

# Poly[ $\mu_2$ -1,4-bis(3-pyridylmethoxy)-benzene-hemi- $\mu_2$ -fumarato-silver(I) monohydrate]

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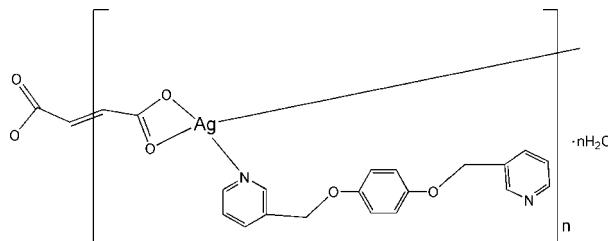
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(C-C) = 0.005$  Å;  $R$  factor = 0.034;  $wR$  factor = 0.107; data-to-parameter ratio = 15.9.

The asymmetric unit of the title structure,  $\{[\text{Ag}(\text{C}_{18}\text{H}_{16}\text{N}_2\text{O}_2)(\text{C}_4\text{H}_2\text{O}_4)_{0.5}]\cdot\text{H}_2\text{O}\}_n$ , contains one  $\text{Ag}^{\text{I}}$  cation, one 1,4-bis(3-pyridylmethoxy)benzene ( $L$ ) ligand, half of a fumarate ligand and one solvent water molecule. The  $\text{Ag}^{\text{I}}$  ion is in a distorted tetrahedral coordination geometry. Each  $L$  ligand bridges two symmetry-related  $\text{Ag}^{\text{I}}$  cations to form extended one-dimensional chains, which are, in turn, bridged by fumarate ligands to create chains of rings. The solvent water molecules donate hydrogen bonds to the carboxylate O atoms of fumarate ligands, generating a two-dimensional supramolecular structure.

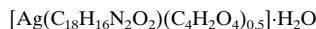
## Related literature

For related literature, see: Allen *et al.* (1987); Fujita *et al.* (1995); Yaghi *et al.* (1995); Zaworotko & Moulton (2001); Corespo *et al.* (1998).



## Experimental

### Crystal data



$M_r = 475.24$

Triclinic,  $P\bar{1}$

$a = 8.5730$  (8) Å

$b = 9.7120$  (9) Å

$c = 12.0990$  (11) Å

$\alpha = 88.845$  (2)°

$\beta = 71.8670$  (10)°

$\gamma = 77.047$  (2)°

$V = 931.65$  (15) Å<sup>3</sup>

$Z = 2$

Mo  $K\alpha$  radiation

$\mu = 1.12$  mm<sup>-1</sup>

$T = 293$  (2) K

$0.42 \times 0.36 \times 0.35$  mm

### Data collection

Bruker APEX CCD area-detector

diffractometer

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

$T_{\min} = 0.632$ ,  $T_{\max} = 0.676$

5611 measured reflections

4127 independent reflections

3629 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.018$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.107$

$S = 1.09$

4127 reflections

259 parameters

3 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 1.17$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.57$  e Å<sup>-3</sup>

**Table 1**  
Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
O1W—H1B···O1	0.85 (5)	2.23 (5)	2.941 (6)	141 (7)
O1W—H1A···O1 <sup>i</sup>	0.85 (6)	2.07 (3)	2.888 (5)	162 (8)

Symmetry code: (i)  $-x + 2, -y, -z + 1$ .

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL-Plus (Sheldrick, 1990); 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: LH2537).

## References

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## **supplementary materials**

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## Poly[ $\mu_2$ -1,4-bis(3-pyridylmethoxy)benzene-hemi- $\mu_2$ -fumarato-silver(I)] monohydrate]

S.-L. Li, H.-Y. Bai and J. Yang

### Comment

The design and synthesis of supramolecular complexes exhibiting novel structures and properties has provided exciting new prospects for chemists (Fujita *et al.*, 1995; Yaghi *et al.*, 1995; Zaworotko & Moulton, 2001). Among various supramolecular compounds, Ag(I) compounds are attractive because of their diverse structural types (Corespo *et al.*, 1998). In this paper, we isolated a new Ag supramolecular compound,  $\{[\text{Ag}(L)(\text{fum})_{0.5}] \cdot \text{H}_2\text{O}\}_n$ , constructed using 1,4-bis(pyridin-3-ylmethoxy)benzene (*L*) and fumarate (fum) ligands.

In the title structure, each Ag<sup>I</sup> cation is four-coordinated and shows a tetrahedral geometry, surrounded by two N atoms from different *L* ligands and two carboxylate oxygen atoms from different fum anions (Fig. 1). The dihedral angle between two pyridine rings in the same *L* ligand is 23.6 (5) $^\circ$ . All bond distances and angles are normal (Allen *et al.*, 1987). The *L* ligands exhibit bis-monodentate coordination modes and link Ag<sup>I</sup> cations to generate an extended chain, which is further linked by fumarate anions to generate a double chainlike structure (Fig. 2). The lattice water molecules donate hydrogen bonds to carboxylate oxygen atoms of fumarate anions from adjacent double-chains, thus forming an interesting two-dimensional supramolecular structure (Fig. 3).

### Experimental

A mixture of *L* (0.30 g, 1 mmol), AgNO<sub>3</sub> (0.17 g, 1 mmol), fumaric acid (0.12 g, 1 mmol) and H<sub>2</sub>O (10 ml) was stirred for 1 h and then sealed in a 25 ml Teflonlined stainless steel container. The container was heated to 423 K and held at that temperature for 72 h, then cooled to room temperature at a rate of 10 K h<sup>-1</sup>. Colorless crystals of the title compound were collected in 56% yield based on Ag.

### Refinement

All H atoms bonded to C atoms were positioned geometrically and refined as riding atoms with C—H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The water H-atoms were located in a difference Fourier map, and were refined freely with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ .

### Figures

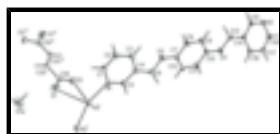


Fig. 1. View of the coordination environment of an Ag atom. Displacement ellipsoids are drawn at the 30% probability level. Symmetry codes: (i)  $x + 2, y - 1, z - 1$ ; (ii)  $1 - x, -y, 1 - z$ .

# supplementary materials

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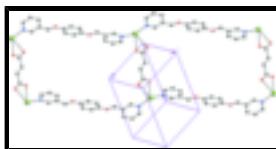


Fig. 2. Ball-stick representation of part of an extended chain of rings.

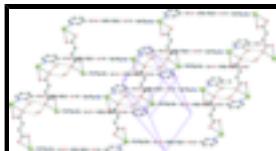


Fig. 3. Ball-stick representation of part of the two-dimensional supramolecular structure. Hydrogen bonds are shown as dashed lines.

## Poly[[ $\mu_2$ -1,4-bis(3-pyridylmethoxy)benzene-hemi- $\mu_2$ -fumarato-silver(I)] hydrate]

### Crystal data

[Ag(C <sub>18</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub> )(C <sub>4</sub> H <sub>2</sub> O <sub>4</sub> ) <sub>0.5</sub> ]·H <sub>2</sub> O	Z = 2
M <sub>r</sub> = 475.24	F <sub>000</sub> = 480
Triclinic, P <sup>−</sup> <sub>1</sub>	D <sub>x</sub> = 1.694 Mg m <sup>−3</sup>
Hall symbol: -P 1	Mo K $\alpha$ radiation
a = 8.5730 (8) Å	$\lambda$ = 0.71069 Å
b = 9.7120 (9) Å	Cell parameters from 4127 reflections
c = 12.0990 (11) Å	$\theta$ = 1.8–28.5°
$\alpha$ = 88.845 (2)°	$\mu$ = 1.12 mm <sup>−1</sup>
$\beta$ = 71.8670 (10)°	T = 293 (2) K
$\gamma$ = 77.047 (2)°	Block, colorless
V = 931.65 (15) Å <sup>3</sup>	0.42 × 0.36 × 0.35 mm

### Data collection

Bruker APEX CCD area-detector diffractometer	4127 independent reflections
Radiation source: fine-focus sealed tube	3629 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.018$
T = 293(2) K	$\theta_{\text{max}} = 28.5^\circ$
$\omega$ scans	$\theta_{\text{min}} = 1.8^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 11$
$T_{\text{min}} = 0.632$ , $T_{\text{max}} = 0.676$	$k = -12 \rightarrow 12$
5611 measured reflections	$l = -15 \rightarrow 8$

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.034$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.107$	$w = 1/[ \sigma^2(F_o^2) + (0.0611P)^2 + 0.3593P ]$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $S = 1.09$        $(\Delta/\sigma)_{\max} = 0.001$   
 4127 reflections       $\Delta\rho_{\max} = 1.17 \text{ e } \text{\AA}^{-3}$   
 259 parameters       $\Delta\rho_{\min} = -0.57 \text{ e } \text{\AA}^{-3}$   
 3 restraints      Extinction correction: none  
 Primary atom site location: structure-invariant direct methods

### 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.64106 (3)	0.45095 (3)	0.55161 (2)	0.04642 (11)
C1	0.4381 (4)	0.4066 (3)	0.8046 (3)	0.0479 (8)
H1	0.5187	0.3215	0.7871	0.058*
C2	0.3196 (5)	0.4286 (4)	0.9124 (3)	0.0547 (9)
H2	0.3224	0.3613	0.9680	0.066*
C3	0.1954 (4)	0.5524 (4)	0.9376 (3)	0.0476 (7)
H3	0.1127	0.5687	1.0101	0.057*
C4	0.1949 (3)	0.6511 (3)	0.8549 (3)	0.0352 (6)
C5	0.3232 (3)	0.6225 (3)	0.7493 (3)	0.0362 (6)
H5	0.3262	0.6902	0.6937	0.043*
C6	0.0622 (4)	0.7879 (3)	0.8736 (3)	0.0391 (6)
H6A	0.1143	0.8682	0.8640	0.047*
H6B	0.0016	0.7916	0.8175	0.047*
C7	-0.1839 (4)	0.9076 (3)	1.0236 (3)	0.0416 (7)
C8	-0.2800 (4)	0.9094 (3)	1.1393 (3)	0.0470 (8)
H8	-0.2509	0.8372	1.1858	0.056*
C9	-0.4204 (4)	1.0199 (3)	1.1857 (3)	0.0448 (7)
H9	-0.4861	1.0209	1.2631	0.054*
C10	-0.4615 (4)	1.1267 (3)	1.1173 (3)	0.0378 (6)
C11	-0.3624 (4)	1.1257 (3)	1.0023 (3)	0.0427 (7)
H11	-0.3894	1.1998	0.9566	0.051*
C12	-0.2235 (4)	1.0157 (3)	0.9544 (3)	0.0418 (7)
H12	-0.1581	1.0148	0.8769	0.050*
C13	-0.7012 (4)	1.2405 (3)	1.2734 (3)	0.0409 (7)
H13A	-0.6349	1.2422	1.3252	0.049*

## supplementary materials

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H13B	-0.7448	1.1556	1.2856	0.049*
C14	-0.8441 (3)	1.3692 (3)	1.2985 (3)	0.0354 (6)
C15	-0.9936 (3)	1.3643 (3)	1.3841 (3)	0.0356 (6)
H15	-1.0021	1.2801	1.4208	0.043*
C16	-0.8321 (4)	1.4946 (3)	1.2444 (3)	0.0444 (7)
H16	-0.7342	1.5014	1.1858	0.053*
C17	-0.9688 (4)	1.6107 (4)	1.2789 (3)	0.0515 (8)
H17	-0.9628	1.6967	1.2444	0.062*
C18	-1.1126 (4)	1.5963 (3)	1.3645 (3)	0.0457 (7)
H18	-1.2037	1.6740	1.3870	0.055*
C19	0.6094 (4)	0.1537 (3)	0.5074 (3)	0.0428 (7)
C20	0.5740 (4)	0.0108 (3)	0.4968 (3)	0.0416 (7)
H20	0.6633	-0.0679	0.4847	0.050*
N1	0.4431 (3)	0.5020 (3)	0.7234 (2)	0.0388 (5)
N2	-1.1269 (3)	1.4750 (3)	1.4167 (2)	0.0372 (5)
O1	0.7521 (4)	0.1564 (3)	0.5123 (4)	0.0778 (10)
O2	0.4997 (3)	0.2597 (2)	0.5080 (3)	0.0596 (7)
O3	-0.0494 (3)	0.7919 (2)	0.9878 (2)	0.0562 (7)
O4	-0.5989 (3)	1.2410 (2)	1.15538 (19)	0.0470 (5)
O1W	1.0451 (6)	-0.0306 (5)	0.3447 (3)	0.0956 (12)
H1A	1.107 (6)	-0.084 (7)	0.378 (5)	0.143*
H1B	0.946 (3)	-0.015 (8)	0.392 (5)	0.143*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ag1	0.02882 (14)	0.05097 (17)	0.04432 (17)	-0.00020 (10)	0.00425 (10)	-0.00846 (11)
C1	0.0378 (16)	0.0375 (15)	0.0535 (19)	0.0032 (12)	-0.0014 (14)	-0.0017 (14)
C2	0.0462 (18)	0.0487 (18)	0.051 (2)	0.0015 (15)	0.0014 (15)	0.0091 (15)
C3	0.0387 (16)	0.0505 (18)	0.0394 (16)	-0.0026 (14)	0.0027 (13)	-0.0011 (13)
C4	0.0270 (13)	0.0354 (14)	0.0377 (15)	-0.0021 (11)	-0.0054 (11)	-0.0094 (11)
C5	0.0308 (13)	0.0347 (14)	0.0372 (15)	-0.0031 (11)	-0.0051 (12)	-0.0056 (11)
C6	0.0317 (14)	0.0396 (14)	0.0357 (15)	0.0029 (11)	-0.0032 (12)	-0.0101 (11)
C7	0.0293 (14)	0.0362 (14)	0.0451 (17)	0.0034 (11)	0.0011 (12)	-0.0083 (12)
C8	0.0381 (16)	0.0410 (16)	0.0443 (17)	0.0069 (13)	0.0009 (14)	0.0013 (13)
C9	0.0352 (15)	0.0450 (16)	0.0370 (16)	0.0042 (13)	0.0036 (13)	-0.0042 (13)
C10	0.0260 (13)	0.0372 (14)	0.0393 (15)	0.0046 (11)	-0.0023 (11)	-0.0095 (11)
C11	0.0346 (15)	0.0451 (16)	0.0386 (16)	0.0049 (12)	-0.0072 (13)	-0.0017 (13)
C12	0.0309 (14)	0.0505 (17)	0.0320 (14)	0.0004 (12)	0.0010 (12)	-0.0076 (12)
C13	0.0269 (13)	0.0400 (15)	0.0434 (16)	0.0025 (11)	-0.0002 (12)	-0.0058 (12)
C14	0.0253 (12)	0.0361 (14)	0.0371 (15)	0.0008 (10)	-0.0038 (11)	-0.0090 (11)
C15	0.0259 (13)	0.0349 (13)	0.0384 (15)	-0.0008 (10)	-0.0031 (11)	-0.0072 (11)
C16	0.0296 (14)	0.0473 (17)	0.0466 (17)	-0.0040 (12)	-0.0017 (13)	-0.0006 (13)
C17	0.0450 (18)	0.0400 (16)	0.057 (2)	-0.0034 (14)	-0.0036 (16)	0.0044 (14)
C18	0.0321 (15)	0.0407 (16)	0.0528 (19)	0.0047 (12)	-0.0058 (14)	-0.0073 (13)
C19	0.0439 (17)	0.0377 (15)	0.0421 (17)	-0.0125 (13)	-0.0046 (13)	0.0008 (12)
C20	0.0426 (16)	0.0311 (13)	0.0450 (17)	-0.0042 (12)	-0.0079 (14)	0.0014 (12)
N1	0.0284 (11)	0.0365 (12)	0.0400 (13)	-0.0002 (9)	0.0010 (10)	-0.0059 (10)

N2	0.0257 (11)	0.0378 (12)	0.0397 (13)	0.0001 (9)	-0.0027 (10)	-0.0107 (10)
O1	0.0632 (18)	0.0588 (17)	0.124 (3)	-0.0218 (14)	-0.043 (2)	0.0142 (18)
O2	0.0475 (14)	0.0339 (11)	0.0852 (19)	-0.0040 (10)	-0.0071 (13)	-0.0046 (11)
O3	0.0423 (13)	0.0443 (12)	0.0509 (14)	0.0131 (10)	0.0132 (11)	0.0001 (10)
O4	0.0330 (11)	0.0467 (12)	0.0403 (12)	0.0127 (9)	0.0029 (9)	-0.0047 (9)
O1W	0.093 (3)	0.109 (3)	0.073 (2)	-0.005 (2)	-0.022 (2)	0.010 (2)

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

Ag1—N2 <sup>i</sup>	2.202 (2)	C10—O4	1.388 (3)
Ag1—N1	2.217 (2)	C11—C12	1.386 (4)
Ag1—O2	2.577 (3)	C11—H11	0.9300
Ag1—Ag1 <sup>ii</sup>	3.0193 (5)	C12—H12	0.9300
C1—N1	1.335 (4)	C13—O4	1.425 (4)
C1—C2	1.367 (5)	C13—C14	1.501 (4)
C1—H1	0.9300	C13—H13A	0.9700
C2—C3	1.382 (5)	C13—H13B	0.9700
C2—H2	0.9300	C14—C16	1.379 (4)
C3—C4	1.372 (4)	C14—C15	1.384 (4)
C3—H3	0.9300	C15—N2	1.343 (3)
C4—C5	1.386 (4)	C15—H15	0.9300
C4—C6	1.512 (4)	C16—C17	1.393 (4)
C5—N1	1.341 (4)	C16—H16	0.9300
C5—H5	0.9300	C17—C18	1.375 (5)
C6—O3	1.411 (4)	C17—H17	0.9300
C6—H6A	0.9700	C18—N2	1.337 (4)
C6—H6B	0.9700	C18—H18	0.9300
C7—C12	1.377 (5)	C19—O2	1.228 (4)
C7—O3	1.382 (3)	C19—O1	1.250 (4)
C7—C8	1.384 (4)	C19—C20	1.502 (4)
C8—C9	1.393 (4)	C20—C20 <sup>iii</sup>	1.309 (6)
C8—H8	0.9300	C20—H20	0.9300
C9—C10	1.366 (4)	N2—Ag1 <sup>iv</sup>	2.202 (2)
C9—H9	0.9300	O1W—H1A	0.85 (6)
C10—C11	1.386 (4)	O1W—H1B	0.85 (5)
N2 <sup>i</sup> —Ag1—N1	153.76 (10)	C10—C11—H11	119.6
N2 <sup>i</sup> —Ag1—O2	116.46 (9)	C7—C12—C11	118.9 (3)
N1—Ag1—O2	89.76 (9)	C7—C12—H12	120.5
N2 <sup>i</sup> —Ag1—Ag1 <sup>ii</sup>	106.01 (7)	C11—C12—H12	120.5
N1—Ag1—Ag1 <sup>ii</sup>	85.94 (7)	O4—C13—C14	108.2 (2)
O2—Ag1—Ag1 <sup>ii</sup>	63.49 (6)	O4—C13—H13A	110.1
N1—C1—C2	122.8 (3)	C14—C13—H13A	110.1
N1—C1—H1	118.6	O4—C13—H13B	110.1
C2—C1—H1	118.6	C14—C13—H13B	110.1
C1—C2—C3	119.0 (3)	H13A—C13—H13B	108.4
C1—C2—H2	120.5	C16—C14—C15	118.0 (3)
C3—C2—H2	120.5	C16—C14—C13	123.5 (3)

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C4—C3—C2	119.5 (3)	C15—C14—C13	118.4 (3)
C4—C3—H3	120.2	N2—C15—C14	123.4 (3)
C2—C3—H3	120.2	N2—C15—H15	118.3
C3—C4—C5	117.7 (3)	C14—C15—H15	118.3
C3—C4—C6	123.3 (3)	C14—C16—C17	119.1 (3)
C5—C4—C6	119.0 (3)	C14—C16—H16	120.5
N1—C5—C4	123.3 (3)	C17—C16—H16	120.5
N1—C5—H5	118.4	C18—C17—C16	119.0 (3)
C4—C5—H5	118.4	C18—C17—H17	120.5
O3—C6—C4	107.4 (2)	C16—C17—H17	120.5
O3—C6—H6A	110.2	N2—C18—C17	122.6 (3)
C4—C6—H6A	110.2	N2—C18—H18	118.7
O3—C6—H6B	110.2	C17—C18—H18	118.7
C4—C6—H6B	110.2	O2—C19—O1	124.1 (3)
H6A—C6—H6B	108.5	O2—C19—C20	118.8 (3)
C12—C7—O3	125.2 (3)	O1—C19—C20	117.1 (3)
C12—C7—C8	120.7 (3)	C20 <sup>iii</sup> —C20—C19	124.6 (4)
O3—C7—C8	114.1 (3)	C20 <sup>iii</sup> —C20—H20	117.7
C7—C8—C9	119.7 (3)	C19—C20—H20	117.7
C7—C8—H8	120.1	C1—N1—C5	117.7 (3)
C9—C8—H8	120.1	C1—N1—Ag1	118.8 (2)
C10—C9—C8	120.0 (3)	C5—N1—Ag1	123.5 (2)
C10—C9—H9	120.0	C18—N2—C15	117.9 (3)
C8—C9—H9	120.0	C18—N2—Ag1 <sup>iv</sup>	122.60 (19)
C9—C10—C11	119.9 (3)	C15—N2—Ag1 <sup>iv</sup>	119.5 (2)
C9—C10—O4	124.3 (3)	C19—O2—Ag1	99.6 (2)
C11—C10—O4	115.8 (3)	C7—O3—C6	117.5 (2)
C12—C11—C10	120.8 (3)	C10—O4—C13	115.5 (2)
C12—C11—H11	119.6	H1A—O1W—H1B	106 (6)
N1—C1—C2—C3	2.4 (6)	O1—C19—C20—C20 <sup>iii</sup>	172.3 (4)
C1—C2—C3—C4	−0.9 (6)	C2—C1—N1—C5	−1.6 (5)
C2—C3—C4—C5	−1.3 (5)	C2—C1—N1—Ag1	−179.4 (3)
C2—C3—C4—C6	178.6 (3)	C4—C5—N1—C1	−0.8 (5)
C3—C4—C5—N1	2.2 (5)	C4—C5—N1—Ag1	176.9 (2)
C6—C4—C5—N1	−177.7 (3)	N2 <sup>i</sup> —Ag1—N1—C1	−109.7 (3)
C3—C4—C6—O3	1.5 (4)	O2—Ag1—N1—C1	68.1 (3)
C5—C4—C6—O3	−178.6 (3)	Ag1 <sup>ii</sup> —Ag1—N1—C1	131.5 (3)
C12—C7—C8—C9	1.5 (5)	N2 <sup>i</sup> —Ag1—N1—C5	72.7 (3)
O3—C7—C8—C9	−179.3 (3)	O2—Ag1—N1—C5	−109.5 (2)
C7—C8—C9—C10	−0.8 (5)	Ag1 <sup>ii</sup> —Ag1—N1—C5	−46.1 (2)
C8—C9—C10—C11	−0.7 (5)	C17—C18—N2—C15	0.8 (5)
C8—C9—C10—O4	179.9 (3)	C17—C18—N2—Ag1 <sup>iv</sup>	−178.9 (3)
C9—C10—C11—C12	1.5 (5)	C14—C15—N2—C18	−0.9 (5)
O4—C10—C11—C12	−179.0 (3)	C14—C15—N2—Ag1 <sup>iv</sup>	178.7 (2)
O3—C7—C12—C11	−179.8 (3)	O1—C19—O2—Ag1	−7.9 (4)
C8—C7—C12—C11	−0.7 (5)	C20—C19—O2—Ag1	173.8 (2)

C10—C11—C12—C7	−0.8 (5)	N2 <sup>i</sup> —Ag1—O2—C19	65.7 (2)
O4—C13—C14—C16	−30.1 (4)	N1—Ag1—O2—C19	−113.2 (2)
O4—C13—C14—C15	152.9 (3)	Ag1 <sup>ii</sup> —Ag1—O2—C19	161.2 (2)
C16—C14—C15—N2	0.1 (5)	C12—C7—O3—C6	4.0 (5)
C13—C14—C15—N2	177.3 (3)	C8—C7—O3—C6	−175.2 (3)
C15—C14—C16—C17	0.9 (5)	C4—C6—O3—C7	−178.9 (3)
C13—C14—C16—C17	−176.2 (3)	C9—C10—O4—C13	−1.1 (5)
C14—C16—C17—C18	−1.0 (6)	C11—C10—O4—C13	179.4 (3)
C16—C17—C18—N2	0.2 (6)	C14—C13—O4—C10	−179.0 (3)
O2—C19—C20—C20 <sup>iii</sup>	−9.4 (6)		

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

*Hydrogen-bond geometry (Å, °)*

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
O1W—H1B···O1	0.85 (5)	2.23 (5)	2.941 (6)	141 (7)
O1W—H1A···O1 <sup>v</sup>	0.85 (6)	2.07 (3)	2.888 (5)	162 (8)

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

## supplementary materials

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Fig. 1

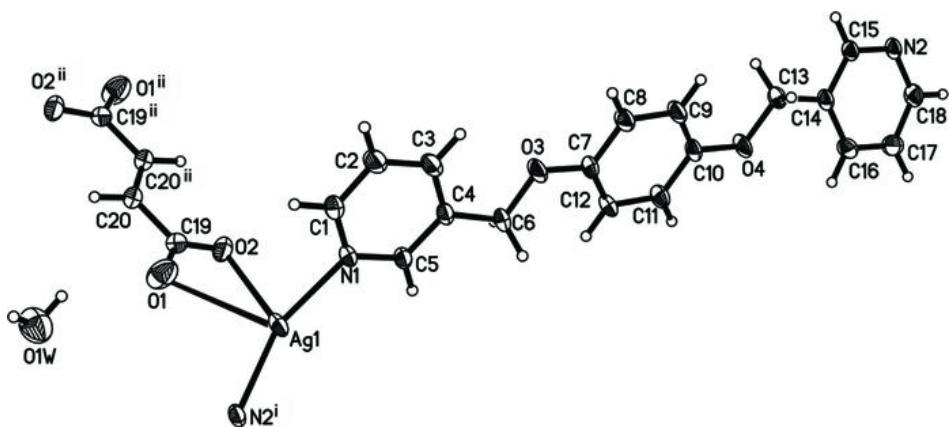
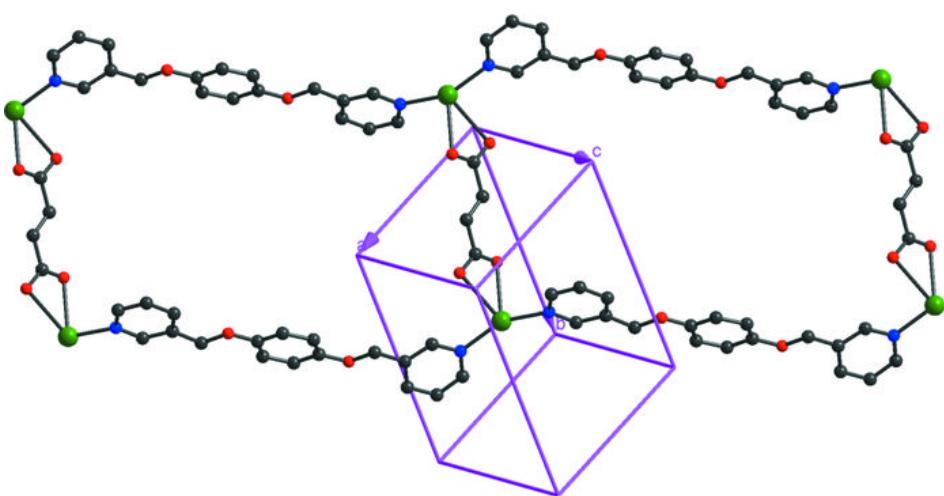


Fig. 2



## **supplementary materials**

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**Fig. 3**

