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Key indicators

Single-crystal X-ray study
T = 180 K
 Mean $\sigma(\text{C}-\text{C}) = 0.009 \text{ \AA}$
R factor = 0.029
wR factor = 0.070
 Data-to-parameter ratio = 23.7

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

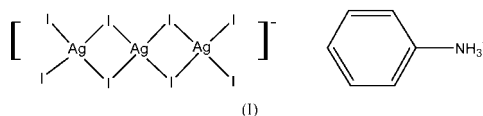
A silver–iodine chain complex: catena-poly[anilinium [silver(I)-di- μ -iodo]], $\{[\text{PhNH}_3][\text{AgI}_2]\}_n$

The title compound, $\{(\text{C}_6\text{H}_8\text{N})[\text{AgI}_2]\}_n$, is the anilinium salt of an iodo–silver complex anion containing infinite $[\text{AgI}_2]_n^{n-}$ chains.

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Comment

The title compound is the anilinium salt of an iodo–silver complex anion of the type reviewed by Jagner & Helgesson (1991). It contains AgI_4 tetrahedra sharing edges, giving infinite chains of formula $[\text{AgI}_2]_n^{n-}$. These run parallel to the *a* axis with the anilinium cations between them (aligned perpendicular to the *a* axis) (Figs. 1 and 2). The Ag–I distances found here are towards the longer end of the known range (2.76–2.90 Å). The degree of polymerization of these anions has been shown to depend on the bulk of the cation, with the present type being the commonest for small cations. It is found, for example, in the tetramethylammonium and strontium salts (Peters *et al.*, 1984; Geller & Dudley, 1978). Related structures have also been identified through the Cambridge Structural Database (Allen, 2002), which shows that no new examples with the present catenation pattern have appeared since these compounds were reviewed in 1991.



Experimental

The title complex was originally prepared accidentally during the synthesis of a silver complex in the presence of an *N,N'*-diphenylamidine contaminated with potassium iodide. The complex was then prepared rationally from anilinium iodide and silver iodide. Anilinium iodide (aqueous HI and aniline in methanol) was dissolved in acetonitrile and silver iodide (Aldrich) added as solid in an equimolar ratio. The mixture was refluxed for 1 h, giving a yellow solution. On cooling to room temperature, the solution was filtered through celite and allowed to evaporate slowly. The initially precipitated solid was removed by filtration and the desired compound obtained as a microcrystalline solid after several days. Similar tetraphenylphosphonium iodoargentate compounds have been prepared by related methods (Helgesson & Jagner, 1990).

Crystal data

$(\text{C}_6\text{H}_8\text{N})[\text{AgI}_2]$
M_r = 455.80
 Orthorhombic, *Cmca*
a = 13.3019 (10) Å
b = 18.6809 (15) Å
c = 16.5245 (15) Å
V = 4106.2 (6) Å³
Z = 16
D_x = 2.949 Mg m⁻³

Mo *K*α radiation
 Cell parameters from 7996 reflections
 $\theta = 3\text{--}20^\circ$
 $\mu = 7.92 \text{ mm}^{-1}$
T = 180 (2) K
 Lath, light yellow
 0.54 × 0.20 × 0.10 mm

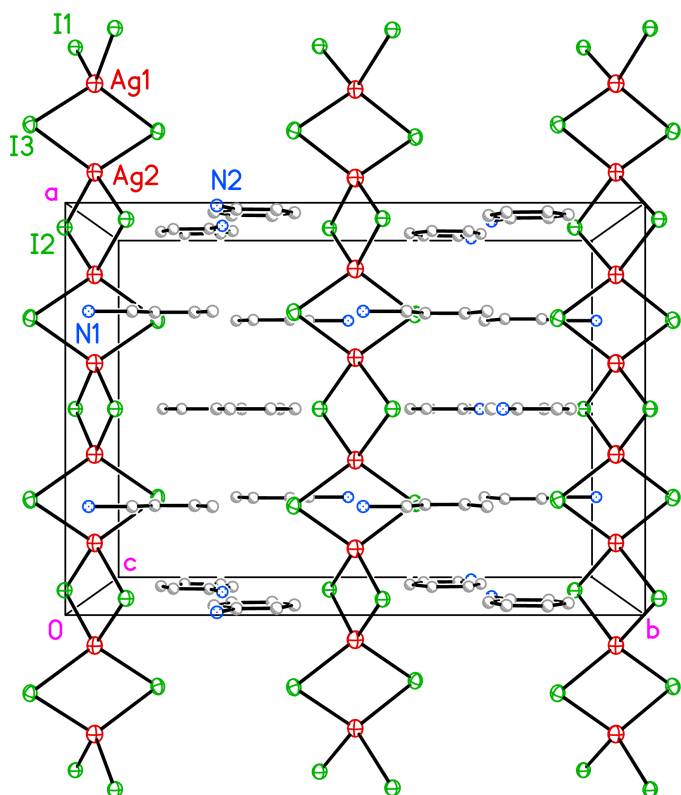


Figure 1
Packing diagram (50% probability displacement ellipsoids), viewed down the *c* axis. Colour code: Ag atoms red; I atoms green; N atoms blue.

Data collection

Siemens SMART area-detector diffractometer	2564 independent reflections
ω scans	2172 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.039$
$T_{\text{min}} = 0.222$, $T_{\text{max}} = 0.453$	$\theta_{\text{max}} = 28.6^\circ$
12054 measured reflections	$h = -17 \rightarrow 17$
	$k = -18 \rightarrow 23$
	$l = -17 \rightarrow 21$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.038P)^2 + 11.3P]$
$R[F^2 > 2\sigma(F^2)] = 0.029$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.070$	$(\Delta/\sigma)_{\text{max}} = 0.008$
$S = 0.98$	$\Delta\rho_{\text{max}} = 0.94 \text{ e } \text{\AA}^{-3}$
2564 reflections	$\Delta\rho_{\text{min}} = -0.88 \text{ e } \text{\AA}^{-3}$
108 parameters	Extinction correction: SHELXL97
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.000123 (14)

Table 1

Selected geometric parameters (\AA , $^\circ$).

Ag1–I3	2.8670 (4)	Ag2–I2 ⁱ	2.8405 (5)
Ag1–I1	2.8785 (5)	Ag2–I3	2.8661 (4)
I3 ⁱⁱⁱ –Ag1–I3	112.60 (2)	I2–Ag2–I3	108.622 (11)
I3 ⁱⁱⁱ –Ag1–I1	119.087 (12)	I3–Ag2–I3 ⁱⁱⁱ	112.66 (2)
I3–Ag1–I1	102.882 (11)	Ag1–I1–Ag1 ⁱⁱⁱ	79.44 (2)
I1–Ag1–I1 ⁱⁱⁱ	100.56 (2)	Ag2 ⁱ –I2–Ag2	70.13 (2)
I2 ⁱ –Ag2–I2	109.87 (2)	Ag2–I3–Ag1	67.366 (15)
I2 ⁱ –Ag2–I3	108.523 (11)		

Symmetry codes: (i) $-x, -y, -z$; (ii) $x, -y, -z$; (iii) $1-x, -y, -z$.

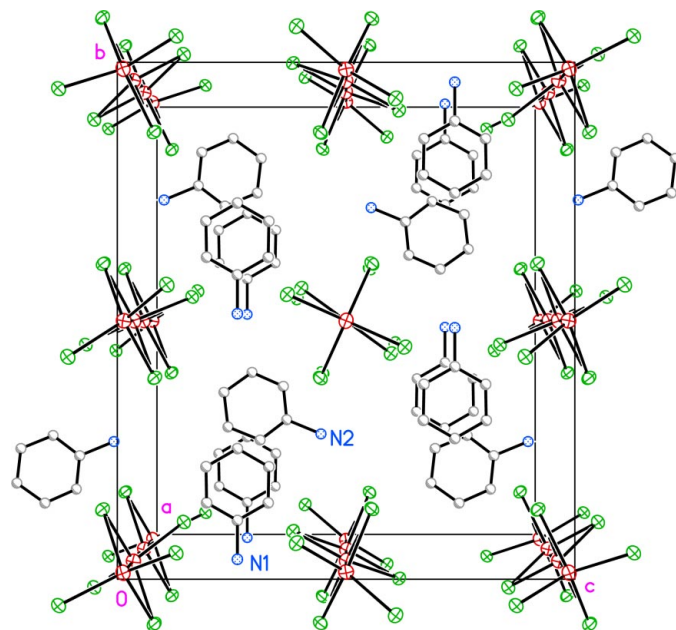


Figure 2
Packing diagram, viewed down the *a* axis. Conventions are as in Fig. 1.

The temperature of the crystal was controlled using the Oxford Cryosystems Cryostream Cooler (Cosier & Glazer, 1986). H atoms were positioned geometrically and refined using a riding model (including free rotation about the C–N bond for the ammonium group), with C–H = 0.98 Å, N–H = 0.91 Å and $U_{\text{iso}}(\text{H}) = 1.2$ (or 1.5 for the ammonium H atoms) times U_{eq} of the carrier atom.

Data collection: SMART (Siemens, 1994); cell refinement: SAINT (Siemens, 1995); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 1997); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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