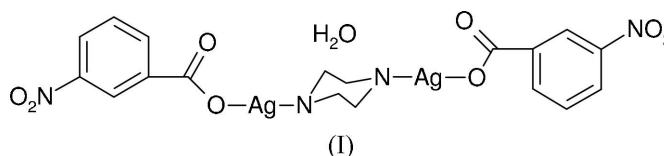


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hailiang_zhu@163.com**Key indicators**Single-crystal X-ray study
T = 298 K
Mean $\sigma(\text{C}-\text{C})$ = 0.007 Å
R factor = 0.051
wR factor = 0.115
Data-to-parameter ratio = 14.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>. **μ -Piperidine- $\kappa^2\text{N}:N'$ -bis[(3-nitrobenzoato- κO)-silver(I)] monohydrate**

The title compound, $[\text{Ag}_2(\text{C}_7\text{H}_4\text{NO}_4)_2(\text{C}_4\text{H}_{10}\text{N}_2)]\cdot\text{H}_2\text{O}$, has two similar dinuclear Ag^{I} complex molecules, each with a crystallographic inversion center; the asymmetric unit contains half of each molecule and a molecule of water. Each Ag atom in the compound is coordinated by one O atom from a 3-nitrobenzoate anion and one N atom from a piperidine bridge, in a slightly distorted linear geometry.

Comment

In the last few years, attention has been paid to the preparation of complexes of the coinage metals, due to their importance in the development of optical materials, polymer conductors, catalyst carriers, *etc.* Silver(I) complexes are interesting and challenging because most of them are water-insoluble and unstable upon exposure to light. Recently, we have reported some silver(I) carboxylate complexes with organic amines (Zhu, Wang, Pan & Wang, 2003; Pan *et al.*, 2003; Zhu, Wang, Sun & Wang, 2003; Zhu, Wang, Lin *et al.*, 2003). As an extension of our work, we report here the crystal structure of a new silver(I) complex, μ -piperidine- $\kappa^2\text{N}:N'$ -bis[(3-nitrobenzoato- κO)-silver(I)] monohydrate, (I).



The title compound is a neutral dinuclear silver(I) compound (Fig. 1). The asymmetric unit contains two half-molecules of the dinuclear silver compound and one water molecule. In both complex molecules, the Ag^{I} atoms are in a distorted linear geometry and are two-coordinated by one O atom from a 3-nitrobenzoate anion and one N atom from a piperidine bridge. All the Ag–O and Ag–N bond lengths (Table 1) are comparable to the corresponding values in the silver(I) complexes we reported recently (You & Zhu, 2004; Chen *et al.*, 2003; Zhu, Sun *et al.*, 2003). The bond angles at the Ag^{I} atoms deviate somewhat from 180° , *viz.* $165.85(15)^\circ$ for Ag1 and $168.12(16)^\circ$ for Ag2.

In the crystal structure, all the O atoms of the water molecules and the uncoordinated O atoms of the carboxylate anions, together with all the N atoms of the piperidine group, are involved in the formation of hydrogen bonds (Table 2).

Experimental

Piperidine and 3-nitrobenzoic acid were available commercially and were used without further purification. Ag_2O (0.5 mmol, 116 mg) and

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3-nitrobenzoic acid (1 mmol, 167 mg) were dissolved in a solution of ammonia (10 ml, 30%) and CH₃CN (10 ml). The mixture was stirred for about 10 min to obtain a clear colorless solution. To this solution was added an ammonia solution (2 ml) of piperidine (0.5 mmol, 43 mg). After keeping the resulting solution in air for a week, with ammonia and CH₃CN evaporating, large colorless crystals were formed. The crystals were isolated, washed three times with water and dried in a desiccator using CaCl₂ (yield 60%). Elemental analysis found: C 33.25, H 2.90, N 8.69%; calculated for C₁₈H₂₀Ag₂N₄O₉: C 33.15, H 3.09, N 8.59%.

Crystal data

[Ag₂(C₇H₄NO₄)₂(C₄H₁₀N₂)]·H₂O
M_r = 652.12
 Monoclinic, *P*2₁/*n*
a = 7.285 (1) Å
b = 24.298 (2) Å
c = 11.945 (1) Å
 β = 93.523 (2)°
V = 2110.4 (4) Å³
Z = 4
D_x = 2.052 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 2560 reflections
 θ = 2.4–25.8°
 μ = 1.92 mm⁻¹
T = 298 (2) K
 Block, yellow
 0.37 × 0.25 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.532, *T_{max}* = 0.767
 17019 measured reflections
 4571 independent reflections
 3873 reflections with *I* > 2σ(*I*)
R_{int} = 0.030
 θ_{max} = 27.0°
h = -9 → 9
k = -30 → 30
l = -15 → 15

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.051
wR(*F*²) = 0.115
S = 1.05
 4571 reflections
 314 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0377P)^2 + 6.6578P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 2.03 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -1.90 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Ag1—O1	2.107 (3)	Ag2—O5	2.132 (3)
Ag1—N2	2.147 (4)	Ag2—N4	2.174 (4)
O1—Ag1—N2	165.85 (15)	O5—Ag2—N4	168.12 (16)

Table 2

Hydrogen-bonding 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>
N4—H4A...O6 ⁱ	0.897 (10)	2.094 (19)	2.968 (5)	165 (5)
N2—H2A...O9 ⁱⁱ	0.895 (10)	2.10 (3)	2.881 (6)	146 (4)
O9—H2...O2 ⁱ	0.841 (10)	1.859 (16)	2.688 (6)	168 (6)
O9—H1...O6	0.841 (10)	1.905 (12)	2.745 (6)	177 (7)

Symmetry codes: (i) 1 - *x*, -*y*, 1 - *z*; (ii) *x*, *y*, 1 + *z*.

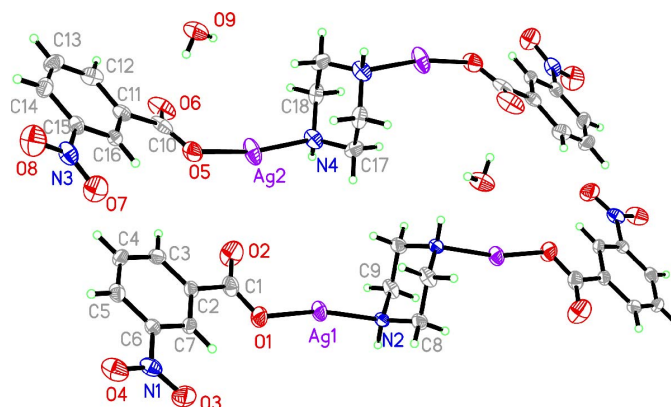


Figure 1

The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

The H atoms of the water molecules and the piperidine N atoms were located in a difference Fourier map and refined isotropically, with the N—H distances restrained to 0.90 (1) Å, and with the O—H and H...H distances restrained to 0.84 (1) and 1.37 (2) Å, respectively. All H atoms attached to C atoms were placed in geometrical positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.97 Å, and with *U_{iso}*(H) = 1.2*U_{eq}*(C). The unsigned maximum residual density is 0.85 Å⁻³ from atom Ag2 and the minimum residual density is 0.83 Å⁻³ from atom Ag2.

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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