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catena-Poly[[silver(I)-μ-2,5-bis(4-pyridyl)-1,3,4-oxadiazole] nitrate], a one-dimensional coordination polymer exhibiting a double-chain supramolecular structure through hydrogen bonds

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In the crystal structure of the title complex, $[Ag(C_{12}H_8N_4O)(NO_3)]_n$, each silver(I) center is coordinated by two N atoms of the pyridine rings of the bridging ligand 2,5-bis(4-pyridyl)-1,3,4-oxadiazole and one oxygen donor of the nitrate anion, giving a trigonal coordination geometry. The ligands bridge the silver(I) centers to form a one-dimensional linear structure, which is further linked into a double-chain motif through intermolecular C—H···O hydrogen bonds.

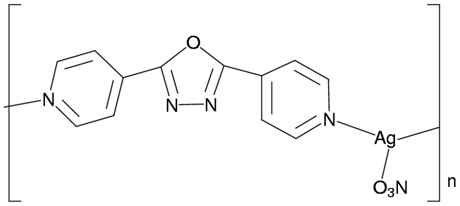
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.040
wR factor = 0.117
Data-to-parameter ratio = 11.6

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

Comment

Great efforts have been devoted to metal-directed coordination supramolecules due to their interesting structural topologies and potential applications as functional materials (Batten & Robson, 1998; Eddaoudi *et al.*, 2001). Using a 'building block' methodology, combination of linear 4,4′-bipyridine-based ligands and metal ions has generated a wide variety of solid-state architectures (Hagrman *et al.*, 1999). Recently, an interesting angular dipyridyl ligand, 2,5-bis(4-pyridyl)-1,3,4-oxadiazole, which could potentially provide both discrete and divergent topologies upon metal complexation under appropriate conditions (Du, Bu *et al.*, 2002; Du, Chen *et al.*, 2002; Du, Liu *et al.*, 2002), has been developed. Here, we report the crystal structure of a silver(I) complex of this ligand, which reveals that it is a neutral one-dimensional coordination polymer, (I).



(I)

As depicted in Fig. 1, the Ag^I center is coordinated by two N atoms of the pyridine rings from two bridging ligands, and one O atom of the nitrate anion. The coordination environment of each Ag^I ion can best be described as trigonal, with the Ag^I ion deviating from the mean coordination plane by *ca* 0.18 Å. The mean atomic displacement from the least-squares plane of the ligand (including all the atoms) is equal to 0.0733 (4) Å. The two pyridine rings in the same ligand molecule are inclined by 4.9 (3) and 4.7 (4)° with respect to the central oxadiazole plane, and by 8.5 (3)° with respect to one another.

As shown in Fig. 2, within this 1:1 ligand–metal polymeric chain, the neighboring Ag···Ag separation is 14.191 (5) Å, and the nearest Ag···Ag distance between the coordination chains is only 3.592 (2) Å. This is slightly longer than the van

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der Waals contact distance for Ag···Ag (3.40 Å), illustrating the lack of direct metal–metal interaction (Hartshorn & Steel, 1998). Of further interest is the fact that each nitrate anion in the chain acts as an acceptor of two intermolecular C—H···O hydrogen bonds (with the pyridine rings of the adjacent coordination chain), forming a unique double-chain supramolecular motif (Fig. 2). The C···O and H···O separations and the bond angles are listed in Table 2; these are in the normal range for weak hydrogen-bonding interactions.

Experimental

A CH_3CN solution of $AgNO_3$ (42.5 mg, 0.25 mmol) was carefully layered on to a $CHCl_3$ solution of the ligand 2,5-bis(4-pyridyl)-1,3,4-oxadiazole (56.0 mg, 0.25 mmol). Colorless block-shaped single crystals of (I), suitable for X-ray diffraction, were obtained after *ca* two weeks at room temperature (yield: 75%). Analysis calculated for the title complex: C 36.57, H 2.05, N 17.77%; found: C 36.48, H 2.06, N 17.82%. FT–IR data (KBr pellet, cm^{-1}): 3178 (*w*), 3096 (*m*), 3049 (*m*), 2934 (*w*), 2430 (*m*), 2332 (*m*), 1993 (*w*), 1971 (*w*), 1876 (*w*), 1747 (*m*), 1612 (*s*), 1564 (*s*), 1540 (*s*), 1485 (*s*), 1427 (*s*), 1402 (*s*), 1356 (*s*), 1336 (*s*), 1302 (*s*), 1215 (*s*), 1121 (*m*), 1097 (*m*), 1061 (*m*), 1039 (*m*), 1012 (*s*), 970 (*m*), 892 (*w*), 846 (*s*), 823 (*m*), 747 (*m*), 727 (*s*), 713 (*s*), 699 (*m*).

Crystal data

$[Ag(C_{12}H_8N_4O)(NO_3)]$
$M_r = 394.10$
Triclinic, $P\overline{1}$
$a = 8.3649$ (11) Å
$b = 8.9480$ (13) Å
$c = 9.8344$ (14) Å
$\alpha = 74.713$ (2)°
$\beta = 77.828$ (3)°
$\gamma = 69.389$ (3)°
$V = 658.90$ (16) Å^3
$Z = 2$
$D_x = 1.986$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2737 reflections
$\theta = 2.5$–25.0°
$\mu = 1.56$ mm^{-1}
$T = 298$ (2) K
Block, colorless
0.15 × 0.15 × 0.15 mm

Data collection

Bruker SMART 1000 diffractometer
ω scans
Absorption correction: multi-scan [*SAINT* (Bruker 1998) and *SADABS* (Sheldrick, 1996)]
$T_{min} = 0.491$, $T_{max} = 0.792$
2737 measured reflections
2303 independent reflections
2016 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 25.0°$
$h = -6 \rightarrow 9$
$k = -7 \rightarrow 10$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.117$
$S = 1.06$
2303 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.087P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.81$ e Å^{-3}
$\Delta\rho_{min} = -0.73$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.216 (3)	Ag1—O11	2.512 (5)
Ag1—N4^i	2.250 (3)		
N1—Ag1—N4^i	139.84 (13)	N4^i—Ag1—O11	87.79 (12)
N1—Ag1—O11	130.27 (12)		

Symmetry code: (i) $1 + x, y, 1 + z$.

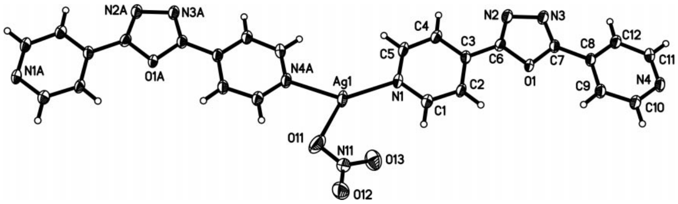

Figure 1
View of the coordination geometry around the Ag^I center in complex (I). Displacement ellipsoids are drawn at the 30% probability level.

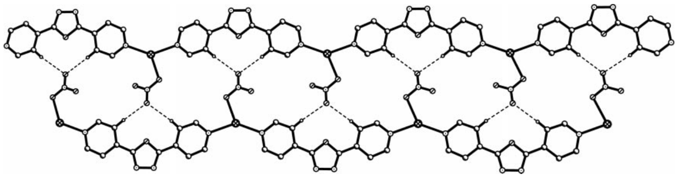

Figure 2
View of the double-chain structure in (I), involving Ag—N coordination interactions and C—H···O hydrogen bonds.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2*A*···O12^i	0.93	2.45	3.350 (4)	163
C9—H9*A*···O12^i	0.93	2.38	3.270 (3)	160

Symmetry code: (i) $2 - x, 2 - y, 1 - z$.

H atoms were placed in geometrically calculated positions and included in the final refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1998)

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