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N,*N*′-Bis(2-aminobenzyl)ethane-1,2-diaminium bis(4-methylbenzenesulfonate)

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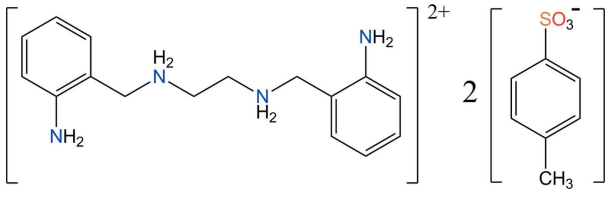
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.056; wR factor = 0.162; data-to-parameter ratio = 13.0.

The title salt, $C_{16}H_{24}N_4^{2+}\cdot 2C_7H_7O_3S^-$, crystallizes with the dication situated on an inversion center and the anion in a general position. The cation contains two ammonium and two free amine groups, and the observed conformation for the chain linking the benzene rings is different from that found in the free tetraamine and in the fully protonated tetraamine. All amine and ammonium H atoms of the cation form hydrogen bonds with eight symmetry-related anions, using the sulfonate O atoms as acceptors. This arrangement for the ions precludes any π–π contacts between benzene rings in the crystal.

Related literature

For reviews on applications of macrocyclic systems, see: Vigato & Tamburini (2004); Radecka-Paryzek *et al.* (2005). For their acid-catalysed synthesis using *p*-toluenesulfonic acid, see: Ionkin *et al.* (2008). For the structures of the free molecule and the fully protonated cation corresponding to the title cation, see: Rodríguez de Barbarín *et al.* (2007) and Garza Rodríguez *et al.* (2009, 2011), respectively.



Experimental

Crystal data

$C_{16}H_{24}N_4^{2+}\cdot 2C_7H_7O_3S^-$
M_r = 614.76
Triclinic, $P\overline{1}$
a = 5.753 (2) Å
b = 9.512 (3) Å
c = 14.493 (5) Å
α = 101.40 (2)°
β = 100.06 (3)°
γ = 97.80 (3)°
V = 753.6 (5) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 298 K
0.60 × 0.16 × 0.16 mm

Data collection

Siemens P4 diffractometer
Absorption correction: ψ scan (*XSCANS*; Siemens, 1996)
T_{min} = 0.512, T_{max} = 0.594
3505 measured reflections
2650 independent reflections
2234 reflections with $I > 2\sigma(I)$
R_{int} = 0.091
2 standard reflections every 98 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.162
S = 1.29
2650 reflections
204 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H11···O2^{i}	0.90 (1)	2.12 (1)	3.012 (3)	177 (3)
N1—H12···O3^{ii}	0.91 (1)	2.27 (3)	3.028 (4)	141 (3)
N8—H81···O3^{iii}	0.91 (1)	1.91 (2)	2.763 (3)	157 (3)
N8—H82···O1^{iv}	0.91 (1)	1.86 (1)	2.739 (3)	160 (3)

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

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: FJ2471).

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