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N,*N*′-Bis(3,4-methylenedioxybenzyl)propane-1,3-diammonium dichloride

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.042
wR factor = 0.099
Data-to-parameter ratio = 13.9

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

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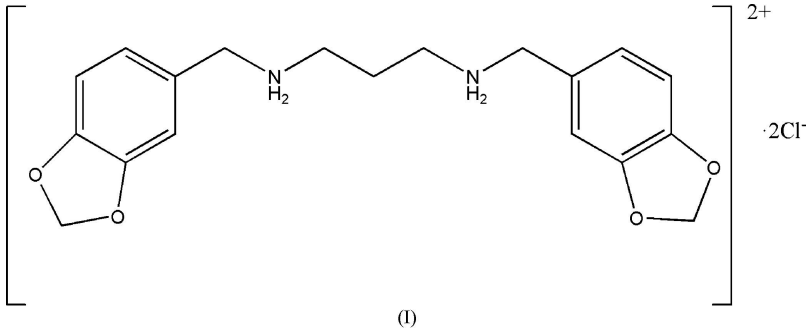
In the title compound, $C_{19}H_{24}N_2O_4^{2+}\cdot 2Cl^-$, the cation has mirror symmetry. The ions are linked by N—H···Cl and C—H···Cl hydrogen bonds into a $[01\bar{1}]$ chain with an $S_2^1(7)S_2^1(7)R_4^2(14)[R_4^2(24)]$ motif, and into a [011] chain with an $S_2^1(7)R_4^2(14)[R_4^2(18)]$ motif.

Comment

We intended to prepare a manganese(II) complex with *N*,*N*′-bis(3,4-methenedioxybenzyl)propane-1,3-diamine. However, we obtained crystals of the title compound, (I), and we report here its crystal structure and supramolecular arrangement (Fig. 1).



(I)

The cation of (I) has mirror symmetry, the mirror plane passing through C10 and its attached H atoms. In the supramolecular structure, there are two $S_2^1(7)$ rings formed by C—H···Cl and N—H···Cl hydrogen bonds (Fig. 1 and Table 1).

In the crystal structure of (I), the ions are linked by N—H···Cl and C—H···Cl hydrogen bonds, so generating a chain of $S_2^1(7)S_2^1(7)R_4^2(14)[R_4^2(24)]$ motif (Garciá-Báez *et al.*, 2002) along the $[01\bar{1}]$ direction (Fig. 2 and Table 1), and also a chain of $S_2^1(7)R_4^2(14)[R_4^2(18)]$ motif along the [011] direction (Fig. 3 and Table 1). The combination of the [011] and $[01\bar{1}]$ chains generates a [100] stack. Neighbouring stacks are connected by van der Waals forces, resulting in a three-dimensional network structure.

Experimental

To a solution containing *N*,*N*′-bis(3,4-methenedioxybenzyl)propane-1,3-diamine (3.42 g, 10 mmol) in ethanol (30 ml), a solution of manganese(II) chloride (1.24 g, 10 mmol) in ethanol (10 ml) was added with stirring for 2 h at room temperature (298–300 K), and then the brown solid obtained was filtered off, washed with 95% ethanol and dried at room temperature. Colourless crystals of (I) suitable for X-ray structure analysis were obtained by slow evaporation of a solution in dimethylformamide over a period of two months (m.p. 493–495 K).

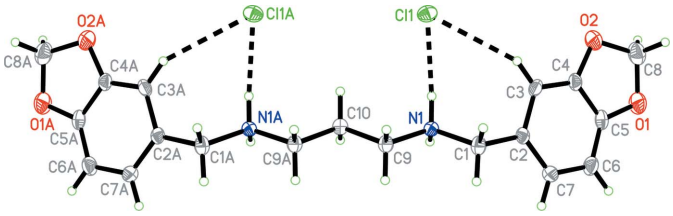


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. Dashed lines indicate hydrogen bonds. [Symmetry code: (A) $1-x, y, z$].

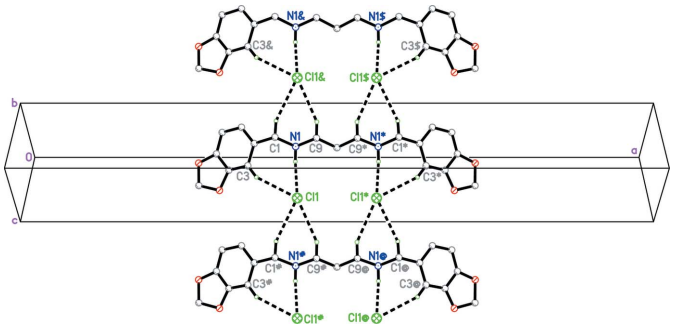


Figure 2
Part of the crystal structure of (I), showing the formation of an $[01\bar{1}]$ chain of $S_2^1(7)S_2^1(7)R_4^2(14)[R_4^2(24)]$ motif. For clarity, H atoms not involved in the motif shown have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry codes: (*) $1-x, y, z$; (#) $x, -1+y, 1+z$; (&) $x, 1+y, -1+z$; ($) $1-x, 1+y, -1+z$; (@) $1-x, -1+y, 1+z$.]

Crystal data

$C_{19}H_{24}N_2O_4^{2+}\cdot 2Cl^-$
M_r = 415.30
Orthorhombic, $Pmn2_1$
a = 38.366 (14) Å
b = 4.8370 (18) Å
c = 5.2980 (19) Å
V = 983.2 (6) Å^3
Z = 2
D_x = 1.403 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 298 (2) K
Column, colourless
0.52 × 0.47 × 0.13 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.836, T_{max} = 0.955
4685 measured reflections
1725 independent reflections
1461 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.099
S = 1.05
1725 reflections
124 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2 + 0.5461P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Absolute structure: Flack (1983), with 736 Freidel pairs
Flack parameter: 0.18 (12)

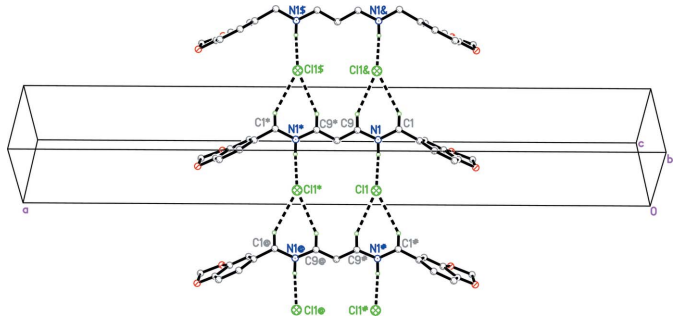


Figure 3
Part of the crystal structure of (I), showing the formation of an [011] chain of $S_2^1(7)R_4^2(14)[R_4^2(18)]$ motif. For clarity, H atoms not involved in the motif shown have been omitted. Dashed lines indicate hydrogen bonds. [Symmetry codes: (*) $1-x, y, z$; (#) $x, -1+y, -1+z$; (&) $x, 1+y, 1+z$; ($) $1-x, 1+y, 1+z$; (@) $1-x, -1+y, -1+z$].

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl1	0.90	2.25	3.134 (4)	169
C3—H3···Cl1	0.93	2.79	3.636 (3)	152
N1—H1B···Cl1^{i}	0.90	2.21	3.111 (4)	176
C1—H1D···Cl1^{ii}	0.97	2.91	3.742 (4)	145
C9—H9A···Cl1^{ii}	0.97	2.85	3.732 (4)	152
C1—H1C···Cl1^{iii}	0.97	2.87	3.790 (5)	158
C9—H9B···Cl1^{iii}	0.97	2.88	3.779 (5)	154

Symmetry codes: (i) $x, y, z-1$; (ii) $x, y+1, z$; (iii) $x, y+1, z-1$.

All H atoms were positioned geometrically and refined as riding on their parent atoms, with N—H = 0.90 Å and C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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