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catena-Poly[[silver(I)-μ-tris(2-aminoethyl)amine-$\kappa^{4}N,N',N'':N'''$] perchlorate]

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The title compound, $\{[Ag(C_6H_{18}N_4)](ClO_4)\}_n$, is a polymeric silver(I) complex. The tris(2-aminoethyl)amine (tren) molecule acts as tridentate ligand. Each Ag^I ion is four-coordinated by three N atoms from one tren ligand and one N atom from a symmetry-related tren ligand. The symmetry-related tren ligand acts as a bridge linking the Ag^I atoms together, forming a polymeric chain. Adjacent chains are linked *via* N—H···O hydrogen bonds to anions, forming a three-dimensional network.

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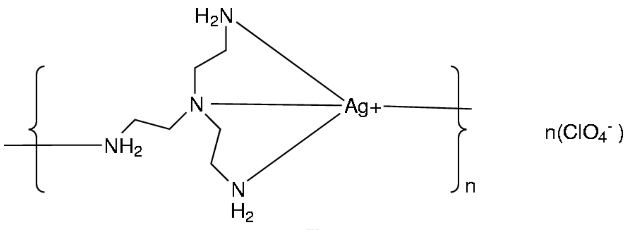
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.011 Å
Disorder in solvent or counterion
R factor = 0.036
wR factor = 0.092
Data-to-parameter ratio = 12.2

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

Comment

The synthesis and design of supramolecular coordination polymeric architectures has received considerable attention and is dominated by the selection of ligand structures and metal ion coordination characteristics (Hoskins & Robson, 1990; Munakata *et al.*, 2001; Ren *et al.*, 2001; Zheng & Chen, 2004). Of these ligands, tris(2-aminoethyl)amine (tren) represents an important family of organic molecules. Tren can interact with many transition metal ions to give rise to a wide variety of supramolecular coordination structures by virtue of the fact that it possesses four coordination sites, tripodal topology and rare μ_2-, μ_3- and μ_4-bridging abilities (Hagen *et al.*, 1988; Masters *et al.*, 1999; Plappert *et al.*, 1997; Sakai *et al.*, 1996). On the other hand, silver(I) also exhibits coordination diversity when coordinated by organic or inorganic ligands (Liu *et al.*, 2004; Yang *et al.*, 2000; Zhu *et al.*, 2003; Zhu, Qiu *et al.*, 2004). We found that different anions can affect the construction of silver(I) coordination polymers with tren; for example, the reaction of $AgNO_3$ with tren gives a two-dimensional polymer (Zhang *et al.*, 2001) and $AgPF_6$ with tren gives a one-dimensional polymer (Plappert *et al.*, 1997). As an extension of our work on the structural characterization of silver(I) complexes, the structure of the title compound, (I), a one-dimensional silver(I) coordination polymer, is reported here.



(I)

The complex consists of a polymeric cation and perchlorate anions. The tris(2-aminoethyl)amine (tren) molecule acts as a tridentate ligand. Each Ag^I ion is four-coordinated by three N

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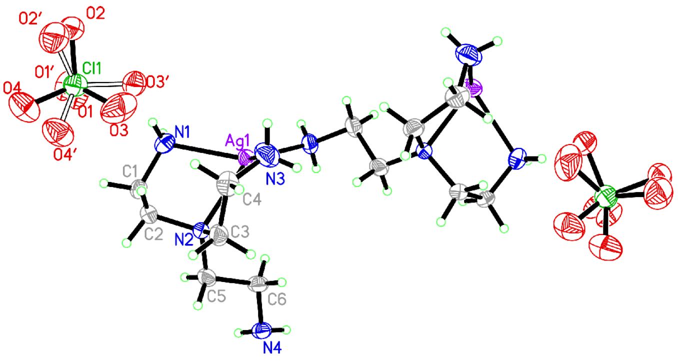

Figure 1
A view of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Both disorder components are shown.

atoms from one tren ligand and one N atom from a symmetry-related tren ligand. The symmetry-related tren ligand acts as a bridge linking the Ag^I atoms together, forming a polymeric chain (Fig. 1). The angles around atom Ag1 range from 74.5 (2) to 141.6 (2)° and thus indicate a severely distorted tetrahedral geometry. The Ag—N [2.255 (6), 2.378 (6), 2.384 (8) and 2.519 (6) Å] bond lengths in the title complex are slightly longer than those [2.201 (2), 2.233 (2) and 2.424 (2) Å] in a similar complex $[Ag(tren)]NO_3$ (Zhang *et al.*, 2001).

In the crystal structure of (I), $[Ag(tren)]^+$ propagates as a zigzag chain along the *a* axis. Adjacent chains interact with the anions *via* intramolecular N—H···O hydrogen bonds (Table 2), forming a three-dimensional network (Fig. 2).

Experimental

$AgClO_4$ (0.21 g, 1 mmol) and tren (0.292 g, 2 mmol) were dissolved in an aqueous ammonia solution (12 ml, 30%) and the mixture was stirred at room temperature for 30 min. The resulting clear colourless solution was allowed to stand in air and, after slow evaporation of the solvent over a period of 11 d, large colourless crystals of (I) were formed at the bottom of the vessel. The crystals were isolated, washed three times with water and dried in a vacuum desiccator using $CaCl_2$ (yield 42%). Analysis found: C 20.32, H 5.18, N 15.82, Cl 10.00%; calculated for $C_6H_{18}AgClN_4O_4$: C 20.38, H 5.13, N 15.85, Cl 10.03%.

Crystal data

$[Ag(C_6H_{18}N_4)](ClO_4)$
M_r = 353.56
Orthorhombic, $Pna2_1$
a = 10.352 (2) Å
b = 8.7608 (18) Å
c = 13.811 (3) Å
V = 1252.5 (4) Å^3
Z = 4
D_x = 1.875 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6726 reflections
θ = 4.5–25.0°
μ = 1.83 mm^{-1}
T = 293 (2) K
Prism, colourless
0.20 × 0.12 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.711, T_{max} = 0.883
6235 measured reflections
2213 independent reflections
1763 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 25.0°
h = −12 → 12
k = −10 → 7
l = −16 → 16

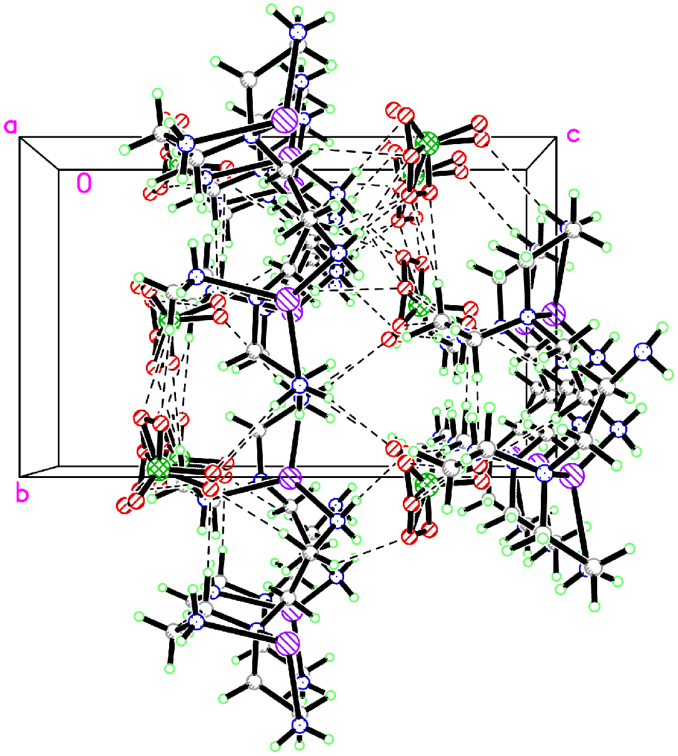

Figure 2
The crystal packing of (I), showing N—H···O hydrogen-bonding interactions as dashed lines.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.092
S = 0.95
2213 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0511P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}
Absolute structure: Flack (1983); 1052 Friedel pairs
Flack parameter = 0.02 (6)

Table 1
Selected geometric parameters (Å, °).

Ag1—N4^i	2.255 (6)	Ag1—N3	2.384 (8)
Ag1—N1	2.378 (6)	Ag1—N2	2.519 (6)
N4^i—Ag1—N1	128.7 (2)	N4^i—Ag1—N2	141.6 (2)
N4^i—Ag1—N3	112.8 (2)	N1—Ag1—N2	74.77 (18)
N1—Ag1—N3	111.8 (3)	N3—Ag1—N2	74.5 (2)

Symmetry code: (i) $\frac{1}{2}+x, \frac{5}{2}-y, z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4N2···O4′^{ii}	0.85	2.39	3.183 (16)	156
N4—H4N2···O3^{ii}	0.85	2.39	3.216 (16)	165
N4—H4N1···O2^{iii}	0.85	2.47	3.297 (15)	165
N3—H3N2···O4′^{iv}	0.85	2.43	3.278 (17)	173
N3—H3N2···O4^{iv}	0.85	2.36	3.111 (12)	148
N1—H1N2···O2′^{v}	0.85	2.20	2.937 (15)	145
N1—H1N1···O1	0.85	2.46	3.211 (13)	148

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

The O atoms of the perchlorate anion were found to be disordered over two positions each (O1/O1′, O2/O2′, O3/O3′ and O4/O4′) with site-occupancy factors of 0.596 (18) and 0.404 (18), respectively. The Cl—O distances were restrained to be equal, with an effective standard deviation of 0.01 Å. Similar restraints were also applied to the O···O distances. All H atoms were placed in geometrically idealized positions (C—H = 0.97 Å and N—H = 0.85 Å) and allowed to ride on their parent atoms with $U_{\rm iso}$(H) = 1.2 $U_{\rm eq}$(C,N).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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