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N,*N*′-Bis(2-azaniumylbenzyl)ethane-1,2-diaminium tetrachloride

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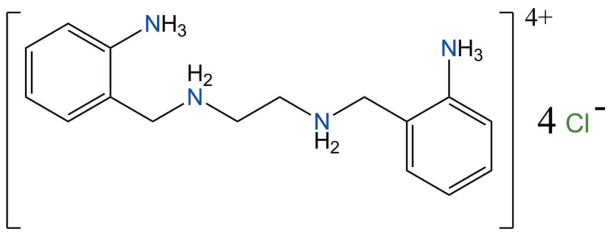
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.033; wR factor = 0.090; data-to-parameter ratio = 18.4.

The title compound, $C_{16}H_{26}N_4^{4+}\cdot 4Cl^-$, is based on a fully protonated tetraamine. In the cation, both benzene rings are connected by an all-*trans* chain, and the rings are almost parallel, with an angle between the mean planes of 8.34 (12)°. The benzene rings are arranged in such a way that the NH_3^+ substituents are oriented *cis* with respect to the central chain. This arrangement is a consequence of multiple N—H···Cl hydrogen bonds, involving all N—H groups in the cation and the four independent Cl^- anions. These contacts have strengths ranging from weak to strong (based on H···Cl separations), and generate a complex three-dimensional crystal structure with no preferential crystallographic orientation for the contacts.

Related literature

For the structure of the free tetraamine, see: Rodríguez de Barbarín *et al.* (2007). For related structures, see: Gakias *et al.* (2005); Garza Rodríguez *et al.* (2009, 2011). For the synthesis of the title hydrochloride, see: Ansell *et al.* (1983); Gruenwedel (1968).



Experimental

Crystal data

$C_{16}H_{26}N_4^{4+}\cdot 4Cl^-$
M_r = 416.21
Triclinic, $P\overline{1}$
a = 8.6827 (13) Å
b = 11.4831 (17) Å
c = 11.7317 (17) Å
α = 117.773 (10)°
β = 101.826 (14)°
γ = 94.387 (16)°
V = 992.8 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.60 mm^{-1}
T = 298 K
0.40 × 0.22 × 0.18 mm

Data collection

Siemens P4 diffractometer
Absorption correction: ψ scan (*XSCANS*; Siemens, 1996)
T_{min} = 0.552, T_{max} = 0.607
6618 measured reflections
4022 independent reflections
3185 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
2 standard reflections every 98 reflections
intensity decay: 1.5%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.090
S = 1.06
4022 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···Cl4	0.89	2.33	3.1067 (18)	146
N1—H1B···Cl1^{i}	0.89	2.30	3.1798 (18)	170
N1—H1C···Cl2^{ii}	0.89	2.26	3.1301 (18)	167
N9—H9A···Cl1	0.90	2.21	3.1046 (17)	172
N9—H9B···Cl2	0.90	2.22	3.0968 (17)	165
N12—H12A···Cl3	0.90	2.18	3.0333 (18)	159
N12—H12B···Cl2^{iii}	0.90	2.35	3.1779 (17)	153
N20—H20A···Cl1^{iv}	0.89	2.29	3.1764 (19)	173
N20—H20B···Cl3^{iv}	0.89	2.56	3.2305 (18)	133
N20—H20C···Cl3	0.89	2.23	3.1139 (18)	173

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

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL-Plus*; molecular graphics: *SHELXTL-Plus* and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXTL-Plus*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2472).

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