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Tetramethylguanidinium chloride

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In the title compound, $C_5H_{14}N_3^+\cdot Cl^-$, the central C atom displays almost ideal trigonal planar geometry. Classical hydrogen bonds of the form $N^+—H\cdots Cl^-$ link the formula units into discrete centrosymmetric dimers.

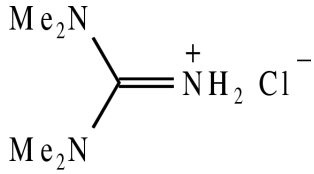
Key indicators

Single-crystal X-ray study
T = 143 K
Mean σ(N–C) = 0.002 Å
R factor = 0.025
wR factor = 0.064
Data-to-parameter ratio = 20.2

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

Comment

The title compound was formed as an unexpected hydrolysis product during a study of guanidinophosphine derivatives (Münchenberg, 1996). Its structure is nevertheless of interest because few salts of this cation have been structurally investigated (CCDC refcodes: BEQQOD, KOYWEA, MATKAT and XERHEH; Version Oct. 2002; Allen & Kennard, 1993), and because of its hydrogen-bonding pattern.



(I)

The formula unit displays no imposed crystallographic symmetry. The geometry at the central atom C1 is almost ideal trigonal planar; the r.m.s. deviation from the least-squares plane of C1, N1, N2 and N3 is 0.006 Å. The methyl groups are rotated out of this plane (torsion angles are in Table 1).

The classical hydrogen bonds of the form $N^+—H\cdots Cl^-$ (Table 2) link the formula units into discrete centrosymmetric dimers (Fig. 1). Further contacts of the form $C—H\cdots Cl^-$, the shortest of which (C4—H4*C*$\cdots$Cl) has a normalized (Steiner, 1998) H$\cdots$Cl distance of only 2.70 Å, may also be interpreted as hydrogen bonds.

Experimental

Crystal data

$C_5H_{14}N_3^+\cdot Cl^-$
M_r = 151.64
Monoclinic, $P2_1/n$
a = 6.979 (4) Å
b = 13.153 (7) Å
c = 9.283 (4) Å
β = 104.73 (4)°
V = 824.1 (7) Å^3
Z = 4
D_x = 1.222 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 50 reflections
θ = 10–11.5°
μ = 0.39 mm^{-1}
T = 143 (2) K
Block, colourless
0.7 × 0.6 × 0.6 mm

Data collection

Stoe Stadi-4 diffractometer
ω/θ scans
Absorption correction: none
3151 measured reflections
1900 independent reflections
1763 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.6°$
$h = -9 \rightarrow 9$
$k = -17 \rightarrow 0$
$l = -12 \rightarrow 6$
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.065$
$S = 1.08$
1900 reflections
94 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0265P)^2 + 0.1898P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.3304 (15)	N3—C1	1.3370 (14)
N2—C1	1.3417 (15)		
N1—C1—N3	120.91 (10)	N3—C1—N2	119.36 (10)
N1—C1—N2	119.70 (10)		
C4—N3—C1—N1	−23.93 (16)	C2—N2—C1—N1	−21.74 (16)
C5—N3—C1—N1	151.32 (11)	C3—N2—C1—N1	145.76 (11)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl	0.918 (17)	2.415 (17)	3.2863 (17)	158.4 (13)
N1—H1B···Cl^{i}	0.866 (17)	2.373 (17)	3.2268 (17)	168.9 (14)
C3—H3B···Cl^{ii}	0.98	2.89	3.773 (2)	150
C4—H4A···Cl^{iii}	0.98	3.00	3.776 (2)	137
C4—H4C···Cl	0.98	2.77	3.574 (2)	139
C5—H5A···Cl^{iv}	0.98	2.96	3.922 (2)	167
C5—H5B···Cl^{iii}	0.98	2.81	3.6492 (19)	144

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

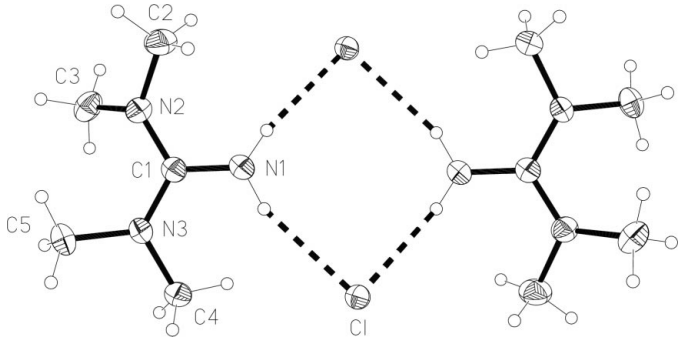


Figure 1
Dimeric unit of the title compound. Hydrogen bonds (Table 2) are indicated as thick dashed lines. Ellipsoids are at the 50% probability level.

H atom positions were obtained from difference syntheses. Methyl groups were refined as idealized rigid groups allowed to rotate about the C—N bonds. H atoms of the NH_2 group were refined freely.

Data collection: *DIF*4 (Stoe & Cie, 1992); cell refinement: *DIF*4; data reduction: *REDU*4 (Stoe & Cie, 1992); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL*97.

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