Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[silver(I)-μ-isonicotinato-κ^2O:N]

Yang-Yi Yang,[a] Zhong-Qi Huang,[a] Gang-Feng Ouyang[a] and Seik Weng Ng[b]*

[a]School of Chemistry and Chemical Engineering, Sun Yat-Sen University, Guangzhou 510275, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.012 Å
R factor = 0.058
wR factor = 0.155
Data-to-parameter ratio = 14.5

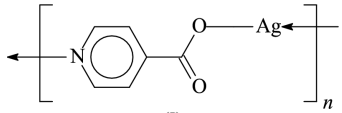
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The crystal structure of silver isonicotinate, $[Ag(C_6H_4NO_2)]_n$, consists of isonicotinate units that are each linked to adjacent Ag atoms through the O and N atoms to furnish a linear chain running parallel to the b axis of the monoclinic unit cell. The Ag atom shows linear coordination [Ag—O = 2.175 (6) Å Ag←N = 2.149 (7) Å and O—Ag←N = 170.4 (3)°].

Received 16 July 2004
Accepted 19 July 2004
Online 24 July 2004

Comment

The reaction of silver tetrafluoroborate and isonicotinic acid furnishes the co-crystal, $[C_5H_4NCO_2Ag]$ $[(C_5H_4NCO_2)(C_5H_4NCO_2H)Ag]$ (2/1); the compound is said to be mesoporous arising from a plywood motif that allows cavities to be connected in the three-dimensional network structure. The Ag atom in the $[C_5H_4NCO_2Ag]_n$ chain shows linear coordination; the atom is covalently bonded to the carboxylate O atom and datively bonded to the N atom of an adjacent anionic group [Ag—O = 2.133 (3) Å, Ag←N = 2.173 (4) Å Å and O—Ag←N = 155.6 (2)°; Cova *et al.*, 2001]. Although channels are present, the cavities are probably not particularly large as a check with *PLATON* (Spek, 2003) did not reveal any solvent-accessible voids.



(I)

The title compound, (I), has only linear $[C_5H_4NCO_2Ag]_n$ chains (Fig. 1); the bond dimensions involving the Ag atom [Ag—O = 2.175 (6) Å, Ag←N = 2.149 (7) Å and O—Ag←N = 170.4 (3)°] are similar to those found in the reported co-crystal. Also, there are no voids in the structure.

Experimental

Silver nitrate (0.085 g, 0.5 mmol) and isonicotinic acid (0.062 g, 0.5 mmol) were dissolved in water (8 ml); the pH of the solution was adjusted to 5 by the addition of trimethylamine. The mixture was placed in a 23 ml Teflon-lined digestion bomb, which was heated at

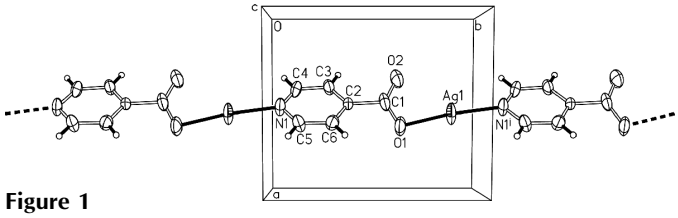


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii. [Symmetry code: (i) x, 1 + y, z.]

413 K for 24 h. The bomb was cooled slowly. The resulting product was collected and washed with water. Rod-shaped crystals were isolated in about 40% yield.

Crystal data

$[Ag(C_6H_4NO_2)]$	$D_x = 2.519$ Mg m^{-3}
$M_r = 229.97$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/a$	Cell parameters from 25 reflections
$a = 7.763$ (6) Å	$\theta = 7$–15°
$b = 9.152$ (4) Å	$\mu = 3.24$ mm^{-1}
$c = 8.619$ (6) Å	$T = 298$ (2) K
$\beta = 98.08$ (6)°	Rod, colorless
$V = 606.3$ (7) Å^3	0.40 × 0.20 × 0.18 mm
$Z = 4$	

Data collection

Siemens *R*3*m* four-circle diffractometer	$R_{int} = 0.061$
ω scans	$\theta_{max} = 27.0^\circ$
Absorption correction: ψ scan (North *et al.*, 1968)	$h = 0 \rightarrow 9$
$T_{min} = 0.287$, $T_{max} = 0.558$	$k = 0 \rightarrow 11$
1416 measured reflections	$l = -11 \rightarrow 10$
1319 independent reflections	2 standard reflections
828 reflections with $I > 2\sigma(I)$	every 150 reflections
	intensity decay: 1%

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.058$	$w = 1/[\sigma^2(F_o^2) + (0.0795P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.155$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.03$	$\Delta\rho_{max} = 1.06$ e Å^{-3}
1319 reflections	$\Delta\rho_{min} = -0.93$ e Å^{-3}
91 parameters	

H atoms were placed at calculated positions in the riding-model approximation (C—H = 0.93 Å) with their displacement parameters tied to those of the parent atoms; $U_{iso}(H) = 1.2U_{eq}(C)$. The final difference Fourier map had a large peak near the Ag atom.

Data collection: *R*3*m Software* (Siemens, 1990); cell refinement: *R*3*m Software*; data reduction: *R*3*m Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

The authors thank the National Key Basic Research and Development Program of China (No. G 2000026302) and the University of Malaya for the generous support of this work.

References

Cova, B., Bricenõ, A. & Atencio, R. (2001). *New J. Chem.* **25**, 1516–1519.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Siemens (1990). *R*3*m Software*. Version 4.0. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst* **36**, 7–13.