

Bis[bis(4-aminopyridine- κN^1)silver(I)] terephthalate decahydrateYu-Guang Li,^a Hai-Liang Zhu,^a
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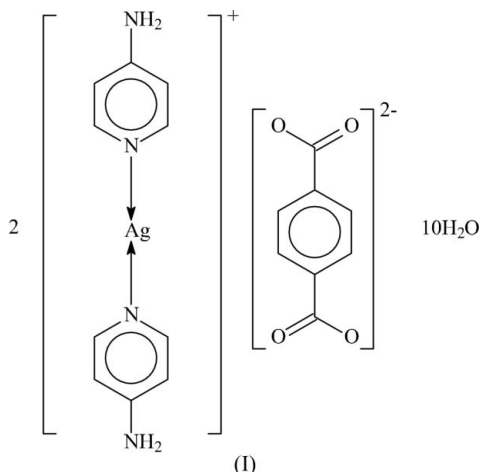
Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(C-C) = 0.004$ Å
 R factor = 0.032
 wR factor = 0.109
Data-to-parameter ratio = 14.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The Ag^I atom in the title compound, $[Ag(C_5H_6N_2)_2]_2 \cdot (C_8H_4O_4) \cdot 10H_2O$, shows linear coordination. The cation and centrosymmetric anion interact indirectly *via* the non-coordinated water molecules, to furnish a tightly held three-dimensional structure.

Comment

A study of the 2-aminopyridine adduct of disilver(I) terephthalate documented the involvement of both the heterocycle and the anion in bonding with silver, resulting in three-coordinate Ag (Zhu, Liu *et al.*, 2003). Surprisingly, the bis(4-aminopyridine)silver cation does not interact directly with the terephthalate ion in the title compound, (I) (Fig. 1), despite the similarity of the heterocyclic ligands. Thus, the Ag atom in (I) shows only linear coordination (Table 1). The cation and dianion, the latter possessing inversion symmetry, interact through $N-H \cdots O$ and $O-H \cdots O$ bonds *via* the non-coordinated water molecules (Table 2) to give rise to a tightly held three-dimensional structure.



The silver trifluoroacetate complex with 4-aminopyridine adopts a similar ion-pair motif but that compound does not incorporate any water molecules of crystallization (Zhu, Zeng *et al.*, 2003).

Experimental

Silver(I) oxide (1 mmol, 232 mg) and terephthalic acid (1 mmol, 166 mg) were dissolved in an aqueous ammonia solution (10 ml). To the clear solution was added a solution of 4-aminopyridine (1 mmol, 94 mg) dissolved in acetonitrile (2 ml). The mixture was set aside for a week for the colorless crystals of (I) to separate from the solution in about 60% yield. Analysis calculated for $C_{28}H_{48}Ag_2N_8O_{14}$: C 35.91, H 5.17, N 11.97%; found: C 35.88, H 5.91, N 11.90%.

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Crystal data

[Ag(C₅H₆N₂)₂]₂(C₈H₄O₄)·10H₂O
M_r = 936.48
 Triclinic, *P* $\bar{1}$
a = 9.1463 (5) Å
b = 10.7369 (6) Å
c = 10.9623 (7) Å
 α = 113.685 (1)°
 β = 93.418 (1)°
 γ = 95.906 (1)°
V = 974.6 (1) Å³

Z = 1
D_x = 1.596 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 3817 reflections
 θ = 2.4–28.1°
 μ = 1.08 mm⁻¹
T = 295 (2) K
 Block, colorless
 0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.625, *T_{max}* = 0.814
 6098 measured reflections

4294 independent reflections
 3955 reflections with *I* > 2σ(*I*)
R_{int} = 0.018
 θ_{\max} = 27.5°
h = -11 → 9
k = -13 → 12
l = -14 → 12

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.032
wR (*F*²) = 0.109
S = 1.12
 4294 reflections
 292 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0673P)^2 + 0.0987P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.49 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.45 \text{ e } \text{Å}^{-3}$
 Extinction correction: SHELXL97
 Extinction coefficient: 0.029 (2)

Table 1

Selected geometric parameters (Å, °).

Ag1–N1	2.118 (2)	Ag1–N3	2.121 (2)
N1–Ag1–N3	174.9 (1)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
N2–H2 <i>n</i> 1...O1 <i>w</i>	0.85 (1)	2.21 (1)	3.039 (3)	166 (3)
N2–H2 <i>n</i> 2...O5 <i>w</i> ⁱⁱ	0.85 (1)	2.22 (1)	3.068 (3)	176 (3)
N4–H4 <i>n</i> 1...O5 <i>w</i> ⁱⁱⁱ	0.86 (1)	2.28 (2)	3.081 (4)	155 (4)
N4–H4 <i>n</i> 2...O1 <i>w</i> ^{iv}	0.84 (1)	2.40 (2)	3.191 (4)	158 (4)
O1 <i>w</i> –H1 <i>w</i> 1...O2 <i>w</i>	0.84 (1)	1.89 (1)	2.727 (3)	178 (3)
O1 <i>w</i> –H1 <i>w</i> 2...O3 <i>w</i> ^v	0.85 (1)	2.04 (1)	2.870 (3)	169 (4)
O2 <i>w</i> –H2 <i>w</i> 1...O1 ^{vi}	0.85 (1)	1.95 (1)	2.778 (2)	164 (3)
O2 <i>w</i> –H2 <i>w</i> 2...O2 ^{vii}	0.84 (1)	1.92 (1)	2.748 (3)	165 (3)
O3 <i>w</i> –H3 <i>w</i> 1...O1	0.85 (1)	1.88 (1)	2.718 (3)	172 (4)
O3 <i>w</i> –H3 <i>w</i> 2...O1 ^{iv}	0.85 (1)	2.09 (2)	2.913 (3)	164 (4)
O4 <i>w</i> –H4 <i>w</i> 1...O2 ^{viii}	0.85 (1)	1.88 (1)	2.718 (3)	172 (4)
O4 <i>w</i> –H4 <i>w</i> 2...O3 <i>w</i>	0.84 (1)	1.92 (1)	2.757 (3)	170 (3)
O5 <i>w</i> –H5 <i>w</i> 1...O4 <i>w</i>	0.84 (1)	2.03 (1)	2.853 (3)	170 (4)
O5 <i>w</i> –H5 <i>w</i> 2...O4 <i>w</i> ⁱⁱ	0.84 (1)	2.06 (1)	2.898 (3)	180 (4)

Symmetry codes: (ii) $-x, -y + 1, -z + 2$; (iii) $-x + 1, -y, -z + 1$; (iv) $x + 1, y - 1, z - 1$; (v) $x, y + 1, z$; (vi) $-x, -y + 1, -z + 1$; (vii) $x - 1, y + 1, z$; (viii) $x - 1, y, z$.

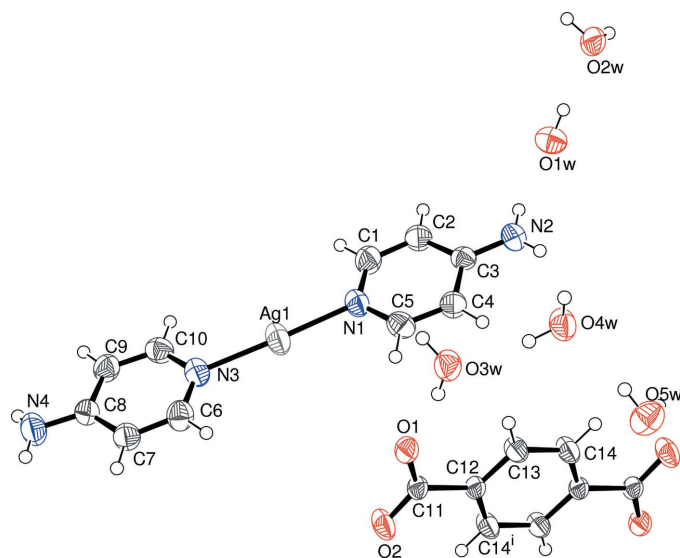


Figure 1

View of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for the H atoms). [Symmetry code: (i) $1 - x, 1 - y, 2 - z$.]

The aromatic H atoms were placed in idealized positions and constrained to ride on their parent atoms, with a C–H distance of 0.93 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The amine and water H atoms were located in difference maps and were refined with distance restraints of N–H = O–H = 0.85 (1) Å; their displacement parameters were freely refined.

Data collection: SMART (Bruker, 2003); cell refinement: SAINT (Bruker, 2003); 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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