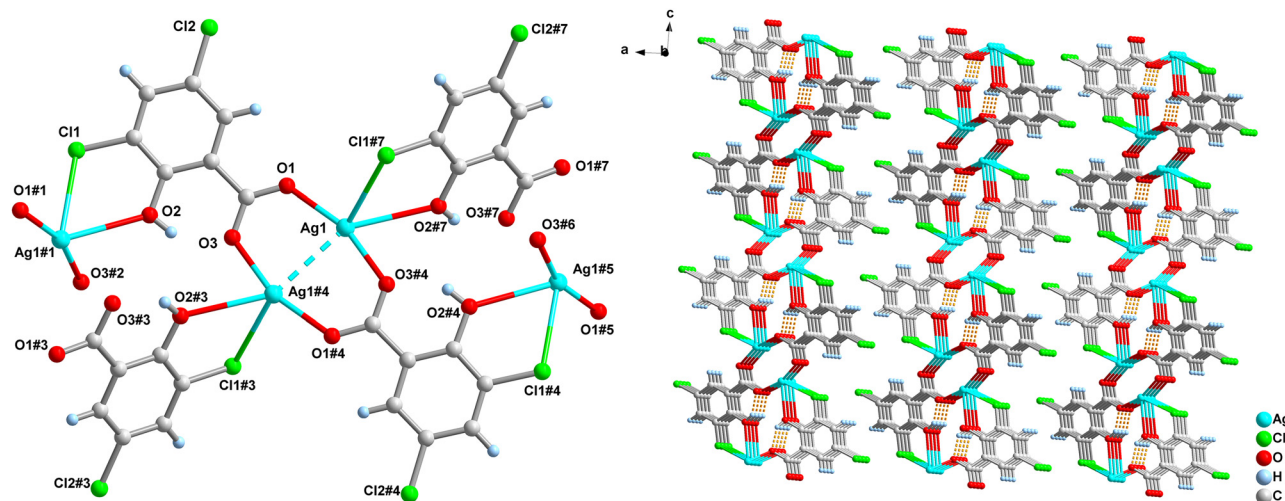


Jin-Ke Jiang and Chun-Yan Niu*

Crystal structure of poly[(μ_3 -3, 5-dichloro-2-hydroxy-benzoato- $\kappa^4 Cl, O:O':O''$) silver(I)], $C_7H_3AgCl_2O_3$



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Abstract

$C_7H_3AgCl_2O_3$, monoclinic, $P2_1/c$ (no. 14), $a = 13.1492(5) \text{ \AA}$, $b = 3.72760(10) \text{ \AA}$, $c = 16.5625(6) \text{ \AA}$, $\beta = 92.1810(10)^\circ$, $V = 811.22(5) \text{ \AA}^3$, $Z = 4$, $R_{\text{gt}}(F) = 0.0229$, $wR_{\text{ref}}(F^2) = 0.0492$, $T = 301(2) \text{ K}$.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colorless needle
Size:	$0.10 \times 0.04 \times 0.03 \text{ mm}$
Wavelength:	Mo $K\alpha$ radiation ($0.71073 \text{ \AA}$)
μ :	3.10 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	27.1° , >99 %
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{uni-que}}$, R_{int} :	27,890, 1795, 0.058
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1623
$N(\text{param})_{\text{refined}}$:	119
Programs:	Bruker [1], SHELX [2, 4], Olex2 [3], Diamond [5]

1 Source of materials

The AgNO_3 (0.170 g, 1 mmol) and Na_2CO_3 (0.052 g, 0.5 mmol) were added in 10 mL H_2O to form a spot of jade-green Ag_2CO_3 precipitate. After several minutes, the DMF solution of

2-hydroxy-3, 5-dichlorobenzoic acid (**HDBA**, 0.207 g, 1 mmol) was mixed with Ag_2CO_3 precipitate to react for 15 min and a few drops of ammonia was added in precursor to make it clear. The solution was maintained at room temperature in a dark room to obtain some crystals after several days.

2 Experimental details

The structure was solved by SHELXT [2] program within Olex2 [3] and refined by SHELXL [4]. The graphics were finished using Diamond [5].

*Corresponding author: Chun-Yan Niu, College of Food Engineering, Jilin Agricultural Science and Technology University, 132101 Jilin Jilin, China; and Jilin Province Brewing Technology Innovation Center, 132101 Jilin Jilin, China, E-mail: cyniu_jlnku@163.com. <https://orcid.org/0009-0008-0161-246X>
Jin-Ke Jiang, College of Biology and Pharmaceutical Engineering, Jilin Agricultural Science and Technology University, 132101 Jilin Jilin, China

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.06825 (2)	0.97028 (7)	0.57215 (2)	0.04894 (9)
Cl1	0.24723 (5)	0.13062 (19)	0.13438 (3)	0.03959 (15)
Cl2	0.50327 (5)	0.1217 (2)	0.39439 (4)	0.04191 (16)
O1	0.15808 (14)	0.6805 (6)	0.48567 (10)	0.0416 (4)
O2	0.10453 (13)	0.4635 (5)	0.24177 (10)	0.0395 (4)
H2	0.066300	0.555208	0.273860	0.059*
O3	0.05119 (13)	0.6967 (6)	0.37795 (11)	0.0434 (5)
C1	0.13651 (18)	0.6245 (6)	0.41305 (14)	0.0290 (5)
C2	0.21530 (17)	0.4583 (6)	0.36220 (13)	0.0264 (5)
C3	0.31102 (17)	0.3769 (6)	0.39720 (13)	0.0278 (5)
H3	0.324844	0.423754	0.451663	0.033*
C4	0.38464 (18)	0.2275 (6)	0.35094 (14)	0.0296 (5)
C5	0.36590 (18)	0.1530 (6)	0.26964 (14)	0.0299 (5)
H5	0.415991	0.050623	0.238856	0.036*
C6	0.27132 (18)	0.2340 (6)	0.23544 (13)	0.0289 (5)
C7	0.19469 (17)	0.3887 (6)	0.27974 (13)	0.0279 (5)

3 Comment

In this paper, we report a silver(I) coordination polymer, which has been synthesized by the volatilization of solution. As is depicted in the left part of the figure, the Ag1 is four-coordinated by two oxygen atoms from two **HDBA** ligands desperately, one oxygen atom from hydroxyl and a chlorine atom coming from the one **HDBA** ligand. The bond distances of Ag–O range from 2.178 to 2.842 Å within the normal range of the literatures which have reported [6–9]. The distance of Ag1–Cl1 is 2.938 Å. At the same time, the distance among silver atoms (Ag1 ... Ag1#4) is 2.942 Å. There is a $\text{Ag}_2\text{O}_4\text{C}_2$ plane among two **HDBA** ligands connected with two silver atoms. Above all, the interactions furnish a layered coordination polymer (*cf.* right part of the figure) (symmetry codes: #1 = $x, 1.5 - y, -0.5 + z$; #2 = $-x, -0.5 + y, 0.5 - z$; #3 = $-x, 0.5 + y,$

$0.5 - z$; #4 = $-x, 2 - y, 1 - z$; #5 = $-x, 0.5 + y, 1.5 - z$; #6 = $x, 2.5 - y, 0.5 + z$; #7 = $x, 1.5 - y, 0.5 + z$).

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