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(1*R*,2*R*)-1,2-Diammoniocyclohexane dichloride

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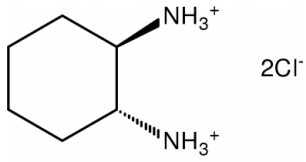
The dication and chloride ions of (1*R*,2*R*)-1,2-diammoniocyclohexane dichloride, $C_6H_{16}N_2^{2+}\cdot 2Cl^-$, (I), lie in general positions. The cyclohexane ring adopts the expected chair conformation, with equatorial ammonio substituents. The cation and chloride ions stack parallel to the *b* axis. All six ammonio H atoms are involved in hydrogen bonds to the chloride ions. The Cl···H contacts range from 2.225 (15) to 2.384 (15) Å.

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.001 Å
R factor = 0.017
wR factor = 0.047
Data-to-parameter ratio = 17.5

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



(I)

Experimental

The title compound was recrystallized from ethanol. It is the serendipitous hydrolysis product of a diimine ligand, for which it is also the precursor.

Crystal data

$C_6H_{16}N_2^{2+}\cdot 2Cl^-$
M_r = 187.11
Orthorhombic, $P2_12_12_1$
a = 8.1138 (2) Å
b = 9.5567 (2) Å
c = 11.9553 (3) Å
V = 927.03 (4) Å^3
Z = 4
D_x = 1.341 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 1549 reflections
θ = 1–30.0°
μ = 0.64 mm^{-1}
T = 150 (2) K
Prism, colourless
0.50 × 0.40 × 0.35 mm

Data collection

KappaCCD diffractometer
CCD rotation images, thick-slice scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.751, T_{max} = 0.800
10 435 measured reflections
2709 independent reflections
2662 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 30.0°
h = −11 → 11
k = −13 → 13
l = −16 → 16

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.047
S = 1.06
2709 reflections
155 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0240P)^2 + 0.1345P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Absolute structure: Flack (1983); 1131 Friedel pairs
Flack parameter = −0.07 (4)

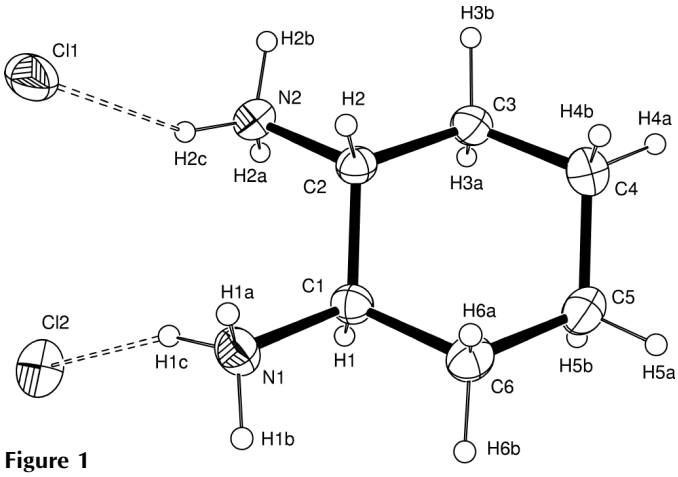


Figure 1
View of the asymmetric unit of (I) (70% probability displacement ellipsoids)

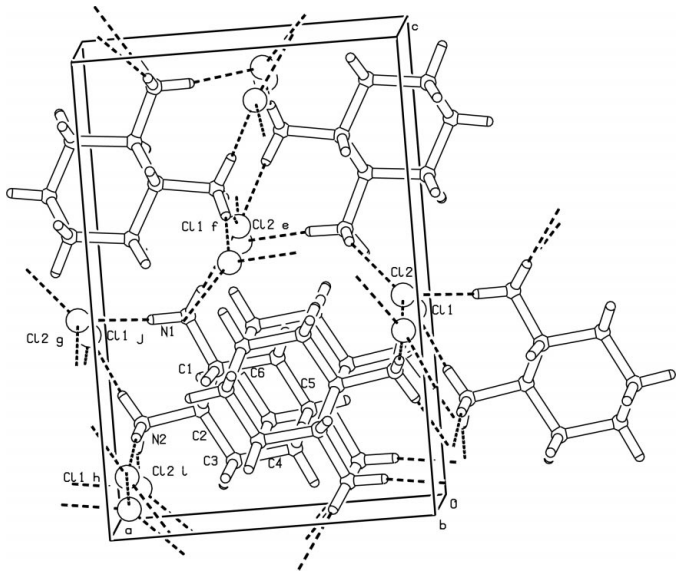


Figure 2
Unit-cell packing diagram of (I) viewed along the *b* axis.

Table 1
Selected geometric parameters (Å, °).

C1—N1	1.5012 (12)	C2—C3	1.5319 (13)
C1—C2	1.5254 (12)	C3—C4	1.5256 (14)
C1—C6	1.5296 (12)	C4—C5	1.5209 (14)
C2—N2	1.4990 (11)	C5—C6	1.5246 (14)
N1—C1—C2	111.63 (7)	C1—C2—C3	111.02 (7)
N1—C1—C6	108.31 (7)	C4—C3—C2	111.25 (8)
C2—C1—C6	111.12 (8)	C5—C4—C3	110.02 (8)
N2—C2—C1	111.73 (7)	C4—C5—C6	110.31 (8)
N2—C2—C3	108.55 (7)	C5—C6—C1	111.44 (8)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···Cl2^{i}	0.924 (15)	2.384 (15)	3.1871 (9)	145.2 (12)
N1—H1*B*···Cl1^{i}	0.922 (15)	2.225 (15)	3.1466 (9)	177.1 (13)
N1—H1*C*···Cl2	0.903 (15)	2.241 (15)	3.0918 (9)	156.9 (12)
N2—H2*A*···Cl1^{ii}	0.878 (16)	2.309 (16)	3.1853 (8)	175.1 (15)
N2—H2*B*···Cl2^{iii}	0.905 (14)	2.277 (14)	3.1303 (9)	157.1 (12)
N2—H2*C*···Cl1	0.883 (17)	2.319 (16)	3.1134 (8)	149.8 (13)

Symmetry codes: (i) $\frac{1}{2}+x, \frac{3}{2}-y, 2-z$; (ii) $1-x, y-\frac{1}{2}, \frac{3}{2}-z$; (iii) $1-x, \frac{1}{2}+y, \frac{3}{2}-z$.

Data collection: *COLLECT* (Nonius, 1997–2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and WinGX (Farrugia, 1999); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999).

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