# metal-organic papers

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#### **Key indicators**

Single-crystal X-ray study T = 291 K Mean  $\sigma$ (I–Ag) = 0.001 Å Disorder in main residue R factor = 0.041 wR factor = 0.117 Data-to-parameter ratio = 11.9

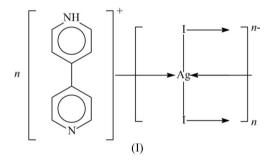
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e. catena-Poly[4,4'-bipyridinium(+) [argentate(I)di-μ-iodo]]

In the crystal structure of the title compound,  $\{(C_{10}H_9N_2)-[AgI_2]\}_n$ , both the cation and anion adopt chain motifs. A hydrogen bond links the positively charged pyridinium end of one cation to the neutral pyridyl end of an adjacent cation; the anions are bridged by two I atoms into a zigzag chain. The Ag atom in the chain exists in a nearly regular tetrahedral environment, on a special position of site symmetry 2.

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### Comment

Several di- $\mu_2$ -iodo-argentate chain motifs with ammonium cations as counter-ions have been reported, for example, the tetramethylammonium (Peters *et al.*, 1984), hexamethylethylenediammonium (Thackeray & Coetzer, 1975), anilinium (Alcock *et al.*, 2003) and ethane-1,2-dipyridinium (Li *et al.*, 2004) salts. The present 4,4'-bipyridinium(+) analog is the crystalline product of the reaction between silver iodide and 4,4'-bipyridine in an attempted synthesis of the 4,4'-bipyridine adduct of silver iodide. The reaction of silver iodide and pyridine, on the other hand, yields the 1:1 silver iodide–pyridine adduct, which has a tetranuclear composition (Engelhardt *et al.*, 1989).



The anionic chain of the title compound, (I), viz. catenapoly[argentate(I)-di- $\mu$ -iodo] adopts an iodine-bridged chain motif (Fig. 1), the polyanion propagating as a zigzag chain along the c axis of the monoclinic unit cell. The metal atom shows a nearly regular tetrahedral geometry, and the two independent Ag-I bonds are not statistically different from each other. The cation also adopts a linear chain motif, and one positively charged pyridinium end of the protonated cation interacts with the neutral pyridyl end of the adjacent cation  $[N \cdot \cdot \cdot N = 2.71 (1) \text{ Å}]$ . The two rings are twisted by 27.4 (4)° with respect to each other. The N-H...N hydrogenbonded cationic chain propagates in the [110] direction. Whereas the 4,4'-bipyridinium(2+) dication is relatively common, the 4,4'-bipyridinium(+) monocation is rarely found in its metal salts, and only a few examples of these crystal structures have been reported (Al-Rasoul & Weakley, 1982;

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Bukowska-Strzyzewska & Tosik, 1978; Chippindale & Turner, 1997; Hirose *et al.*, 2002; Krishnamohan Sharma & Rogers, 1999; Li *et al.*, 2001, 2004; Liang *et al.*, 2001; Rammo *et al.*, 1994; Su *et al.*, 1998; Weakley, 1984; Xu *et al.*, 2002).

## **Experimental**

Silver iodide (0.024 g, 0.1 mmol), potassium iodide (0.100 g, 0.6 mmol), 4,4'-bipyridine (0.016 g, 0.1 mmol) and triphenylphosphite (1 ml) were dissolved in a DMF/methanol mixture (10 ml) to give a clear solution. Red crystals separated from the solution in about a week.

#### Crystal data

$(C_{10}H_9N_2)[AgI_2]$	$D_x = 2.607 \text{ Mg m}^{-3}$		
$M_r = 518.86$	Mo $K\alpha$ radiation		
Monoclinic, $C2/c$	Cell parameters from 2830		
a = 13.6038 (9) Å	reflections		
b = 13.9457 (9)Å	$\theta = 2.9-29.2^{\circ}$		
c = 7.1524 (7) Å	$\mu = 6.17 \text{ mm}^{-1}$		
$\beta = 103.031 \ (1)^{\circ}$	T = 291 (2)  KBlock, red		
$V = 1322.0 (2) \text{ Å}^3$			
Z = 4	$0.38 \times 0.27 \times 0.16 \ \mathrm{mm}$		
Data collection			
Bruker APEX-II area-detector	1463 independent reflections		
diffractometer	1392 reflections with $I > 2\sigma(I)$		

 $R_{\rm int} = 0.026$ 

 $\theta_{\rm max} = 27.5^{\circ}$ 

 $l = -9 \rightarrow 9$ 

 $h = -17 \rightarrow 16$ 

 $k = -16 \rightarrow 17$ 

 $\varphi$  and  $\omega$  scans Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  $T_{min} = 0.128, T_{max} = 0.373$ 3879 measured reflections

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_0^2) + (0.066P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.041$	+ 8.4861P]
$wR(F^2) = 0.117$	where $P = (F_0^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{\rm max} = 0.001$
1463 reflections	$\Delta \rho_{\rm max} = 1.71 \ {\rm e} \ {\rm \AA}^{-3}$
123 parameters	$\Delta \rho_{\rm min} = -1.09 \ {\rm e} \ {\rm \AA}^{-3}$
H-atom parameters constrained	

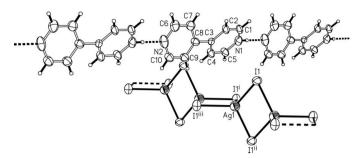
#### Table 1

Selected geometric parameters (Å, °).

Ag1–I1	2.8759 (6)	Ag1-I1 <sup>i</sup>	2.8882 (6)
$\substack{I1-Ag1-I1^i\\I1-Ag1-I1^{ii}}$	113.05 (2) 103.26 (1)	I1-Ag1-I1 <sup>iii</sup>	114.88 (3)

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

The 4,4'-bipyridinium(+) cation is disordered over an inversion center, and it was refined as two pyridyl rings that are linked by a 1.50 (1) Å C–C bond. In both rings, the N–C distances were restrained to 1.35 (1) Å and the C–C distances to 1.39 (1) Å. The rings were also restrained to be almost flat, the six atoms in each ring not being allowed to deviate from the plane by more than 0.01 Å. Carbon-bound H atoms were placed at calculated positions (C–H = 0.93 Å), and they were included in the refinement in the riding-model approximation, with  $U_{\rm iso}(H)$  values set at 1.2 times  $U_{\rm eq}(C)$ . The positive charge was arbitrarily placed on atom N1 (instead of atom N2); the N–H distance was fixed at 0.86 Å, and the displacement parameter was similarly tied to  $U_{\rm eq}(N)$ . The final difference Fourier map had a large peak and a large hole, both at about 1 Å from atom Ag1 but was otherwise featureless.



#### Figure 1

ORTEP plot (Johnson, 1976) of a portion of the polymeric structure of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii [symmetry codes: (i) x, 1 - y,  $\frac{1}{2} + z$ ; (ii) 1 - x, 1 - y, -z; (iii) 1 - x, y,  $\frac{1}{2} - z$ ]. The disorder is not shown.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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