metal-organic papers

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Key indicators

Single-crystal X-ray study T = 292 KMean $\sigma(C-C) = 0.008 \text{ Å}$ R factor = 0.043 wR factor = 0.110 Data-to-parameter ratio = 16.2

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

An orthorhombic polymorph of poly[µ-2-aminobenzoato-silver(I)]

The orthorhombic (space group $Pna2_1$) title compound, [Ag(C₇H₆NO₂)]_n, is a polymorph of the known monoclinic ($P2_1/n$) variant of this stoichiometry [Smith, Lynch & Kennard (1999). *Aust. J. Chem.* **52**, 325–327]. In the title compound, the Ag atom shows linear coordination to one O and one N atom [Ag-O = 2.138 (5) Å, Ag-N = 2.153 (4) Å and O-Ag-N = 173.55 (18)°]. In the monoclinic form, the Ag coordination to two O atoms and one N atom can be described as Y-shaped or distorted trigonal planar. Weak Ag···Ag interactions, aromatic π - π stacking and N-H···O hydrogen-bond interactions help to establish the crystal packing in the title compound.

Comment

Silver(I) adducts with carboxylate ligands are now an extremely topical area of research and a number of structures have been characterized (Smith *et al.*, 1996, 1998; You & Zhu, 2004; Zhu *et al.*, 2004). The monoclinic structure of silver(I) 2aminobenzoate, $[Ag(C_7H_6NO_2)]$, was reported by Smith *et al.* (1999), as a zigzag coordination polymer in which the 2aminobenzoate anion behaves as an *N*,*O*,*O'*-tridentate ligand. Here we report the synthesis and structure of the title compound, (I) (Fig. 1), an orthorhombic modification of the same stoichiometry.



In (I), two silver(I) atoms are linked *via* a 2-aminobenzoate ion, acting as a bridge, extending into a zigzag chain. Each Ag atom is two-coordinated by one N atom and one O atom from two 2-aminobenzoate ligands (Table 1) in a near-linear geometry $[N-Ag-O = 173.55 (18)^{\circ}]$. The carboxylate C–O distances in (I) are roughly equal, suggesting delocalization of the negative charge. In the monoclinic form (Smith *et al.*,

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Figure 1

The structure of (I), expanded to show the Ag coordination, showing 50% probability displacement ellipsoids (arbitrary spheres for the H atoms). Atoms labelled with suffixes A, B and C are at symmetry positions $(x - \frac{1}{2}, -y + \frac{1}{2}, z), (x - 1, y, z), \text{ and } (x + \frac{1}{2}, -y + \frac{1}{2}, z - 1), \text{ respectively.}$



Figure 2

The two-dimensional sheet structure of (I) arising from the $Ag \cdots Ag$ interactions, viewed along c.

1999), the stereochemistry about each Ag centre is distorted AgO₂N trigonal planar [Ag-O = 2.223 (4) and 2.408 (4) Å, and Ag-N = 2.301 (5) Å], with the three angles subtended at the Ag atom being 89.8 (2), 126.2 (2) and 142.9 (2)°.

The Ag···Ag distance in (I) of 3.1061 (4) Å is longer than the equivalent separations of 2.9128 (9) and 2.9887 (10) Å observed in the monoclinic form; all these are much shorter than the sum of the van der Waals radii of two Ag atoms (3.44 Å).

In (I), the bridging ligand results in zigzag chains propagating in [101]. The chains are crosslinked via weak $Ag \cdots Ag$ interactions into a two-dimensional sheet structure propa-

Experimental

Ag₂O (0.1 mmol, 23.2 mg) and 2-aminobenzoic acid (0.2 mmol, 27.4 mg) were dissolved in an aqueous ammonia solution (10 ml), and the resulting solution was stirred for ca 15 min to give a clear colorless solution. To this solution was added an acetonitrile solution (5 ml). The mixture was stirred for 1 h, and the resulting colorless solution was kept in the dark at room temperature for 8 d. Colorless blockshaped crystals of (I) formed on slow evaporation of the solvent; these were dried in a vacuum desiccator over anhydrous CaCl₂ (yield 55%). Elemental analysis calculated for C₇H₆AgNO₂: C 34.46, H 2.48, N 5.74%; found: C 34.32, H 2.51, N 5.81%.

Z = 4

 $D_r = 2.293 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

 $\mu = 2.79 \text{ mm}^{-1}$

T = 292 (2) K

Block, colorless

 $0.36 \times 0.30 \times 0.10 \text{ mm}$

Flack parameter: 0.01 (7)

Crystal data

 $[Ag(C_7H_6NO_2)]$ $M_r = 244.00$ Orthorhombic, Pna21 a = 5.9486 (8) Å b = 24.227 (3) Å c = 4.9042 (6) Å V = 706.77 (16) Å³

Data collection

Bruker APEX CCD diffractometer 7681 measured reflections 1621 independent reflections (i) scans Absorption correction: multi-scan 1568 reflections with $I > 2\sigma(I)$ (SADABS; Sheldrick, 1996) $R_{\rm int}=0.091$ $\theta_{\rm max} = 27.5^{\circ}$ $T_{\rm min}=0.433,\ T_{\rm max}=0.768$

Refinement R

Refinement on F^2	$w = 1/[\sigma^2(F_0^2) + (0.0739P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	+ 0.1709P]
$wR(F^2) = 0.110$	where $P = (F_0^2 + 2F_c^2)/3$
S = 1.10	$(\Delta/\sigma)_{\rm max} < 0.001$
1621 reflections	$\Delta \rho_{\rm max} = 1.69 \ {\rm e} \ {\rm \AA}^{-3}$
100 parameters	$\Delta \rho_{\rm min} = -1.53 \text{ e } \text{\AA}^{-3}$
H-atom parameters constrained	Absolute structure: Flack (1983)
	713 Friedel pairs

Table 1

Selected geometric parameters (Å, °).

Ag1-O1 ⁱ	2.138 (5)	C7-O1	1.264 (7)
Ag1-N1	2.153 (4)	C7-O2	1.247 (6)
O1 ⁱ -Ag1-N1	173.55 (18)		
	1 1 1 1 4		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$\frac{N1 - H1A \cdots O1}{N1 - H1B \cdots O2^{ii}}$	0.90	1.86	2.644 (6)	144
	0.90	2.09	2.917 (6)	152

Symmetry code: (ii) x - 1, y, z.

All H atoms were placed in geometrically idealized positions (C– H = 0.93 Å and N–H = 0.90 Å) and refined as riding, with U_{iso} (H) = $1.2U_{eq}$ (carrier).

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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