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Poly[(μ_3-quinoline-6-carboxylato-κ^3N:O:O')silver(I)]

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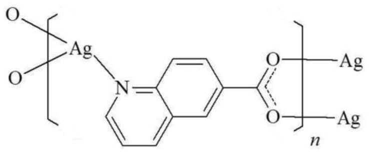
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.027; wR factor = 0.075; data-to-parameter ratio = 13.2.

In the title coordination polymer, $[Ag(C_{10}H_6NO_2)]_n$, the Ag^I cation is coordinated by two O atoms and one N atom from three 6-quinolinecarboxylate anions in a distorted T-shaped $AgNO_2$ geometry, in which the O—Ag—O angle is 160.44 (9)°. The 6-quinolinecarboxylate anion bridges three Ag$^+$ cations, forming a nearly planar polymeric sheet parallel to (101). The distance between Ag$^+$ cations bridged by the carboxyl group is 2.9200 (5) Å. In the crystal, π–π stacking is observed between parallel quinoline ring systems, the centroid–centroid distance being 3.7735 (16) Å.

Related literature

For background to coordination polymers with organic ligands, see: Kitagawa *et al.* (2004); Chiang *et al.* (2008); Yeh *et al.* (2008, 2009); Hsu *et al.* (2009). For related pyridinecarboxylate structures, see: Yeh *et al.* (2004); Ockwig *et al.* (2005); Chen *et al.* (2008); Hirano *et al.* (2002) and for related 6-quinolinecarboxylate structures, see: Lin & Maggard (2007); Du *et al.* (2008*a*,*b*); Hu *et al.* (2008); Xu *et al.* (2009).



Experimental

Crystal data

$[Ag(C_{10}H_6NO_2)]$
M_r = 280.03
Monoclinic, $C2/c$
a = 13.0008 (10) Å
b = 14.3900 (11) Å
c = 9.3431 (7) Å
β = 103.446 (1)°
V = 1700.0 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.34 mm^{-1}
T = 294 K
0.39 × 0.28 × 0.25 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.471, T_{max} = 1.000
4717 measured reflections
1674 independent reflections
1543 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.075
S = 1.08
1674 reflections
127 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.94 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ag—O1^i	2.2067 (19)	Ag—N	2.397 (2)
Ag—O2^{ii}	2.252 (2)		

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

Data collection: *APEX2* (Bruker, 2010); cell refinement: *SAINT* (Bruker, 2010); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5546).

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supplementary materials

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Poly[(μ_3-quinoline-6-carboxylato-κ^3*N*:*O*:*O*′)silver(I)]

Chun-Wei Yeh, Ay Jong, Chi-Hui Tsou, Fu-Chang Huang and Maw-Cherng Suen

Comment

The synthesis of metal coordination polymers has been a subject of intense research due to their interesting structural chemistry and potential applications in gas storage, separation, catalysis, magnetism, luminescence, and drug delivery (Kitagawa *et al.*, 2004). Roles of anion, solvent and ligand comformations in self-assembly of coordination complexes containing polydentate nitrogen ligands are very intersting (Chiang *et al.*, 2008; Yeh *et al.*, 2008; Hsu *et al.*, 2009; Yeh *et al.*, 2009). In the past, the pyridinecarboxylate ligands have been subjected to many studies of its coordination ability to metal centers (Yeh *et al.*, 2004; Ockwig *et al.*, 2005; Chen *et al.*, 2008; Hirano *et al.*, 2002). The various metal complexes containing 6-quinolinecarboxylate (*L*-) ligands have been reported, which show various multi-dimensional frameworks (Lin & Maggard, 2007; Du *et al.*, 2008*a,b*; Hu *et al.*, 2008; Xu *et al.*, 2009). The Ag^+ cations are coordinated with two N atoms from two 1,2-bis(4,4-dimethyl-4,5-dihydrooxazol-2-yl)ethane (*L*) ligands (Fig. 1). The Ag···Ag distances separated by the bridging *L*- anions are 2.9200 (5), 9.974 (1) and 10.469 (1) Å, while the unit of dinuclear Ag^+ are forming (4,4) polymeric nets (Fig. 2). The two-dimensional polymeric nets are interlinking through Ag···O interactions [2.954 (2) Å] and pi—pi stacking interactions in the crystal structure (Fig. 3).

Experimental

An aqueous solution (5.0 ml) of $AgNO_3$ (1.0 mmol) was layered carefully over a methanolic solution (5.0 ml) of 6-quinolinecarboxylic acid (1.0 mmol) in a tube and kept it in the dark. Colourless crystals were obtained after several weeks.

Refinement

All the H atoms were constrained to ideal geometries, with C—H = 0.93 Å (aromatic) and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

Computing details

Data collection: *APEX2* (Bruker, 2010); cell refinement: *SAINT* (Bruker, 2010); data reduction: *SAINT* (Bruker, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

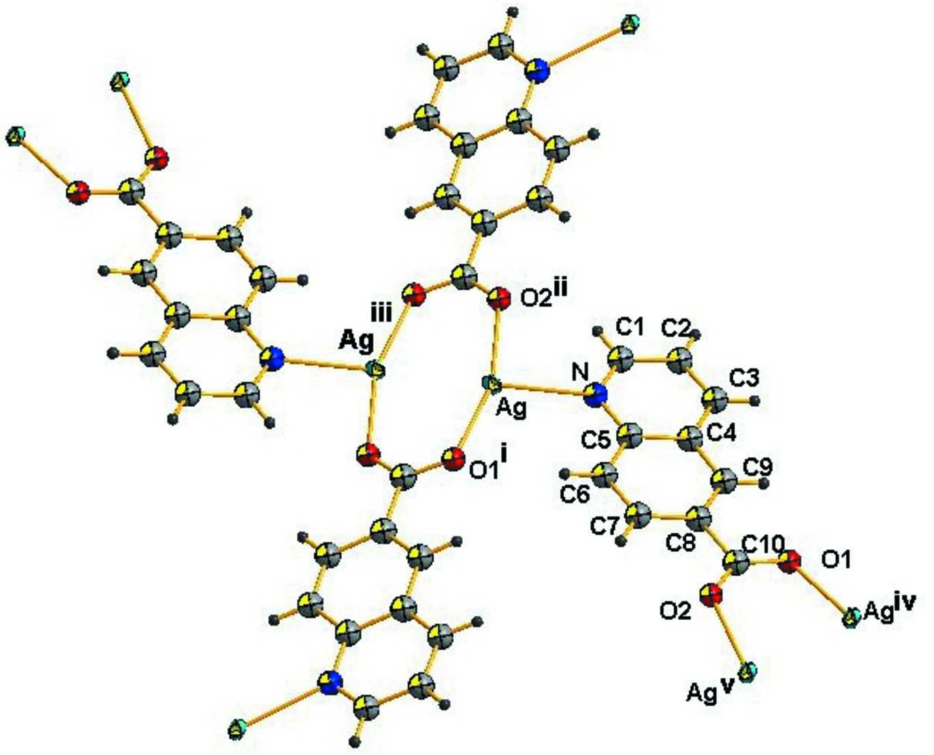

Figure 1

A portion of the two-dimensional grid. Ellipsoids are drawn at 30% probability level. Symmetry codes: (i) -*x* + 1/2,*y* + 1/2,-*z* + 1/2;(ii) *x* + 1/2,-*y* + 1/2,*z* - 1/2; (iii) -*x* + 1,-*y* + 1,-*z*; (iv) -*x* + 1/2,*y* - 1/2,-*z* + 1/2; (v) *x* - 1/2,-*y* + 1/2,*z* + 1/2.

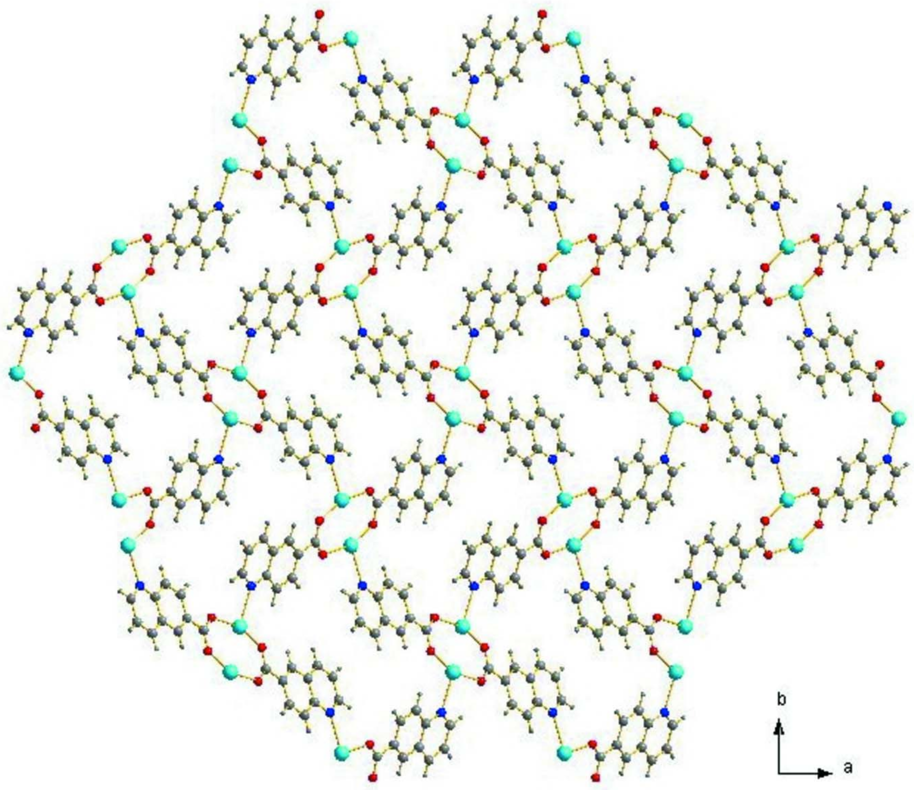

Figure 2

The view shows the pleated (4,4) net along (001) direction.

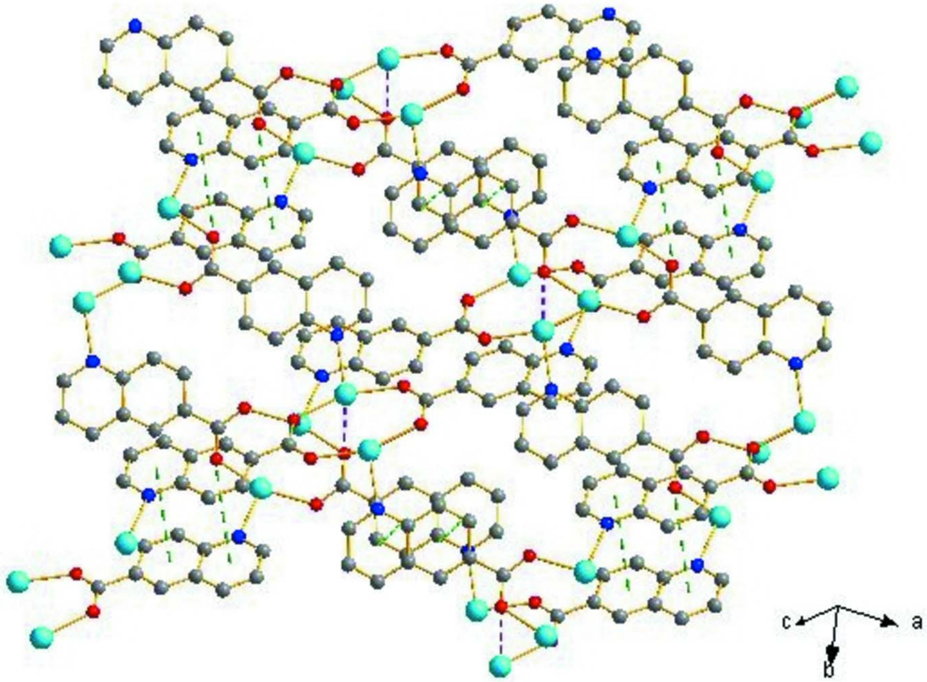

Figure 3

The packing diagram shows the Ag···O interactions and *π*-*π* stacking interactions between the two-dimensional networks.

Poly[(μ_3-quinoline-6-carboxylato-κ^3N:O:O')silver(I)]

Crystal data

[Ag($C_{10}H_6NO_2$)]	$F(000) = 1088$
$M_r = 280.03$	$D_x = 2.188$ Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *Kα* radiation, $\lambda = 0.71073$ Å
Hall symbol: -C 2yc	Cell parameters from 3671 reflections
$a = 13.0008$ (10) Å	$\theta = 2.2$–$26.0°$
$b = 14.3900$ (11) Å	$\mu = 2.34$ mm^{-1}
$c = 9.3431$ (7) Å	$T = 294$ K
$\beta = 103.446$ (1)°	Block, colourless
$V = 1700.0$ (2) Å^3	0.39 × 0.28 × 0.25 mm
$Z = 8$	

Data collection

Bruker APEXII CCD diffractometer	4717 measured reflections
Radiation source: fine-focus sealed tube	1674 independent reflections
Graphite monochromator	1543 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\rm int} = 0.021$
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	$\theta_{\rm max} = 26.0°$, $\theta_{\rm min} = 2.1°$
	$h = -16 \rightarrow 7$
	$k = -17 \rightarrow 17$
$T_{\rm min} = 0.471$, $T_{\rm max} = 1.000$	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.075$
$S = 1.08$
1674 reflections
127 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 2.6516P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.37$ e Å^{-3}
$\Delta\rho_{\min} = -0.94$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
Ag	0.47914 (2)	0.410289 (16)	0.06057 (3)	0.04647 (13)
O1	0.12021 (17)	−0.00759 (14)	0.3242 (2)	0.0426 (5)
O2	0.1053 (2)	0.12550 (16)	0.4404 (3)	0.0530 (6)
N	0.42688 (18)	0.25041 (16)	0.0564 (2)	0.0345 (5)
C1	0.4658 (2)	0.2003 (2)	−0.0380 (3)	0.0422 (7)
H1A	0.5138	0.2286	−0.0840	0.051*
C2	0.4390 (3)	0.1078 (2)	−0.0724 (4)	0.0460 (7)
H2A	0.4675	0.0765	−0.1412	0.055*
C3	0.3706 (2)	0.0635 (2)	−0.0040 (3)	0.0398 (6)
H3A	0.3529	0.0015	−0.0243	0.048*
C4	0.3274 (2)	0.11373 (19)	0.0982 (3)	0.0303 (5)
C5	0.3568 (2)	0.20801 (18)	0.1252 (3)	0.0298 (5)
C6	0.3125 (2)	0.25912 (18)	0.2252 (3)	0.0328 (5)
H6A	0.3305	0.3213	0.2434	0.039*
C7	0.2435 (2)	0.21763 (19)	0.2955 (3)	0.0326 (5)
H7A	0.2150	0.2522	0.3610	0.039*
C8	0.2145 (2)	0.12338 (19)	0.2705 (3)	0.0297 (5)
C9	0.2555 (2)	0.07253 (19)	0.1723 (3)	0.0320 (5)
H9A	0.2360	0.0107	0.1544	0.038*
C10	0.1398 (2)	0.07663 (19)	0.3510 (3)	0.0324 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag	0.0560 (2)	0.03486 (17)	0.0611 (2)	0.00687 (9)	0.03898 (14)	−0.00040 (9)
O1	0.0516 (12)	0.0344 (11)	0.0518 (11)	−0.0060 (9)	0.0324 (10)	−0.0010 (9)

O2	0.0695 (15)	0.0394 (12)	0.0698 (15)	−0.0088 (11)	0.0563 (13)	−0.0094 (11)
N	0.0351 (12)	0.0319 (12)	0.0425 (12)	−0.0010 (9)	0.0209 (10)	0.0046 (9)
C1	0.0440 (16)	0.0419 (16)	0.0501 (15)	−0.0009 (13)	0.0304 (13)	0.0016 (13)
C2	0.0533 (19)	0.0432 (16)	0.0529 (18)	0.0022 (14)	0.0354 (15)	−0.0056 (13)
C3	0.0457 (16)	0.0351 (14)	0.0453 (15)	−0.0009 (13)	0.0246 (13)	−0.0048 (12)
C4	0.0313 (13)	0.0293 (12)	0.0342 (13)	0.0022 (10)	0.0159 (10)	0.0024 (10)
C5	0.0293 (12)	0.0313 (13)	0.0319 (12)	0.0013 (10)	0.0135 (10)	0.0040 (10)
C6	0.0377 (14)	0.0260 (12)	0.0380 (13)	−0.0021 (10)	0.0158 (11)	−0.0021 (10)
C7	0.0359 (13)	0.0328 (14)	0.0334 (12)	0.0022 (11)	0.0168 (10)	−0.0018 (10)
C8	0.0306 (12)	0.0300 (13)	0.0327 (12)	0.0021 (11)	0.0158 (10)	0.0041 (10)
C9	0.0364 (14)	0.0270 (12)	0.0377 (13)	−0.0004 (10)	0.0193 (11)	0.0009 (10)
C10	0.0323 (13)	0.0349 (14)	0.0358 (13)	0.0022 (11)	0.0196 (11)	0.0046 (10)

Geometric parameters (Å, º)

Ag—O1^{i}	2.2067 (19)	C2—H2A	0.9300
Ag—O2^{ii}	2.252 (2)	C3—C4	1.414 (4)
Ag—N	2.397 (2)	C3—H3A	0.9300
Ag—Ag^{iii}	2.9200 (5)	C4—C5	1.416 (4)
O1—C10	1.252 (3)	C4—C9	1.415 (4)
O1—Ag^{iv}	2.2067 (19)	C5—C6	1.413 (4)
O2—C10	1.252 (4)	C6—C7	1.366 (4)
O2—Ag^{v}	2.252 (2)	C6—H6A	0.9300
N—C1	1.327 (4)	C7—C8	1.412 (4)
N—C5	1.374 (3)	C7—H7A	0.9300
C1—C2	1.395 (5)	C8—C9	1.375 (4)
C1—H1A	0.9300	C8—C10	1.517 (4)
C2—C3	1.367 (5)	C9—H9A	0.9300

O1^{i}—Ag—O2^{ii}	160.44 (9)	C5—C4—C9	119.7 (2)
O1^{i}—Ag—N	109.04 (8)	C3—C4—C9	121.8 (3)
O2^{ii}—Ag—N	90.51 (8)	N—C5—C4	121.6 (2)
O1^{i}—Ag—Ag^{iii}	84.15 (5)	N—C5—C6	119.7 (2)
O2^{ii}—Ag—Ag^{iii}	77.68 (6)	C4—C5—C6	118.8 (2)
N—Ag—Ag^{iii}	156.92 (6)	C7—C6—C5	120.3 (2)
C10—O1—Ag^{iv}	122.44 (18)	C7—C6—H6A	119.8
C10—O2—Ag^{v}	128.3 (2)	C5—C6—H6A	119.8
C1—N—C5	117.8 (2)	C6—C7—C8	121.3 (2)
C1—N—Ag	112.45 (18)	C6—C7—H7A	119.3
C5—N—Ag	129.42 (18)	C8—C7—H7A	119.3
N—C1—C2	123.9 (3)	C9—C8—C7	119.4 (2)
N—C1—H1A	118.0	C9—C8—C10	119.2 (2)
C2—C1—H1A	118.0	C7—C8—C10	121.4 (2)
C3—C2—C1	119.5 (3)	C8—C9—C4	120.4 (3)
C3—C2—H2A	120.3	C8—C9—H9A	119.8
C1—C2—H2A	120.3	C4—C9—H9A	119.8
C2—C3—C4	118.8 (3)	O1—C10—O2	126.1 (3)
C2—C3—H3A	120.6	O1—C10—C8	117.1 (2)

C4—C3—H3A	120.6	O2—C10—C8	116.9 (2)
C5—C4—C3	118.4 (2)		

Symmetry codes: (i) $-x+1/2, y+1/2, -z+1/2$; (ii) $x+1/2, -y+1/2, z-1/2$; (iii) $-x+1, -y+1, -z$; (iv) $-x+1/2, y-1/2, -z+1/2$; (v) $x-1/2, -y+1/2, z+1/2$.