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catena-Poly[[(1,10-phenanthroline-κ^2N,N')-silver(I)]-μ-chloro]

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Key indicators

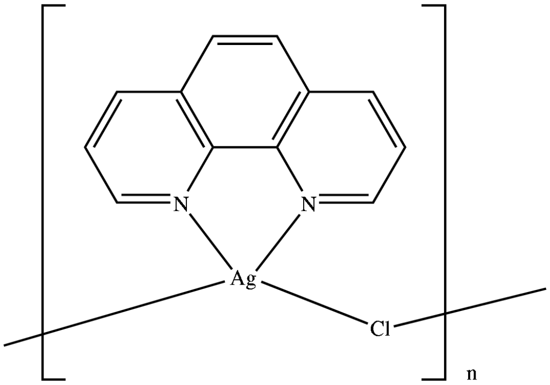
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.010 Å
R factor = 0.036
wR factor = 0.066
Data-to-parameter ratio = 16.2

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

In the title compound, $[AgCl(C_{12}H_8N_2)]_n$, the Ag atom is four-coordinate in a highly distorted tetrahedral environment formed by two N atoms of phenanthroline and two Cl atoms. The Ag atoms are bridged by Cl atoms and the compound forms a one-dimensional polymer. Ag and Cl atoms lie on twofold rotation axes.

Comment

Aromatic heterocycles are interesting compounds due to their ability to stack with nucleobases to enhance complex formation with DNA, which is the principal target in the chemotherapy of tumors (Shehata, 2001). On the other hand, silver has been focused on because of its antitumor and antibacterial activity. We aimed to synthesize the title compound, *catena*-poly[[(1,10-phenanthroline-κ^2N,N')silver(I)]-μ-chloro], (I), and analyse its crystal structure to clarify the coordination mode of 1,10-phenanthroline (phen) and silver. Its antibacterial activity has already been studied (Coyle *et al.*, 2004).



(I)

The crystal structure of (I) is shown in Fig. 1. Ag and Cl atoms lie on twofold rotation axes. One phen molecule coordinates to each Ag atom as a bidentate ligand, and around the Ag atom, five-membered rings [Ag1/N1/C5/C5^{ii}/N1^{ii}; symmetry code: (ii) $1 - x$, y, $-z$] are formed. Two N atoms (N1 and N1^{ii}) of phen and two Cl atoms [Cl1 and Cl1^{i}; symmetry code: (i) x, y, $1 + z$] are coordinated to Ag, forming a highly distorted tetrahedral environment around it. Ag atoms of adjacent units are bridged by one Cl atom and the compound forms a one-dimensional polymer along the c axis. The crystal structure is stabilized by stacking interactions between neighboring phen ligands [the distance between the plane N1/C1–C6/N1^{ii}/C1^{ii}–C6^{ii} and atom N1^{i} is 3.385 (7) Å, and between the same plane and N1^{iv} is 3.430 (6) Å; symmetry code: (i) x, y, $1 + z$; (iv) $1 - x$, y, $1 - z$] and C—H$\cdots$Cl

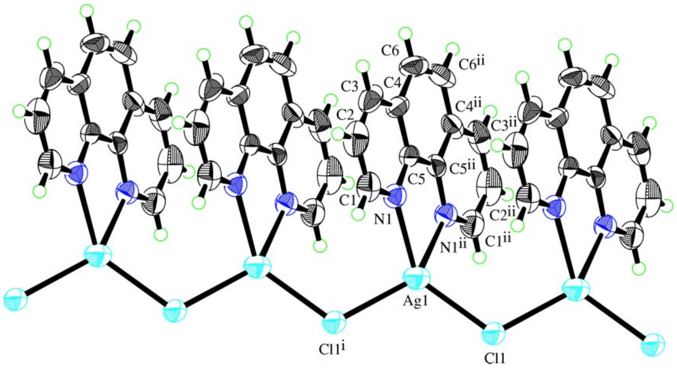


Figure 1
*ORTEP*II (Johnson, 1976) drawing of (I). Displacement ellipsoids for non-H atoms are shown at the 50% probability level. [symmetry codes: (i) $x, y, 1 + z$; (ii) $1 - x, y, -z$.]

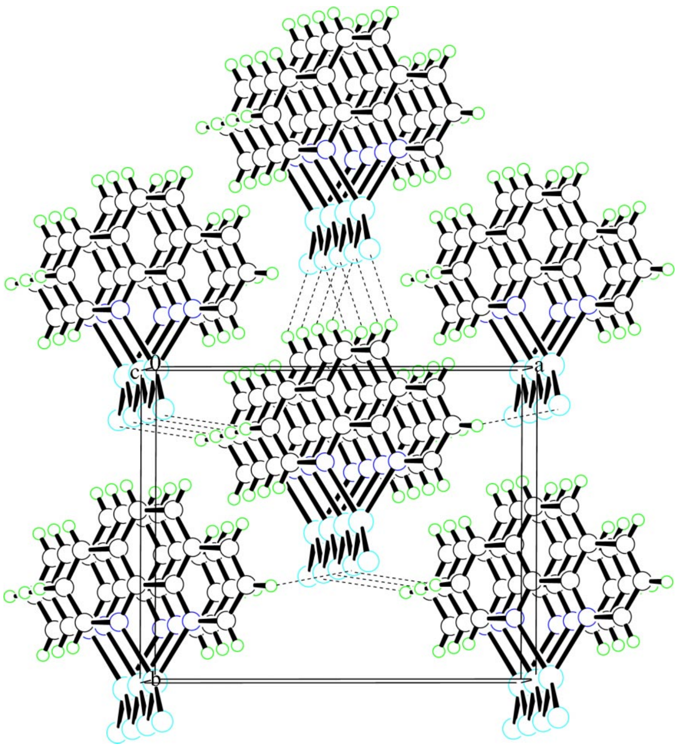


Figure 2
Packing view of (I). Dashed lines represent C—H···Cl hydrogen-bonding interactions.

hydrogen-bonding interactions between adjacent parallel chains (Table 2 and Fig. 2).

Crystal structures of Ag–phen complexes have been reported previously (Leschke *et al.*, 2002; Paramonov *et al.*, 2003), in which the Ag atom is coordinated by two phen molecules to form propeller-like structures. The title compound, (I), is the first structure in which Ag and phen form a linear-chain polymer.

Experimental

Red prismatic crystals of the title compound were obtained at room temperature by the slow evaporation of a mixture of a dimethylformamide solution of 1,10-phenanthroline, silver(I) chloride and malonic acid (molar ratio 1:1:1).

Crystal data

$[AgCl(C_{12}H_8N_2)]$
$M_r = 323.52$
Monoclinic, $C2$
$a = 12.566\ (14)$ Å
$b = 10.235\ (11)$ Å
$c = 4.279\ (4)$ Å
$\beta = 104.92\ (4)^\circ$
$V = 531.7\ (8)$ Å^3
$Z = 2$

$D_x = 2.020$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2250 reflections
$\theta = 3.4$–27.4°
$\mu = 2.11$ mm^{-1}
$T = 296.1$ K
Prism, red
$0.10 \times 0.10 \times 0.10$ mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.456$, $T_{max} = 0.810$
2616 measured reflections

1215 independent reflections
686 reflections with $F^2 > 2\sigma(F^2)$
$R_{int} = 0.043$
$\theta_{max} = 27.4^\circ$
$h = -16 \rightarrow 16$
$k = -13 \rightarrow 13$
$l = -5 \rightarrow 5$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.066$
$S = 0.89$
1215 reflections
75 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0268P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ e Å^{-3}
Absolute structure: Flack (1983), 564 Friedel pairs
Flack parameter = 0.53 (6)

Table 1
Selected geometric parameters (Å, °).

Ag1—Cl1	2.535 (3)	Ag1—N1	2.396 (5)
Cl1—Ag1—Cl1^{i}	115.10 (5)	Cl1—Ag1—N1^{ii}	99.0 (1)
Cl1—Ag1—N1	136.5 (1)	N1—Ag1—N1^{ii}	69.6 (2)

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···Cl1^{v}	0.93	2.88	3.765 (8)	159
C6—H6···Cl1^{vi}	0.93	2.96	3.716 (7)	140

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

H atoms are placed in calculated positions (C—H = 0.93 Å) and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$. The Flack (1983) parameter indicates inversion twinning.

Data collection and cell refinement: *PROCESS-AUTO* (Rigaku/MSC, 2004); data reduction: *CrystalStructure* (Rigaku/MSC, 2004) and *CRYSTALS* (Watkin *et al.*, 1996); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999) and *DIRDIF*99 (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *CrystalStructure*.

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