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(*E*)-4-[4-(Dimethylamino)styryl]-1-isopropylpyridinium diiodidoargentate(I)

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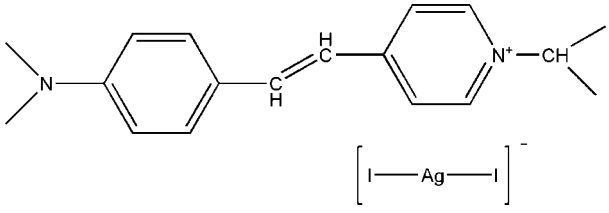
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.011 Å; R factor = 0.053; wR factor = 0.184; data-to-parameter ratio = 23.3.

The title compound, $(C_{18}H_{23}N_2)[AgI_2]$, contains linear anions. In the crystal structure, weak nonclassical C—H···I hydrogen bonds link adjacent cations and anions.

Related literature

For related structures, see: Ke *et al.* (2005); Kildea & White (1984); Li *et al.* (2004).



Experimental

Crystal data

$(C_{18}H_{23}N_2)[AgI_2]$
M_r = 629.05
Monoclinic, $P2_1/n$
a = 8.9356 (18) Å
b = 14.226 (3) Å
c = 16.988 (3) Å
β = 92.34 (3)°
V = 2157.7 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.80 mm^{-1}
T = 293 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID imaging-plate diffractometer
Absorption correction: ψ scan (*TEXRAY*; Molecular Structure Corporation, 1999)
T_{min} = 0.684, T_{max} = 0.691
20713 measured reflections
4947 independent reflections
2862 reflections with $I > 2\sigma(I)$
R_{int} = 0.054

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.184
S = 1.10
4947 reflections
212 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.24 e Å^{-3}
$\Delta\rho_{min}$ = −1.09 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—I2	2.8847 (11)	Ag1—I1	2.9200 (10)
I2—Ag1—I1	176.04 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···I1^{i}	0.93	3.05	3.879 (5)	150

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

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: SJ2367).

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supplementary materials

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(*E*)-4-[4-(Dimethylamino)styryl]-1-isopropylpyridinium diiodidoargentate(I)

Y.-F. Liu, M. Lin, C.-C. Huang and J.-Z. Chen

Comment

The synthesis of organic–inorganic complex materials has been extensively reported in recent years and shown to provide an efficacious method for the design of new materials. Owing to their potential applications as new functional solid materials, many complexes such as $[(C_{22}H_{50}N_2)(Ag_2I_4)]_n$ (Li *et al.*, 2004), $(C_8H_{20}N)(Ag_2I_3)_n$ (Ke *et al.*, 2005) and $(C_6H_{14}NO_2)(Ag_5Br_8)$ (Kildea & White, 1984) have been prepared. In the search for a new organic–inorganic materials, we present here the synthesis and the structure of the title compound (I), Fig 1.

The structure consists of an organic 4-(4-(dimethylamino)stryl-1-isopropylpyridinium cation and an inorganic $(AgI_2)^-$ anion. In the anion, each silver atom is bound to two iodine atoms in a nearly linear geometry with I_1—Ag_1—I_2 177.41 (3)°. The two Ag—I bond lengths are 2.9200 (10) Å and 2.8847 (11) Å, with an average of 2.9024 Å. These are slightly longer than the average of 2.8784 Å reported for $C_8H_{20}N)(Ag_2I_3)$ (Ke *et al.*, 2005).

In the crystal structure, Fig. 2, weak non-classical C_{11}—$H_{11}\cdots I_1^{i}$ hydrogen bonds (i = −1/2 + *x*, 1/2 − *y*, 1/2 + *z*) link adjacent cations and anions.

Experimental

4-(4-(dimethylamino)stryl-1-isopropylpyridinium iodide (0.195 g, 0.5 mmol) and AgI (0.117 g, 0.5 mmol) were dissolved in 8 ml DMF. The solution was stirred until clear, and the pH adjusted to 5.5 by the addition of 10% HI/DMF. The solution was filtered and kept at room temperature for five days to obtain brown block-like crystals.

Refinement

The H atoms were placed in idealized positions and treated as riding with d(C—H) = 0.93 Å, U_{iso}= 1.2U_{eq}(C) for aromatic 0.96 Å, U_{iso} = 1.5U_{eq}(C) for CH_3 atoms and 0.98 Å, U_{iso} = 1.2U_{eq}(C) for the CH atoms.

Figures

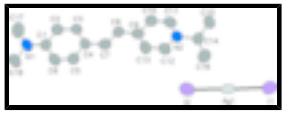

Fig. 1. The molecular structure of (I), with atom labels and 50% probability displacement ellipsoids for non-H atoms.

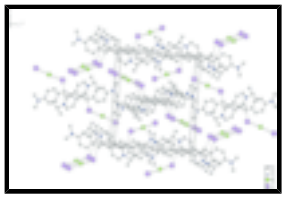

Fig. 2. Crystal packing for (I) with C—H···I hydrogen bonds drawn as dotted lines.

(*E*)-4-[4-(Dimethylamino)styryl]-1-isopropylpyridinium diiodidoargentate(I)

Crystal data

$(C_{18}H_{23}N_2)[AgI_2]$	F_{000} = 1192
M_r = 629.05	D_x = 1.936 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 12724 reflections
a = 8.9356 (18) Å	θ = 3.1–27.5º
b = 14.226 (3) Å	μ = 3.80 mm^{-1}
c = 16.988 (3) Å	T = 293 (2) K
β = 92.34 (3)º	Block, brown
V = 2157.7 (7) Å^3	0.10 × 0.10 × 0.10 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID imaging-plate diffractometer	4947 independent reflections
Radiation source: fine-focus sealed tube	2862 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.054
T = 293(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.1º
Absorption correction: ψ scan (TEXRAY; Molecular Structure Corporation, 1999)	h = −10→11
T_{min} = 0.684, T_{max} = 0.691	k = −16→18
20713 measured reflections	l = −22→22

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.053	H-atom parameters constrained
$wR(F^2)$ = 0.184	$w = 1/[\sigma^2(F_o^2) + (0.0839P)^2 + 1.7625P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{max} < 0.001$
4947 reflections	$\Delta\rho_{max}$ = 1.24 e Å^{-3}
212 parameters	$\Delta\rho_{min}$ = −1.09 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Ag1	0.43451 (6)	0.37865 (5)	0.21087 (3)	0.0675 (2)
I1	0.61642 (8)	0.21820 (5)	0.16627 (4)	0.0970 (3)
I2	0.27107 (8)	0.54058 (5)	0.26277 (4)	0.1020 (3)
N1	−0.6719 (8)	0.9749 (5)	0.5741 (4)	0.081 (2)
N2	−0.1385 (6)	0.3379 (4)	0.4027 (4)	0.0611 (14)
C1	−0.6132 (8)	0.8939 (5)	0.5480 (4)	0.0623 (17)
C2	−0.5300 (8)	0.8344 (5)	0.5997 (4)	0.0651 (18)
H2	−0.5143	0.8512	0.6523	0.078*
C3	−0.4716 (8)	0.7510 (5)	0.5724 (4)	0.0611 (17)
H3	−0.4190	0.7121	0.6078	0.073*
C4	−0.4885 (8)	0.7230 (5)	0.4946 (4)	0.0589 (16)
C5	−0.5726 (9)	0.7822 (5)	0.4451 (4)	0.0674 (19)
H5	−0.5887	0.7645	0.3927	0.081*
C6	−0.6321 (10)	0.8642 (5)	0.4692 (5)	0.074 (2)
H6	−0.6863	0.9014	0.4332	0.089*
C7	−0.4232 (8)	0.6400 (5)	0.4648 (5)	0.0655 (18)
H7	−0.4435	0.6283	0.4116	0.079*
C8	−0.3366 (8)	0.5761 (5)	0.5025 (4)	0.0606 (17)
H8	−0.3166	0.5851	0.5561	0.073*
C9	−0.2726 (8)	0.4955 (5)	0.4674 (4)	0.0608 (17)
C10	−0.1702 (9)	0.4393 (5)	0.5101 (4)	0.070 (2)
H10	−0.1454	0.4546	0.5622	0.084*
C11	−0.1058 (9)	0.3628 (6)	0.4774 (5)	0.074 (2)
H11	−0.0378	0.3271	0.5076	0.089*
C12	−0.2360 (9)	0.3897 (5)	0.3599 (5)	0.071 (2)
H12	−0.2571	0.3737	0.3076	0.085*
C13	−0.3063 (9)	0.4666 (5)	0.3917 (5)	0.072 (2)
H13	−0.3777	0.4993	0.3612	0.087*
C14	−0.0663 (9)	0.2531 (6)	0.3643 (5)	0.073 (2)
H14A	−0.1448	0.2190	0.3341	0.088*
C15	0.0047 (12)	0.1887 (7)	0.4188 (6)	0.097 (3)
H15A	0.0959	0.2159	0.4402	0.146*
H15B	0.0271	0.1313	0.3920	0.146*

H15C	−0.0612	0.1757	0.4607	0.146*
C16	0.0414 (12)	0.2936 (7)	0.3065 (6)	0.103 (3)
H16A	0.1294	0.3163	0.3347	0.155*
H16B	−0.0061	0.3446	0.2781	0.155*
H16C	0.0690	0.2456	0.2701	0.155*
C17	−0.6485 (13)	1.0061 (7)	0.6547 (6)	0.106 (3)
H17A	−0.6969	0.9634	0.6893	0.159*
H17B	−0.6900	1.0679	0.6603	0.159*
H17C	−0.5431	1.0078	0.6681	0.159*
C18	−0.7621 (11)	1.0351 (6)	0.5204 (6)	0.089 (3)
H18A	−0.7039	1.0526	0.4765	0.134*
H18B	−0.7917	1.0906	0.5479	0.134*
H18C	−0.8497	1.0014	0.5018	0.134*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0614 (3)	0.0983 (5)	0.0419 (3)	−0.0166 (3)	−0.0102 (2)	0.0125 (3)
I1	0.1135 (5)	0.1104 (5)	0.0666 (4)	−0.0017 (4)	−0.0036 (3)	−0.0106 (3)
I2	0.1068 (5)	0.1060 (5)	0.0929 (5)	0.0012 (4)	0.0002 (4)	0.0203 (4)
N1	0.102 (5)	0.067 (4)	0.070 (4)	0.026 (4)	−0.018 (4)	−0.005 (3)
N2	0.065 (3)	0.060 (3)	0.058 (4)	0.004 (3)	−0.004 (3)	0.002 (3)
C1	0.060 (4)	0.071 (4)	0.055 (4)	0.011 (4)	−0.003 (3)	−0.006 (3)
C2	0.071 (4)	0.075 (5)	0.048 (4)	0.009 (4)	−0.007 (3)	0.001 (3)
C3	0.065 (4)	0.068 (4)	0.050 (4)	0.013 (4)	0.002 (3)	0.010 (3)
C4	0.065 (4)	0.055 (4)	0.056 (4)	0.006 (3)	−0.002 (3)	0.000 (3)
C5	0.080 (5)	0.071 (5)	0.050 (4)	0.010 (4)	−0.007 (4)	−0.009 (3)
C6	0.090 (5)	0.068 (5)	0.063 (5)	0.022 (4)	−0.018 (4)	0.000 (4)
C7	0.072 (4)	0.068 (4)	0.056 (4)	−0.005 (4)	−0.002 (3)	−0.002 (4)
C8	0.072 (4)	0.062 (4)	0.049 (4)	−0.002 (4)	0.004 (3)	−0.001 (3)
C9	0.068 (4)	0.061 (4)	0.053 (4)	−0.006 (3)	0.001 (3)	0.007 (3)
C10	0.087 (5)	0.072 (5)	0.050 (4)	0.010 (4)	−0.009 (4)	−0.003 (3)
C11	0.086 (5)	0.080 (5)	0.055 (5)	0.012 (4)	−0.013 (4)	0.009 (4)
C12	0.079 (5)	0.072 (5)	0.060 (5)	0.013 (4)	−0.018 (4)	−0.001 (4)
C13	0.079 (5)	0.064 (5)	0.072 (5)	0.015 (4)	−0.015 (4)	−0.012 (4)
C14	0.079 (5)	0.076 (5)	0.064 (5)	0.019 (4)	0.009 (4)	−0.003 (4)
C15	0.115 (7)	0.078 (6)	0.101 (7)	0.036 (5)	0.027 (6)	0.018 (5)
C16	0.117 (8)	0.105 (7)	0.092 (7)	0.025 (6)	0.041 (6)	0.014 (6)
C17	0.135 (8)	0.091 (6)	0.090 (7)	0.031 (6)	−0.010 (6)	−0.028 (5)
C18	0.104 (6)	0.068 (5)	0.095 (7)	0.027 (5)	−0.003 (5)	0.009 (5)

Geometric parameters (Å, °)

Ag1—I2	2.8847 (11)	C9—C13	1.372 (10)
Ag1—I1	2.9200 (10)	C9—C10	1.396 (10)
N1—C1	1.349 (9)	C10—C11	1.360 (11)
N1—C17	1.447 (11)	C10—H10	0.9300
N1—C18	1.468 (10)	C11—H11	0.9300
N2—C12	1.333 (9)	C12—C13	1.382 (11)

N2—C11	1.339 (9)	C12—H12	0.9300
N2—C14	1.526 (10)	C13—H13	0.9300
C1—C6	1.407 (10)	C14—C15	1.433 (11)
C1—C2	1.410 (10)	C14—C16	1.516 (12)
C2—C3	1.384 (10)	C14—H14A	0.9800
C2—H2	0.9300	C15—H15A	0.9600
C3—C4	1.382 (10)	C15—H15B	0.9600
C3—H3	0.9300	C15—H15C	0.9600
C4—C5	1.388 (10)	C16—H16A	0.9600
C4—C7	1.420 (10)	C16—H16B	0.9600
C5—C6	1.352 (10)	C16—H16C	0.9600
C5—H5	0.9300	C17—H17A	0.9600
C6—H6	0.9300	C17—H17B	0.9600
C7—C8	1.339 (10)	C17—H17C	0.9600
C7—H7	0.9300	C18—H18A	0.9600
C8—C9	1.423 (11)	C18—H18B	0.9600
C8—H8	0.9300	C18—H18C	0.9600
I2—Ag1—I1	176.04 (3)	N2—C11—H11	119.4
C1—N1—C17	122.1 (7)	C10—C11—H11	119.4
C1—N1—C18	120.3 (7)	N2—C12—C13	121.5 (7)
C17—N1—C18	117.6 (7)	N2—C12—H12	119.2
C12—N2—C11	118.9 (7)	C13—C12—H12	119.2
C12—N2—C14	118.8 (6)	C9—C13—C12	121.1 (7)
C11—N2—C14	122.3 (6)	C9—C13—H13	119.4
N1—C1—C6	122.5 (7)	C12—C13—H13	119.4
N1—C1—C2	120.7 (7)	C15—C14—C16	112.7 (7)
C6—C1—C2	116.9 (7)	C15—C14—N2	114.4 (7)
C3—C2—C1	120.2 (7)	C16—C14—N2	105.5 (7)
C3—C2—H2	119.9	C15—C14—H14A	108.0
C1—C2—H2	119.9	C16—C14—H14A	108.0
C4—C3—C2	122.6 (6)	N2—C14—H14A	108.0
C4—C3—H3	118.7	C14—C15—H15A	109.5
C2—C3—H3	118.7	C14—C15—H15B	109.5
C3—C4—C5	116.1 (7)	H15A—C15—H15B	109.5
C3—C4—C7	123.3 (7)	C14—C15—H15C	109.5
C5—C4—C7	120.6 (7)	H15A—C15—H15C	109.5
C6—C5—C4	123.3 (7)	H15B—C15—H15C	109.5
C6—C5—H5	118.3	C14—C16—H16A	109.5
C4—C5—H5	118.3	C14—C16—H16B	109.5
C5—C6—C1	120.9 (7)	H16A—C16—H16B	109.5
C5—C6—H6	119.5	C14—C16—H16C	109.5
C1—C6—H6	119.5	H16A—C16—H16C	109.5
C8—C7—C4	129.2 (7)	H16B—C16—H16C	109.5
C8—C7—H7	115.4	N1—C17—H17A	109.5
C4—C7—H7	115.4	N1—C17—H17B	109.5
C7—C8—C9	125.5 (7)	H17A—C17—H17B	109.5
C7—C8—H8	117.2	N1—C17—H17C	109.5
C9—C8—H8	117.2	H17A—C17—H17C	109.5
C13—C9—C10	115.5 (7)	H17B—C17—H17C	109.5

C13—C9—C8	123.9 (7)	N1—C18—H18A	109.5
C10—C9—C8	120.6 (7)	N1—C18—H18B	109.5
C11—C10—C9	121.7 (7)	H18A—C18—H18B	109.5
C11—C10—H10	119.2	N1—C18—H18C	109.5
C9—C10—H10	119.2	H18A—C18—H18C	109.5
N2—C11—C10	121.3 (7)	H18B—C18—H18C	109.5
C17—N1—C1—C6	−178.3 (9)	C7—C8—C9—C13	−8.2 (12)
C18—N1—C1—C6	1.3 (13)	C7—C8—C9—C10	172.6 (7)
C17—N1—C1—C2	2.2 (13)	C13—C9—C10—C11	1.8 (12)
C18—N1—C1—C2	−178.2 (8)	C8—C9—C10—C11	−179.0 (7)
N1—C1—C2—C3	179.3 (7)	C12—N2—C11—C10	0.1 (12)
C6—C1—C2—C3	−0.2 (12)	C14—N2—C11—C10	179.2 (7)
C1—C2—C3—C4	1.4 (12)	C9—C10—C11—N2	−0.2 (13)
C2—C3—C4—C5	−2.2 (11)	C11—N2—C12—C13	−1.7 (12)
C2—C3—C4—C7	176.8 (7)	C14—N2—C12—C13	179.2 (7)
C3—C4—C5—C6	1.9 (12)	C10—C9—C13—C12	−3.3 (12)
C7—C4—C5—C6	−177.1 (8)	C8—C9—C13—C12	177.5 (8)
C4—C5—C6—C1	−0.9 (14)	N2—C12—C13—C9	3.4 (13)
N1—C1—C6—C5	−179.6 (8)	C12—N2—C14—C15	−164.5 (8)
C2—C1—C6—C5	0.0 (12)	C11—N2—C14—C15	16.4 (11)
C3—C4—C7—C8	−0.7 (13)	C12—N2—C14—C16	71.1 (10)
C5—C4—C7—C8	178.3 (8)	C11—N2—C14—C16	−108.0 (9)
C4—C7—C8—C9	−178.4 (7)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···I1^{i}	0.93	3.05	3.879 (5)	150

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*+1/2.

Fig. 1

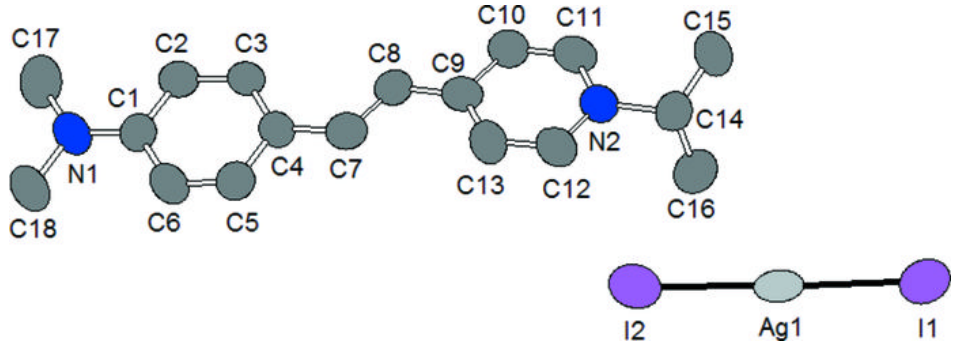
C17
C2
C3
C10
C11
C15
C8
C9
C1
C14
N1
N2
C4
C7
C13
C12
C18
C6
C5
C16
I2
Ag1
I1

Fig. 2