Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Diamminesilver(I) picrate

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Received 4 October 2004
Accepted 8 October 2004
Online 16 October 2004

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.027
wR factor = 0.072
Data-to-parameter ratio = 9.4

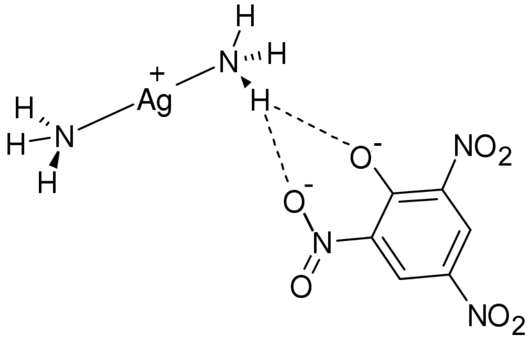
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $[Ag(NH_3)_2](C_6H_2N_3O_7)$, the Ag^I ion is bicoordinated in a linear configuration by two N atoms from two inversion-related ammine ligands. In the crystal structure, the picrate anions, with twofold rotation symmetry, are linked to the diamminesilver(I) cations through intermolecular N—H$\cdots$O hydrogen bonds, forming two-dimensional layers parallel to the *ac* plane.

Comment

The synthesis or construction of supramolecular coordination architecture is currently receiving considerable attention (Melcer *et al.*, 2001; Fei *et al.*, 2001; Xu *et al.*, 2001; Zhu *et al.*, 2004). The construction of a wide variety of network cation topologies has been achieved through ligand design and the use of different counter-anions. The balance between the formation of different structures is often subtle. Factors that affect the coordination polymer topology include not only the anion-based interactions but also the configurations of the ligands. The latter factor is particularly notable in Ag^I coordination polymers (You, Zhu *et al.*, 2004; You, Yang *et al.*, 2004). Owing to the flexible coordination sphere of Ag^I, coordination numbers from two to six are all possible, and because of the relatively weak nature of many Ag^I–ligand interactions such compounds are particularly susceptible to the influence of weaker supramolecular forces (Khlobystov *et al.*, 2001).

Recently, we have reported a polynuclear Ag^I complex with 1,2-diaminoethane as the ligand and picrate as the counter-anion, *viz.* *catena*-poly[(silver(I)-μ-ethylenediamine)-2,4,6-trinitrophenolate], (II) (Zhu *et al.*, 2003). In order to study the effects of the ligand in the construction of silver(I) coordination polymers, the structure of the title compound, (I), is reported here.



(I)

doi: 10.1107/S1600536804025425

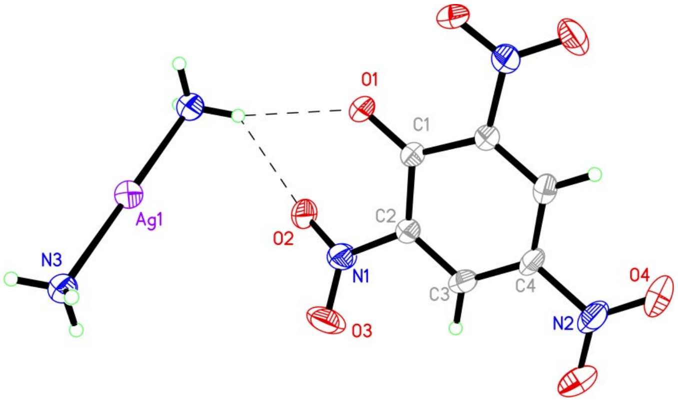


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Dashed lines indicate N—H···O hydrogen bonds.

Compound (I) has a discrete diammine–Ag^I complex cation with picrate as the counter-anion (Fig. 1). The asymmetric unit contains half each of a diamminesilver(I) cation and a picrate anion. The diamminesilver(I) cation lies on an inversion centre. The picrate anion has crystallographic twofold symmetry, with atoms O1, C1, C4 and N2 lying on the twofold axis. The Ag^I ion is in a perfectly linear coordination environment and is bicoordinated by two N atoms [N3 and $N3^i$; symmetry code: (i) $1 - x, 1 - y, 1 - z$] from two symmetry-related ammine ligands. Compound (II) is a polymeric ethylenediamine–Ag^I complex, with linear coordination geometry for the Ag^I ion. In (I), the Ag1—N3 bond length [2.113 (2) Å] is slightly shorter than the average value of 2.124 (5) Å observed in (II). All other bond lengths in (I) are within the normal ranges (Allen *et al.*, 1987).

In the crystal structure, cations and anions are linked together by intermolecular N—H···O hydrogen bonds (Table 1). The ammine ligand acts as a multiple hydrogen-bond donor, whereas the phenolate O atom and the O atoms of the 2,6-nitro groups of the picrate anion act as hydrogen-bond acceptors. The same pattern can be observed in complex (II). In (I), the N—H···O hydrogen bonds link the cations and anions into two-dimensional sheets parallel to the *ac* plane (Fig. 2), while in the crystal packing of (II), the N—H···O hydrogen bonding leads to a three-dimensional network. This may be caused by the different types of ligands present in the two compounds.

Experimental

Ag_2O (0.5 mmol, 116.1 mg) and picric acid (1.0 mmol, 229.2 mg) were dissolved in a 30% ammonia solution (20 ml). The mixture was stirred for 20 min to give a clear solution. After allowing the colourless solution to stand in air for 12 d, colourless block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent.

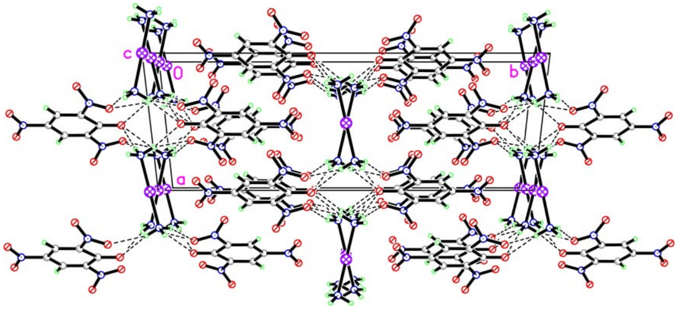


Figure 2
The crystal packing of (I), viewed along the *c* axis. Dashed lines indicate N—H···O hydrogen bonds.

Crystal data

$[Ag(NH_3)_2](C_6H_2N_3O_7)$
$M_r = 370.04$
Monoclinic, $C2/c$
$a = 10.046$ (5) Å
$b = 21.735$ (10) Å
$c = 7.189$ (3) Å
$\beta = 131.879$ (4)°
$V = 1168.7$ (9) Å^3
$Z = 4$
$D_x = 2.103$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2263 reflections
$\theta = 3.0$–26.4°
$\mu = 1.77$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.34 × 0.31 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.585$, $T_{max} = 0.753$
3050 measured reflections
1038 independent reflections
892 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 25.0°$
$h = -10 \rightarrow 11$
$k = -25 \rightarrow 19$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.072$
$S = 1.10$
1038 reflections
110 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 0.3947P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.88$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.058 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H1···$O1^i$	0.89	2.42	3.294 (3)	169
N3—H2···$O2^{ii}$	0.89	2.16	3.019 (8)	162
N3—H2···$O2'^{ii}$	0.89	2.18	3.061 (8)	173
N3—H3···$O1^{iii}$	0.89	2.28	3.149 (3)	165
N3—H3···$O2^{iii}$	0.89	2.46	3.087 (7)	128
N3—H3···$O2'^{iii}$	0.89	2.27	2.848 (7)	122

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

After location, all H atoms were placed in idealized positions and constrained to ride on their parent atoms, with N—H and C—H distances of 0.89 and 0.93 Å, respectively, and with U_{iso}(H) values fixed at 0.08 Å^2. One of the nitro groups is found to have rotational disorder; the occupancies of the disordered positions O2 and O2′ (or O3 and O3′) were initially refined to 0.490 (19) and 0.510 (19), respectively, and were later fixed at 0.5.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: ; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

The authors thank the Education Office of Anhui Province, the People's Republic of China, for research grant No. 2004kj300zd.

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