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# The chain structure of *catena*-poly[[di-$\mu$-benzoato-$\kappa^4O$:$O'$-disilver(I)]-$\mu$-1,4-diazabicyclo[2.2.2]octane-$\kappa^2N$:$N'$]

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The crystal structure determination of the title complex, $[Ag_2(C_7H_5O_2)_2(C_6H_{12}N_2)]_n$, reveals a slightly distorted T geometry for the $Ag^I$ atom, coordinated by an N atom from a 1,4-diazabicyclo[2.2.2]octane ligand and two O atoms from two benzoate anions. The dibenzoatodisilver(I) and 1,4-diazabicyclo[2.2.2]octane units lie across crystallographic inversion centres. The carboxyl groups in the complex behave in a $\eta^1$:$\eta^1$:$\mu_2$ fashion, bridging adjacent Ag atoms to form one-dimensional chains.

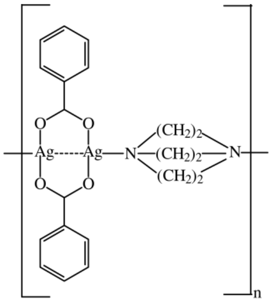
**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.013 Å
Disorder in main residue
$R$ factor = 0.055
$wR$ factor = 0.148
Data-to-parameter ratio = 16.0

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

## Comment

Inorganic–organic supramolecular architectures derived from building blocks that are linked by coordinate covalent bonds (Lehn, 1995) constitute an active field that impinges on the synthesis of interesting topological structures and potential functional materials. So far, a number of one-, two- and three-dimensional coordination networks have already been generated with linear *N,N'*-bidentate spacers (Barren & Robson, 1998; Yaghi *et al.*, 1998; Munakata *et al.*, 1999; Hagrman *et al.*, 1999). However, factors influencing the formation of coordination polymers are still not well understood, in spite of the fact that the self-assembly of these architectures has been documented to be highly influenced by various factors such as the nature of the metal ions (Carlucci *et al.*, 1995), templates (Tong, Ye *et al.*, 1998), and experimental conditions (Tong, Chen *et al.*, 1998; Hennigar *et al.*, 1997; Yaghi & Li, 1995). Much work is required to extend the knowledge of the relevant structural types and establish proper synthetic strategies leading to the desired species. Recently, we have synthesized a series of imidazole-containing compounds, which are used in the synthesis of transition metal complexes as structural models of some metalloenzymes and in crystal engineering (Long *et al.*, 1999; Yang *et al.*, 2000, 2001). In the course of our systematic study of metal complexes, we have isolated the title compound, (I), and report here its preparation and crystal structure.



(I)

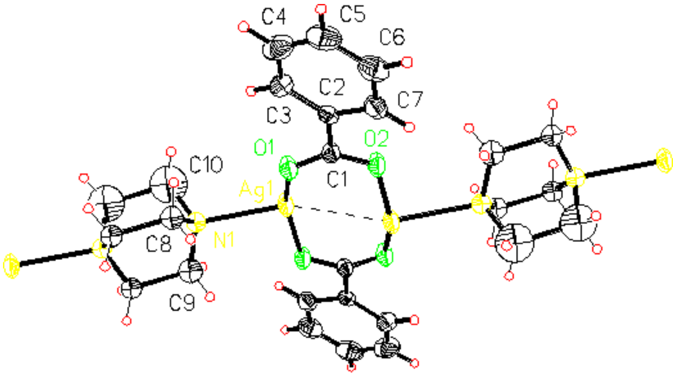


**Figure 1**
The structure of (I), showing the atom-numbering scheme for the contents of the asymmetric unit. Displacement ellipsoids are drawn at the 35% probability level. Only one orientation of the disordered triethylenediamine moiety is shown.

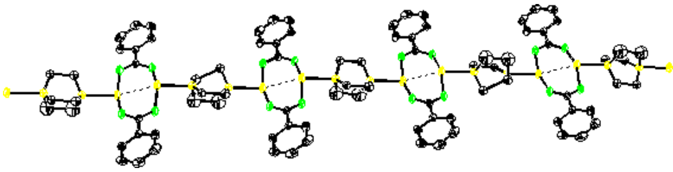


**Figure 2**
A view of the polymeric chain. Only one orientation of the disordered triethylenediamine moiety is shown.

The X-ray structure determination shows that in (I), the dibenzoatodisilver(I) and 1,4-diazabicyclo[2.2.2]octane units lie across crystallographic inversion centres and hence the asymmetric unit consists of one-half each of these units (Fig. 1), the diamine being disordered. The Ag atom in the complex is coordinated in a slightly distorted T geometry by two O atoms from the carboxylate group of two benzoate anions and an N atom from a 1,4-diazabicyclo[2.2.2]octane group, with angles ranging from 94.7 (2) to 158.2 (2)°. The Ag—O [2.216 (6) and 2.219 (5) Å] and Ag—N [2.415 (5) Å] bond distances are consistent with those in related compounds. In the crystal structure, the carboxyl groups of benzoate anions arrange in a $\eta^1$:$\eta^1$:$\mu_2$ fashion, bridging adjacent Ag atoms to form one-dimensional chains along the *c* axis (Fig. 2) with an Ag$\cdots$Ag distance of 2.852 (2) Å. This value is well below the sum of the van der Waals radii of two Ag atoms (3.44 Å; Bondi, 1964), indicating some degree of weak metal–metal interaction.

## Experimental

A $CH_3CN$ solution (10 ml) of 1,4-diazabicyclo[2.2.2]octane (1 mmol, 0.112 g) was added dropwise to a stirred MeCN–$H_2O$ solution (10 ml) of Ag($O_2CC_6H_5$) (0.229 g, 1 mmol). After 5 d at room temperature, the solution precipitated colourless block-shaped crystals of (I) in 65% yield.

*Crystal data*

$C_{20}H_{22}Ag_2N_2O_4$
$M_r$ = 570.14
Monoclinic, $P2_1/n$
$a$ = 6.243 (5) Å
$b$ = 16.459 (5) Å
$c$ = 10.084 (5) Å
$\beta$ = 101.13 (4)°
$V$ = 1016.7 (10) Å$^3$
$Z$ = 2

$D_x$ = 1.862 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta$ = 4.0–27.0°
$\mu$ = 1.95 mm$^{-1}$
$T$ = 293 (2) K
Block, colourless
0.42 × 0.38 × 0.34 mm

*Data collection*

Siemens *R*3*m* diffractometer
$\omega$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.457, $T_{max}$ = 0.515
2672 measured reflections
2460 independent reflections
1298 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.027
$\theta_{max}$ = 28.0°
$h = 0 \rightarrow 8$
$k = 0 \rightarrow 21$
$l = -13 \rightarrow 13$
2 standard reflections every 118 reflections intensity decay: none

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.148
$S$ = 1.02
2460 reflections

154 parameters
H-atom parameters constrained
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.79 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.56 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Ag1—O1 | 2.216 (6) | Ag1—N1 | 2.415 (5) |
| Ag1—O2$^i$ | 2.219 (5) | Ag1—Ag1$^i$ | 2.8520 (17) |
| | | | |
| O1—Ag1—O2$^i$ | 158.2 (2) | O2$^i$—Ag1—N1 | 94.73 (19) |
| O1—Ag1—N1 | 96.16 (19) | | |

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

The 1,4-diazabicyclo[2.2.2]octane moiety, which lies across an inversion centre, is disordered over two orientations, each with an occupancy of 0.5. All H atoms were positioned geometrically (C—H = 0.96 Å) and refined using the riding-model approximation, with $U_{iso}$(H) = 1.2$U_{eq}$ of the parent atom.

Data collection: *R3m Software* (Siemens, 1990); cell refinement: *R3m Software*; data reduction: *SHELXTL-Plus* (Sheldrick, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1998); software used to prepare material for publication: *SHELXL*97.

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