

catena-Poly[[bis[(2-carboxybenzoato- κ O)silver(I)](Ag—Ag)]bis(μ -isonicotinic acid- κ^2 N:O)]

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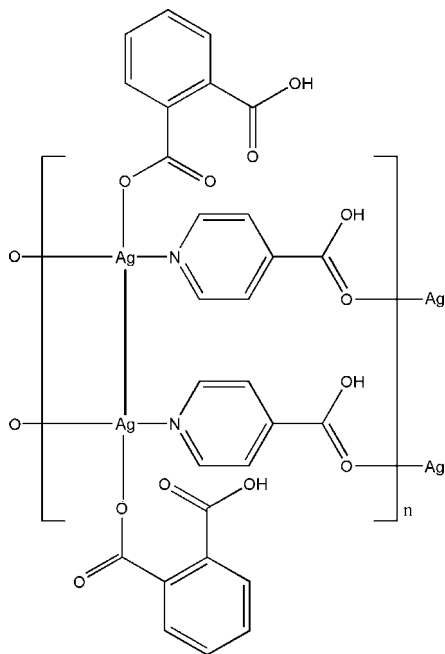
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.043; wR factor = 0.120; data-to-parameter ratio = 15.3.

The title compound, $[\text{Ag}(\text{C}_8\text{H}_5\text{O}_4)(\text{C}_6\text{H}_5\text{NO}_2)]_n$, contains one Ag^{I} atom, one phthalate ligand and one isonicotinic acid molecule in the asymmetric unit. Each Ag atom is three-coordinated in a T-shaped geometry by two O atoms and one N atom from one phthalate ligand and two isonicotinic acid ligands. The isonicotinic acid ligand bridges two Ag atoms, forming a one-dimensional chain. Adjacent chains are linked by Ag—Ag interactions, leading to a double-chain. These double-chains are further linked *via* hydrogen bonds into a two-dimensional layer.

Related literature

 For related literature, see: He *et al.* (2007); Xie *et al.* (2005).


Experimental

Crystal data

$[\text{Ag}(\text{C}_8\text{H}_5\text{O}_4)(\text{C}_6\text{H}_5\text{NO}_2)]$
 $M_r = 396.10$
 Monoclinic, $C2/c$
 $a = 13.540$ (3) Å
 $b = 8.160$ (2) Å
 $c = 24.223$ (5) Å
 $\beta = 99.546$ (15)°

$V = 2639$ (1) Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 1.56$ mm⁻¹
 $T = 293$ (2) K
 $0.37 \times 0.32 \times 0.27$ mm

Data collection

Siemens P4 four-circle diffractometer
 Absorption correction: ψ scan (North *et al.*, 1968)
 $T_{\text{min}} = 0.597$, $T_{\text{max}} = 0.680$
 3909 measured reflections

3037 independent reflections
 1879 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$
 3 standard reflections every 97 reflections
 intensity decay: 1.0%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.119$
 $S = 1.00$
 3037 reflections

199 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.99$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.71$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ag1—N1	2.179 (4)	Ag1—O2 ⁱ	2.621 (3)
Ag1—O3	2.185 (3)	Ag1—Ag1 ⁱⁱ	3.2123 (11)
N1—Ag1—O3	164.57 (14)	O3—Ag1—O2 ⁱ	101.74 (11)
N1—Ag1—O2 ⁱ	93.52 (12)		

 Symmetry codes: (i) $x, y - 1, z$; (ii) $-x + 1, y, -z + \frac{3}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1A \cdots O6 ⁱⁱⁱ	0.82	1.80	2.616 (5)	175
O5—H5A \cdots O4	0.82	1.57	2.390 (5)	180

 Symmetry code: (iii) $x, -y + 1, z - \frac{1}{2}$.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2121).

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supplementary materials

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***catena*-Poly[[bis[(2-carboxybenzoato- κ O)silver(I)](*Ag*-*Ag*)]bis(μ -isonicotinic acid- κ^2 N:O)]**

X.-F. Li, Y. An and Y.-S. Yin

Comment

Silver ion reacts with isonicotinic acid and imidazole under hydrothermal conditions to form $[\text{Ag}_8(\text{in})_6(\text{NO}_3)_2]$ and $[\text{Ag}(\text{in})(\text{Hin})]_{0.5}[\text{Ag}(\text{in})]$ (Hin = isonicotinic acid) (Xie *et al.*, 2005). With phthalic acid in place of imidazole, the reaction yields the title compound.

In the title compound, the Ag^{I} atom is three-coordinated by two O atoms and one N atom from one phthalate ligand and two isonicotinic acid ligands in a T-like geometry, with an O—Ag—N bond angle being $164.57(14)^\circ$ (Fig. 1; Table 1), giving a chain structure. Furthermore, the adjacent chains are linked by $\text{Ag}\cdots\text{Ag}$ interactions (He *et al.*, 2007) to form a one-dimensional double-chain (Fig. 2). These double-chains are further linked *via* O—H \cdots O hydrogen bonds (Table 2) into a two-dimensional layer. The hydrogen bonding interactions enhance the stability of the complex.

Experimental

A mixture of $\text{Ag}(\text{NO}_3)$ (0.085 g, 0.5 mmol), isonicotinic acid (0.123 g, 1 mmol), phthalic acid (0.166 g, 1 mmol) and water (10 ml) was sealed in a 23 ml Teflon-lined reactor, which was heated at 473 K for 4 d and then cooled to room temperature at a rate of 5 K h^{-1} (yield 72%). Analysis calculated for $\text{C}_{14}\text{H}_{10}\text{AgNO}_6$: C 42.45, H 2.54, N 3.54%; found: C 42.39, H 2.61, N 3.48%.

Refinement

H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 and O—H = 0.82 \AA and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{O})$.

Figures

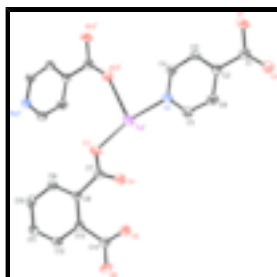


Fig. 1. The coordination geometry of the Ag atom in the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $x, -1 + y, z$.]



Fig. 2. The one-dimensional double-chain connected by $\text{Ag}\cdots\text{Ag}$ interactions.

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Crystal data

[Ag(C₈H₅O₄)(C₆H₅NO₂)]

$M_r = 396.10$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 13.540\ (3)\ \text{\AA}$

$b = 8.160\ (2)\ \text{\AA}$

$c = 24.223\ (5)\ \text{\AA}$

$\beta = 99.546\ (15)^\circ$

$V = 2639\ (1)\ \text{\AA}^3$

$Z = 8$

$F_{000} = 1568$

$D_x = 1.994\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 28 reflections

$\theta = 5.2\text{--}12.4^\circ$

$\mu = 1.56\ \text{mm}^{-1}$

$T = 293\ (2)\ \text{K}$

Block, purple

$0.37 \times 0.32 \times 0.27\ \text{mm}$

Data collection

Siemens P4 four-circle
diffractometer

Radiation source: medium-focus sealed tube

Monochromator: graphite

$T = 293(2)\ \text{K}$

ω - 2θ scans

Absorption correction: ψ scan
(North *et al.*, 1968)

$T_{\min} = 0.597$, $T_{\max} = 0.680$

3909 measured reflections

3037 independent reflections

1879 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.034$

$\theta_{\max} = 27.5^\circ$

$\theta_{\min} = 1.7^\circ$

$h = -17 \rightarrow 1$

$k = -1 \rightarrow 10$

$l = -31 \rightarrow 31$

3 standard reflections

every 97 reflections

intensity decay: 1.0%

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.119$

$S = 1.00$

3037 reflections

199 parameters

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

$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.99\ \text{e \AA}^{-3}$

$\Delta\rho_{\min} = -0.71\ \text{e \AA}^{-3}$

Extinction correction: none

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.40822 (3)	0.04719 (5)	0.698630 (15)	0.05417 (17)
C1	0.4164 (4)	0.7535 (6)	0.58243 (19)	0.0405 (11)
C2	0.4211 (3)	0.5872 (5)	0.60835 (17)	0.0347 (10)
C3	0.4339 (4)	0.4453 (6)	0.57882 (17)	0.0397 (10)
H3A	0.4417	0.4514	0.5415	0.048*
C4	0.4348 (4)	0.2962 (6)	0.60478 (18)	0.0413 (11)
H4A	0.4430	0.2020	0.5844	0.050*
C5	0.4137 (4)	0.4183 (6)	0.68640 (19)	0.0442 (12)
H5B	0.4070	0.4087	0.7239	0.053*
C6	0.4119 (4)	0.5724 (6)	0.66396 (19)	0.0455 (12)
H6A	0.4046	0.6644	0.6856	0.055*
C7	0.3575 (4)	-0.0952 (6)	0.80056 (17)	0.0383 (11)
C8	0.3373 (3)	-0.2215 (5)	0.84252 (16)	0.0307 (9)
C9	0.3225 (3)	-0.3796 (6)	0.82196 (17)	0.0368 (10)
H9A	0.3240	-0.3975	0.7842	0.044*
C10	0.3056 (4)	-0.5119 (6)	0.8547 (2)	0.0437 (11)
H10A	0.2958	-0.6164	0.8394	0.052*
C11	0.3036 (4)	-0.4842 (6)	0.9109 (2)	0.0453 (12)
H11A	0.2927	-0.5711	0.9340	0.054*
C12	0.3177 (4)	-0.3304 (6)	0.93258 (18)	0.0403 (11)
H12A	0.3159	-0.3145	0.9704	0.048*
C13	0.3346 (3)	-0.1963 (5)	0.89994 (17)	0.0321 (9)
C14	0.3497 (4)	-0.0355 (6)	0.93203 (18)	0.0411 (11)
N1	0.4245 (3)	0.2820 (5)	0.65827 (15)	0.0414 (9)
O1	0.3992 (3)	0.7496 (5)	0.52779 (12)	0.0626 (11)
H1A	0.3896	0.8431	0.5156	0.094*
O2	0.4267 (3)	0.8778 (4)	0.60899 (13)	0.0513 (9)
O3	0.3817 (3)	-0.1459 (4)	0.75691 (13)	0.0579 (10)
O4	0.3483 (3)	0.0565 (4)	0.80925 (14)	0.0619 (11)
O5	0.3438 (3)	0.1015 (4)	0.90631 (14)	0.0579 (10)
H5A	0.3454	0.0858	0.8730	0.087*
O6	0.3672 (3)	-0.0408 (4)	0.98320 (13)	0.0641 (11)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0797 (3)	0.0432 (2)	0.0430 (2)	0.0001 (2)	0.02032 (19)	0.01176 (18)
C1	0.046 (3)	0.038 (3)	0.037 (2)	0.002 (2)	0.007 (2)	0.002 (2)
C2	0.037 (2)	0.037 (2)	0.030 (2)	-0.001 (2)	0.0055 (18)	0.0028 (18)
C3	0.055 (3)	0.036 (2)	0.028 (2)	-0.003 (2)	0.008 (2)	0.0023 (19)
C4	0.055 (3)	0.037 (2)	0.034 (2)	0.000 (2)	0.012 (2)	-0.0002 (19)
C5	0.061 (3)	0.039 (3)	0.034 (2)	-0.002 (2)	0.012 (2)	0.0022 (19)
C6	0.065 (3)	0.042 (3)	0.031 (2)	0.005 (3)	0.014 (2)	-0.002 (2)
C7	0.046 (3)	0.042 (3)	0.027 (2)	-0.001 (2)	0.0060 (19)	0.0026 (19)

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C8	0.038 (2)	0.028 (2)	0.0250 (18)	-0.0007 (19)	0.0035 (17)	0.0007 (17)
C9	0.050 (3)	0.034 (2)	0.0278 (19)	-0.001 (2)	0.0098 (19)	-0.0021 (18)
C10	0.045 (3)	0.027 (2)	0.057 (3)	-0.003 (2)	0.004 (2)	-0.001 (2)
C11	0.058 (3)	0.037 (3)	0.042 (2)	-0.005 (2)	0.009 (2)	0.010 (2)
C12	0.051 (3)	0.040 (3)	0.030 (2)	-0.003 (2)	0.007 (2)	0.0033 (19)
C13	0.038 (2)	0.028 (2)	0.031 (2)	0.002 (2)	0.0056 (18)	0.0000 (17)
C14	0.053 (3)	0.036 (3)	0.035 (2)	-0.004 (2)	0.012 (2)	-0.006 (2)
N1	0.053 (2)	0.038 (2)	0.0349 (18)	-0.0020 (19)	0.0101 (18)	0.0034 (17)
O1	0.112 (3)	0.042 (2)	0.0295 (16)	-0.002 (2)	-0.0001 (19)	0.0104 (15)
O2	0.075 (3)	0.0364 (18)	0.0425 (18)	0.0043 (19)	0.0082 (17)	0.0005 (16)
O3	0.101 (3)	0.0417 (19)	0.0379 (17)	0.004 (2)	0.0313 (19)	0.0044 (16)
O4	0.116 (3)	0.0339 (18)	0.0379 (17)	-0.003 (2)	0.019 (2)	0.0053 (15)
O5	0.107 (3)	0.0303 (17)	0.0380 (17)	-0.006 (2)	0.017 (2)	-0.0037 (15)
O6	0.117 (3)	0.047 (2)	0.0278 (15)	-0.004 (2)	0.0086 (19)	-0.0078 (16)

Geometric parameters (\AA , $^\circ$)

Ag1—N1	2.179 (4)	C7—O4	1.265 (6)
Ag1—O3	2.185 (3)	C7—C8	1.504 (6)
Ag1—O2 ⁱ	2.621 (3)	C8—C9	1.385 (6)
Ag1—Ag1 ⁱⁱ	3.2123 (11)	C8—C13	1.412 (5)
C1—O2	1.197 (6)	C9—C10	1.380 (6)
C1—O1	1.306 (5)	C9—H9A	0.9300
C1—C2	1.492 (6)	C10—C11	1.387 (7)
C2—C6	1.379 (6)	C10—H10A	0.9300
C2—C3	1.386 (6)	C11—C12	1.361 (7)
C3—C4	1.368 (6)	C11—H11A	0.9300
C3—H3A	0.9300	C12—C13	1.391 (6)
C4—N1	1.331 (5)	C12—H12A	0.9300
C4—H4A	0.9300	C13—C14	1.521 (6)
C5—N1	1.325 (6)	C14—O6	1.223 (5)
C5—C6	1.368 (7)	C14—O5	1.276 (6)
C5—H5B	0.9300	O1—H1A	0.8200
C6—H6A	0.9300	O5—H5A	0.8200
C7—O3	1.229 (5)		
N1—Ag1—O3	164.57 (14)	C9—C8—C7	115.3 (3)
N1—Ag1—O2 ⁱ	93.52 (12)	C13—C8—C7	127.1 (4)
O3—Ag1—O2 ⁱ	101.74 (11)	C10—C9—C8	123.4 (4)
N1—Ag1—Ag1 ⁱⁱ	102.98 (11)	C10—C9—H9A	118.3
O3—Ag1—Ag1 ⁱⁱ	71.85 (11)	C8—C9—H9A	118.3
O2—C1—O1	123.4 (4)	C9—C10—C11	117.9 (4)
O2—C1—C2	123.5 (4)	C9—C10—H10A	121.0
O1—C1—C2	113.1 (4)	C11—C10—H10A	121.0
C6—C2—C3	118.0 (4)	C12—C11—C10	120.3 (4)
C6—C2—C1	119.1 (4)	C12—C11—H11A	119.8
C3—C2—C1	122.9 (4)	C10—C11—H11A	119.8
C4—C3—C2	119.8 (4)	C11—C12—C13	122.2 (4)
C4—C3—H3A	120.1	C11—C12—H12A	118.9

C2—C3—H3A	120.1	C13—C12—H12A	118.9
N1—C4—C3	122.0 (4)	C12—C13—C8	118.6 (4)
N1—C4—H4A	119.0	C12—C13—C14	114.1 (4)
C3—C4—H4A	119.0	C8—C13—C14	127.3 (4)
N1—C5—C6	124.3 (4)	O6—C14—O5	120.8 (4)
N1—C5—H5B	117.9	O6—C14—C13	118.3 (4)
C6—C5—H5B	117.9	O5—C14—C13	120.9 (4)
C5—C6—C2	118.0 (5)	C5—N1—C4	117.8 (4)
C5—C6—H6A	121.0	C5—N1—Ag1	118.6 (3)
C2—C6—H6A	121.0	C4—N1—Ag1	123.3 (3)
O3—C7—O4	121.4 (4)	C1—O1—H1A	109.5
O3—C7—C8	117.0 (4)	C7—O3—Ag1	114.1 (3)
O4—C7—C8	121.6 (4)	C14—O5—H5A	109.5
C9—C8—C13	117.6 (4)		
O2—C1—C2—C6	16.8 (8)	C9—C8—C13—C12	0.2 (7)
O1—C1—C2—C6	-162.7 (4)	C7—C8—C13—C12	-178.0 (4)
O2—C1—C2—C3	-163.7 (5)	C9—C8—C13—C14	179.3 (4)
O1—C1—C2—C3	16.8 (7)	C7—C8—C13—C14	1.1 (8)
C6—C2—C3—C4	1.3 (7)	C12—C13—C14—O6	15.3 (7)
C1—C2—C3—C4	-178.2 (5)	C8—C13—C14—O6	-163.8 (5)
C2—C3—C4—N1	-0.5 (8)	C12—C13—C14—O5	-164.4 (5)
N1—C5—C6—C2	0.4 (8)	C8—C13—C14—O5	16.5 (8)
C3—C2—C6—C5	-1.3 (7)	C6—C5—N1—C4	0.4 (8)
C1—C2—C6—C5	178.3 (5)	C6—C5—N1—Ag1	-173.0 (4)
O3—C7—C8—C9	-16.1 (6)	C3—C4—N1—C5	-0.4 (7)
O4—C7—C8—C9	162.6 (5)	C3—C4—N1—Ag1	172.6 (4)
O3—C7—C8—C13	162.1 (5)	O3—Ag1—N1—C5	4.1 (8)
O4—C7—C8—C13	-19.2 (8)	Ag1 ⁱⁱ —Ag1—N1—C5	-64.4 (4)
C13—C8—C9—C10	-0.1 (7)	O3—Ag1—N1—C4	-168.9 (5)
C7—C8—C9—C10	178.3 (4)	Ag1 ⁱⁱ —Ag1—N1—C4	122.6 (4)
C8—C9—C10—C11	-0.1 (8)	O4—C7—O3—Ag1	0.9 (6)
C9—C10—C11—C12	0.3 (8)	C8—C7—O3—Ag1	179.6 (3)
C10—C11—C12—C13	-0.2 (8)	N1—Ag1—O3—C7	0.2 (8)
C11—C12—C13—C8	-0.1 (7)	Ag1 ⁱⁱ —Ag1—O3—C7	72.7 (4)
C11—C12—C13—C14	-179.3 (5)		

Symmetry codes: (i) $x, y-1, z$; (ii) $-x+1, y, -z+3/2$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1A \cdots O6 ⁱⁱⁱ	0.82	1.80	2.616 (5)	175
O5—H5A \cdots O4	0.82	1.57	2.390 (5)	180

Symmetry codes: (iii) $x, -y+1, z-1/2$.

Fig. 1

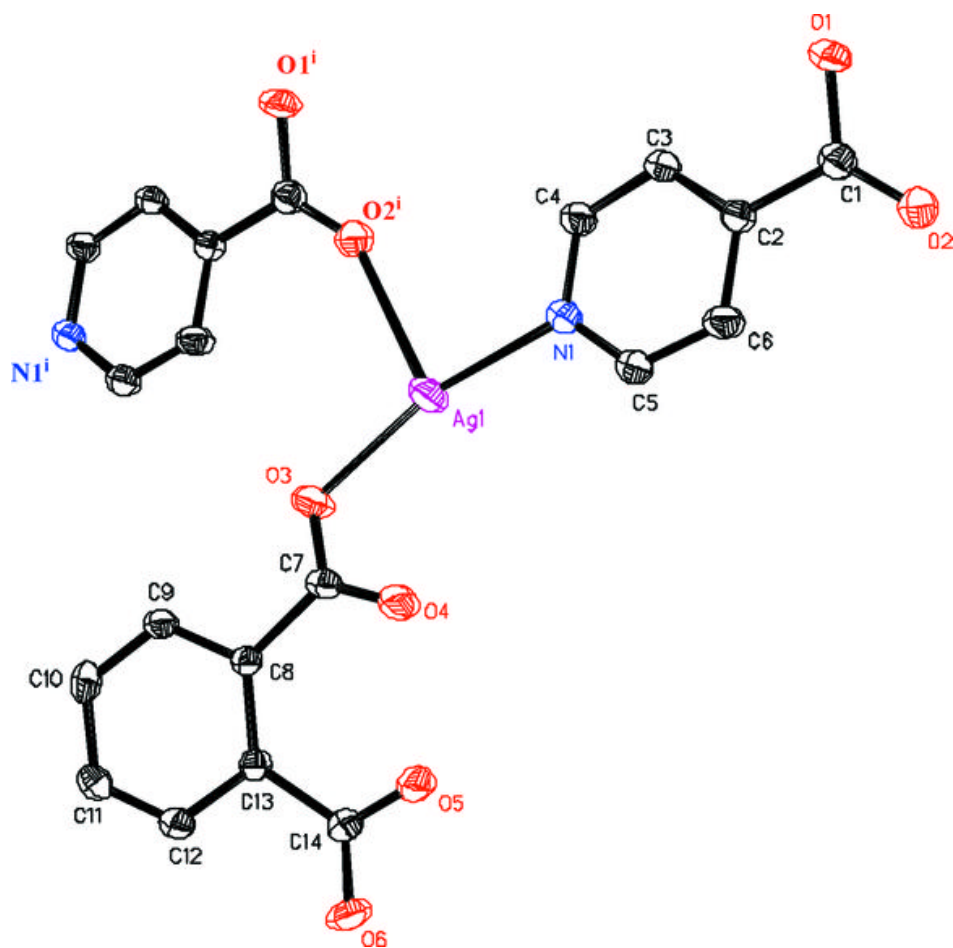


Fig. 2

