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catena-Poly[[silver(I)-μ-4,4′-bipyridine-κ^2N:N'] perchlorate]

Li-Shi Wang,[a] Jin-Feng Zhang[b] and Shi-Ping Yang[c]*

[a]School of Chemistry, South China University of Technology, Guangzhou 510641, People's Republic of China, [b]Children's Hospital of Shanghai, Shanghai 200040, People's Republic of China, and [c]School of Chemistry, Shanghai Teachers' University, Shanghai 200234, People's Republic of China

Correspondence e-mail: shipingy@shtu.edu.cn

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
Disorder in solvent or counterion
R factor = 0.045
wR factor = 0.133
Data-to-parameter ratio = 20.2

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

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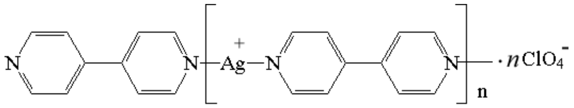
The crystal structure determination of the title complex, {[Ag($C_{10}H_8N_2$)]ClO_4}$_n$, reveals an approximately linear geometry for the Ag^I atom [N—Ag—N = 174.77 (14)°], coordinated by two N atoms from two 4,4′-bipyridine molecules, which form one-dimensional chains.

Comment

Inorganic–organic supramolecular architectures derived from building blocks that are linked by coordinate covalent bonds (Lehn, 1995) constitute an active research field that impinges on the synthesis of interesting topological structures and potential functional materials. So far, a number of one-, two- and three-dimensional coordination networks have already been generated with linear *N*,*N*′-bidentate spacers (Batten & Robson, 1998; Yaghi *et al.*, 1998; Munakata *et al.*, 1999; Hagrman *et al.*, 1999). However, the factors influencing the formation of coordination polymers are still not well understood, in spite of the fact that the self-assembly of these architectures has been documented to be highly influenced by various factors, such as the nature of the metal ions (Carlucci *et al.*, 1995), templates (Tong, Ye *et al.*, 1998) and experimental conditions (Tong, Chen *et al.*, 1998; Hennigar *et al.*, 1997; Yaghi & Li, 1995). Much work is required to extend the knowledge of the relevant structural types and establish proper synthetic strategies leading to the desired species. Recently, we have synthesized a series of imidazole-containing compounds, which are used in the synthesis of transition metal complexes as structural models of some metalloenzymes and in crystal engineering (Long *et al.*, 1999; Yang *et al.*, 2000, 2001). In the course of our ongoing studies of metal complexes, we have isolated the title compound, (I), and report here its preparation and crystal structure.



(I)

The Ag atom in (I) (Fig. 1) is coordinated, in a near-linear geometry, by two N atoms from two 4,4′-bipyridine molecules, the N—Ag—N angle being 174.77 (14)°. The Ag—N bond distances [2.145 (4) and 2.147 (4) Å] are consistent with those in related compounds (Tong *et al.*, 2000). The bond lengths and angles in the pyridine rings are normal and the dihedral angle between the N1- and N2-containing rings is 10.5 (2)°, indicating approximate coplanarity. The 4,4′-bipyridine molecules coordinate to two Ag atoms to form one-dimensional chains

(Fig. 2). The shortest Ag$\cdots$Ag distance between Ag atoms in adjacent chains is 3.598 (4) Å. This value is longer than the sum of the van der Waals radii of two Ag atoms (3.44 Å; Bondi, 1964), indicating that no metal–metal interactions occur in (I).

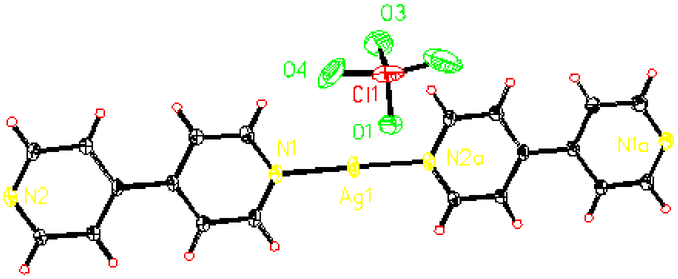


Figure 1
View of (I), with displacement ellipsoids drawn at the 35% probability level (small spheres for the H atoms). Only one component of the disordered perchlorate ion is shown. Atoms marked with the suffix ‘a’ are generated by the symmetry operation (x, $1 + y$, $z - 1$).

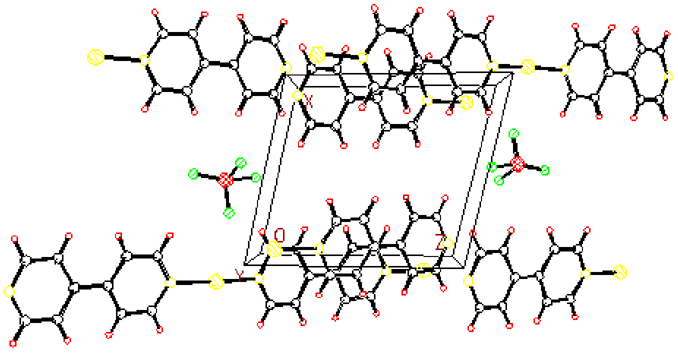


Figure 2
The molecular packing of (I), viewed down the b axis. Only one component of the disordered perchlorate ion is shown.

Experimental

An acetonitrile solution (10 ml) of 4,4′-bipyridine (1 mmol, 0.156 g) was added dropwise to a stirred MeCN/H_2O solution (1:1, 10 ml) of $Ag(ClO_4)$ (0.208 g, 1 mmol). After 3 d at room temperature, the solution precipitated colourless block-shaped crystals of (I) in 75% yield.

Crystal data

$[Ag(C_{10}H_8N_2)]ClO_4$
$M_r = 363.51$
Triclinic, $P\overline{1}$
$a = 8.181$ (8) Å
$b = 8.747$ (4) Å
$c = 8.921$ (7) Å
$\alpha = 80.35$ (1)°
$\beta = 74.64$ (1)°
$\gamma = 73.48$ (1)°
$V = 587.2$ (8) Å^3
$Z = 2$
$D_x = 2.056$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 2.0$–27.0°
$\mu = 1.95$ mm^{-1}
$T = 293$ (2) K
Block, colourless
0.21 × 0.15 × 0.10 mm

Data collection

Siemens *R*3*m* diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.725$, $T_{\max} = 0.836$
3411 measured reflections
3400 independent reflections
2770 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.014$
$\theta_{\max} = 30.0°$
$h = 0 \rightarrow 11$
$k = -11 \rightarrow 12$
$l = -12 \rightarrow 12$
2 standard reflections every 118 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.133$
$S = 1.07$
3400 reflections
168 parameters
H-atom parameters constrained
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 1.02$ e Å^{-3}
$\Delta\rho_{\min} = -1.07$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag—N2$^{\rm i}$	2.145 (3)	Ag—N1	2.147 (3)
N2$^{\rm i}$—Ag—N1	174.77 (14)		

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

All H atoms were positioned geometrically (C—H = 0.93 Å) and refined using the riding-model approximation, with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(carrier atom). The perchlorate anion is disordered over two adjacent positions (atoms Cl1/O1–O4 and Cl1′/O1′–O4′), with equal occupancies for the two components. The Cl—O and O$\cdots$O distances were restrained to be 1.37 (1) and 2.32 (2) Å, respectively. The highest peak and deepest hole in the difference Fourier map are located 0.44 and 0.53 Å, respectively, from atoms O4′ and O4.

Data collection: *R3m Software* (Siemens, 1990); cell refinement: *R3m Software*; data reduction: *SHELXTL-Plus* (Sheldrick, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1998); software used to prepare material for publication: *SHELXL*97.

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