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Polymeric (ethylenediamine)silver(I) 2,4,6-trinitrophenolate

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In the title compound, *catena*-poly[[silver(I)-μ-ethylenediamine] 2,4,6-trinitrophenolate], $\{[Ag(C_2H_8)](C_6H_2N_3O_7)\}_n$, the Ag atom is bicoordinated, in a linear configuration, by two different N atoms from two symmetry-related ethylenediamine ligands, resulting in a linear polymeric helical chain with an $[–Ag—N—C—C—N–]_n$ backbone. In the crystal structure, the components are connected by weak interactions between Ag and O atoms from the phenolate anion and the nitro groups. There are also weak hydrogen-bonding interactions between the NH_2 groups and some of the O atoms of the anions, forming a three-dimensional network.

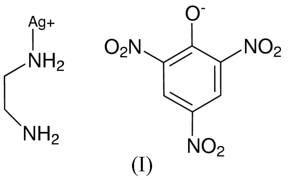
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.061
wR factor = 0.102
Data-to-parameter ratio = 13.0

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

Comment

The title complex, (I), is an analogue of the compound we reported on recently, *viz.* silver ethylenediamine 3-nitrobenzoate (Usman *et al.*, 2003).



(I)

In (I), atom Ag1 is bicoordinated, in a slightly distorted linear configuration, by two different N atoms [N1 and N2^{i}; symmetry code: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, z-\frac{1}{2}$] from two symmetry-related ethylenediamine ligands (Fig. 1). The Ag1—N1 and Ag1—N2^{i} bond lengths are 2.123 (5) and 2.126 (5) Å, respectively, which are slightly shorter than those observed in the silver ethylenediamine 3-nitrobenzoate analogue [2.140 (2) and 2.141 (2) Å]. The N1—Ag1—N2^{i} angle is 172.70 (18)°, which is less than that [177.1 (1)°] observed in the 3-nitrobenzoate analogue. This configuration gives rise to a

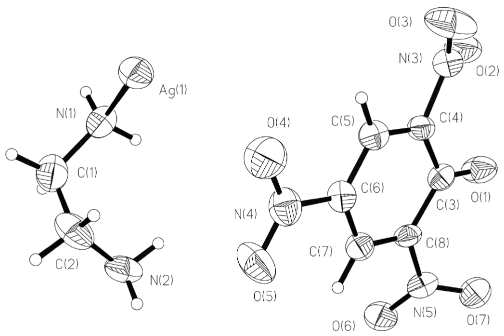


Figure 1
The asymmetric unit of the title compound, (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

linear polymeric chain in (I), with an [–Ag—N—C—C—N–]$_n$ backbone (Fig. 2).

The remainder of the bond lengths in (I) are within the normal ranges (Allen *et al.*, 1987). The C—O bond length of the phenolate is typical for a double bond, implying that the negative charge located on the phenolate O atom is delocalized. The N—O bond distances of the nitro groups of the trinitrophenolate anion are typical for double bonds.

In each repeat unit, the two components, *viz*. the ethylenediamine-coordinated silver cation and the 2,4,6-trinitrophenolate anion, are linked by weak Ag···O interactions [2.927 (6)–3.643 (6) Å]. Hydrogen bonds between the NH_2 H atoms and some of the O atoms of the anions result in the formation of a three-dimensional network (Fig. 2 and Table 1). The distance between the centroids of neighbouring, parallel, aromatic rings of the 2,4,6-trinitrophenolate anions is 3.504 (3) Å (symmetry code: $-x$, $2-y$, $2-z$). The π–π stacking of the benzene planes also contributes to the three-dimensional structure of the complex.

Experimental

Ethylenediamine and 2,4,6-trinitrophenol are available commercially and were used without further purification. Ag_2O (0.5 mmol, 116 mg) and 2,4,6-trinitrophenol (1 mmol, 229 mg) were dissolved in an aqueous solution of ammonia (10 ml). The mixture was stirred for ~10 min to obtain a clear solution. To this solution was added ethylenediamine (2 mmol, 120 mg) in an ammonia solution (2 ml). After keeping the resulting solution in air for one month, large brown single crystals were formed on slow evaporation. The crystals were isolated, washed with water three times and dried in a vacuum desiccator using $CaCl_2$ (yield 42%).

Crystal data

$[Ag(C_2H_8)](C_6H_2N_3O_7)$
M_r = 396.08
Monoclinic, $P2_1/n$
a = 7.844 (2) Å
b = 19.406 (4) Å
c = 8.376 (2) Å
β = 93.72 (3)°
V = 1272.3 (5) Å^3
Z = 4
D_x = 2.068 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5661 reflections
θ = 2.5–25.4°
μ = 1.63 mm^{-1}
T = 293 (2) K
Prism, brown
0.54 × 0.25 × 0.16 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.575, T_{max} = 0.787
5663 measured reflections
2492 independent reflections
2031 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 26.0°
$h = -9 \rightarrow 6$
$k = -20 \rightarrow 23$
$l = -10 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.102
S = 1.20
2492 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.009
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

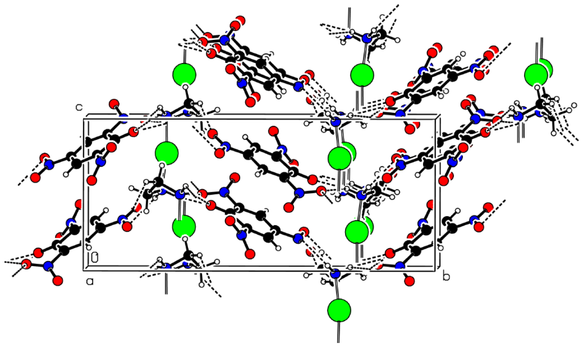


Figure 2
The crystal packing of (I), showing the hydrogen-bonding interactions as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1C···O1^{ii}	0.90	2.02	2.908 (6)	169
N1—H1C···O7^{ii}	0.90	2.53	2.976 (6)	111
N1—H1D···O5^{iii}	0.90	2.30	3.087 (6)	147
N2—H2C···O7^{iv}	0.90	2.45	3.121 (6)	131
N2—H2D···O1^{ii}	0.90	2.06	2.904 (6)	155

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

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with N—H and C—H distances of 0.90 and 0.96 Å, respectively, and U_{iso}(H) values of 0.08 Å^2.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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