

## Poly[[diaquabis( $\mu_3$ -3-carboxylato-4-hydroxybenzenesulfonato)tri- $\mu_2$ -pyrazine-tetrasilver(I)] dihydrate]

Ying-Ying Liu, Shen-Tang Wang and Yong-Sheng Yan\*

Department of Chemistry and Chemical Engineering, Jiangsu University, Zhenjiang 212013, People's Republic of China  
Correspondence e-mail: yys@ujs.edu.cn

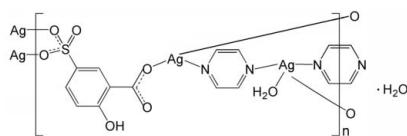
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Key indicators: single-crystal X-ray study;  $T = 293\text{ K}$ ; mean  $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$ ;  $R$  factor = 0.033;  $wR$  factor = 0.073; data-to-parameter ratio = 13.2.

The title coordination polymer,  $\{[\text{Ag}_4(\text{C}_7\text{H}_4\text{O}_6\text{S})_2(\text{C}_4\text{H}_4\text{N}_2)_3\cdot(\text{H}_2\text{O})_2]\cdot2\text{H}_2\text{O}\}_n$ , contains two independent  $\text{Ag}^{\text{I}}$  ions. One  $\text{Ag}^{\text{I}}$  ion is coordinated by one O atom from a 3-carboxylato-4-hydroxybenzenesulfonate ( $L$ ) ligand, two N atoms from two pyrazine ligands and a water molecule. The other  $\text{Ag}^{\text{I}}$  ion is coordinated by two O atoms from two  $L$  ligands and one N atom from a pyrazine ligand. One of the pyrazine ligands lies on an inversion center. The  $L$  and pyrazine ligands link the  $\text{Ag}^{\text{I}}$  ions into polymeric layers parallel to the  $ac$  plane. The layers are connected by intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds. An intramolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bond is also present in the  $L$  ligand.

### Related literature

For a related structure, see: Nie & Qu (2011).



### Experimental

#### Crystal data

$[\text{Ag}_4(\text{C}_7\text{H}_4\text{O}_6\text{S})_2(\text{C}_4\text{H}_4\text{N}_2)_3\cdot(\text{H}_2\text{O})_2]\cdot2\text{H}_2\text{O}$	$\beta = 73.436(4)^{\circ}$
$M_r = 1176.14$	$\gamma = 82.882(5)^{\circ}$
Triclinic, $P\bar{1}$	$V = 843.2(7)\text{ \AA}^3$
$a = 7.646(5)\text{ \AA}$	$Z = 1$
$b = 10.340(4)\text{ \AA}$	Mo $K\alpha$ radiation
$c = 11.375(4)\text{ \AA}$	$\mu = 2.50\text{ mm}^{-1}$
$\alpha = 78.751(3)^{\circ}$	$T = 293\text{ K}$
	$0.21 \times 0.15 \times 0.12\text{ mm}$

#### Data collection

Bruker APEX CCD diffractometer	7253 measured reflections
Absorption correction: multi-scan ( <i>SADABS</i> ; Sheldrick, 1996)	3387 independent reflections
$T_{\min} = 0.622$ , $T_{\max} = 0.754$	2190 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.058$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.073$	$\Delta\rho_{\text{max}} = 0.70\text{ e \AA}^{-3}$
$S = 0.88$	$\Delta\rho_{\text{min}} = -1.09\text{ e \AA}^{-3}$
3387 reflections	
256 parameters	
5 restraints	

**Table 1**  
Selected bond lengths ( $\text{\AA}$ ).

$\text{Ag1}-\text{N1}$	2.180 (3)	$\text{Ag2}-\text{N3}$	2.262 (3)
$\text{Ag1}-\text{O3}^{\text{i}}$	2.621 (3)	$\text{Ag2}-\text{O1}^{\text{ii}}$	2.516 (4)
$\text{Ag1}-\text{O6}$	2.153 (3)	$\text{Ag2}-\text{OW2}$	2.576 (4)
$\text{Ag2}-\text{N2}$	2.245 (3)		

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

**Table 2**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^{\circ}$ ).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{OW1}-\text{H1A}\cdots\text{O5}$	0.88 (2)	1.89 (2)	2.751 (4)	168 (6)
$\text{OW1}-\text{H1B}\cdots\text{O5}^{\text{iii}}$	0.89 (2)	2.00 (2)	2.883 (5)	173 (6)
$\text{OW2}-\text{H2A}\cdots\text{O2}^{\text{iii}}$	0.88 (2)	1.91 (3)	2.757 (5)	161 (6)
$\text{OW2}-\text{H2B}\cdots\text{OW1}^{\text{iv}}$	0.89 (2)	2.03 (3)	2.794 (6)	143 (2)
$\text{O4}-\text{H4A}\cdots\text{O6}$	0.82	1.84	2.556 (4)	146

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2474).

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## **supplementary materials**

*Acta Cryst.* (2011). E67, m1545 [doi:10.1107/S1600536811041626]

## Poly[[diaquabis( $\mu_3$ -3-carboxylato-4-hydroxybenzenesulfonato)tri- $\mu_2$ -pyrazine-tetrasilver(I)] dihydrate]

**Y.-Y. Liu, S.-T. Wang and Y.-S. Yan**

### Comment

As part of an investigation of the applications of transition metal complexes, there is a need to prepare further examples of these compounds. In this paper, the structure of the title compound is described.

As shown in Fig. 1, there exist two crystallographically independent  $\text{Ag}^{\text{I}}$  ions. Ag1 atom is three-coordinated (Table 1), having an approximate T-shaped geometry composed of one sulfonate O atom, one carboxylate O atom from two 3-carboxylate-4-hydroxybenzenesulfonate (*L*) ligands and one N atom from a pyrazine ligand. Ag2 atom is coordinated by one sulfonate O atom of an *L* ligand, two N atoms from two pyrazine ligands and one water molecule (Nie & Qu, 2011). The  $\text{Ag}^{\text{I}}$  ions are bridged by the *L* and pyrazine ligands, forming a two-dimensional polymeric layer (Fig. 2). The layers are connected by intermolecular O—H···O hydrogen bonds (Table 2). An intramolecular O—H···O hydrogen bond is present in the *L* ligand.

### Experimental

To a mixture of 5-sulfosalicylic acid (0.109 g, 0.5 mmol) and NaOH (0.040 g, 1.0 mmol) in water (5 ml) was added  $\text{AgNO}_3$  (0.170 g, 1.0 mmol), giving a clear solution. Then ethanol (15 ml) was added to the solution, and white precipitate appeared. The precipitate was collected and dissolved in water. To the solution was added pyrazine (0.081 g, 1 mmol) in methanol (5 ml) and white precipitate formed. The precipitate was dissolved by dropwise addition of acetonitrile. Colorless crystals were obtained from the filtrate after standing in a dark room for several days (yield: 0.150 g, 51%).

### Refinement

H atoms bound to C atoms and hydroxyl O atom were positioned geometrically and refined using a riding model, with C—H = 0.93 and O—H = 0.82 Å and with  $U_{\text{iso}}(\text{H}) = 1.2(1.5 \text{ for hydroxyl})U_{\text{eq}}(\text{C}, \text{O})$ . Water H atoms were located from a difference Fourier map and refined with a restraint of O—H = 0.88 Å and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ .

### Figures

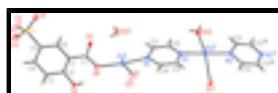


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i)  $-x, -y, -1 - z$ ; (ii)  $1 - x, -y, 1 - z$ ; (iii)  $1 - x, 1 - y, 1 - z$ .]

# supplementary materials

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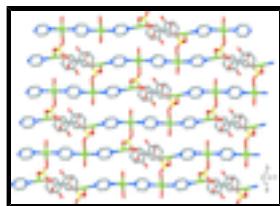


Fig. 2. View of the two-dimensional layer in the title compound.

## Poly[[diaquabis( $\mu_3$ -3-carboxylato-4-hydroxybenzenesulfonato)tri- $\mu_2$ -pyrazine-tetrasilver(I)] dihydrate]

### Crystal data

$[\text{Ag}_4(\text{C}_7\text{H}_4\text{O}_6\text{S})_2(\text{C}_4\text{H}_4\text{N}_2)_3(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$	$Z = 1$
$M_r = 1176.14$	$F(000) = 574$
Triclinic, $P\bar{1}$	$D_x = 2.316 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 7.646 (5) \text{ \AA}$	Cell parameters from 2192 reflections
$b = 10.340 (4) \text{ \AA}$	$\theta = 3.2\text{--}27.5^\circ$
$c = 11.375 (4) \text{ \AA}$	$\mu = 2.50 \text{ mm}^{-1}$
$\alpha = 78.751 (3)^\circ$	$T = 293 \text{ K}$
$\beta = 73.436 (4)^\circ$	Block, colorless
$\gamma = 82.882 (5)^\circ$	$0.21 \times 0.15 \times 0.12 \text{ mm}$
$V = 843.2 (7) \text{ \AA}^3$	

### Data collection

Bruker APEX CCD diffractometer	3387 independent reflections
Radiation source: fine-focus sealed tube graphite	2190 reflections with $I > 2\sigma(I)$
$\varphi$ and $\omega$ scans	$R_{\text{int}} = 0.058$
Absorption correction: multi-scan ( <i>SADABS</i> ; Sheldrick, 1996)	$\theta_{\text{max}} = 27.5^\circ, \theta_{\text{min}} = 3.2^\circ$
$T_{\text{min}} = 0.622, T_{\text{max}} = 0.754$	$h = -9 \rightarrow 9$
7253 measured reflections	$k = -12 \rightarrow 13$
	$l = -12 \rightarrow 14$

### Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.033$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.073$	H atoms treated by a mixture of independent and constrained refinement
$S = 0.88$	$w = 1/[\sigma^2(F_o^2) + (0.0213P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
3387 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
256 parameters	$\Delta\rho_{\text{max}} = 0.70 \text{ e \AA}^{-3}$

5 restraints

$$\Delta\rho_{\min} = -1.09 \text{ e } \text{\AA}^{-3}$$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.29090 (6)	0.17665 (4)	-0.29686 (4)	0.03972 (13)
Ag2	0.39877 (5)	0.41619 (4)	0.22945 (4)	0.03870 (13)
C1	0.1323 (5)	0.1138 (4)	-0.6235 (4)	0.0216 (9)
C2	0.2275 (6)	-0.0059 (4)	-0.6494 (4)	0.0253 (10)
C3	0.1985 (6)	-0.0669 (4)	-0.7399 (4)	0.0288 (10)
H3	0.2663	-0.1448	-0.7589	0.035*
C4	0.0686 (6)	-0.0115 (4)	-0.8019 (4)	0.0263 (10)
H4	0.0493	-0.0518	-0.8630	0.032*
C5	-0.0332 (5)	0.1047 (4)	-0.7726 (4)	0.0219 (9)
C6	-0.0001 (5)	0.1680 (4)	-0.6871 (4)	0.0214 (9)
H6	-0.0656	0.2474	-0.6709	0.026*
C7	0.1616 (6)	0.1842 (5)	-0.5288 (4)	0.0266 (10)
C8	0.3541 (6)	0.1792 (5)	-0.0457 (4)	0.0311 (11)
H8	0.3830	0.0903	-0.0517	0.037*
C9	0.3716 (6)	0.2241 (4)	0.0570 (4)	0.0299 (11)
H9	0.4142	0.1646	0.1171	0.036*
C10	0.2678 (6)	0.4298 (5)	-0.0175 (4)	0.0317 (11)
H10	0.2345	0.5181	-0.0100	0.038*
C11	0.2525 (6)	0.3863 (5)	-0.1201 (5)	0.0322 (11)
H11	0.2101	0.4459	-0.1802	0.039*
C12	0.5470 (6)	0.3813 (5)	0.4676 (4)	0.0288 (10)
H12	0.5817	0.2972	0.4474	0.035*
C13	0.4107 (6)	0.5879 (5)	0.4325 (4)	0.0294 (11)
H13	0.3477	0.6518	0.3871	0.035*
N1	0.2969 (5)	0.2599 (4)	-0.1363 (3)	0.0280 (9)
N2	0.3295 (5)	0.3496 (4)	0.0728 (4)	0.0281 (9)
N3	0.4568 (5)	0.4690 (4)	0.3978 (3)	0.0288 (9)
O1	-0.3073 (6)	0.2729 (4)	-0.7854 (4)	0.0730 (16)
O2	-0.1208 (6)	0.2172 (5)	-0.9749 (4)	0.0738 (14)
O3	-0.3110 (6)	0.0589 (4)	-0.8372 (5)	0.0805 (17)
O4	0.3512 (4)	-0.0688 (3)	-0.5882 (3)	0.0359 (8)
H4A	0.3588	-0.0253	-0.5370	0.054*
O5	0.0833 (5)	0.2950 (3)	-0.5153 (3)	0.0421 (9)
O6	0.2710 (4)	0.1232 (3)	-0.4660 (3)	0.0353 (8)
S1	-0.20943 (15)	0.16850 (10)	-0.84628 (11)	0.0261 (3)
OW1	0.0538 (5)	0.4656 (4)	-0.3518 (4)	0.0460 (10)
H1A	0.072 (8)	0.403 (5)	-0.397 (5)	0.069*
H1B	0.021 (8)	0.542 (3)	-0.393 (5)	0.069*
OW2	0.2451 (5)	0.6472 (4)	0.1729 (4)	0.0449 (9)
H2A	0.230 (8)	0.686 (5)	0.100 (3)	0.067*
H2B	0.128 (3)	0.648 (3)	0.218 (4)	0.067*

## supplementary materials

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ag1	0.0586 (3)	0.0419 (3)	0.0292 (2)	-0.00358 (19)	-0.0243 (2)	-0.01205 (18)
Ag2	0.0527 (2)	0.0423 (3)	0.0330 (3)	0.00471 (18)	-0.0272 (2)	-0.01620 (19)
C1	0.026 (2)	0.019 (2)	0.022 (2)	0.0003 (17)	-0.009 (2)	-0.0059 (18)
C2	0.028 (2)	0.022 (2)	0.025 (3)	0.0019 (18)	-0.011 (2)	0.0001 (19)
C3	0.034 (2)	0.023 (2)	0.030 (3)	0.0092 (19)	-0.012 (2)	-0.010 (2)
C4	0.033 (2)	0.025 (3)	0.026 (3)	-0.0005 (19)	-0.012 (2)	-0.011 (2)
C5	0.026 (2)	0.022 (2)	0.020 (2)	0.0034 (18)	-0.010 (2)	-0.0069 (18)
C6	0.026 (2)	0.019 (2)	0.020 (2)	0.0019 (17)	-0.009 (2)	-0.0044 (18)
C7	0.033 (2)	0.029 (3)	0.021 (3)	-0.004 (2)	-0.013 (2)	-0.004 (2)
C8	0.040 (3)	0.025 (3)	0.032 (3)	0.003 (2)	-0.016 (2)	-0.007 (2)
C9	0.035 (2)	0.029 (3)	0.030 (3)	0.001 (2)	-0.017 (2)	-0.004 (2)
C10	0.041 (3)	0.028 (3)	0.032 (3)	0.006 (2)	-0.020 (2)	-0.010 (2)
C11	0.040 (3)	0.031 (3)	0.031 (3)	-0.001 (2)	-0.022 (2)	-0.002 (2)
C12	0.039 (3)	0.022 (3)	0.026 (3)	0.003 (2)	-0.011 (2)	-0.006 (2)
C13	0.039 (3)	0.026 (3)	0.026 (3)	0.003 (2)	-0.015 (2)	-0.005 (2)
N1	0.031 (2)	0.032 (2)	0.024 (2)	-0.0006 (17)	-0.0104 (18)	-0.0063 (18)
N2	0.030 (2)	0.033 (2)	0.026 (2)	-0.0027 (17)	-0.0116 (19)	-0.0080 (18)
N3	0.034 (2)	0.033 (2)	0.022 (2)	-0.0005 (17)	-0.0131 (19)	-0.0043 (18)
O1	0.076 (3)	0.092 (3)	0.077 (3)	0.056 (3)	-0.058 (3)	-0.059 (3)
O2	0.066 (3)	0.111 (4)	0.036 (3)	0.010 (3)	-0.025 (2)	0.012 (2)
O3	0.082 (3)	0.041 (3)	0.143 (5)	-0.019 (2)	-0.087 (4)	0.020 (3)
O4	0.0398 (18)	0.035 (2)	0.041 (2)	0.0159 (15)	-0.0263 (18)	-0.0129 (16)
O5	0.066 (2)	0.029 (2)	0.047 (2)	0.0100 (17)	-0.037 (2)	-0.0191 (17)
O6	0.0442 (19)	0.039 (2)	0.033 (2)	0.0043 (16)	-0.0252 (18)	-0.0135 (16)
S1	0.0345 (6)	0.0234 (6)	0.0274 (7)	0.0032 (5)	-0.0195 (5)	-0.0074 (5)
OW1	0.068 (3)	0.041 (2)	0.036 (2)	0.001 (2)	-0.026 (2)	-0.0095 (18)
OW2	0.059 (2)	0.039 (2)	0.039 (2)	0.0057 (18)	-0.020 (2)	-0.0083 (18)

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

Ag1—N1	2.180 (3)	C8—H8	0.9300
Ag1—O3 <sup>i</sup>	2.621 (3)	C9—N2	1.332 (5)
Ag1—O6	2.153 (3)	C9—H9	0.9300
Ag2—N2	2.245 (3)	C10—N2	1.346 (6)
Ag2—N3	2.262 (3)	C10—C11	1.368 (6)
Ag2—O1 <sup>ii</sup>	2.516 (4)	C10—H10	0.9300
Ag2—OW2	2.576 (4)	C11—N1	1.343 (6)
C1—C2	1.395 (6)	C11—H11	0.9300
C1—C6	1.408 (5)	C12—N3	1.343 (5)
C1—C7	1.491 (6)	C12—C13 <sup>iii</sup>	1.369 (6)
C2—O4	1.360 (5)	C12—H12	0.9300
C2—C3	1.388 (6)	C13—N3	1.340 (5)
C3—C4	1.382 (6)	C13—C12 <sup>iii</sup>	1.369 (6)
C3—H3	0.9300	C13—H13	0.9300

C4—C5	1.392 (6)	O1—S1	1.415 (3)
C4—H4	0.9300	O2—S1	1.444 (5)
C5—C6	1.366 (5)	O3—S1	1.423 (4)
C5—S1	1.778 (4)	O4—H4A	0.8200
C6—H6	0.9300	OW1—H1A	0.88 (2)
C7—O5	1.241 (5)	OW1—H1B	0.89 (2)
C7—O6	1.281 (5)	OW2—H2A	0.88 (2)
C8—N1	1.335 (6)	OW2—H2B	0.89 (2)
C8—C9	1.383 (6)		
O6—Ag1—N1	171.57 (13)	N2—C10—C11	122.4 (4)
N2—Ag2—N3	175.29 (14)	N2—C10—H10	118.8
N2—Ag2—O1 <sup>ii</sup>	95.52 (12)	C11—C10—H10	118.8
N3—Ag2—O1 <sup>ii</sup>	84.24 (12)	N1—C11—C10	121.9 (4)
N2—Ag2—OW2	89.83 (12)	N1—C11—H11	119.1
N3—Ag2—OW2	92.92 (12)	C10—C11—H11	119.1
O1 <sup>ii</sup> —Ag2—OW2	147.05 (16)	N3—C12—C13 <sup>iii</sup>	121.9 (4)
C2—C1—C6	118.4 (3)	N3—C12—H12	119.0
C2—C1—C7	122.6 (4)	C13 <sup>iii</sup> —C12—H12	119.0
C6—C1—C7	119.0 (4)	N3—C13—C12 <sup>iii</sup>	122.3 (4)
O4—C2—C1	122.5 (3)	N3—C13—H13	118.8
O4—C2—C3	116.8 (4)	C12 <sup>iii</sup> —C13—H13	118.8
C1—C2—C3	120.8 (4)	C8—N1—C11	116.0 (4)
C4—C3—C2	119.8 (4)	C8—N1—Ag1	117.5 (3)
C4—C3—H3	120.1	C11—N1—Ag1	126.5 (3)
C2—C3—H3	120.1	C9—N2—C10	115.6 (4)
C3—C4—C5	119.8 (3)	C9—N2—Ag2	118.8 (3)
C3—C4—H4	120.1	C10—N2—Ag2	125.1 (3)
C5—C4—H4	120.1	C13—N3—C12	115.8 (4)
C6—C5—C4	120.6 (3)	C13—N3—Ag2	123.5 (3)
C6—C5—S1	120.4 (3)	C12—N3—Ag2	120.7 (3)
C4—C5—S1	119.1 (3)	S1—O1—Ag2 <sup>iv</sup>	139.7 (2)
C5—C6—C1	120.5 (4)	C2—O4—H4A	109.5
C5—C6—H6	119.7	C7—O6—Ag1	123.7 (3)
C1—C6—H6	119.7	O1—S1—O3	115.8 (3)
O5—C7—O6	124.1 (3)	O1—S1—O2	110.9 (3)
O5—C7—C1	120.2 (4)	O3—S1—O2	110.4 (3)
O6—C7—C1	115.6 (4)	O1—S1—C5	106.73 (19)
N1—C8—C9	121.9 (4)	O3—S1—C5	105.6 (2)
N1—C8—H8	119.1	O2—S1—C5	106.9 (2)
C9—C8—H8	119.1	H1A—OW1—H1B	110 (6)
N2—C9—C8	122.2 (4)	Ag2—OW2—H2A	128 (4)
N2—C9—H9	118.9	Ag2—OW2—H2B	107.5 (17)
C8—C9—H9	118.9	H2A—OW2—H2B	100 (5)
C6—C1—C2—O4	-176.7 (4)	C11—C10—N2—C9	-1.2 (7)
C7—C1—C2—O4	1.4 (7)	C11—C10—N2—Ag2	170.5 (4)
C6—C1—C2—C3	3.1 (7)	O1 <sup>ii</sup> —Ag2—N2—C9	35.7 (4)
C7—C1—C2—C3	-178.8 (4)	OW2—Ag2—N2—C9	-176.9 (4)

## supplementary materials

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O4—C2—C3—C4	177.1 (4)	O1 <sup>ii</sup> —Ag2—N2—C10	-135.8 (4)
C1—C2—C3—C4	-2.7 (7)	OW2—Ag2—N2—C10	11.6 (4)
C2—C3—C4—C5	-0.4 (7)	C12 <sup>iii</sup> —C13—N3—C12	0.2 (8)
C3—C4—C5—C6	3.1 (7)	C12 <sup>iii</sup> —C13—N3—Ag2	-177.7 (3)
C3—C4—C5—S1	-176.0 (4)	C13 <sup>iii</sup> —C12—N3—C13	-0.2 (8)
C4—C5—C6—C1	-2.6 (7)	C13 <sup>iii</sup> —C12—N3—Ag2	177.8 (3)
S1—C5—C6—C1	176.4 (3)	O1 <sup>ii</sup> —Ag2—N3—C13	147.0 (4)
C2—C1—C6—C5	-0.4 (7)	OW2—Ag2—N3—C13	-0.1 (4)
C7—C1—C6—C5	-178.6 (4)	O1 <sup>ii</sup> —Ag2—N3—C12	-30.8 (4)
C2—C1—C7—O5	174.9 (5)	OW2—Ag2—N3—C12	-177.9 (4)
C6—C1—C7—O5	-7.0 (7)	O5—C7—O6—Ag1	15.5 (7)
C2—C1—C7—O6	-4.6 (7)	C1—C7—O6—Ag1	-165.0 (3)
C6—C1—C7—O6	173.5 (4)	Ag2 <sup>iv</sup> —O1—S1—O3	-50.2 (6)
N1—C8—C9—N2	1.2 (7)	Ag2 <sup>iv</sup> —O1—S1—O2	76.5 (5)
N2—C10—C11—N1	0.5 (7)	Ag2 <sup>iv</sup> —O1—S1—C5	-167.4 (4)
C9—C8—N1—C11	-1.8 (7)	C6—C5—S1—O1	-8.2 (5)
C9—C8—N1—Ag1	176.7 (3)	C4—C5—S1—O1	170.9 (4)
C10—C11—N1—C8	1.0 (7)	C6—C5—S1—O3	-132.0 (4)
C10—C11—N1—Ag1	-177.4 (4)	C4—C5—S1—O3	47.1 (5)
C8—C9—N2—C10	0.3 (7)	C6—C5—S1—O2	110.5 (4)
C8—C9—N2—Ag2	-171.9 (3)	C4—C5—S1—O2	-70.4 (4)

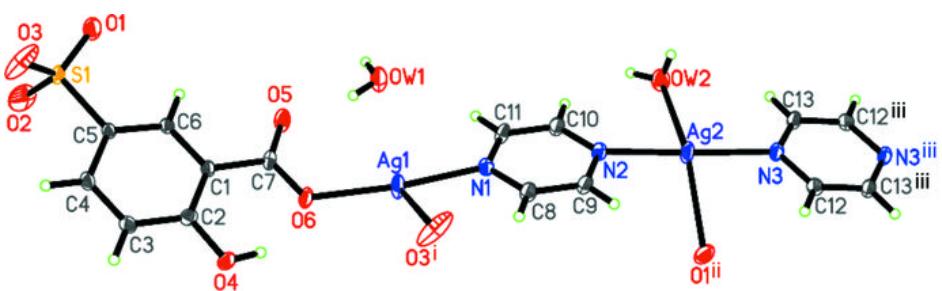
Symmetry codes: (i)  $-x, -y, -z-1$ ; (ii)  $x+1, y, z+1$ ; (iii)  $-x+1, -y+1, -z+1$ ; (iv)  $x-1, y, z-1$ .

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

$D\cdots H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
OW1—H1A <sup>v</sup> —O5	0.88 (2)	1.89 (2)	2.751 (4)
OW1—H1B <sup>v</sup> —O5 <sup>v</sup>	0.89 (2)	2.00 (2)	2.883 (5)
OW2—H2A <sup>v</sup> —O2 <sup>v</sup>	0.88 (2)	1.91 (3)	2.757 (5)
OW2—H2B <sup>v</sup> —OW1 <sup>vi</sup>	0.89 (2)	2.03 (3)	2.794 (6)
O4—H4A <sup>v</sup> —O6	0.82	1.84	2.556 (4)

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

Fig. 1



## **supplementary materials**

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**Fig. 2**

