

Poly[dipotassium $[(\mu_6-2,2',2'',2''')\text{-}\{[\text{pyrazine-2,3,5,6-tetra-yltetrakis(methylene)}]\text{tetrakis(sulfanediy)}]\text{tetraacetato}]\text{disilver(I)}]$ 5.2-hydrate]

Jessica Pacifico^a and Helen Stoeckli-Evans^{b*}

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Keywords: crystal structure; pyrazine; carboxylate; tetrakis; silver–potassium–organic framework.

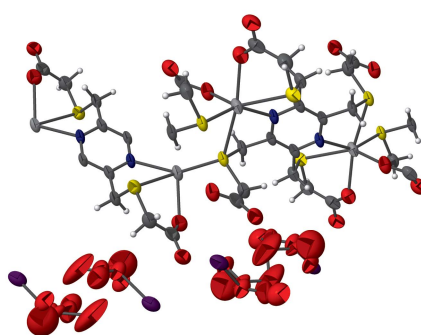
CCDC reference: 2143798

Structural data: full structural data are available from iucrdata.iucr.org

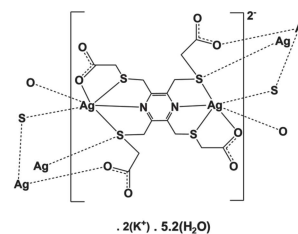
^aInstitute of Chemistry, University of Neuchâtel, Av. de Bellevaux 51, CH-2000 Neuchâtel, Switzerland, and ^bInstitute of Physics, University of Neuchâtel, rue Emile-Argand 11, CH-2000 Neuchâtel, Switzerland. *Correspondence e-mail: helen.stoeckli-evans@unine.ch

The reaction of AgNO_3 with the ligand $2,2',2'',2'''\text{-}\{[\text{pyrazine-2,3,5,6-tetra-yltetrakis(methylene)}]\text{tetrakis(sulfanediy)}]\text{tetraacetic acid}$ in the presence of a potassium acetate buffer lead to the formation of a silver(I)–potassium–organic framework, poly[dipotassium $[(\mu_6-2,2',2'',2''')\text{-}\{[\text{pyrazine-2,3,5,6-tetra-yltetrakis(methylene)}]\text{tetrakis(sulfanediy)}]\text{tetraacetato}]\text{disilver(I)}]$ 5.2-hydrate], $\{\text{K}_2[\text{Ag}_2(\text{C}_{16}\text{H}_{16}\text{N}_2\text{O}_8\text{S}_4)] \cdot 5.2\text{H}_2\text{O}\}_n$, (**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 $\text{Ag} \cdots \text{S} \cdots \text{Ag}$ zigzag bonds, forming a network lying parallel to the *bc* plane. The networks are linked by $\text{O}_{\text{carboxylate}} \cdots \text{K}^+ \cdots \text{O}_{\text{carboxylate}}$ bridging bonds to form a framework. The disordered water molecules are present near to the K^+ cations.

3D view



Chemical scheme



Structure description

The title ligand, tetrakis-substituted pyrazine carboxylic acid, $2,2',2'',2'''\text{-}\{[\text{pyrazine-2,3,5,6-tetra-yltetrakis(methylene)}]\text{tetrakis(sulfanediy)}]\text{tetraacetic acid}$ (**H₄L1**), is one of a series of tetrakis-substituted pyrazine ligands containing N_xS_4 and $\text{N}_2\text{S}_4\text{O}_8$ donor atoms (Pacifico, 2003).

H₄L1 is the tetraacetic acid analogue of $3,3',3'',3'''\text{-}\{[\text{pyrazine-2,3,5,6-tetra-yltetrakis(methylene)}]\text{tetrakis(sulfanediy)}]\text{tetrapropionic acid}$ (**H₄L2**), for which two triclinic polymorphs and two potassium–organic frameworks have been reported (Pacifico &

Table 1
Selected geometric parameters (Å, °).

Ag1–N1	2.550 (5)	K1–O1	3.289 (6)
Ag1–O1 ⁱ	2.470 (5)	K1–O2	2.729 (6)
Ag1–O4 ⁱⁱ	2.466 (6)	K1–O3 ^{iv}	2.724 (6)
Ag1–S1	2.926 (2)	K1–O3 ^v	2.751 (6)
Ag1–S1 ⁱⁱⁱ	2.604 (2)	K1–O4 ^{vi}	2.608 (6)
Ag1–S2 ⁱⁱ	2.824 (2)		
O4 ⁱⁱ –Ag1–O1 ⁱ	90.01 (19)	S1 ⁱⁱⁱ –Ag1–S1	87.60 (4)
O4 ⁱⁱ –Ag1–N1	110.25 (18)	S2 ⁱⁱ –Ag1–S1	122.15 (6)
O1 ⁱ –Ag1–N1	84.78 (17)	Ag1 ⁱ –S1–Ag1	129.26 (7)
O4 ⁱⁱ –Ag1–S1 ⁱⁱⁱ	96.08 (14)	O4 ^{vi} –K1–O3 ^{iv}	94.50 (18)
O1 ⁱ –Ag1–S1 ⁱⁱⁱ	108.15 (12)	O4 ^{vi} –K1–O2	89.60 (19)
N1–Ag1–S1 ⁱⁱⁱ	150.87 (13)	O3 ^{iv} –K1–O2	170.9 (2)
O4 ⁱⁱ –Ag1–S2 ⁱⁱ	69.66 (14)	O4 ^{vi} –K1–O3 ^v	116.0 (2)
O1 ⁱ –Ag1–S2 ⁱⁱ	138.52 (12)	O3 ^{iv} –K1–O3 ^v	86.76 (14)
N1–Ag1–S2 ⁱⁱ	70.23 (12)	O2–K1–O3 ^v	98.72 (18)
S1 ⁱⁱⁱ –Ag1–S2 ⁱⁱ	109.63 (5)	O4 ^{vi} –K1–O1	71.53 (16)
O4 ⁱⁱ –Ag1–S1	165.62 (14)	O3 ^{iv} –K1–O1	146.36 (18)
O1 ⁱ –Ag1–S1	75.65 (14)	O2–K1–O1	42.72 (15)
N1–Ag1–S1	70.04 (12)	O3 ^v –K1–O1	73.37 (15)
N1–C1–C3–S1	–61.4 (7)	S2–C7–C8–O4	1.5 (10)
N1 ⁱⁱ –C2–C6–S2	–70.4 (7)		

Symmetry codes: (i) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x, -y + 1, -z + 1$; (iii) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$; (iv) $-x + 1, -y + 1, -z + 1$; (v) $x, -y + \frac{3}{2}, z - \frac{1}{2}$; (vi) $x, -y + \frac{1}{2}, z - \frac{1}{2}$.

Stoekli-Evans, 2021*b*). Reaction of **H₄L1** with NiCl₂ lead to the formation of a binuclear complex, $\{[(\text{H}_2\text{O})_2\text{Ni}_2(\text{C}_{16}\text{H}_{20}\text{N}_2\text{O}_8\text{S}_4)] \cdot 7(\text{H}_2\text{O})\}$, whose crystal structure has been reported (Pacífico & Stoekli-Evans, 2021*b*).

The reaction of **H₄L1** (Pacífico & Stoekli-Evans, 2021*a*) with AgNO₃ in the presence of a potassium acetate buffer resulted in deprotonation of the ligand and the formation of a heterobimetallic silver(I)–potassium–organic framework (**I**).

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

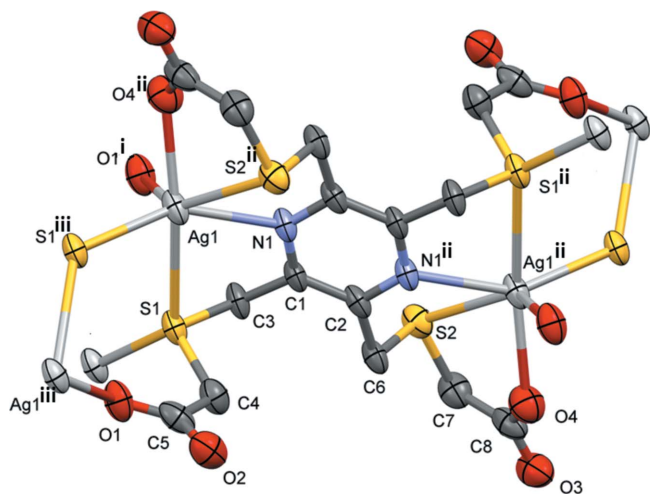


Figure 1
The molecular structure of the silver complex dianion of compound **I**, with atom labelling. Displacement ellipsoids are drawn at the 50% probability level. For clarity, the potassium cation and the disordered water molecules have been omitted. [Symmetry codes: (i) $-x, y + \frac{1}{2}, -z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

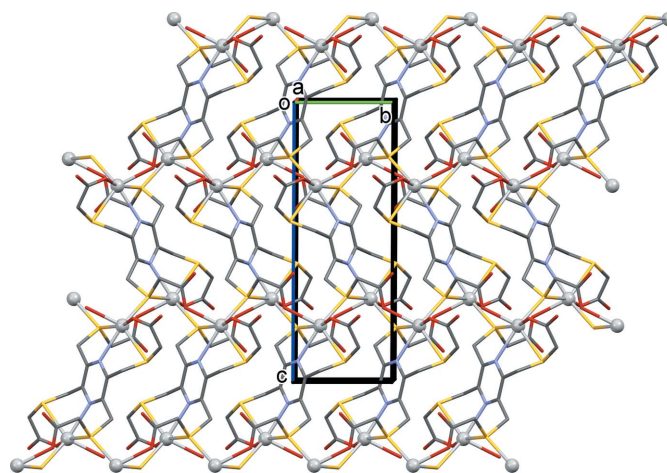


Figure 2
A view along the *a*-axis of the network of the silver complex dianions in compound **I**. The silver atoms are shown as silver balls. For clarity, the potassium ions, the disordered water molecules, and the C-bound H atoms have been omitted.

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 2.321 (89) Å, median 2.304 Å and a skew 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–S2ⁱⁱ 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/C2ⁱⁱ/C6ⁱⁱ/S2ⁱⁱ has an envelope conformation with atom S2ⁱⁱ as the flap, and ring Agⁱⁱ/S2/C7/C8/O4 has an envelope conformation with atom Ag1ⁱⁱⁱ 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⁺...O_{carboxylate} 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*-[(*μ*₄-3,5,6-tricarboxypyrazine-2-carboxylato)potassium] (CSD refcode

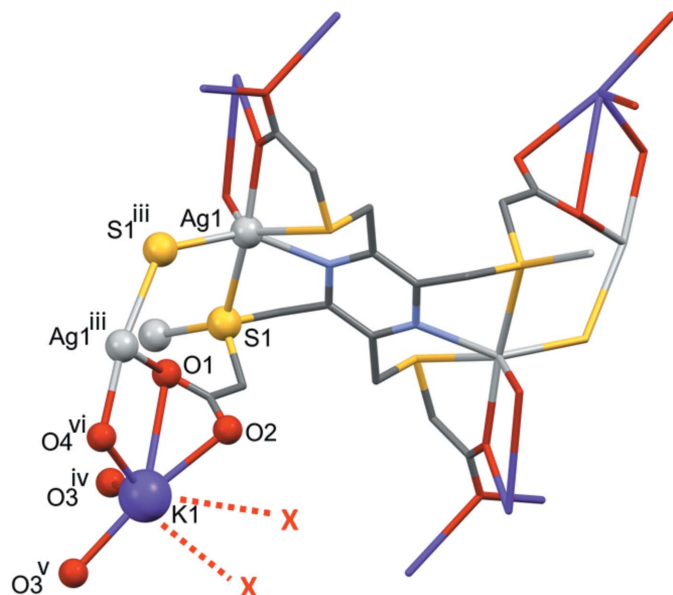


Figure 3

A view of the environment of the potassium cation in compound **I**. [X(red) regions of disordered water molecules; symmetry codes: (iii) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$; (iv) $-x + 1, -y + 1, -z + 1$; (v) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (vi) $x, -y + \frac{3}{2}, z - \frac{1}{2}$]

UBUPAK; Masci *et al.*, 2010), and *catena*-[$(\mu$ -6-carboxypyridine-2-carboxylato)potassium] (MUMPIW; Li *et al.*, 2020), the $K^+ \cdots O$ 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 MUMPIW. In UBUPAK the K^+ cation has a coordination number of 8 (KO_8) and a distorted dodecahedral geometry, while in MUMPIW the K^+ ion has a coordination number of 7 (KO_6N) and has an edge-sharing pentagonal antiprism geometry. In **I**, the stronger $K \cdots O$ bond lengths are shorter and, owing to the presence of the disordered water

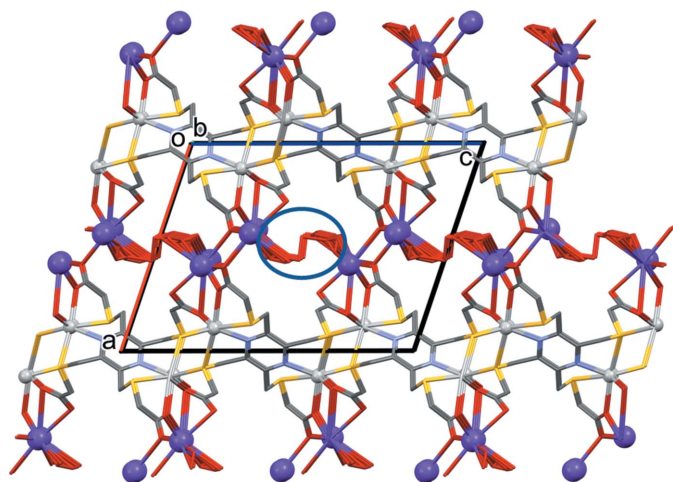


Figure 4

A view along the *b*-axis of the crystal packing of compound **I**. The silver atoms are shown as small silver balls and the potassium ions as large purple balls. The blue ellipse indicates the region occupied by the disordered water molecules. For clarity, the C-bound H atoms have been omitted.

Table 2

Experimental details.

Crystal data	
Chemical formula	$K_2[Ag_2(C_{16}H_{16}N_2O_8S_4)] \cdot 5.2H_2O$
M_r	880.17
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	153
a, b, c (Å)	13.386 (3), 6.0085 (7), 17.843 (3)
β (°)	108.657 (15)
V (Å ³)	1359.7 (4)
Z	2
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	2.12
Crystal size (mm)	0.24 × 0.13 × 0.05
Data collection	
Diffractometer	Stoe <i>IPDS 2</i>
Absorption correction	Multi-scan (<i>MULABS</i> ; Spek, 2020)
T_{min}, T_{max}	0.611, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9305, 2316, 2088
R_{int}	0.043
$(\sin \theta/\lambda)_{max}$ (Å ⁻¹)	0.591
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.048, 0.114, 1.17
No. of reflections	2316
No. of parameters	218
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å ⁻³)	1.14, -1.10

Computer programs: *X-AREA* (Stoe & Cie, 2002), *X-RED32* (Stoe & Cie, 2002), *SHELXS97* (Sheldrick, 2008), *PLATON* (Spek, 2020) and *Mercury* (Macrae *et al.*, 2020), *SHELXL2018/3* (Sheldrick, 2015), *PLATON* (Spek, 2020) and *publCIF* (Westrip, 2010).

molecules, it is not clear what the K^+ ion coordination number or geometry are.

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

Synthesis and crystallization

The synthesis of the ligand **H₄L1** has been described (Pacífico & Stoeckli-Evans, 2021a).

Synthesis of poly{ $(\mu$ -2,2',2'',2''')-[pyrazine-2,3,5,6-tetra-yltetrakis(methylene)] tetrakis(sulfanediyl)tetracetato}-bis[silver(I)]-bis[potassium] 5.2(hydrate)} (I**):**

$AgNO_3$ (20.5 mg, 0.121 mmol, 2 eq) and **H₄L1** (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 $C_{16}H_{16}Ag_2N_2O_8S_4, K_2, 5.2(H_2O)$, $M_w = 880.175 \text{ g mol}^{-1}$: 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.

IR (KBr disc, cm^{-1}) ν : 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_2O). 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 $-1.10 \text{ e}\text{\AA}^3$ are at distances of 0.96 and 0.91 Å, respectively, from atom Ag1.

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References

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full crystallographic data

IUCrData (2022). 7, x220077 [https://doi.org/10.1107/S2414314622000773]

Poly[dipotassium [(μ_6 -2,2',2'',2'''-{[pyrazine-2,3,5,6-tetrayltetrakis(methylene)]tetrakis(sulfanediyl)}tetraacetato)disilver(I)] 5.2-hydrate]

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Poly[dipotassium [(μ_6 -2,2',2'',2'''-{[pyrazine-2,3,5,6-tetrayltetrakis(methylene)]tetrakis(sulfanediyl)}tetraacetato)disilver(I)] 5.2-hydrate]

Crystal data

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

$M_r = 880.17$

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) Å³

$Z = 2$

$F(000) = 852$

$D_x = 2.097$ Mg m⁻³

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

Cell parameters from 17882 reflections

$\theta = 1.6$ – 24.9 °

$\mu = 2.12$ mm⁻¹

$T = 153$ K

Rod, yellow

$0.24 \times 0.13 \times 0.05$ mm

Data collection

Stoe IPDS 2

diffractometer

Radiation source: fine-focus sealed tube

Plane graphite monochromator

$\varphi + \omega$ scans

Absorption correction: multi-scan

(*MULABS*; Spek, 2020)

$T_{\min} = 0.611$, $T_{\max} = 1.000$

9305 measured reflections

2316 independent reflections

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

$R_{\text{int}} = 0.043$

$\theta_{\max} = 24.8$ °, $\theta_{\min} = 2.4$ °

$h = -15 \rightarrow 15$

$k = -7 \rightarrow 6$

$l = -20 \rightarrow 21$

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

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

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.14$ e Å⁻³

$\Delta\rho_{\min} = -1.10$ e Å⁻³

Extinction correction: (SHELXL2018/3;

Sheldrick, 2015),

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

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 $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	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)	
H3A	0.116280	0.769845	0.388415	0.047*	
H3B	−0.006596	0.766385	0.338485	0.047*	
C4	0.1990 (6)	0.3419 (12)	0.3732 (4)	0.0486 (18)	
H4A	0.258373	0.444967	0.377860	0.058*	
H4B	0.192240	0.321755	0.426414	0.058*	
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)	
H6A	0.208510	0.805366	0.497629	0.048*	
H6B	0.239747	0.706121	0.585903	0.048*	
C7	0.2611 (6)	1.1711 (12)	0.6282 (5)	0.0508 (18)	
H7A	0.303971	1.179423	0.592207	0.061*	
H7B	0.244080	1.325716	0.638995	0.061*	
C8	0.3293 (6)	1.0693 (13)	0.7059 (5)	0.052 (2)	
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)	0.0602 (12)	0.0891 (14)	0.0039 (9)	0.0400 (10)	0.0048 (10)
S1	0.0579 (11)	0.0325 (8)	0.0332 (8)	-0.0005 (7)	0.0266 (8)	-0.0006 (7)
S2	0.0552 (11)	0.0347 (9)	0.0531 (11)	-0.0041 (8)	0.0261 (9)	-0.0089 (8)
O1	0.082 (4)	0.037 (3)	0.050 (3)	0.003 (3)	0.034 (3)	-0.002 (2)
O2	0.069 (4)	0.053 (3)	0.067 (3)	0.011 (3)	0.033 (3)	0.015 (3)
O3	0.059 (4)	0.059 (4)	0.075 (4)	-0.012 (3)	0.030 (3)	-0.018 (3)
O4	0.070 (4)	0.057 (3)	0.064 (4)	-0.007 (3)	0.030 (3)	0.005 (3)
N1	0.057 (4)	0.031 (3)	0.028 (3)	-0.002 (3)	0.024 (2)	-0.001 (2)
C1	0.050 (4)	0.028 (3)	0.030 (3)	0.000 (3)	0.025 (3)	-0.004 (3)
C2	0.055 (4)	0.027 (3)	0.039 (3)	0.001 (3)	0.031 (3)	-0.001 (3)
C3	0.064 (4)	0.032 (3)	0.030 (3)	-0.003 (3)	0.028 (3)	-0.001 (3)
C4	0.063 (5)	0.045 (4)	0.045 (4)	0.002 (4)	0.028 (4)	0.004 (3)
C5	0.059 (5)	0.034 (4)	0.065 (5)	0.003 (3)	0.040 (4)	0.010 (4)
C6	0.059 (4)	0.032 (3)	0.039 (3)	-0.005 (3)	0.030 (3)	-0.007 (3)
C7	0.065 (5)	0.036 (4)	0.058 (5)	-0.010 (3)	0.030 (4)	-0.005 (3)
C8	0.057 (5)	0.045 (4)	0.069 (5)	-0.013 (4)	0.039 (4)	-0.019 (4)
O1W	0.081 (17)	0.052 (12)	0.066 (14)	0.000 (13)	0.000 (13)	0.017 (11)
O2W	0.084 (15)	0.055 (14)	0.060 (13)	-0.001 (11)	0.003 (11)	-0.004 (11)
O3W	0.123 (15)	0.18 (2)	0.065 (10)	0.040 (14)	0.024 (9)	-0.005 (12)
O4W	0.113 (17)	0.077 (13)	0.111 (16)	0.001 (12)	0.016 (13)	0.011 (12)
O5W	0.044 (11)	0.043 (12)	0.062 (13)	0.006 (9)	-0.015 (9)	0.000 (10)
O6W	0.22 (4)	0.16 (3)	0.21 (3)	0.05 (3)	0.06 (3)	-0.01 (3)
O7W	0.21 (5)	0.21 (5)	0.16 (4)	0.08 (5)	-0.09 (4)	-0.02 (4)

Geometric parameters (Å, °)

Ag1—N1	2.550 (5)	O4—C8	1.241 (9)
Ag1—O1 ⁱ	2.470 (5)	N1—C1	1.324 (8)
Ag1—O4 ⁱⁱ	2.466 (6)	N1—C2 ⁱⁱ	1.334 (8)
Ag1—S1	2.926 (2)	C1—C2	1.399 (9)
Ag1—S1 ⁱⁱⁱ	2.604 (2)	C1—C3	1.509 (8)
Ag1—S2 ⁱⁱ	2.824 (2)	C2—C6	1.489 (10)
Ag1—K1 ⁱ	4.113 (2)	C3—H3A	0.9900
K1—O2W ^{iv}	2.46 (2)	C3—H3B	0.9900
K1—O1	3.289 (6)	C4—C5	1.512 (10)
K1—O2	2.729 (6)	C4—H4A	0.9900
K1—O3 ^v	2.724 (6)	C4—H4B	0.9900
K1—O3 ^{vi}	2.751 (6)	C6—H6A	0.9900
K1—O4 ^{vii}	2.608 (6)	C6—H6B	0.9900
K1—O1W ^{viii}	2.84 (3)	C7—C8	1.523 (12)
K1—O3W ^{iv}	2.848 (17)	C7—H7A	0.9900
K1—O4W ^{iv}	3.05 (2)	C7—H7B	0.9900
K1—C5	3.162 (7)	O1W—O6W ^{iv}	0.93 (4)
K1—O5W ^{iv}	3.26 (2)	O1W—O5W ^{iv}	1.22 (4)
K1—O6W ^{ix}	3.30 (4)	O2W—O5W	1.13 (3)
S1—C3	1.803 (6)	O2W—O3W	1.19 (3)
S1—C4	1.824 (8)	O2W—O6W	1.81 (4)
S2—C7	1.808 (8)	O3W—O4W	1.55 (3)

S2—C6	1.811 (7)	O5W—O6W	0.94 (4)
O1—C5	1.263 (9)	O5W—O7W ^x	1.66 (6)
O2—C5	1.256 (9)	O7W—O7W ^{xi}	1.53 (11)
O3—C8	1.262 (9)		
O4 ⁱⁱ —Ag1—O1 ⁱ	90.01 (19)	C7—S2—C6	103.3 (4)
O4 ⁱⁱ —Ag1—N1	110.25 (18)	C7—S2—Ag1 ⁱⁱ	98.5 (3)
O1 ⁱ —Ag1—N1	84.78 (17)	C6—S2—Ag1 ⁱⁱ	86.3 (2)
O4 ⁱⁱ —Ag1—S1 ⁱⁱⁱ	96.08 (14)	C5—O1—Ag1 ⁱⁱⁱ	127.6 (5)
O1 ⁱ —Ag1—S1 ⁱⁱⁱ	108.15 (12)	C5—O1—K1	73.1 (4)
N1—Ag1—S1 ⁱⁱⁱ	150.87 (13)	Ag1 ⁱⁱⁱ —O1—K1	90.02 (15)
O4 ⁱⁱ —Ag1—S2 ⁱⁱ	69.66 (14)	C5—O2—K1	98.2 (4)
O1 ⁱ —Ag1—S2 ⁱⁱ	138.52 (12)	C8—O3—K1 ^v	113.7 (5)
N1—Ag1—S2 ⁱⁱ	70.23 (12)	C8—O3—K1 ^{xii}	126.4 (5)
S1 ⁱⁱⁱ —Ag1—S2 ⁱⁱ	109.63 (5)	K1 ^v —O3—K1 ^{xii}	115.0 (2)
O4 ⁱⁱ —Ag1—S1	165.62 (14)	C8—O4—Ag1 ⁱⁱ	124.0 (6)
O1 ⁱ —Ag1—S1	75.65 (14)	C8—O4—K1 ^{xiii}	127.6 (5)
N1—Ag1—S1	70.04 (12)	Ag1 ⁱⁱ —O4—K1 ^{xiii}	108.3 (2)
S1 ⁱⁱⁱ —Ag1—S1	87.60 (4)	C1—N1—C2 ⁱⁱ	119.9 (6)
S2 ⁱⁱ —Ag1—S1	122.15 (6)	C1—N1—Ag1	120.9 (4)
O4 ⁱⁱ —Ag1—K1 ⁱ	37.02 (14)	C2 ⁱⁱ —N1—Ag1	114.4 (4)
O1 ⁱ —Ag1—K1 ⁱ	53.08 (13)	N1—C1—C2	121.4 (5)
N1—Ag1—K1 ⁱ	105.00 (13)	N1—C1—C3	115.9 (6)
S1 ⁱⁱⁱ —Ag1—K1 ⁱ	103.54 (5)	C2—C1—C3	122.7 (6)
S2 ⁱⁱ —Ag1—K1 ⁱ	101.25 (5)	N1 ⁱⁱ —C2—C1	118.7 (6)
S1—Ag1—K1 ⁱ	128.60 (5)	N1 ⁱⁱ —C2—C6	115.6 (6)
Ag1 ⁱ —S1—Ag1	129.26 (7)	C1—C2—C6	125.6 (5)
O2W ^{iv} —K1—O4 ^{vii}	169.6 (6)	C1—C3—S1	112.2 (4)
O2W ^{iv} —K1—O3 ^v	86.3 (6)	C1—C3—H3A	109.2
O4 ^{vii} —K1—O3 ^v	94.50 (18)	S1—C3—H3A	109.2
O2W ^{iv} —K1—O2	88.2 (6)	C1—C3—H3B	109.2
O4 ^{vii} —K1—O2	89.60 (19)	S1—C3—H3B	109.2
O3 ^v —K1—O2	170.9 (2)	H3A—C3—H3B	107.9
O2W ^{iv} —K1—O3 ^{vi}	74.4 (6)	C5—C4—S1	109.6 (5)
O4 ^{vii} —K1—O3 ^{vi}	116.0 (2)	C5—C4—H4A	109.7
O3 ^v —K1—O3 ^{vi}	86.76 (14)	S1—C4—H4A	109.7
O2—K1—O3 ^{vi}	98.72 (18)	C5—C4—H4B	109.7
O2W ^{iv} —K1—O1W ^{viii}	103.5 (8)	S1—C4—H4B	109.7
O4 ^{vii} —K1—O1W ^{viii}	66.6 (6)	H4A—C4—H4B	108.2
O3 ^v —K1—O1W ^{viii}	79.4 (6)	O2—C5—O1	126.8 (7)
O2—K1—O1W ^{viii}	94.8 (6)	O2—C5—C4	115.7 (7)
O3 ^{vi} —K1—O1W ^{viii}	166.2 (6)	O1—C5—C4	117.4 (7)
O2W ^{iv} —K1—O3W ^{iv}	24.4 (6)	O2—C5—K1	58.7 (4)
O4 ^{vii} —K1—O3W ^{iv}	145.2 (5)	O1—C5—K1	84.4 (4)
O3 ^v —K1—O3W ^{iv}	91.9 (4)	C4—C5—K1	132.6 (5)
O2—K1—O3W ^{iv}	80.2 (4)	C2—C6—S2	105.7 (5)
O3 ^{vi} —K1—O3W ^{iv}	98.4 (5)	C2—C6—H6A	110.6
O1W ^{viii} —K1—O3W ^{iv}	81.2 (8)	S2—C6—H6A	110.6

O2W ^{iv} —K1—O4W ^{iv}	54.0 (7)	C2—C6—H6B	110.6
O4 ^{vii} —K1—O4W ^{iv}	115.6 (4)	S2—C6—H6B	110.6
O3 ^v —K1—O4W ^{iv}	90.3 (5)	H6A—C6—H6B	108.7
O2—K1—O4W ^{iv}	80.6 (5)	C8—C7—S2	117.4 (5)
O3 ^{vi} —K1—O4W ^{iv}	128.4 (4)	C8—C7—H7A	108.0
O1W ^{viii} —K1—O4W ^{iv}	51.4 (7)	S2—C7—H7A	108.0
O3W ^{iv} —K1—O4W ^{iv}	30.2 (6)	C8—C7—H7B	108.0
O2W ^{iv} —K1—C5	94.6 (6)	S2—C7—H7B	108.0
O4 ^{vii} —K1—C5	87.3 (2)	H7A—C7—H7B	107.2
O3 ^v —K1—C5	165.0 (2)	O4—C8—O3	124.6 (9)
O2—K1—C5	23.16 (17)	O4—C8—C7	120.7 (7)
O3 ^{vi} —K1—C5	79.11 (18)	O3—C8—C7	114.8 (7)
O1W ^{viii} —K1—C5	114.7 (6)	O4—C8—K1 ^v	117.4 (5)
O3W ^{iv} —K1—C5	95.1 (5)	O3—C8—K1 ^v	46.6 (4)
O4W ^{iv} —K1—C5	102.4 (5)	C7—C8—K1 ^v	102.3 (4)
O2W ^{iv} —K1—O5W ^{iv}	16.3 (6)	O4—C8—K1 ^{xiii}	36.1 (4)
O4 ^{vii} —K1—O5W ^{iv}	169.7 (4)	O3—C8—K1 ^{xiii}	92.8 (5)
O3 ^v —K1—O5W ^{iv}	95.3 (4)	C7—C8—K1 ^{xiii}	147.2 (5)
O2—K1—O5W ^{iv}	81.2 (5)	K1 ^v —C8—K1 ^{xiii}	83.44 (19)
O3 ^{vi} —K1—O5W ^{iv}	61.4 (4)	O6W ^{iv} —O1W—O5W ^{iv}	50 (3)
O1W ^{viii} —K1—O5W ^{iv}	118.5 (7)	O6W ^{iv} —O1W—K1 ^{xiv}	112 (4)
O3W ^{iv} —K1—O5W ^{iv}	37.5 (6)	O5W ^{iv} —O1W—K1 ^{xiv}	155 (2)
O4W ^{iv} —K1—O5W ^{iv}	67.6 (5)	O5W—O2W—O3W	119 (3)
C5—K1—O5W ^{iv}	82.5 (4)	O5W—O2W—O6W	27 (2)
O2W ^{iv} —K1—O1	112.9 (6)	O3W—O2W—O6W	143 (2)
O4 ^{vii} —K1—O1	71.53 (16)	O5W—O2W—K1 ^{xv}	126.2 (17)
O3 ^v —K1—O1	146.36 (18)	O3W—O2W—K1 ^{xv}	96.4 (16)
O2—K1—O1	42.72 (15)	O6W—O2W—K1 ^{xv}	117.0 (16)
O3 ^{vi} —K1—O1	73.37 (15)	O2W—O3W—O4W	138 (2)
O1W ^{viii} —K1—O1	119.2 (6)	O2W—O3W—K1 ^{xv}	59.1 (13)
O3W ^{iv} —K1—O1	117.2 (5)	O4W—O3W—K1 ^{xv}	82.0 (11)
O4W ^{iv} —K1—O1	123.3 (5)	O3W—O4W—K1 ^{xv}	67.8 (10)
C5—K1—O1	22.47 (17)	O6W—O5W—O2W	121 (4)
O5W ^{iv} —K1—O1	98.4 (4)	O6W—O5W—O1W ^{xv}	49 (3)
O2W ^{iv} —K1—O6W ^{ix}	95.0 (8)	O2W—O5W—O1W ^{xv}	131 (2)
O4 ^{vii} —K1—O6W ^{ix}	76.0 (7)	O6W—O5W—O7W ^x	111 (4)
O3 ^v —K1—O6W ^{ix}	66.1 (7)	O2W—O5W—O7W ^x	122 (3)
O2—K1—O6W ^{ix}	107.3 (7)	O1W ^{xv} —O5W—O7W ^x	101 (3)
O3 ^{vi} —K1—O6W ^{ix}	151.6 (7)	O6W—O5W—K1 ^{xv}	107 (3)
O1W ^{viii} —K1—O6W ^{ix}	15.1 (8)	O2W—O5W—K1 ^{xv}	37.5 (13)
O3W ^{iv} —K1—O6W ^{ix}	75.6 (9)	O1W ^{xv} —O5W—K1 ^{xv}	95.3 (16)
O4W ^{iv} —K1—O6W ^{ix}	48.4 (8)	O7W ^x —O5W—K1 ^{xv}	140 (2)
C5—K1—O6W ^{ix}	128.6 (7)	O1W ^{xv} —O6W—O5W	82 (4)
O5W ^{iv} —K1—O6W ^{ix}	111.1 (7)	O1W ^{xv} —O6W—O2W	98 (4)
O1—K1—O6W ^{ix}	134.3 (7)	O5W—O6W—O2W	32 (2)
C3—S1—C4	99.7 (3)	O1W ^{xv} —O6W—K1 ^{xvi}	53 (3)
C3—S1—Ag1 ⁱ	97.3 (2)	O5W—O6W—K1 ^{xvi}	131 (4)
C4—S1—Ag1 ⁱ	110.7 (2)	O2W—O6W—K1 ^{xvi}	151 (2)

C3—S1—Ag1	92.9 (2)	O7W ^{xi} —O7W—O5W ^x	96 (3)
C4—S1—Ag1	116.3 (3)		
C2 ⁱⁱ —N1—C1—C2	0.9 (10)	K1 ^{xii} —O3—C8—C7	70.3 (8)
Ag1—N1—C1—C2	-153.3 (5)	K1 ^{xii} —O3—C8—K1 ^v	153.8 (8)
C2 ⁱⁱ —N1—C1—C3	-175.4 (6)	K1 ^v —O3—C8—K1 ^{xiii}	78.2 (4)
Ag1—N1—C1—C3	30.4 (7)	K1 ^{xii} —O3—C8—K1 ^{xiii}	-128.0 (4)
N1—C1—C2—N1 ⁱⁱ	-0.9 (10)	S2—C7—C8—O4	1.5 (10)
C3—C1—C2—N1 ⁱⁱ	175.2 (6)	S2—C7—C8—O3	-178.3 (5)
N1—C1—C2—C6	-177.5 (6)	S2—C7—C8—K1 ^v	134.0 (4)
C3—C1—C2—C6	-1.4 (10)	S2—C7—C8—K1 ^{xiii}	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 ^{xv} —O2W—O3W—O4W	24 (3)
Ag1 ⁱ —S1—C3—C1	-178.7 (5)	O5W—O2W—O3W—K1 ^{xv}	138 (3)
Ag1—S1—C3—C1	51.1 (5)	O6W—O2W—O3W—K1 ^{xv}	155 (4)
C3—S1—C4—C5	165.4 (5)	O2W—O3W—O4W—K1 ^{xv}	-21 (3)
Ag1 ⁱ —S1—C4—C5	-93.0 (5)	O3W—O2W—O5W—O6W	157 (4)
Ag1—S1—C4—C5	67.3 (5)	K1 ^{xv} —O2W—O5W—O6W	-78 (4)
K1—O2—C5—O1	53.3 (8)	O3W—O2W—O5W—O1W ^{xv}	-143 (3)
K1—O2—C5—C4	-125.8 (5)	O6W—O2W—O5W—O1W ^{xv}	60 (4)
Ag1 ⁱⁱⁱ —O1—C5—O2	33.0 (11)	K1 ^{xv} —O2W—O5W—O1W ^{xv}	-18 (5)
K1—O1—C5—O2	-43.5 (7)	O3W—O2W—O5W—O7W ^x	7 (4)
Ag1 ⁱⁱⁱ —O1—C5—C4	-147.9 (5)	O6W—O2W—O5W—O7W ^x	-150 (6)
K1—O1—C5—C4	135.6 (6)	K1 ^{xv} —O2W—O5W—O7W ^x	132 (3)
Ag1 ⁱⁱⁱ —O1—C5—K1	76.5 (5)	O3W—O2W—O5W—K1 ^{xv}	-125 (4)
S1—C4—C5—O2	-159.1 (5)	O6W—O2W—O5W—K1 ^{xv}	78 (4)
S1—C4—C5—O1	21.6 (8)	O2W—O5W—O6W—O1W ^{xv}	120 (4)
S1—C4—C5—K1	130.8 (5)	O7W ^x —O5W—O6W—O1W ^{xv}	-87 (4)
N1 ⁱⁱ —C2—C6—S2	-70.4 (7)	K1 ^{xv} —O5W—O6W—O1W ^{xv}	81 (4)
C1—C2—C6—S2	106.2 (6)	O1W ^{xv} —O5W—O6W—O2W	-120 (4)
C7—S2—C6—C2	165.8 (5)	O7W ^x —O5W—O6W—O2W	153 (5)
Ag1 ⁱⁱ —S2—C6—C2	68.0 (4)	K1 ^{xv} —O5W—O6W—O2W	-39 (2)
C6—S2—C7—C8	-69.2 (6)	O2W—O5W—O6W—K1 ^{xvi}	142 (3)
Ag1 ⁱⁱ —S2—C7—C8	18.9 (6)	O1W ^{xv} —O5W—O6W—K1 ^{xvi}	22 (2)
Ag1 ⁱⁱ —O4—C8—O3	150.8 (6)	O7W ^x —O5W—O6W—K1 ^{xvi}	-65 (5)
K1 ^{xiii} —O4—C8—O3	-32.5 (10)	K1 ^{xv} —O5W—O6W—K1 ^{xvi}	103 (4)
Ag1 ⁱⁱ —O4—C8—C7	-29.0 (9)	O5W—O2W—O6W—O1W ^{xv}	-60 (5)
K1 ^{xiii} —O4—C8—C7	147.7 (6)	O3W—O2W—O6W—O1W ^{xv}	-94 (5)
Ag1 ⁱⁱ —O4—C8—K1 ^v	-154.8 (3)	K1 ^{xv} —O2W—O6W—O1W ^{xv}	58 (5)
K1 ^{xiii} —O4—C8—K1 ^v	21.9 (8)	O3W—O2W—O6W—O5W	-34 (6)
Ag1 ⁱⁱ —O4—C8—K1 ^{xiii}	-176.7 (9)	K1 ^{xv} —O2W—O6W—O5W	118 (4)
K1 ^v —O3—C8—O4	96.7 (8)	O5W—O2W—O6W—K1 ^{xvi}	-72 (5)
K1 ^{xii} —O3—C8—O4	-109.5 (8)	O3W—O2W—O6W—K1 ^{xvi}	-106 (5)
K1 ^v —O3—C8—C7	-83.5 (7)	K1 ^{xv} —O2W—O6W—K1 ^{xvi}	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) $-x+1, -y+1, -z+1$; (vi) $x, -y+3/2, z-1/2$; (vii) $x, -y+1/2, z-1/2$; (viii) $x, y-1, z$; (ix) $-x+1, y-3/2, -z+1/2$; (x) $-x+1, -y+1, -z$; (xi) $-x+1, -y, -z$; (xii) $x, -y+3/2, z+1/2$; (xiii) $x, -y+1/2, z+1/2$; (xiv) $x, y+1, z$; (xv) $-x+1, y+1/2, -z+1/2$; (xvi) $-x+1, y+3/2, -z+1/2$.