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catena-Poly[1-ethyl-4-methylpyridinium [argentate(I)-di-μ-iodido]]

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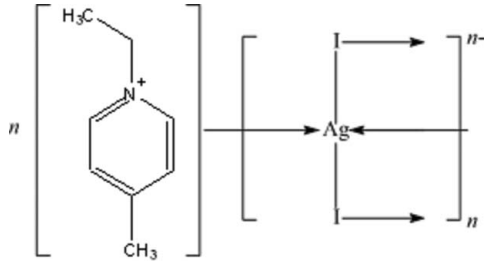
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.013 Å; R factor = 0.036; wR factor = 0.096; data-to-parameter ratio = 24.8.

The title compound, $\{(C_8H_{12}N)[AgI_2]\}_n$, was synthesized by a self-assembling reaction of 1-ethyl-4-methylpyridinium iodide and silver(I) iodide. The anion adopts a one-dimensional chain structure with the Ag atom in the chain in a nearly regular tetrahedral environment. The crystal packing is stabilized by electrostatic interactions and by a C—H···I hydrogen bond between a methylene H atom of the ethyl substituent and an I atom.

Related literature

For the crystal structure of four-coordinate $[Ag_2I_4]$ chain compounds, see: Thackeray & Coetzer (1975), Peters *et al.* (1984), Alcock *et al.* (2003), Li *et al.* (2004) and Niu *et al.* (2005). For related literature, see: Horn *et al.* (2003); Huang & Xie (1988).



Experimental

Crystal data

$(C_8H_{12}N)[AgI_2]$
M_r = 483.86
Tetragonal, $P4_2bc$
a = 18.205 (3) Å
c = 7.371 (2) Å
V = 2442.9 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 6.66 mm^{-1}
T = 293 (2) K
0.30 × 0.22 × 0.20 mm

Data collection

Rigaku Weissenberg IP diffractometer
Absorption correction: multi-scan (*TEXRAY*; Molecular Structure Corporation, 1999)
T_{min} = 0.140, T_{max} = 0.250 (expected range = 0.148–0.264)
21995 measured reflections
2749 independent reflections
2267 reflections with $I > 2\sigma(I)$
R_{int} = 0.053

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.096
S = 1.12
2749 reflections
111 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}
Absolute structure: Flack (1983), 1233 Friedel pairs
Flack parameter: 0.06 (6)

Table 1
Selected geometric parameters (Å, °).

Ag1—I1	2.842 (1)	Ag2—I2	2.873 (1)
Ag1—I1^{i}	2.849 (1)	Ag2—I2^{ii}	2.871 (1)
I1^{iii}—Ag1—I1^{i}	117.20 (2)	I2^{ii}—Ag2—I2^{v}	100.23 (5)
I1^{iii}—Ag1—I1	99.45 (6)	I2^{v}—Ag2—I2	114.31 (1)
I1—Ag1—I1^{i}	112.43 (2)	I2^{vi}—Ag2—I2	100.12 (5)
I1^{i}—Ag1—I1^{iv}	99.13 (6)		

Symmetry codes: (i) $y-\frac{1}{2}, x+\frac{1}{2}, z-\frac{1}{2}$; (ii) $-y+1, x+1, z+\frac{1}{2}$; (iii) $-x+1, -y+2, z$; (iv) $-y+\frac{3}{2}, -x+\frac{3}{2}, z-\frac{1}{2}$; (v) $y-1, -x+1, z+\frac{1}{2}$; (vi) $-x, -y+2, z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7B···I1	0.97	3.05	3.93 (1)	151

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2023).

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supplementary materials

Acta Cryst. (2007). E**63**, m2846-m2847 [**doi:10.1107/S1600536807052269**]

catena-Poly[1-ethyl-4-methylpyridinium [argentate(I)-di-μ-iodido]]

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Comment

In the title compound, each silver atom coordinated by four iodine atoms forms [AgI_4] tetrahedrons (Fig. 1). The [AgI_4] tetrahedron is highly distorted with Ag—I distances and I—Ag—I angles compared to an ideal tetrahedron (Table 1). This *trans* edge-sharing [AgI_4] tetrahedron results in two types of one-dimensional $[(AgI_2)^-]_n$ anion chains which are along the crystallographic *c* axis. The further stability comes from a weak C—H···I hydrogen bond (Horn *et al.*, 2003) between a methylene H of the cation part and I atom of anion part to give a 3-D network (Table 2 & Fig. 2).

Experimental

The title compound was synthesized by self-assembling reaction of silver iodide and *N*-ethyl-4-methylpyridinium iodide (Huang & Xie, 1988). *N*-Ethyl-4-methylpyridinium iodide (0.25 g, 1.0 mmol) and silver iodide (0.23 g, 1 mmol) were dissolved in DMF (15 ml). After being stirred at room temperature for 20 min. Finally, a kind of yellow clear solution was formed and filtered. Then the solution was allowed to evaporate at room temperature for one week. The title compound was obtained as a kind of yellow crystals [yield 0.15 g (31% based on Ag)]. Anal. Calcd. for $C_8H_{12}NAgI_2$ (483.86): C19.88, H 2.47, N 2.90%. Found: C,19.84, H 2.48, N 2.89%.

Refinement

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å for aromatic H atoms, 0.97 Å for methylene H atoms and 0.96 Å for methyl H atoms, respectively, and with U_{iso}(H) = 1.2Ueq(C) for aromatic and methylene H atoms, U_{iso}(H) = 1.5Ueq(C) for methyl H atoms. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Figures

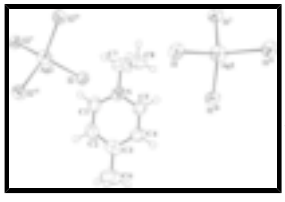

Fig. 1. The molecular structure of the title compound, showing displacement ellipsoides drawn at the 50% probability level. [Symmetry code: (i) 3/2 − *y*, 3/2 − *x*, *z* − 1/2 (ii) 1 − *x*, 2 − *y*, *z* (iii) *y* − 1/2, *x* + 1/2, *z* − 1/2 (iv) 1 − *y*, *x* + 1, *z* + 1/2 (v) −*x*, 2 − *y*, *z* (vi)*y* − 1, 1 − *x*, *z* + 1/2.]

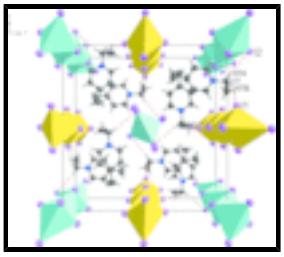

Fig. 2. The packing diagrame of title compound with C—H···I hydrogen bonds (dotted line).

catena-Poly[1-ethyl-4-methylpyridinium [argentate(I)-di-μ-iodido]]

Crystal data

$(C_8H_{12}N)[AgI_2]$	$Z = 8$
$M_r = 483.86$	$F_{000} = 1760$
Tetragonal, $P4_2bc$	$D_x = 2.631$ Mg m^{-3}
Hall symbol: P 4c -2ab	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 18.205$ (3) Å	Cell parameters from 25 reflections
$b = 18.205$ (3) Å	$\theta = 12$–18°
$c = 7.371$ (2) Å	$\mu = 6.66$ mm^{-1}
$\alpha = 90^\circ$	$T = 293$ (2) K
$\beta = 90^\circ$	Club, yellow
$\gamma = 90^\circ$	0.30 × 0.22 × 0.20 mm
$V = 2442.9$ (9) Å^3	

Data collection

Rigaku Weissenberg IP diffractometer	2749 independent reflections
Radiation source: rotor target	2267 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.053$
Detector resolution: None pixels mm^{-1}	$\theta_{max} = 27.5^\circ$
$T = 293(2)$ K	$\theta_{min} = 3.2^\circ$
scintillation counter scans	$h = -23 \rightarrow 23$
Absorption correction: multi-scan (TEXRAY; Molecular Structure Corporation, 1999)	$k = -23 \rightarrow 23$
$T_{min} = 0.140$, $T_{max} = 0.250$	$l = -9 \rightarrow 9$
21995 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.036$	$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 1.1814P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.096$	$(\Delta/\sigma)_{max} < 0.001$

S = 1.12	$\Delta\rho_{max}$ = 0.55 e Å^{-3}
2749 reflections	$\Delta\rho_{min}$ = −0.75 e Å^{-3}
111 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983)
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.06 (6)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
I1	0.38094 (3)	0.99613 (3)	1.14714 (10)	0.05327 (15)
I2	0.10725 (3)	0.94396 (3)	1.23364 (12)	0.05458 (15)
Ag1	0.5000	1.0000	0.8979 (2)	0.0671 (3)
Ag2	0.0000	1.0000	1.48388 (18)	0.0665 (3)
N	0.2267 (4)	0.8906 (4)	0.7893 (8)	0.0460 (15)
C1	0.1605 (4)	0.8590 (5)	0.7740 (11)	0.055 (2)
H1	0.1190	0.8872	0.7510	0.066*
C2	0.1552 (5)	0.7847 (5)	0.7928 (12)	0.058 (2)
H2	0.1092	0.7627	0.7835	0.069*
C3	0.2152 (5)	0.7414 (5)	0.8250 (11)	0.053 (2)
C4	0.2822 (5)	0.7770 (5)	0.8414 (12)	0.054 (2)
H4	0.3243	0.7499	0.8655	0.064*
C5	0.2870 (4)	0.8504 (5)	0.8227 (11)	0.0485 (18)
H5	0.3324	0.8735	0.8332	0.058*
C6	0.2094 (7)	0.6606 (6)	0.8389 (15)	0.080 (3)
H6A	0.1998	0.6471	0.9626	0.121*
H6B	0.2547	0.6386	0.8001	0.121*
H6C	0.1700	0.6436	0.7632	0.121*
C7	0.2338 (5)	0.9718 (5)	0.7626 (14)	0.062 (2)
H7A	0.1854	0.9936	0.7517	0.074*
H7B	0.2581	0.9935	0.8666	0.074*
C8	0.2772 (7)	0.9867 (5)	0.5952 (15)	0.078 (3)
H8A	0.2826	1.0388	0.5796	0.117*
H8B	0.2521	0.9664	0.4921	0.117*
H8C	0.3248	0.9645	0.6060	0.117*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1	0.0493 (2)	0.0602 (3)	0.0503 (3)	0.0061 (2)	−0.0008 (3)	−0.0007 (3)
I2	0.0519 (3)	0.0537 (3)	0.0581 (3)	0.0063 (2)	−0.0008 (3)	−0.0024 (3)
Ag1	0.0722 (8)	0.0698 (8)	0.0593 (5)	−0.0005 (5)	0.000	0.000
Ag2	0.0693 (7)	0.0660 (7)	0.0641 (6)	−0.0027 (8)	0.000	0.000
N	0.047 (3)	0.047 (3)	0.044 (4)	0.006 (3)	0.005 (3)	0.000 (3)
C1	0.042 (4)	0.066 (5)	0.058 (6)	0.005 (4)	0.009 (3)	−0.008 (4)
C2	0.044 (4)	0.066 (5)	0.063 (5)	−0.014 (4)	0.009 (4)	−0.008 (4)
C3	0.075 (6)	0.050 (4)	0.035 (3)	−0.013 (4)	−0.001 (4)	−0.001 (3)
C4	0.061 (5)	0.044 (4)	0.056 (5)	0.008 (4)	−0.013 (4)	0.001 (4)
C5	0.042 (4)	0.052 (4)	0.052 (4)	0.004 (3)	−0.007 (4)	−0.003 (4)
C6	0.116 (9)	0.056 (6)	0.070 (6)	−0.010 (6)	−0.029 (7)	0.008 (5)
C7	0.081 (6)	0.042 (4)	0.063 (5)	0.010 (4)	−0.002 (5)	−0.004 (4)
C8	0.109 (9)	0.049 (5)	0.076 (7)	−0.011 (5)	−0.001 (6)	0.009 (4)

Geometric parameters (Å, °)

Ag1—I1	2.842 (1)	C4—C5	1.35 (1)
Ag1—I1^{i}	2.849 (1)	C4—H4	0.9300
Ag2—I2	2.873 (1)	C5—H5	0.9300
Ag2—I2^{ii}	2.871 (1)	C6—H6A	0.9600
N—C1	1.34 (1)	C6—H6B	0.9600
N—C5	1.34 (1)	C6—H6C	0.9600
N—C7	1.50 (1)	C7—C8	1.490 (15)
C1—C2	1.36 (2)	C7—H7A	0.9700
C1—H1	0.9300	C7—H7B	0.9700
C2—C3	1.37 (1)	C8—H8A	0.9600
C2—H2	0.9300	C8—H8B	0.9600
C3—C4	1.39 (1)	C8—H8C	0.9600
C3—C6	1.48 (1)		
I1^{iii}—Ag1—I1^{i}	117.20 (2)	C3—C4—H4	119.6
I1^{iii}—Ag1—I1	99.45 (6)	N—C5—C4	120.5 (8)
I1—Ag1—I1^{i}	112.43 (2)	N—C5—H5	119.8
I1^{i}—Ag1—I1^{iv}	99.13 (6)	C4—C5—H5	119.8
I2^{ii}—Ag2—I2^{v}	100.23 (5)	C3—C6—H6A	109.5
I2^{v}—Ag2—I2	114.31 (1)	C3—C6—H6B	109.5
I2^{vi}—Ag2—I2	100.12 (5)	H6A—C6—H6B	109.5
Ag1—I1—Ag1^{vii}	80.71 (2)	C3—C6—H6C	109.5
Ag2^{viii}—I2—Ag2	79.83 (2)	H6A—C6—H6C	109.5
C1—N—C5	121.1 (7)	H6B—C6—H6C	109.5
C1—N—C7	119.4 (7)	C8—C7—N	109.5 (7)
C5—N—C7	119.5 (7)	C8—C7—H7A	109.8
N—C1—C2	118.8 (8)	N—C7—H7A	109.8

N—C1—H1	120.6	C8—C7—H7B	109.8
C2—C1—H1	120.6	N—C7—H7B	109.8
C1—C2—C3	122.2 (8)	H7A—C7—H7B	108.2
C1—C2—H2	118.9	C7—C8—H8A	109.5
C3—C2—H2	118.9	C7—C8—H8B	109.5
C2—C3—C4	116.6 (8)	H8A—C8—H8B	109.5
C2—C3—C6	122.0 (9)	C7—C8—H8C	109.5
C4—C3—C6	121.5 (9)	H8A—C8—H8C	109.5
C5—C4—C3	120.8 (8)	H8B—C8—H8C	109.5
C5—C4—H4	119.6		
$Ag1^{vii}$—I1—Ag1—$I1^{iii}$	0.0	C7—N—C1—C2	177.9 (8)
$Ag1^{vii}$—I1—Ag1—$I1^{i}$	124.75 (3)	C1—C2—C3—C6	−177.8 (9)
$Ag1^{vii}$—I1—Ag1—$I1^{iv}$	−121.36 (4)	C6—C3—C4—C5	177.9 (9)
$Ag2^{viii}$—I2—Ag2—$I2^{ii}$	−122.65 (3)	C7—N—C5—C4	−177.9 (8)
$Ag2^{viii}$—I2—Ag2—$I2^{v}$	122.65 (3)	C1—N—C7—C8	−113.0 (9)
$Ag2^{viii}$—I2—Ag2—$I2^{vi}$	0.0	C5—N—C7—C8	65.0 (11)

Symmetry codes: (i) *y*−1/2, *x*+1/2, *z*−1/2; (ii) −*y*+1, *x*+1, *z*+1/2; (iii) −*x*+1, −*y*+2, *z*; (iv) −*y*+3/2, −*x*+3/2, *z*−1/2; (v) *y*−1, −*x*+1, *z*+1/2; (vi) −*x*, −*y*+2, *z*; (vii) −*y*+3/2, −*x*+3/2, *z*+1/2; (viii) *y*−1, −*x*+1, *z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7B···I1	0.97	3.05	3.93 (1)	151

Fig. 1

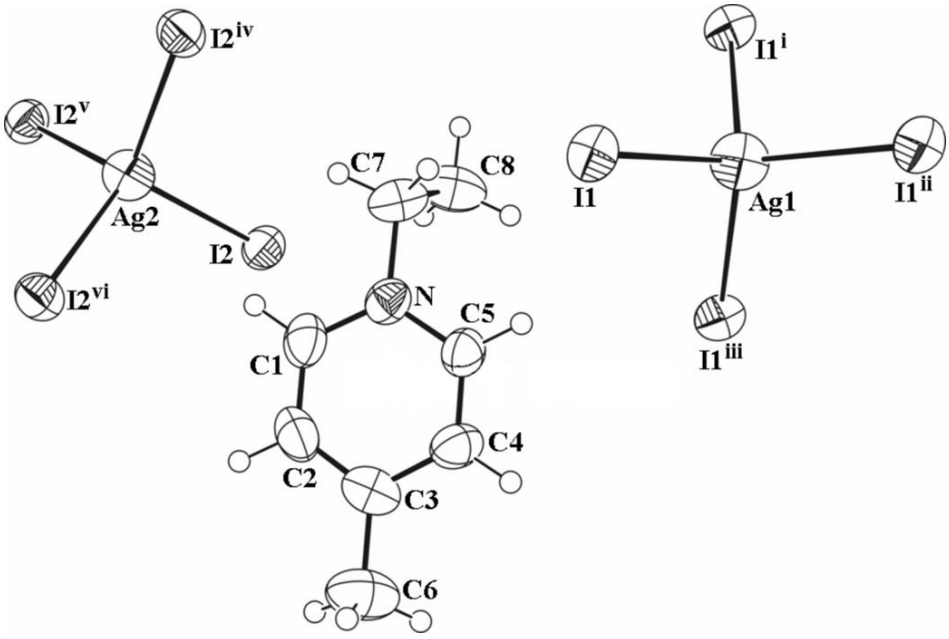
I2iv
I2v
Ag2
I2
I2vi
C7
C8
N
C5
C1
C4
C2
C3
C6
I1i
I1
Ag1
I1ii
I1iii

Fig. 2