) |
| N2—H22···Cl1$^{ii}$ | 0.88 (2) | 2.30 (2) | 3.1853 (13) | 178 (1) |
| N5—H52···Cl1$^{iii}$ | 0.89 (2) | 2.58 (2) | 3.4104 (13) | 156 (2) |
| N5—H53···Cl1$^{iv}$ | 0.85 (2) | 2.61 (2) | 3.4344 (13) | 164 (2) |

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

H atoms were located in difference maps and their positions were freely refined; $U_{iso}$(H) = 1.2$U_{eq}$(carrier).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ATOMS* (Dowty, 2000); software used to prepare material for publication: *CRYSTALS*.

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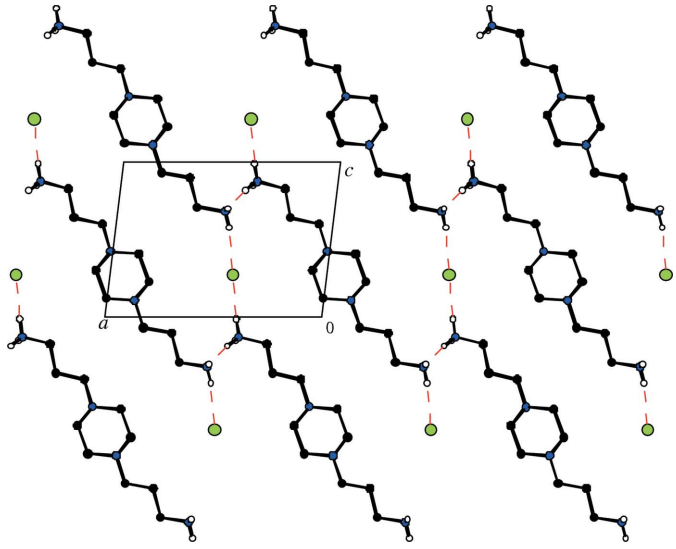


**Figure 2**
View of a layer parallel to the (010) plane, showing the network of hydrogen bonds (dashed lines). Hydrogen atoms not participating in hydrogen bonding have been omitted for clarity.

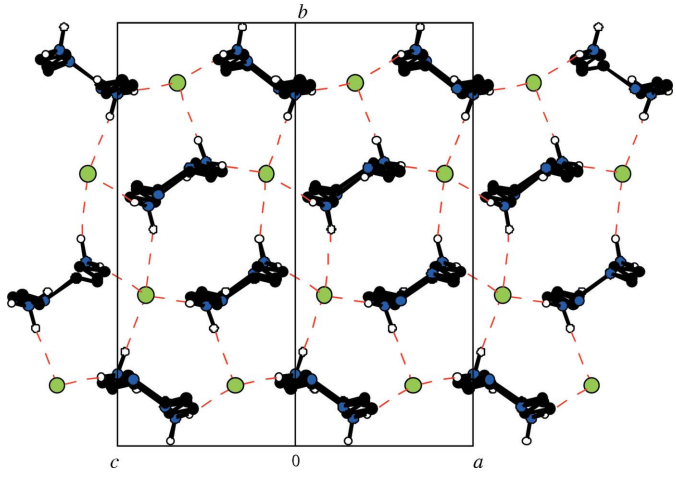


**Figure 3**
View of the packing in (I). Drawing conventions as in Fig. 2.

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