metal-organic papers

catena-Poly[[silver(I)-μ-1,4-bis(2-methyl-1H-imidazol-1-ylmethyl)benzene-$\kappa^2 N^3 : N^{3'}$] nitrate]

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In the title complex, $\{[Ag(C_{16}H_{18}N_4)]NO_3\}_n$, the cationic part forms infinite chains where the Ag^I ions are coordinated in a slightly bent fashion by two N-donor atoms of imidazole rings of two distinct ligand molecules. The nitrate anions interact weakly with the silver cations to form infinite strands running in the c-axis direction, approximately perpendicular to the cationic chains. The resulting layers are stabilized by offset π–π interactions between benzene rings. Furthermore, a set of C—H···O and π–π interactions (imidazole rings) between adjacent layers results in the formation of a three-dimensional assembly.

Comment

During the course of our ongoing studies of metal complexes with flexible ditopic ligands (Dobrzańska, 2005; Dobrzańska, Lloyd et al., 2005; Dobrzańska, Raubenheimer & Barbour, 2005; Dobrzańska et al., 2006; Dobrzańska & Lloyd, 2006), we have isolated the title compound, (I), which consists of infinite cationic chains (Fig. 1) and nitrate counter-ions.

(I)
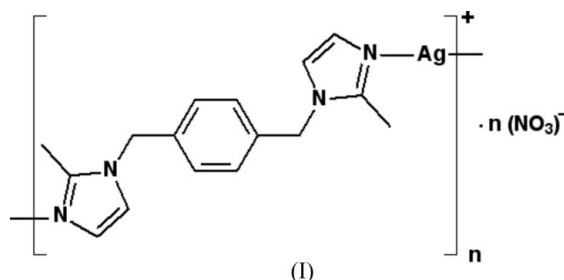
Bidendate 1,4-bis(2-methylimidazol-1-ylmethyl)benzene adopts the trans configuration with respect to the plane of the aromatic spacer and acts as a linkage between Ag^I ions [Ag···Ag separation of 14.847 (4) Å]. The deviation from linearity about the Ag ion is significant [N—Ag—N = 155.78 (17)°] and results from weak interactions of Ag ions with nitrate ions that function as bidentate (O1, O3) as well as bridging (O1, O3) units. In this manner, four Ag—O 'quasi' bonds are formed via three nitrate anions (two of which are
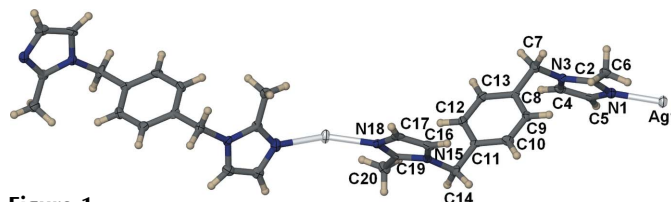
Figure 1
Fragment of an infinite cationic chain in the crystal structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 70% probability level.

generated by symmetry) and complete the overall environment about each Ag ion with the following Ag···O distances: bidentate Ag···O1 = 2.652 (4) Å and Ag···O3 = 3.042 (6) Å; bridging Ag1^i···O1—N21—O3···Ag1^{ii} = 2.991 (4) and 2.995 (5) Å [symmetry codes: (i) $x, \frac{1}{2} - y, \frac{1}{2} + z$; (ii) $x, \frac{1}{2} - y, z - \frac{1}{2}$].

The presence of interactions between Ag and nitrate ions leads to the formation of infinite strands {Ag···NO$_3$}$_n$ along the [001] direction, with an Ag···Ag distance of 4.785 (1) Å. Furthermore, π–π stacking between benzene rings (centroid–centroid distance = 3.847 Å) results in the formation of an undulating layer (Fig. 2) which is schematically presented in Fig. 3.

The final three-dimensional assembly is stabilized by C—H···O hydrogen bonds with C···O distances in the range 3.39–3.89 Å (Table 1) and offset π–π (imidazole rings) interactions (centroid–centroid distances 3.707 and 4.246 Å) between neighboring layers (Fig. 4).

Experimental

A methanol solution of AgNO$_3$ was added to a methanol solution of 1,4-bis(2-methylimidazol-1-ylmethyl)benzene in a 1:1 molar ratio. Colorless crystals suitable for single-crystal X-ray diffraction were obtained by slow evaporation.

Crystal data

[Ag(C$_{16}$H$_{18}$N$_4$)]NO$_3$	$Z = 4$
$M_r = 436.22$	$D_x = 1.790$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 14.885$ (4) Å	$\mu = 1.27$ mm^{-1}
$b = 14.459$ (4) Å	$T = 100$ (2) K
$c = 7.693$ (2) Å	Block, colorless
$\beta = 102.115$ (4)°	$0.12 \times 0.10 \times 0.09$ mm
$V = 1618.7$ (8) Å^3	

Data collection

Bruker APEX CCD area-detector diffractometer	9697 measured reflections
	3702 independent reflections
ω scans	2785 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)	$R_{int} = 0.056$
	$\theta_{max} = 28.3°$
$T_{min} = 0.862$, $T_{max} = 0.894$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.069$	$+ 3.538P]$
$wR(F^2) = 0.136$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{max} < 0.001$
3702 reflections	$\Delta\rho_{max} = 1.34$ e Å^{-3}
228 parameters	$\Delta\rho_{min} = -1.34$ e Å^{-3}
H-atom parameters constrained	

Table 1
C—H···O2 interactions stabilizing the overall three-dimensional assembly of (I) (Å, °).

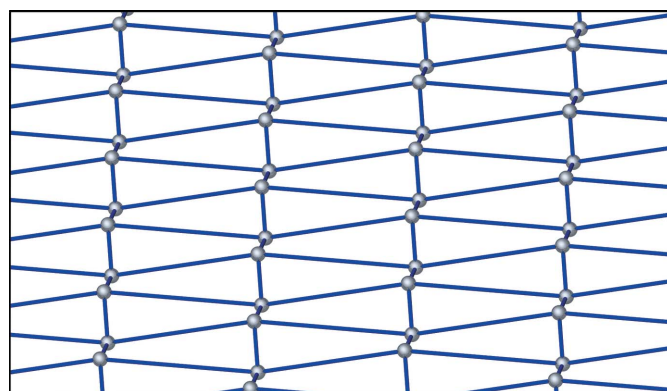| D—H···A	D—H	H···A	D···A	D—H···A
C10—H10···O2^i	0.95	2.64	3.387 (7)	136
C14—H14b···O2^i	0.99	3.17	3.886 (8)	130
C13—H13···O2^{ii}	0.95	2.66	3.404 (8)	135
C7—H7b···O2^{ii}	0.99	3.07	3.778 (8)	129

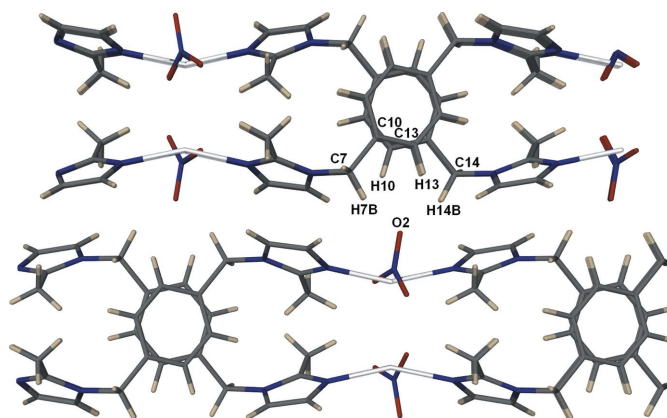Symmetry codes: (i) $-x, -y + 1, -z$; (ii) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$.
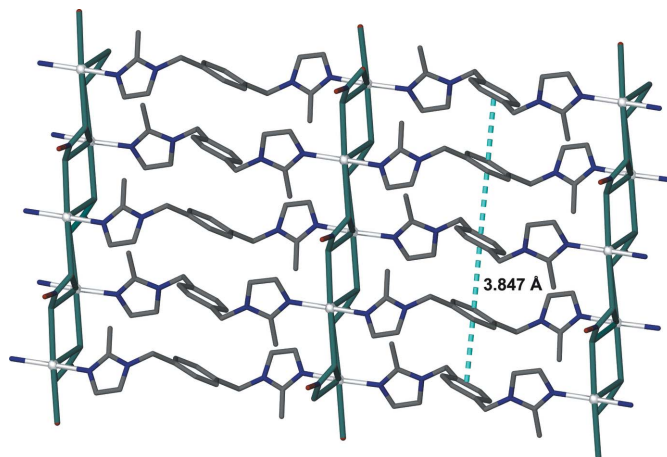
Figure 2
Capped-stick representation, showing layers formed by {Ag···NO$_3$}$_n$ interactions (green strands) and π–π stacking (blue dashed lines) in (I).

Figure 3
Schematic projection of the two-dimensional network.

Figure 4
A packing diagram of (I), viewed along [001], with labeled atoms participating in the stabilization of the overall three-dimensional assembly.

H atoms were positioned geometrically, with C—H = 0.95, 0.99 and 0.98 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where $x = 1.5$ for methyl H and $x = 1.2$ for all other H. The highest peak and deepest hole are located 0.93 and 0.99 Å, respectively, from atom Ag1.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve

structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001; Atwood & Barbour, 2003); software used to prepare material for publication: *X-SEED*.

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