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## Structure Reports

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## Li Wang ${ }^{\mathrm{a}, \mathrm{b}}$ * and Yamei Pei ${ }^{\text {b }}$

${ }^{\text {a }}$ College of Life Sciences, Shenzhen University, Shenzhen 518060, People's Republic of China, and ${ }^{\mathbf{b}}$ Department of Chemistry, Central China Normal University, Wuhan, Hubei 430079, People's Republic of China

Correspondence e-mail:
wl_928@mail.ccnu.edu.cn

## Key indicators

Single-crystal X-ray study
$T=292 \mathrm{~K}$
Mean $\sigma(\mathrm{C}-\mathrm{C})=0.014 \AA$
$R$ factor $=0.047$
$w R$ factor $=0.171$
Data-to-parameter ratio $=11.7$
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

[^0]
## catena-Poly[silver(I)- $\mu$-L-phenylalaninato- $\left.\kappa^{2} N: O\right]$

In the title one-dimensional polymeric structure, $\left[\mathrm{Ag}\left(\mathrm{C}_{9} \mathrm{H}_{10} \mathrm{NO}_{2}\right)\right]_{n}$, the $\mathrm{Ag}^{\mathrm{I}}$ atom is bis-coordinated by an O and an N atom. Intermolecular $\mathrm{N}-\mathrm{H} \cdots \mathrm{O}[\mathrm{H} \cdots \mathrm{O}=$ 2.07 (3) $\AA$ ] and $\mathrm{C}-\mathrm{H} \cdots \mathrm{O}(\mathrm{H} \cdots \mathrm{O}=2.54-2.58 \AA)$ hydrogen bonds and a weak $\mathrm{C}-\mathrm{H} \cdots \pi$ (arene) interaction link the polymeric chains into an extended three-dimensional framework.

## Comment

Amino acids are interesting biological ligands which have multiple functional groups. A systematic investigation of the coordination behaviour of amino acids is necessary in order to reveal the role played by amino acids in important chemical processes involving metal ions (Yamauchi et al., 2002). The structures of a series of amino acid complexes with silver(I) have previously been reported (Acland \& Freeman, 1971; Démaret \& Abraham, 1987; Erxleben, 2002; Nomiya \& Yokoyama, 2002). We present here the crystal structure of the title compound, (I).

(I)

Compound (I) forms a one-dimensional polymer along the [100] direction, with the $\mathrm{Ag}^{\mathrm{I}}$ atom coordinated by one carboxylate O atom and a symmetry-related amido N atom (Fig. 1 and Table 1), and with all phenyl rings located on the same side of the chain.

In the crystal structure, intermolecular $\mathrm{N}-\mathrm{H} \cdots \mathrm{O}$ and $\mathrm{C}-$ $\mathrm{H} \cdots \mathrm{O}$ hydrogen bonds and a $\mathrm{C}-\mathrm{H} \cdots \pi$ (arene) interaction link the polymeric chains into a three-dimensional network (Fig. 2 and Table 1).

## Experimental

To an aqueous solution ( 10 ml ) of $\mathrm{AgNO}_{3}(0.5 \mathrm{~mol}, 0.09 \mathrm{~g}$ ), an equimolar amount of L -phenylalanine was added and the mixture was stirred for 5 h . The solution was kept at room temperature. Colourless prism-shaped crystals of (I) suitable for X-ray analysis were obtained over several days in $60 \%$ yield.

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Figure 1
Part of the title polymer，propagating along the［100］direction，showing $30 \%$ probability displacement ellipsoids（ H atoms as small spheres）． Atoms labelled with the suffixes＇$a$＇and＇$b$＇are related by the symmetry operators $(-1+x, y, z)$ and $(1+x, y, z)$ ，respectively．


Figure 2
Part of the crystal structure of（I），with hydrogen bonds and $\mathrm{C}-\mathrm{H} \cdots \pi$ interactions shown as dashed lines．Only H atoms which are involved in the hydrogen－bonding or $\mathrm{C}-\mathrm{H} \cdots \pi$ interactions are shown．

## Crystal data

$\left[\mathrm{Ag}\left(\mathrm{C}_{9} \mathrm{H}_{10} \mathrm{NO}_{2}\right)\right]$
$M_{r}=272.05$
Monoclinic，$P 2_{1}$
$a=7.2244$（13）$\AA$
$b=6.4049$（12）A
$c=10.1620$（19）$\AA$
$\beta=106.692(3)^{\circ}$ 。
$V=450.40(14) \AA^{3}$
Data collection
Bruker SMART CCD area－detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction：multi－scan （SADABS；Sheldrick，1996）
$T_{\text {min }}=0.810, T_{\text {max }}=0.879$

## Refinement

```
Refinement on \(F^{2}\)
\(R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.047\)
\(w R\left(F^{2}\right)=0.171\)
\(S=1.24\)
1362 reflections
116 parameters
H atoms treated by a mixture of
    independent and constrained
    refinement
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## $Z=2$

$D_{x}=2.006 \mathrm{Mg} \mathrm{m}^{-3}$
Mo $K \alpha$ radiation
$\mu=2.20 \mathrm{~mm}^{-1}$
$T=292$（2）K
Prism，colourless
$0.10 \times 0.10 \times 0.06 \mathrm{~mm}$

1859 measured reflections
1362 independent reflections
1305 reflections with $I>2 \sigma(I)$
$R_{\text {int }}=0.017$
$\theta_{\text {max }}=25.0^{\circ}$

$$
\begin{aligned}
& w=1 /\left[\sigma^{2}\left(F_{\mathrm{o}}{ }^{2}\right)+(0.1016 P)^{2}\right. \\
& +0.9012 P] \\
& \text { where } P=\left(F_{\mathrm{o}}{ }^{2}+2 F_{\mathrm{c}}{ }^{2}\right) / 3 \\
& (\Delta / \sigma)_{\text {max }}=0.001 \text { 。 } \\
& \Delta \rho_{\max }=1.45 \mathrm{e}^{-3} \\
& \Delta \rho_{\text {min }}=-1.03 \mathrm{e}^{-3} \\
& \text { Absolute structure: Flack (1983), } \\
& \text { with } 500 \text { Friedel pairs } \\
& \text { Flack parameter: } 0.02 \text { (11) }
\end{aligned}
$$

Table 1
Selected geometric parameters $\left(\AA,^{\circ}\right)$ ．

| $\mathrm{Ag} 1-\mathrm{N} 1^{\mathrm{i}}$ | $2.146(8)$ | $\mathrm{Ag} 1-\mathrm{O} 1$ | $2.184(9)$ |
| :--- | :--- | :--- | :--- |
|  |  |  |  |
| $\mathrm{N} 1^{\mathrm{i}}-\mathrm{Ag} 1-\mathrm{O} 1$ | $166.6(4)$ | $\mathrm{C} 9-\mathrm{O} 1-\mathrm{Ag} 1$ | $103.7(7)$ |
| $\mathrm{C} 8-\mathrm{N} 1-\mathrm{Ag}^{\mathrm{ii}}$ | $113.8(5)$ |  |  |

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

Table 2
Hydrogen－bond geometry $\left(\AA,{ }^{\circ}\right)$ ．
$C g 1$ is the centroid of ring C1－C6

| $D-\mathrm{H} \cdots A$ | $D-\mathrm{H}$ | $\mathrm{H} \cdots A$ | $D \cdots A$ | $D-\mathrm{H} \cdots A$ |
| :--- | :--- | :--- | :--- | :--- |
| $\mathrm{C} 7-\mathrm{H} 7 A \cdots \mathrm{O} 2^{\text {iii }}$ | 0.97 | 2.58 | $3.490(13)$ | 157 |
| $\mathrm{C} 2-\mathrm{H} 2 \cdots 1^{\text {iv }}$ | 0.93 | 2.54 | $3.445(11)$ | 165 |
| $\mathrm{~N} 1-\mathrm{H} 1 B \cdots \mathrm{O} 2^{\mathrm{v}}$ | $0.86(6)$ | $2.07(7)$ | $2.832(16)$ | $148(4)$ |
| C5 $^{\mathrm{H}} 5 \cdots \mathrm{Cg} 1^{\text {vi }}$ | 0.93 | 2.56 | $3.443(1)$ | 159 |

Symmetry codes：（iii）$-x, y+\frac{1}{2},-z$ ；（iv）$x+1, y+1, z$ ；（v）$-x, y-\frac{1}{2},-z$ ；（vi） $-x+1, y-\frac{1}{2},-z+1$ ．

All H atoms bonded to C atoms were placed in idealized positions in a riding－model approximation，with $\mathrm{C}-\mathrm{H}$ distances in the range $0.93-0.98 \AA$ ，and with $U_{\text {iso }}(\mathrm{H})=1.2 U_{\text {eq }}(\mathrm{C})$ ．The coordinates of atom H8 were refined $[\mathrm{C} 8-\mathrm{H} 8=0.98(12) \AA]$ ，with $U_{\text {iso }}(\mathrm{H})=1.2 U_{\text {eq }}(\mathrm{C})$ ． N－bound atoms $\mathrm{H} 1 A$ and $\mathrm{H} 1 B$ were located in a difference Fourier map and refined with a distance restraint of $\mathrm{N}-\mathrm{H}=0.86$（1）$\AA$ ，with $U_{\text {iso }}(\mathrm{H})=1.2 U_{\text {eq }}(\mathrm{N})$ ．Because of the larger than normal displacement parameters for atoms C2，C3 and C4，it appears that the phenyl ring （C1－C6）may be slightly disordered，although this was not modelled． In the final stages of refinement，the benzene ring was constrained to an ideal planar regular hexagon，with fixed $\mathrm{C}-\mathrm{C}$ distances，and the atoms were restrained to approximately isotropic behaviour．

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

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