

Poly[[diaquabis(μ_3 -3-carboxylato-4-hydroxybenzenesulfonato)tri- μ_2 -pyrazine-tetrasilver(I)] dihydrate]

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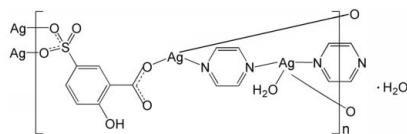
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Key indicators: single-crystal X-ray study; $T = 293\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$; R factor = 0.033; wR factor = 0.073; data-to-parameter ratio = 13.2.

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 Ag^{I} ions. One Ag^{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 Ag^{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 Ag^{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 (\AA).

| | | | |
|---------------------|-----------|----------------------|-----------|
| Ag1—N1 | 2.180 (3) | Ag2—N3 | 2.262 (3) |
| Ag1—O3 ⁱ | 2.621 (3) | Ag2—O1 ⁱⁱ | 2.516 (4) |
| Ag1—O6 | 2.153 (3) | Ag2—OW2 | 2.576 (4) |
| Ag2—N2 | 2.245 (3) | | |

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

Table 2
Hydrogen-bond geometry (\AA , $^\circ$).

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

References

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supporting information

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

Poly[[diaqua $\text{bis}(\mu_3\text{-}3\text{-carboxylato}\text{-}4\text{-hydroxybenzenesulfonato})\text{tri-}\mu_2\text{-pyrazine-tetrasilver(I)}\text{] dihydrate}]$

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

S1. 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.

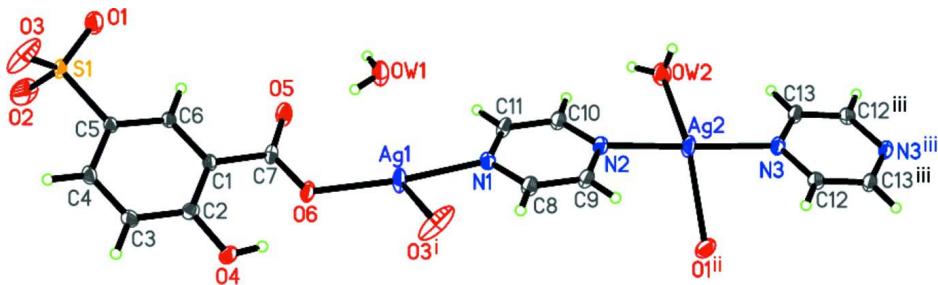
As shown in Fig. 1, there exist two crystallographically independent Ag^{l} ions. Ag^{l} atom is three-coordinated (Table 1), having an approximate T-shaped geometry composed of one sulfonate O atom, one carboxylate O atom from two 3-carboxylate-4-hydroxybenzenesulfonate (*L*) ligands and one N atom from a pyrazine ligand. Ag^{l} 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 Ag^{l} 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 \cdots O hydrogen bonds (Table 2). An intramolecular O—H \cdots O hydrogen bond is present in the *L* ligand.

S2. Experimental

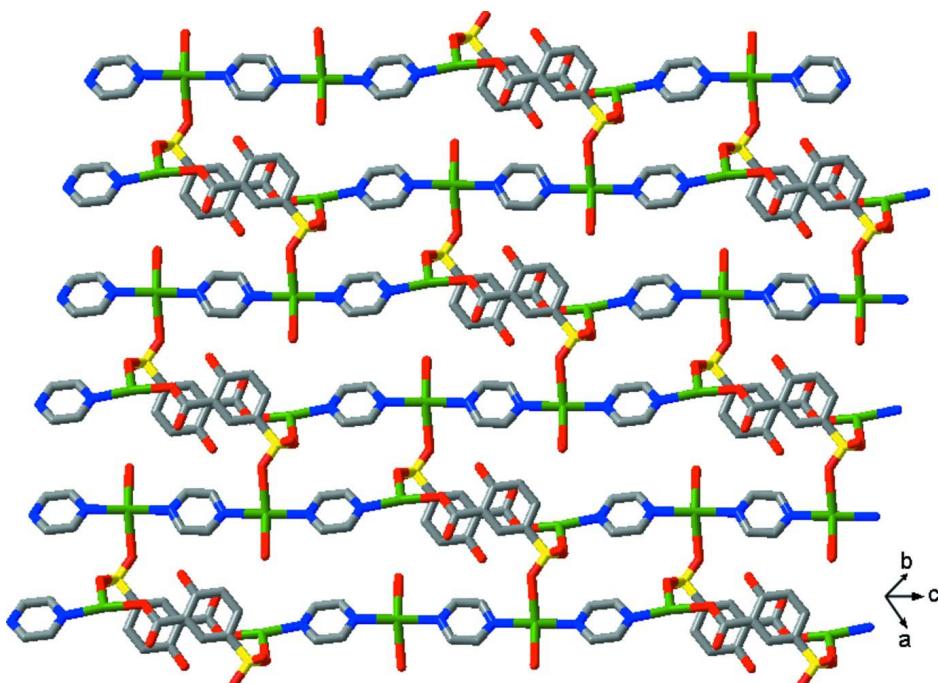
To a mixture of 5-sulfosalicylic acid (0.109 g, 0.5 mmol) and NaOH (0.040 g, 1.0 mmol) in water (5 ml) was added AgNO_3 (0.170 g, 1.0 mmol), giving a clear solution. Then ethanol (15 ml) was added to the solution, and white precipitate appeared. The precipitate was collected and dissolved in water. To 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%).

S3. 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 $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$.

**Figure 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) $1 - x, 1 - y, 1 - z$.]

**Figure 2**

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

Poly[[diaquabis(μ_3 -3-carboxylato-4-hydroxybenzenesulfonato)tri- μ_2 -pyrazine-tetrasilver(I)] dihydrate]

Crystal data



$M_r = 1176.14$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.646 (5)$ Å

$b = 10.340 (4)$ Å

$c = 11.375 (4)$ Å

$\alpha = 78.751 (3)^\circ$

$\beta = 73.436 (4)^\circ$

$\gamma = 82.882 (5)^\circ$

$V = 843.2 (7)$ Å³

$Z = 1$

$F(000) = 574$

$D_x = 2.316 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2192 reflections

$\theta = 3.2\text{--}27.5^\circ$

$\mu = 2.50 \text{ mm}^{-1}$

$T = 293$ K

Block, colorless

$0.21 \times 0.15 \times 0.12$ mm

Data collection

Bruker APEX CCD
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 φ and ω scans
Absorption correction: multi-scan
(*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.622$, $T_{\max} = 0.754$

7253 measured reflections
3387 independent reflections
2190 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.058$
 $\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 3.2^\circ$
 $h = -9 \rightarrow 9$
 $k = -12 \rightarrow 13$
 $l = -12 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.073$
 $S = 0.88$
3387 reflections
256 parameters
5 restraints
Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map
Hydrogen site location: inferred from
neighbouring sites
H atoms treated by a mixture of independent
and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0213P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.70 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.09 \text{ e } \text{\AA}^{-3}$

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

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|-------------|--------------|----------------------------------|
| 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* |

Atomic displacement parameters (\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 (\AA , $\text{^{\circ}}$)

| | | | |
|---------------------------|-------------|-----------------------------|-----------|
| Ag1—N1 | 2.180 (3) | C8—H8 | 0.9300 |
| Ag1—O3 ⁱ | 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 ⁱⁱ | 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 ⁱⁱⁱ | 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 ⁱⁱⁱ | 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 ⁱⁱ | 95.52 (12) | C11—C10—H10 | 118.8 |
| N3—Ag2—O1 ⁱⁱ | 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 ⁱⁱ —Ag2—OW2 | 147.05 (16) | N3—C12—C13 ⁱⁱⁱ | 121.9 (4) |
| C2—C1—C6 | 118.4 (3) | N3—C12—H12 | 119.0 |
| C2—C1—C7 | 122.6 (4) | C13 ⁱⁱⁱ —C12—H12 | 119.0 |
| C6—C1—C7 | 119.0 (4) | N3—C13—C12 ⁱⁱⁱ | 122.3 (4) |
| O4—C2—C1 | 122.5 (3) | N3—C13—H13 | 118.8 |
| O4—C2—C3 | 116.8 (4) | C12 ⁱⁱⁱ —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 ^{iv} | 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 ⁱⁱ —Ag2—N2—C9 | 35.7 (4) |
| C7—C1—C2—C3 | -178.8 (4) | OW2—Ag2—N2—C9 | -176.9 (4) |
| O4—C2—C3—C4 | 177.1 (4) | O1 ⁱⁱ —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 ⁱⁱⁱ —C13—N3—C12 | 0.2 (8) |
| C3—C4—C5—C6 | 3.1 (7) | C12 ⁱⁱⁱ —C13—N3—Ag2 | -177.7 (3) |
| C3—C4—C5—S1 | -176.0 (4) | C13 ⁱⁱⁱ —C12—N3—C13 | -0.2 (8) |
| C4—C5—C6—C1 | -2.6 (7) | C13 ⁱⁱⁱ —C12—N3—Ag2 | 177.8 (3) |
| S1—C5—C6—C1 | 176.4 (3) | O1 ⁱⁱ —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 ⁱⁱ —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 ^{iv} —O1—S1—O3 | -50.2 (6) |
| N1—C8—C9—N2 | 1.2 (7) | Ag2 ^{iv} —O1—S1—O2 | 76.5 (5) |
| N2—C10—C11—N1 | 0.5 (7) | Ag2 ^{iv} —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 (\AA , $^\circ$)

| $D\text{—H}\cdots A$ | $D\text{—H}$ | $H\cdots A$ | $D\cdots A$ | $D\text{—H}\cdots A$ |
|-----------------------------|--------------|-------------|-------------|----------------------|
| $OW1\text{—H1A}\cdots O5$ | 0.88 (2) | 1.89 (2) | 2.751 (4) | 168 (6) |
| $OW1\text{—H1B}\cdots O5^v$ | 0.89 (2) | 2.00 (2) | 2.883 (5) | 173 (6) |
| $OW2\text{—H2A}\cdots O2^v$ | 0.88 (2) | 1.91 (3) | 2.757 (5) | 161 (6) |

| | | | | |
|-----------------------------|----------|----------|-----------|---------|
| OW2—H2B···OW1 ^{vi} | 0.89 (2) | 2.03 (3) | 2.794 (6) | 143 (2) |
| O4—H4A···O6 | 0.82 | 1.84 | 2.556 (4) | 146 |

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