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Bis[aqua(4-chlorobenzoato)silver(I)](*Ag—Ag*)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.055
wR factor = 0.130
Data-to-parameter ratio = 19.6

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

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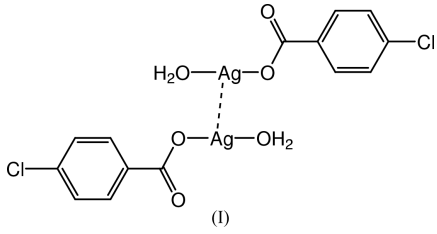
The title compound, $[Ag_2(C_7H_6ClO_3)_2(H_2O)_2]$, is a centrosymmetric dimeric complex held together by a short Ag···Ag contact. The Ag^I atom is coordinated by two O atoms, one from the water molecule and the other from the benzoate moiety, in a nearly linear geometry. The crystal structure is composed of molecular columns which are stabilized by two types of O—H···O hydrogen bonds. Intermolecular Ag···Ag and Ag···O short contacts are also observed.

Comment

The study of the structures and properties of *d*-metal-carboxylates is an important research branch of chemistry. Among different 'hot' topics currently being studied, silver(I)–carboxylate complexes have been widely reported (Zhu *et al.*, 1999; Zheng *et al.*, 2001; Zheng *et al.*, 2001). In these studies, we have reported and structurally characterized a few silver(I) complexes containing carboxylate anions; some of the complexes have special properties. Recently, we reported the crystal structure of a silver complex with 4-fluorobenzoate, and it was found that this complex has significant antitumor activity (Zhu *et al.*, 2003). We have also prepared an analogous silver(I)–carboxylate complex, *viz*. the title compound, (I), whose crystal structure is reported here.



(I)

In the title complex, the Ag atom is coordinated by two O atoms, one from the water molecule and the other from the benzoate moiety, in a nearly linear geometry, O1—Ag1—O1*W* being 174.1 (2)°. The Ag—O bond distances [Ag1—O1 2.103 (5) Å and Ag1—O1*W* 2.109 (5) Å] are significantly shorter than those in other silver(I) complexes with terephthalate [2.175 (3)–2.191 (2) Å; Zhu *et al.*, 2003]. The benzoate moiety is planar, with the carboxylate O atoms deviating by −0.027 (5) Å (O1) and −0.031 (6) Å (O2) from the mean plane.

The asymmetric unit consists of one half of the dimeric complex (Fig. 1), the other half being generated by an inversion center. The dimer is held together by a short Ag···Ag($-x$, $1-y$, $-z$) contact [3.118 (1) Å]. This contact is much shorter than that in the silver(I) complexes with terephthalate [3.277 (7)–3.489 (7) Å].

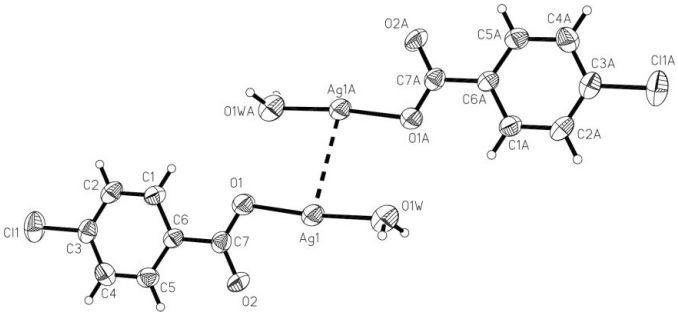


Figure 1
The structure of the title complex, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

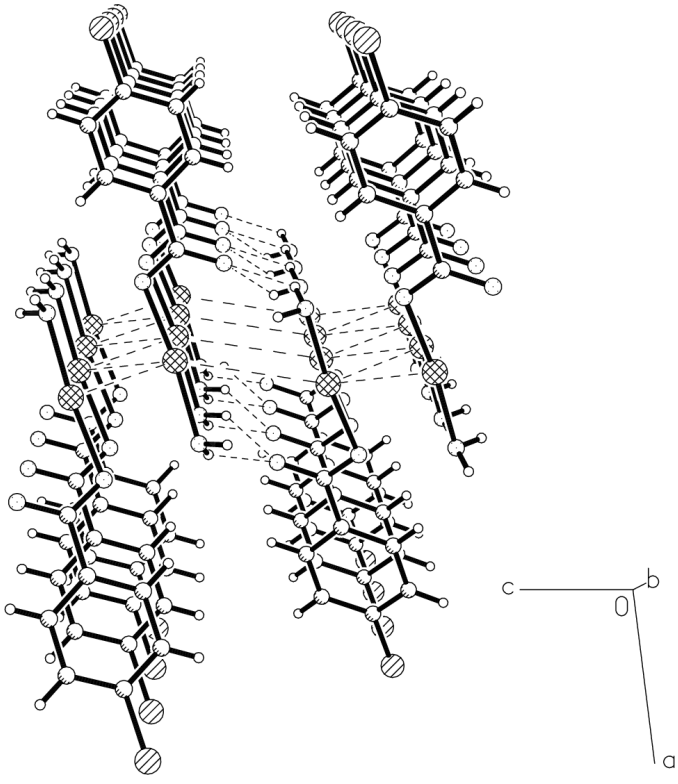


Figure 2
Packing diagram of the complex, viewed down the *b* axis, showing the column formation. The dashed lines denote the O—H···O intermolecular interactions and Ag···Ag short contacts.

In the crystal structure, the molecules are interconnected, in columns parallel to *b*, by intermolecular O1*W*—H1*W*···O2^{i} and O1*W*—H2*W*···O2^{ii} hydrogen bonds (Fig. 2; for symmetry codes see Table 2). The molecular columns are further interconnected by intermolecular Ag···Ag and Ag···O short-contacts (Table 3).

Experimental

Ag_2O (0.5 mmol, 116 mg) and 4-chlorobenzoic acid (1 mmol, 156 mg) were dissolved in aqueous ammonia (10 ml), stirring for *ca* 10 min to obtain a clear solution. After the solution had stood in air for two days with ammonia gas escaping, colorless crystals were deposited, collected and washed with water. These crystals were then dried in a vacuum desiccator over $CaCl_2$ (yield 66%). Analysis of the title complex ($C_{14}H_{12}AgCl_2O_6$) calculated: C 29.87, H 2.15%; found: C 30.05, H 2.18%.

Crystal data

$[Ag_2(C_7H_6ClO_3)_2(H_2O)_2]$	D_x = 2.139 Mg m^{-3}
M_r = 562.88	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 1762 reflections
a = 35.978 (5) Å	θ = 3.3–28.3°
b = 4.0535 (6) Å	μ = 2.57 mm^{-1}
c = 12.3204 (19) Å	T = 293 (2) K
β = 103.439 (3)°	Block, colorless
V = 1747.6 (5) Å^3	0.40 × 0.20 × 0.20 mm
Z = 4	

Data collection

Siemens SMART CCD area-detector diffractometer	2139 independent reflections
	1343 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.031
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 28.3°
	$h = -47 \rightarrow 29$
T_{min} = 0.426, T_{max} = 0.627	$k = -5 \rightarrow 5$
5101 measured reflections	$l = -15 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 8.4499P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.055	
$wR(F^2)$ = 0.130	
S = 1.09	$(\Delta/\sigma)_{max} < 0.001$
2139 reflections	$\Delta\rho_{max}$ = 1.09 e Å^{-3}
109 parameters	$\Delta\rho_{min}$ = −0.57 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å).

Cl1—C3	1.740 (7)	O2—C7	1.240 (7)
O1—C7	1.259 (8)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1*W*···O2^{i}	0.94	2.16	2.946 (8)	141
O1*W*—H2*W*···O2^{ii}	1.00	2.04	2.925 (8)	146

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

Table 3
Intermolecular Ag···Ag and Ag···O short-contact geometry (Å).

Ag1···Ag1^{i}	3.768 (1)	Ag1···O2^{iv}	3.628 (6)
Ag1···Ag1^{iii}	3.334 (1)	Ag1···O1*W*^{i}	3.475 (5)
Ag1···Ag1^{iv}	4.054 (1)		

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

All H atoms were placed geometrically, with C—H = 0.93 Å and O—H = 0.94–1.00 Å. They were treated as riding atoms, with U_{iso}(H) = 1.2U_{eq}(C) and U_{iso}(H) = 1.5U_{eq}(O). The maximum and minimum electron-density peaks are located at 1.00 and 1.19 Å from Ag1 and H2*W*, respectively.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL, PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

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