The reaction of AgNO₃ with the ligand 2,2',2'',2'''-[[pyrazine-2,3,5,6-tetrayltetraakis(methylene)]tetrakis(sulfanediyl)]tetraacetic acid in the presence of a potassium acetate buffer lead to the formation of a silver(I)–potassium–organic framework, poly[dipotassium [{μ₆-2,2',2'',2'''-[[pyrazine-2,3,5,6-tetrayltetraakis(methylene)]tetrakis(sulfanediyl)]tetraacetato}disilver(I)] 5.2-hydrate], {K₂[Ag₂(C₁₆H₁₆N₂O₈S₄)]/C₁₅.2H₂O}ₙ, (I). The asymmetric unit is composed of half a binuclear silver complex located about a center of symmetry, a potassium cation and 2.6 disordered water molecules. The whole binuclear silver complex is generated by inversion symmetry with the pyrazine ring being located about an inversion centre. The ligand coordinates in a bis-tetradentate manner. The binuclear silver complex anions are linked via bridging Ag···S···Ag zigzag bonds, forming a network lying parallel to the bc plane. The networks are linked by O(carboxylate)···K⁺···O(carboxylate) bridging bonds to form a framework. The disordered water molecules are present near to the K⁺ cations.

Structure description

The title ligand, tetrakis-substituted pyrazine carboxylic acid, 2,2',2'',2'''-[[pyrazine-2,3,5,6-tetrayltetraakis(methylene)]tetrakis(sulfanediyl)]tetraacetic acid (H₄L₁), is one of a series of tetrakis-substituted pyrazine ligands containing N₄S₄ and N₂S₄O₈ donor atoms (Pacifico, 2003).

H₄L₁ is the tetraacetic acid analogue of 3,3',3''',3'''-[[pyrazine-2,3,5,6-tetrayltetraakis(methylene)]tetrakis(sulfanediyl)]tetrapropionic acid (H₄L₂), for which two triclinic polymorphs and two potassium–organic frameworks have been reported (Pacifico &
The asymmetric unit of I consists of half a binuclear silver complex, with the ligand coordinating in a bis-tetradentate manner (Fig. 1), a potassium cation and 2.6 disordered water molecules. Selected bond lengths and bond angles involving atom Ag1 are given in Table 1. The binuclear silver complex anions are linked via bridging Ag⋯S⋯Ag zigzag bonds to form a network lying parallel to the bc plane (Fig. 2). The silver ion has a sixfold AgS3O2N coordination sphere. The bond lengths involving Ag1 fall within the limits observed for the various type of bond when searching the Cambridge Structural Database (CSD, last update September 2021; Groom et al., 2016). For example, there were over 600 hits for the Ag—N pyrazine bond length that varies from 2.02 to 2.739 Å [mean value 2.312 (89) Å, median 2.304 Å and a skew value of 0.866]. In I this value is 2.550 (5) Å. For Ag—O carboxylate there were over 2,800 hits with the bond lengths varying from 1.967 to 3.089 Å [mean value 2.377 (147) Å, median 2.352 Å and a skew value of 0.532]. In I the Ag—O carboxylate bond lengths are almost equal; 2.470 (5) and 2.466 (6) Å. Finally for the Ag—S(CH2)2— bond-length type there were over 1,000 hits with the bond length varying from 2.361 to 3.583 Å [mean value 2.596 (98) Å, median 2.565 Å and a skew value of 1.645]. In I the Ag—S(CH2)2— bond lengths vary from 2.604 (2) to 2.926 (2) Å, both values involve the bridging atom S1, while distance Ag1—S2 is 2.824 (2) Å (Table 1).

The three chelate rings are far from flat, as indicated by the torsion angles given in Table 1. This is also shown by the mean planes of the chelate rings calculated using PLATON (Spek, 2020): ring Ag1/N1/C2/C3/S1 is twisted on bond S1—C3, ring Ag1/N1/C2′/C6′/S2′ has an envelope conformation with atom S2′ as the flap, and ring Ag1′/S2/C7/O4 has an envelope conformation with atom Ag1′ as the flap [symmetry code: (ii) −x, −y + 1, −z + 1].

Selected bond lengths and bond angles involving atom K1 are also given in Table 1. The strongest K+⋯Ocarboxylate bonds lengths vary from 2.608 (6) to 2.751 (6) Å, and there is one weak contact K1⋯O1 at 3.289 (6) Å (Fig. 3). A search of the CSD for carboxylato–potassium complexes revealed that in the potassium–organic frameworks catena-[(μ4-3,5,6-trichloroxypyrazine-2-carboxylato)potassium] (CSD refcode IUCrData (2022). 7, x220077) the potassium cation and the disordered water molecules, and the C-bound H atoms have been omitted.

![Figure 1](https://example.com/figure1.png)

**Figure 1**
The molecular structure of the silver complex dianion of compound I, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level. For clarity, the potassium cation and the disordered water molecules have been omitted. [Symmetry codes: (i) −x, y + 1/2, −z + 1/2; (ii) −x, −y + 1, −z + 1; (iii) −x, y − 1/2, −z + 1/2]

![Figure 2](https://example.com/figure2.png)

**Figure 2**
A view along the a-axis of the network of the silver complex dianions in compound I. The silver atoms are shown as silver balls. For clarity, the potassium ions, the disordered water molecules, and the C-bound H atoms have been omitted.

![Table 1](https://example.com/table1.png)

**Table 1**
Selected geometric parameters (Å, °).

| Bond/Angle | Value |
|-----------|-------|
| Ag1—N1    | 2.550 (5) |
| Ag1—O11   | 2.470 (5) |
| Ag1—O1ii  | 2.466 (6) |
| Ag1—S1    | 2.926 (2) |
| Ag1—S1ii  | 2.604 (2) |
| Ag1—S2ii  | 2.824 (2) |
| O4i—Ag1—O1i | 84.78 (17) |
| O4i—Ag1—N1i | 70.04 (12) |
| O4ii—Ag1—S1ii | 96.08 (14) |
| N1—Ag1—S1i | 70.04 (12) |
| N1—Ag1—S1ii | 75.65 (14) |
| N1—Ag1—S2ii | 70.04 (12) |
| O1i—Ag1—O1i | 84.78 (17) |
| O1i—Ag1—N1i | 70.04 (12) |
| O2—K1—O1 | 42.72 (15) |
| O3iv—K1—O1 | 146.36 (18) |
| O4iv—K1—O1 | 116.0 (2) |
| O4ii—K1—O3iv | 94.50 (18) |
| N1—Ag1—S1i | 70.04 (12) |
| N1—Ag1—S1ii | 75.65 (14) |
| N1—Ag1—S2ii | 70.04 (12) |
| S2—C7—C8—O4 | 1.5 (10) |
| K1—Ag1—S2ii | 122.15 (6) |
| K1—O4vi | 2.608 (6) |
| K1—O3v | 2.751 (6) |

Symmetry codes: (i) −x, y + 1/2, −z + 1/2; (ii) −x, −y + 1, −z + 1; (iii) −x, y − 1/2, −z + 1/2.
The disordered water molecules are present near to the K\textsuperscript{+} cations.

In the crystal of I, the networks of the binuclear silver complex anions are linked by the bridging O\textsubscript{carboxylate}⋯K\textsuperscript{+}⋯O\textsubscript{carboxylate} bonds to form a framework (Fig. 4; Table 1). The disordered water molecules are present near to the K\textsuperscript{+} cations.

Synthesis and crystallization

The synthesis of the ligand H\textsubscript{4}L\textsubscript{1} has been described (Pacifico & Stoeckli-Evans, 2021a).

**Synthesis of poly[(μ-2,2′,2″-[[pyrazine-2,3,5,6-tetra-yltetrais(methylene)] tetakis(sulfanediyl)tetraacetato]−bis[silver(I)]-bis[potassium] 5.2(hydrate)] (I):**

\[ \text{AgNO}_3 \text{ (20.5 mg, 0.121 mmol, 2 eq) and H}_4\text{L}_1 \text{ (30 mg, 0.060 mmol, 1 eq) were mixed in 20 ml of a 1M potassium acetate buffer solution. The mixture was left at 323 K under stirring and nitrogen conditions for 1 h. The mixture was then filtered and left to evaporate in air for six weeks, yielding yellow rod-like crystals of compound I (m.p. 553 K decomposition).} \]

**Analysis for C\textsubscript{16}H\textsubscript{16}Ag\textsubscript{2}N\textsubscript{2}O\textsubscript{8}S\textsubscript{4}, K\textsubscript{2}, 5.2(H\textsubscript{2}O), M\textsubscript{w} = 880.175 g mol\textsuperscript{−1}; Calculated (%): C 21.88, H 2.99, N 3.18. Found (%): C 23.03, H 2.91, N 3.03. The small deviation is probably due to the loss of water molecules of crystallization.**

**ESI−MS: unstable under mass spectroscopy experimental conditions.**

---

**Table 1**

| Crystal data   | Chemical formula | K_2[A_2(C_16H_16N_2O_8S_4)]5.2H_2O |
|----------------|------------------|-------------------------------------|
| M_e           |                  | 880.17                              |
| Crystal system |                  | Monoclinic, P_2_1/c                 |
| Space group    |                  |                                     |
| Temperature (K)|                  | 153                                 |
| a, b, c (Å)    |                  | 13.386 (3), 6.0085 (7), 17.843 (3)   |
| β (°)          |                  | 108.657 (15)                        |
| V (Å\textsuperscript{3}) |              | 1359.7 (4)                         |
| Z              |                  | 2                                   |
| Radiation type |                  | Mo Kα                               |
| μ (mm\textsuperscript{−1}) |            | 2.12                                |
| Crystal size (mm) |                | 0.24 × 0.13 × 0.05                  |

**Data collection**

|                  |                  |                                      |
|------------------|------------------|-------------------------------------|
|                |                  | Stoe IPDS 2                         |
| Diffraetometer  |                  | Multi-scan (MULABS; Speck, 2020)    |
| Absorption correction |              |                                      |
| T_{min}, T_{max} |                  | 0.611, 1.000                        |
| No. of measured, independent and observed | | 9305, 2316, 2088                  |
| R_{int}         |                  | 0.094                               |
| (sin θ/λ)_{max} (Å\textsuperscript{−1}) | | 0.591                             |

**Refinement**

|                  |                  |                                      |
|------------------|------------------|-------------------------------------|
|                |                  |                                      |
|                |                  | 0.048, 0.114, 1.17                  |
| No. of reflections |                | 2316                                |
| No. of parameters |                  | 218                                 |
| H-atom treatment |                  | H-atom parameters constrained      |
| Δρ_{max}, Δρ_{min} (e Å\textsuperscript{−3}) | | 1.14, −1.10                     |

**Computer programs:** X-AREA (Stoe & Cie, 2002), X-RED32 (Stoe & Cie, 2002), SHELX97 (Sheldrick, 2008), SHELXL2018/3 (Sheldrick, 2015), PLATON (Speck, 2020) and Mercury (Macrae et al., 2020), SHELXL, 2018/3, PLATON (Speck, 2020) and pubICIF (Westrip, 2010).

---

UBUPAK; Masci et al., 2010, and catena-[(μ-6-carboxy-pyridine-2-carboxylato)potassium] (MUPWIW; Li et al., 2020), the K\textsuperscript{+}⋯O bond lengths vary from 2.7951 (11) to 2.8668 (13) Å in UBUPAK and from 2.8197 (14) to 3.0449 (15) Å in MUPWIW. In UBUPAK the K\textsuperscript{+} cation has a coordination number of 8 (KO\textsubscript{8}) and has an edge-sharing pentagonal dodecahedral geometry, while in MUPWIW the K\textsuperscript{+} ion has a coordination number of 7 (KO\textsubscript{7}N) and has a distorted dodecahedral antiprism geometry. In I, the stronger K⋯O bond lengths are shorter and, owing to the presence of the disordered water molecules, it is not clear what the K\textsuperscript{+} ion coordination number or geometry are.
IR (KBr disc, cm\(^{-1}\)) \(\nu\): 3401(s), 2938(m), 1599(s), 1385(s), 1223(m).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The occupancy factors for the disordered water molecules were initially freely refined and then fixed at rounded values; the final total is 5.2(H\(_2\)O). It was not possible to locate the H atoms of the disordered water molecules of crystallization. The residual electron density peaks of 1.14 and \(-1.10 \text{ eÅ}^3\) are at distances of 0.96 and 0.91 Å, respectively, from atom Ag1.

Acknowledgements

HSE is grateful to the University of Neuchâtel for their support over the years.

Funding information

Funding for this research was provided by: Swiss National Science Foundation; University of Neuchatel.

References

Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B72, 171–179.

Li, C., Wang, K., Li, J. & Zhang, Q. (2020). *Nanoscale*, 12, 7870–7874.

Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* 53, 226–235.

Masci, B., Pasquale, S. & Thuéry, P. (2010). *Cryst. Growth Des.* 10, 2004–2010.

Pacifico, J. (2003). PhD thesis, University of Neuchâtel, Switzerland.

Pacifico, J. & Stoeckli-Evans, H. (2021a). *Acta Cryst.* E77, 480–490.

Pacifico, J. & Stoeckli-Evans, H. (2021b). *IUCrData*, x211295.

Sheldrick, G. M. (2008). *Acta Cryst.* A64, 112–122.

Sheldrick, G. M. (2015). *Acta Cryst.* C71, 3–8.

Spek, A. L. (2020). *Acta Cryst.* E76, 1–11.

Stoe & Cie (2002). X-AREA and X-RED32. Stoe & Cie GmbH, Darmstadt, Germany.

Westrip, S. P. (2010). *J. Appl. Cryst.* 43, 920–925.
full crystallographic data

Poly[dipotassium [(\(\mu_6\)-2,2',2'',2''''-[[pyrazine-2,3,5,6-tetrayltetrakis(methylene)]tetrakis(sulfanediyl)]tetraacetato)disilver(I)] 5.2-hydrate]

Jessica Pacifico and Helen Stoeckli-Evans

Crystal data

K\(_2\)[Ag\(_2\)(C\(_{16}\)H\(_{16}\)N\(_2\)O\(_8\)S\(_4\))]5.2H\(_2\)O

\(M_r = 880.17\)

Monoclinic, \(P2_1/c\)

\(a = 13.386\) (3) Å

\(b = 6.0085\) (7) Å

\(c = 17.843\) (3) Å

\(\beta = 108.657\) (15)

\(V = 1359.7\) (4) Å\(^3\)

\(Z = 2\)

F(000) = 852

\(D_x = 2.097\) Mg m\(^{-3}\)

Mo K\(\alpha\) radiation, \(\lambda = 0.71073\) Å

Cell parameters from 17882 reflections

\(\theta = 1.6^-{24.9}^\circ\)

\(\mu = 2.12\) mm\(^{-1}\)

\(T = 153\) K

Rod, yellow

0.24 × 0.13 × 0.05 mm

Data collection

Stoe IPDS 2
diffractometer

Radiation source: fine-focus sealed tube

Plane graphite monochromator

\(\phi + \omega\) scans

Absorption correction: multi-scan

(MULABS; Spek, 2020)

\(T_{\text{min}} = 0.611, T_{\text{max}} = 1.000\)

9305 measured reflections

2316 independent reflections

2088 reflections with \(I > 2\sigma(I)\)

\(R_{\text{int}} = 0.043\)

\(\theta_{\text{max}} = 24.8^\circ, \theta_{\text{min}} = 2.4^\circ\)

\(h = -15\rightarrow15\)

\(k = -7\rightarrow6\)

\(l = -20\rightarrow21\)

Refinement

Refinement on \(F^2\)

Least-squares matrix: full

\(R[F^2 > 2\sigma(F^2)] = 0.048\)

\(wR(F^2) = 0.114\)

\(S = 1.17\)

2316 reflections

218 parameters

0 restraints

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

\(w = 1/[\sigma^2(F_c^2) + (0.0335P)^2 + 8.3123P]\)

where \(P = (F_c^2 + 2F_s^2)/3\)

\((\Delta\sigma)_{\text{max}} < 0.001\)

\(\Delta\rho_{\text{max}} = 1.14\) e Å\(^{-3}\)

\(\Delta\rho_{\text{min}} = -1.10\) e Å\(^{-3}\)

Extinction correction: (SHELXL2018/3; Sheldrick, 2015),

\(F_c^2 = kF_c[1+0.001x\sigma(F_c^2)^{2/3}/sin(2\theta)]^{1/4}\)

Extinction coefficient: 0.0058 (8)
**Special details**

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement.** The C-bound H atoms were included in calculated positions and treated as riding on their parent C atom: C —H = 0.99 Å with $U_{iso}(H) = 1.2U_{eq}(C)$.

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

|       | x           | y           | z           | $U_{iso}/U_{eq}$ | Occ. (<1) |
|-------|-------------|-------------|-------------|------------------|-----------|
| Ag1   | −0.11736 (5) | 0.22235 (9) | 0.29645 (3) | 0.0422 (2)       |           |
| K1    | 0.42397 (15) | −0.0830 (3) | 0.31383 (13)| 0.0662 (6)       |           |
| S1    | 0.07736 (14) | 0.4594 (3)  | 0.30640 (9) | 0.0383 (4)       |           |
| S2    | 0.13892 (15) | 1.0313 (3)  | 0.57635 (11)| 0.0456 (5)       |           |
| O1    | 0.1777 (5)   | 0.0832 (8)  | 0.2686 (3)  | 0.0534 (13)      |           |
| O2    | 0.2813 (5)   | −0.0081 (9) | 0.3913 (3)  | 0.0602 (15)      |           |
| O3    | 0.4123 (4)   | 1.1764 (10) | 0.7406 (4)  | 0.0625 (15)      |           |
| O4    | 0.3022 (5)   | 0.8947 (10) | 0.7311 (3)  | 0.0617 (15)      |           |
| N1    | −0.0564 (4)  | 0.4506 (9)  | 0.4235 (3)  | 0.0363 (13)      |           |
| C1    | 0.0288 (5)   | 0.5773 (10) | 0.4399 (3)  | 0.0335 (14)      |           |
| C2    | 0.0881 (5)   | 0.6285 (10) | 0.5180 (4)  | 0.0367 (15)      |           |
| C3    | 0.0533 (6)   | 0.6731 (11) | 0.3695 (4)  | 0.0392 (15)      |           |
| C4    | 0.0190 (6)   | 0.3419 (12) | 0.3732 (4)  | 0.0486 (18)      |           |
| C5    | 0.2207 (6)   | 0.1200 (12) | 0.3415 (5)  | 0.0478 (18)      |           |
| C6    | 0.1824 (6)   | 0.7758 (11) | 0.5427 (4)  | 0.0397 (15)      |           |
| C7    | 0.2611 (6)   | 1.1711 (12) | 0.6282 (5)  | 0.0508 (18)      |           |
| C8    | 0.303971 (6) | 1.179423 (13)| 0.592207 (5)| 0.061 (15)       |           |
| O1W   | 0.479 (2)    | 0.483 (5)   | 0.3773 (16) | 0.072 (7)        | 0.3       |
| O2W   | 0.4522 (18)  | 0.660 (4)   | 0.0890 (13) | 0.071 (6)        | 0.3       |
| O3W   | 0.4365 (15)  | 0.538 (4)   | 0.0344 (9)  | 0.123 (7)        | 0.5       |
| O4W   | 0.4421 (18)  | 0.285 (3)   | 0.0195 (13) | 0.105 (7)        | 0.4       |
| O5W   | 0.4629 (16)  | 0.844 (4)   | 0.0802 (13) | 0.057 (5)        | 0.3       |
| O6W   | 0.451 (3)    | 0.951 (7)   | 0.115 (2)   | 0.198 (17)       | 0.5       |
| O7W   | 0.556 (4)    | 0.047 (9)   | 0.009 (3)   | 0.23 (3)         | 0.3       |

**Atomic displacement parameters ($\AA^2$)**

|       | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$    | $U^{13}$    | $U^{23}$    |
|-------|-------------|-------------|-------------|-------------|-------------|-------------|
| Ag1   | 0.0620 (4)  | 0.0363 (3)  | 0.0386 (3)  | −0.0055 (2) | 0.0305 (3)  | −0.0060 (2) |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
|   | K1 0.0607 (11) | K1 0.0602 (12) | K1 0.0891 (14) | K1 0.0039 (9) | K1 0.0400 (10) | K1 0.0048 (10) |
|   | S1 0.0579 (11) | S1 0.0325 (8) | S1 0.0332 (8) | S1 -0.0005 (7) | S1 0.0266 (8) | S1 -0.0006 (7) |
|   | S2 0.0552 (11) | S2 0.0347 (9) | S2 0.0531 (11) | S2 -0.0041 (8) | S2 0.0261 (9) | S2 -0.0089 (8) |
|   | O1 0.082 (4) | O1 0.037 (3) | O1 0.050 (3) | O1 0.003 (3) | O1 0.034 (3) | O1 -0.002 (2) |
|   | O2 0.069 (4) | O2 0.053 (3) | O2 0.067 (3) | O2 0.011 (3) | O2 0.033 (3) | O2 0.015 (3) |
|   | O3 0.059 (4) | O3 0.059 (4) | O3 0.075 (4) | O3 -0.012 (3) | O3 0.030 (3) | O3 -0.018 (3) |
|   | O4 0.070 (4) | O4 0.057 (3) | O4 0.064 (4) | O4 -0.007 (3) | O4 0.030 (3) | O4 0.005 (3) |
|   | N1 0.057 (4) | N1 0.031 (3) | N1 0.028 (3) | N1 -0.002 (3) | N1 0.024 (2) | N1 -0.001 (2) |
|   | C1 0.050 (4) | C1 0.028 (3) | C1 0.030 (3) | C1 0.000 (3) | C1 0.025 (3) | C1 -0.004 (3) |
|   | C2 0.055 (4) | C2 0.027 (3) | C2 0.039 (3) | C2 0.001 (3) | C2 0.031 (3) | C2 -0.001 (3) |
|   | C3 0.064 (4) | C3 0.032 (3) | C3 0.030 (3) | C3 -0.003 (3) | C3 0.028 (3) | C3 -0.001 (3) |
|   | C4 0.063 (5) | C4 0.045 (4) | C4 0.045 (4) | C4 0.002 (4) | C4 0.028 (4) | C4 0.004 (3) |
|   | C5 0.059 (5) | C5 0.034 (4) | C5 0.065 (5) | C5 0.003 (3) | C5 0.040 (4) | C5 0.010 (4) |
|   | C6 0.059 (4) | C6 0.032 (3) | C6 0.039 (3) | C6 -0.005 (3) | C6 0.030 (3) | C6 -0.007 (3) |
|   | C7 0.065 (5) | C7 0.036 (4) | C7 0.058 (5) | C7 -0.010 (3) | C7 0.030 (4) | C7 -0.005 (3) |
|   | C8 0.057 (5) | C8 0.045 (4) | C8 0.069 (5) | C8 -0.013 (4) | C8 0.039 (4) | C8 -0.019 (4) |
|   | O1W 0.081 (17) | O1W 0.052 (12) | O1W 0.066 (14) | O1W 0.000 (13) | O1W 0.000 (13) | O1W 0.017 (11) |
|   | O2W 0.084 (15) | O2W 0.055 (14) | O2W 0.060 (13) | O2W -0.001 (11) | O2W 0.003 (11) | O2W -0.004 (11) |
|   | O3W 0.123 (15) | O3W 0.18 (2) | O3W 0.065 (10) | O3W 0.040 (14) | O3W 0.024 (9) | O3W -0.005 (12) |
|   | O4W 0.113 (17) | O4W 0.077 (13) | O4W 0.111 (16) | O4W 0.001 (12) | O4W 0.016 (13) | O4W 0.011 (12) |
|   | O5W 0.044 (11) | O5W 0.043 (12) | O5W 0.062 (13) | O5W 0.006 (9) | O5W -0.015 (9) | O5W 0.000 (10) |
|   | O6W 0.22 (4) | O6W 0.16 (3) | O6W 0.21 (3) | O6W 0.05 (3) | O6W 0.06 (3) | O6W -0.01 (3) |
|   | O7W 0.21 (5) | O7W 0.21 (5) | O7W 0.16 (4) | O7W 0.08 (5) | O7W -0.09 (4) | O7W -0.02 (4) |

Geometric parameters (Å, °)
S2—C6 1.811 (7) O5W—O6W 0.94 (4)
O1—C5 1.263 (9) O5W—O7W 1.66 (6)
O2—C5 1.256 (9) O7W—O7W 1.53 (11)
O3—C8 1.262 (9)

O4ii—Ag1—O1i 90.01 (19) C7—S2—C6 103.3 (4)
O4ii—Ag1—N1 110.25 (18) C7—S2—Ag1ii 98.5 (3)
O1i—Ag1—N1 84.78 (17) C6—S2—Ag1ii 86.3 (2)
O4ii—Ag1—S1iii 96.08 (14) C5—O1—Ag1iii 127.6 (5)
O1i—Ag1—S1iii 108.15 (12) C5—O1—K1 73.1 (4)
N1—Ag1—S1iii 150.87 (13) Ag1iii—O1—K1 90.02 (15)
O4ii—Ag1—S2ii 69.66 (14) C5—O2—K1 98.2 (4)
O1i—Ag1—S2ii 138.52 (12) C8—O3—K1v 113.7 (5)
N1—Ag1—S2ii 70.23 (12) C8—O3—K1xii 126.4 (5)
S1iii—Ag1—S2ii 109.63 (5) K1v—O3—K1xii 115.0 (2)
O4ii—Ag1—S1 165.62 (14) C8—O4—Ag1ii 124.0 (6)
O1i—Ag1—S1 75.65 (14) C8—O4—K1xiii 127.6 (5)
N1—Ag1—S1 87.60 (4) Ag1ii—O4—K1xiii 108.3 (2)
S2ii—Ag1—S1 122.15 (6) C1—N1—C2ii 119.9 (6)
O4ii—Ag1—K1 37.02 (14) C1—N1—Ag1 120.9 (4)
O1i—Ag1—K1i 53.08 (13) N1—C1—C2 112.4 (5)
N1—Ag1—K1i 105.00 (13) N1—C1—C3 115.9 (6)
S1iii—Ag1—K1i 103.54 (5) C2—C1—C3 122.7 (6)
S2ii—Ag1—K1i 101.25 (5) N1ii—C2—C1 118.7 (6)
S1—Ag1—K1i 128.60 (5) N1ii—C2—C6 115.6 (6)
Ag1i—Si—Ag1 129.26 (7) C1—C2—C6 125.6 (5)
O2Wi—K1—O4 169.6 (6) C1—C3—S1 112.2 (4)
O2Wv—K1—O3i 86.3 (6) C1—C3—H3A 109.2
O4iv—K1—O3i 94.50 (18) S1—C3—H3A 109.2
O2Wv—K1—O2 88.2 (6) C1—C3—H3B 109.2
O4iv—K1—O2 89.60 (19) S1—C3—H3B 109.2
O3v—K1—O2 170.9 (2) H3A—C3—H3B 107.9
O2Wvi—K1—O3vi 74.4 (6) C5—C4—S1 109.6 (5)
O4vi—K1—O3vi 116.0 (2) C5—C4—H4A 109.7
O3v—K1—O3vi 86.76 (14) S1—C4—H4A 109.7
O2—K1—O3vi 98.72 (18) C5—C4—H4B 109.7
O2Wv—K1—O1Wvii 103.5 (8) S1—C4—H4B 109.7
O4iv—K1—O1Wviii 66.6 (6) S4A—C4—H4B 108.2
O3v—K1—O1Wviii 79.4 (6) O2—C5—O1 126.8 (7)
O2—K1—O1Wviii 94.8 (6) O2—C5—C4 115.7 (7)
O3—K1—O1Wviii 166.2 (6) O1—C5—C4 117.4 (7)
O2Wvi—K1—O3Wv 24.4 (6) O2—C5—K1 58.7 (4)
O4vi—K1—O3Wv 145.2 (5) O1—C5—K1 84.4 (4)
O3v—K1—O3Wv 91.9 (4) C4—C5—K1 132.6 (5)
O2—K1—O3Wv 80.2 (4) C2—C6—S2 105.7 (5)
O3vi—K1—O3Wv 98.4 (5) C2—C6—H6A 110.6
O1W—K1—O3Wv 81.2 (8) S2—C6—H6A 110.6
$O_2^{iv}v—K_1—O_4^{iv}v$ 54.0 (7)  
$O_4^{iv}v—K_1—O_4^{iv}v$ 115.6 (4)  
$O_3^{iii}—K_1—O_4^{iv}v$ 90.3 (5)  
$O_2—K_1—O_4^{iv}v$ 80.6 (5)  
$O_3^{iii}—K_1—O_4^{iv}v$ 128.4 (4)  
$O_1^{viii}—K_1—O_4^{iv}v$ 51.4 (7)  
$O_3^{v}—K_1—O_4^{iv}v$ 30.2 (6)  
$O_2^{iv}—K_1—C_5$ 94.6 (6)  
$O_4^{iv}v—K_1—C_5$ 87.3 (2)  
$O_3^{iii}—K_1—C_5$ 165.0 (2)  
$O_2—K_1—C_5$ 23.16 (17)  
$O_3^{v}—K_1—C_5$ 79.11 (18)  
$O_1^{viii}—K_1—C_5$ 114.7 (6)  
$O_3^{iii}—K_1—C_5$ 95.1 (5)  
$O_4^{iv}—K_1—C_5$ 102.4 (5)  
$O_2^{iv}—K_1—O_5^{iv}v$ 16.3 (6)  
$O_4^{iv}v—K_1—O_5^{iv}v$ 169.7 (4)  
$O_3^{v}—K_1—O_5^{iv}v$ 95.3 (4)  
$O_2—K_1—O_5^{iv}v$ 81.2 (5)  
$O_3^{iii}—K_1—O_5^{iv}v$ 61.4 (4)  
$O_1^{viii}—K_1—O_5^{iv}v$ 118.5 (7)  
$O_3^{v}—K_1—O_5^{iv}v$ 37.5 (6)  
$O_4^{iv}—K_1—O_5^{iv}v$ 67.6 (5)  
$C_5—K_1—O_5^{iv}v$ 82.5 (4)  
$O_2^{iv}—K_1—O_1$ 112.9 (6)  
$O_4^{iv}—K_1—O_1$ 71.53 (16)  
$O_3^{v}—K_1—O_1$ 146.36 (18)  
$O_2—K_1—O_1$ 42.72 (15)  
$O_3^{iii}—K_1—O_1$ 73.37 (15)  
$O_1^{viii}—K_1—O_1$ 119.2 (6)  
$O_3^{v}—K_1—O_1$ 117.2 (5)  
$O_4^{iv}—K_1—O_1$ 123.3 (5)  
$C_5—K_1—O_1$ 22.47 (17)  
$O_5^{iv}—K_1—O_1$ 98.4 (4)  
$O_2^{iv}—K_1—O_6^{iv}x$ 95.0 (8)  
$O_4^{iv}—K_1—O_6^{iv}x$ 76.0 (7)  
$O_3^{v}—K_1—O_6^{iv}x$ 66.1 (7)  
$O_2—K_1—O_6^{iv}x$ 107.3 (7)  
$O_3^{iii}—K_1—O_6^{iv}x$ 151.6 (7)  
$O_1^{viii}—K_1—O_6^{iv}x$ 15.1 (8)  
$O_3^{v}—K_1—O_6^{iv}x$ 75.6 (9)  
$O_4^{iv}—K_1—O_6^{iv}x$ 48.4 (8)  
$C_5—K_1—O_6^{iv}x$ 128.6 (7)  
$O_5^{iv}—K_1—O_6^{iv}x$ 111.1 (7)  
$O_1—K_1—O_6^{iv}x$ 134.3 (7)  
$C_3—S_1—C_4$ 99.7 (3)  
$C_3—S_1—A_{gi}^{i}$ 97.3 (2)  
$C_4—S_1—A_{gi}^{i}$ 110.7 (2)
| Bond/Angle | Value 1/StdDev | Bond/Angle | Value 2/StdDev |
|------------|--------------|------------|--------------|
| C3—S1—Ag1 | 92.9 (2)     | O7W\textsuperscript{iv}—O7W—O5W\textsuperscript{v} | 96 (3) |
| C4—S1—Ag1 | 116.3 (3)    |            |              |
| C2\textsuperscript{i}—N1—C1—C2 | 0.9 (10) | K1\textsuperscript{ii}—O3—C8—C7 | 70.3 (8) |
| Ag1—N1—C1—C2 | −153.3 (5) | K1\textsuperscript{ii}—O3—C8—K1\textsuperscript{v} | 153.8 (8) |
| C2\textsuperscript{ii}—N1—C1—C3 | −175.4 (6) | K1\textsuperscript{v}—O3—C8—K1\textsuperscript{iii} | 78.2 (4) |
| Ag1—N1—C1—C3 | 30.4 (7) | K1\textsuperscript{ii}—O3—C8—K1\textsuperscript{viii} | −128.0 (4) |
| N1—C1—C2—N1\textsuperscript{ii} | −0.9 (10) | S2—C7—C8—O4 | 1.5 (10) |
| C3—C1—C2—N1\textsuperscript{ii} | 175.2 (6) | S2—C7—C8—K1\textsuperscript{vii} | −178.3 (5) |
| N1—C1—C2—C6 | −177.5 (6) | S2—C7—C8—K1\textsuperscript{viii} | 134.0 (4) |
| C3—C1—C2—C6 | −1.4 (10) | S2—C7—C8—K1\textsuperscript{v} | 37.0 (11) |
| N1—C1—C3—S1 | −61.4 (7) | O5W—O2W—O3W—O4W | 162 (3) |
| C2—C1—C3—S1 | 122.3 (6) | O6W—O2W—O3W—O4W | 179 (3) |
| C4—S1—C3—C1 | −66.2 (6) | K1\textsuperscript{vii}—O2W—O3W—O4W | 24 (3) |
| Ag1—S1—C3—C1 | −178.7 (5) | O5W—O2W—O3W—K1\textsuperscript{vii} | 138 (3) |
| Ag1—S1—C3—C1 | 51.1 (5) | O6W—O2W—O3W—K1\textsuperscript{vii} | 165 (4) |
| C3—C1—C4—C5 | 165.4 (5) | O2W—O3W—O4W—K1\textsuperscript{viii} | −21 (3) |
| Ag1—S1—C4—C5 | −93.0 (5) | O3W—O2W—O5W—O6W | 157 (4) |
| Ag1—S1—C4—C5 | 67.3 (5) | K1\textsuperscript{vii}—O2W—O5W—O6W | −78 (4) |
| K1—O2—C5—O1 | 53.3 (8) | O3W—O2W—O5W—O1W\textsuperscript{iv} | −143 (3) |
| K1—O2—C5—C4 | −125.8 (5) | O6W—O2W—O5W—O1W\textsuperscript{iv} | 60 (4) |
| Ag1\textsuperscript{iii}—O1—C5—O2 | 33.0 (11) | K1\textsuperscript{vii}—O2W—O5W—O1W\textsuperscript{iv} | −18 (3) |
| K1—O1—C5—O2 | −43.5 (7) | O3W—O2W—O5W—O7W\textsuperscript{v} | 7 (4) |
| Ag1\textsuperscript{iii}—O1—C5—C4 | −147.9 (5) | O6W—O2W—O5W—O7W\textsuperscript{v} | −150 (6) |
| K1—O1—C5—C4 | 135.6 (6) | K1\textsuperscript{vii}—O2W—O5W—O7W\textsuperscript{v} | 132 (3) |
| Ag1\textsuperscript{iii}—O1—C5—K1 | 76.5 (5) | O3W—O2W—O5W—K1\textsuperscript{vii} | −125 (4) |
| S1—C4—C5—O2 | −159.1 (5) | O6W—O2W—O5W—K1\textsuperscript{vii} | 78 (4) |
| S1—C4—C5—O1 | 21.6 (8) | O2W—O5W—O6W—O1W\textsuperscript{v} | 120 (4) |
| S1—C4—C5—K1 | 130.8 (5) | O7W\textsuperscript{iv}—O5W—O6W—O1W\textsuperscript{v} | −87 (4) |
| N1—C2—C6—S2 | −70.4 (7) | K1\textsuperscript{vii}—O5W—O6W—O1W\textsuperscript{v} | 81 (4) |
| C1—C2—C6—S2 | 106.2 (6) | O1W\textsuperscript{iv}—O5W—O6W—O2W | −120 (4) |
| C7—S2—C6—C2 | 165.8 (5) | O7W\textsuperscript{v}—O5W—O6W—O2W | 153 (5) |
| Ag1—S2—C6—C2 | 68.0 (4) | K1\textsuperscript{vii}—O5W—O6W—O2W | −39 (2) |
| C6—S2—C7—C8 | −69.2 (6) | O2W—O5W—O6W—K1\textsuperscript{vii} | 142 (3) |
| Ag1—S2—C7—C8 | 18.9 (6) | O1W\textsuperscript{iv}—O5W—O6W—K1\textsuperscript{vii} | 22 (2) |
| Ag1—O4—C8—O3 | 150.8 (6) | O7W\textsuperscript{v}—O5W—O6W—K1\textsuperscript{vii} | −65 (5) |
| K1\textsuperscript{vii}—O4—C8—O3 | −32.5 (10) | K1\textsuperscript{vii}—O5W—O6W—K1\textsuperscript{vii} | 103 (4) |
| Ag1—O4—C8—C7 | −29.0 (9) | O5W—O2W—O6W—O1W\textsuperscript{v} | −60 (5) |
| K1—O4—C8—C7 | 147.7 (6) | O3W—O2W—O6W—O1W\textsuperscript{v} | −94 (5) |
| Ag1—O4—C8—K1\textsuperscript{v} | −154.8 (3) | K1\textsuperscript{vii}—O2W—O6W—O1W\textsuperscript{v} | 58 (5) |
| K1\textsuperscript{vii}—O4—C8—K1\textsuperscript{v} | 21.9 (8) | O3W—O2W—O6W—O5W | −34 (6) |
| Ag1—O4—C8—K1\textsuperscript{viii} | −176.7 (9) | K1\textsuperscript{vii}—O2W—O6W—O5W | 118 (4) |
| K1—O3—C8—O4 | 96.7 (8) | O5W—O2W—O6W—K1\textsuperscript{vii} | −72 (5) |
| K1\textsuperscript{v}—O3—C8—O4 | −109.5 (8) | O3W—O2W—O6W—K1\textsuperscript{vii} | −106 (5) |
| K1\textsuperscript{v}—O3—C8—C7 | −83.5 (7) | K1\textsuperscript{vii}—O2W—O6W—K1\textsuperscript{vii} | 45 (5) |

Symmetry codes: (i) $-x, y+1/2, -z+1/2$; (ii) $-x, -y+1, -z+1$; (iii) $-x, y-1/2, -z+1/2$; (iv) $-x+1, y-1/2, -z+1/2$; (v) $x, -y+1, -z+1$; (vi) $x, y+1/2, z-1/2$; (vii) $x, y+1/2, z-1/2$; (viii) $x, y-1, z$; (ix) $-x+1, y-3/2, z-1/2$; (x) $-x, -y+1, -z$; (xi) $-x+1, -y, -z$; (xii) $x, -y+3/2, z+1/2$; (xiii) $x, -y+1, z+1/2$; (xiv) $x, y+1, z$; (xv) $-x+1, y+1/2, -z+1/2$; (xvi) $-x+1, y+3/2, -z+1/2$. 

\(IUCrData\) (2022). 7, x220077