metal-organic compounds

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Poly[triaqua(µ₄-5-sulfosalicylato)potassium(I)]

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Key indicators: single-crystal X-ray study; T = 223 K; mean σ (C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.129; data-to-parameter ratio = 11.4.

In the title polymeric complex, $[K(C_7H_5O_6S)(H_2O)_3]_n$, the anions use their sulfonyl and double-bond carbonyl O atoms to link to four K⁺ cations in a μ_4 -bonding mode. The compound has a three-dimensional framework which consists of dinuclear $[K_2O_{10}]$ fragments linked by sulfonate and carboxylic O atoms from the sulfosalicylate (ssa⁻) ligand. In the three-dimensional network, there are different types of channels along the *a*, *b* and *c* axes. In the crystal structure, classical intermolecular $O-H \cdots O$ hydrogen bonds also stabilize the three-dimensional structure.

Related literature

For related literature, see: Braga *et al.* (1998); Distler & Sevov (1998); Drumel *et al.* (1995); Gao *et al.* (2005); Henderson *et al.* (2003); Hix *et al.* (2001); Kennedy *et al.* (2004, 2006); Kitagawa *et al.* (2004); Lloret *et al.* (1998); Ma *et al.* (2005); Moulton & Zaworotko (2001); Sheldrick (2000); Yaghi *et al.* (1997, 2003).



Experimental

Crystal data

 $\begin{bmatrix} K(C_7H_5O_6S)(H_2O)_3 \end{bmatrix} \\ M_r = 310.32 \\ Triclinic, P\overline{1} \\ a = 7.2648 (2) \text{ Å} \\ b = 7.2760 (2) \text{ Å} \\ c = 11.9225 (4) \text{ Å} \\ \alpha = 87.394 (2)^{\circ} \\ \beta = 81.907 (2)^{\circ} \end{bmatrix}$

Data collection

Siemens SMART CCD areadetector diffractometer Absorption correction: multi-scan (SADABS; Sheldrick, 1996) $T_{\rm min} = 0.693, T_{\rm max} = 0.827$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$	
$wR(F^2) = 0.129$	
S = 1.01	
2149 reflections	
188 parameters	
11 restraints	

Selected geometric parameters (Å, °).

$K1 - O2^i$	2.6686 (15)	K1-O9	2.9338 (16)
$K1 - O5^{ii}$	2.7315 (14)	$K1 - O8^{iii}$	2.9394 (18)
K1-O8	2.7345 (16)	$K1 - O6^{iv}$	2.9556 (14)
K1-O6	2.7604 (15)	K1-O7	3.2456 (19)
$O2^{i}-K1-O5^{ii}$	75.99 (5)	O6-K1-O9	129.16 (4)
$O2^{i}-K1-O8$	123.24 (5)	$O5^{ii} - K1 - O8^{iii}$	61.99 (5)
$05^{ii} - K1 - O8$	142.02 (5)	$O6-K1-O8^{iii}$	142.48 (5)
$O5^{ii}-K1-O6$	136.33 (5)	$O2^{i}-K1-O6^{iv}$	125.55 (5)
O8-K1-O6	78.32 (5)	$O6-K1-O6^{iv}$	72.10 (4)
$O2^{i} - K1 - O9$	69.64 (4)		

 $\gamma = 72.313 \ (2)^{\circ}$

Z = 2

V = 594.44 (3) Å³

Mo $K\alpha$ radiation

 $0.60 \times 0.38 \times 0.30 \text{ mm}$

5725 measured reflections

2149 independent reflections

2002 reflections with $I > 2\sigma(I)$

H atoms treated by a mixture of

independent and constrained

 $\mu = 0.66 \text{ mm}^{-1}$

T = 223 (2) K

 $R_{\rm int} = 0.017$

refinement $\Delta \rho_{\text{max}} = 0.56 \text{ e } \text{\AA}^{-3}$

 $\Delta \rho_{\rm min} = -0.66 \text{ e } \text{\AA}^{-3}$

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

Table 2Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdots A$	$D \cdots A$	$D - \mathbf{H} \cdot \cdot \cdot A$
$O1 - H1B \cdots O2$	0.840 (10)	1.839 (18)	2.586 (2)	147 (3)
$O3-H3A\cdots O9^{i}$	0.845 (10)	1.838 (11)	2.674 (2)	170 (2)
$O7-H7A\cdots O6^{iv}$	0.847 (10)	2.092 (13)	2.917 (2)	164 (3)
$O7 - H7B \cdot \cdot \cdot O4^{ii}$	0.843 (10)	2.021 (12)	2.852 (2)	168 (2)
$O8-H8A\cdots O5^{v}$	0.862 (10)	2.55 (3)	2.926 (2)	108 (2)
O8−H8A···O7 ^{iv}	0.862 (10)	2.50 (2)	2.997 (2)	117.9 (18)
$O8-H8B\cdots O4^{vi}$	0.870 (10)	2.037 (11)	2.879 (2)	163 (2)
$O9-H9A\cdots O3^{i}$	0.847 (9)	1.945 (16)	2.674 (2)	144 (2)
$O9-H9B\cdots O7^{vi}$	0.859 (10)	1.910 (11)	2.763 (2)	172 (2)

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1994); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1994); 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: HJ3040).

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Poly[triaqua(μ_4 -5-sulfosalicylato)potassium(I)]

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Comment

The rational design and synthesis of metal-organic high-dimensional networks are of great interest because of their intriguing structural diversity and their potential applications as functional solid materials (Moulton *et al.*,2001; Yaghi *et al.*,2003; Kitagawa *et al.*,2004). The study of solid-state metal-organic coordination frameworks has concentrated on transition metal complexes, while little attention being paid to the s-block metals, such as Na and K (Braga *et al.*,1998; Henderson *et al.*, 2003; Sheldrick *et al.*, 2000). Pharmaceuticals, dyes, and pigments typically utilize alkali and alkaline earth cations in preference to transition metals as, in broad terms, the s-block metals have advantages of nontoxicity, cheapness, and often aqueous solubility (Alan *et al.*,2006). So far most of these materials are formed with N-containing ligands, such as 4,4'-bipyridine and pyrazine(Yaghi *et al.*,1997; Lloret *et al.*,1998). The study on ligands containing different coordinating groups is relatively limited(Distler *et al.*,1998; Hix *et al.*,2001; Drumel *et al.*,1995), and we are interested in coordination polymers containing such ligands. It has been demonstrated that the 5-sulfosalicylic acid(Hssa) is a multifunctional ligand(Ma *et al.*, 2005; Gao *et al.*,2005), which has three potential coordinating groups -OH, $-CO_2H$ and $-SO_3H$. Both $-CO_2H$ and $-SO_3H$ are versatile coordination polymers constructed using the Hssa ligand and main group metals with three-dimensional open framework is very rare. In this paper, the first potassium complex with an interesting 3-D framework structure, [K(ssa)(H₂O)₃](Hssa=5-sulfosalicylic acid) I, was synthesized in aqueous solution and characterizated by single-crystal diffraction.

There is one crystallographically unique potassium ions in the structure (Fig. 1 and Table 1). The K⁺ ion is 8-coordinated by four water molecules (O7, O8, O9 and O8C, symmetry code C: -x - 1, -y, -z + 2), three sulfonate oxygen atoms (O6, O6D and O5E, symmetry code D: -x, -y, -z + 2; E: x, y - 1, z) and one double-bond carboxylic oxygen atom (O2B, symmetry code B:-x, -y, -z + 1) from four different ssa⁻ anions. The K—O(water) distances and potassium sulfonate oxygen distances range from 2.732 (2) to 3.242 (2) and 2.731 (2) to 2.757 (2) Å, respectively, which are similar to reported values (Kennedy *et al.*,2004). The potassium carboxylic oxygen distance is 2.668 (2) Å, while the O—K—O bond angles are in the range of 34.55 (3) to 163.77 (4)°.

In compound (I), $-SO_3H$ group is deprotonated, but the $-CO_2H$ and -OH groups are neutral. The K1 and its symmetryrelated ion (K1C, symmetry code C: -x - 1, -y, -z + 2) are linked by two μ_2 -O from water ligands (O8 and O8C, symmetry code C: -x - 1, -y, -z + 2) to form a dinuclear unit (K₂O₁₀), in which the K1···K1C (symmetry code C: -x - 1, -y, -z + 2) distance is 4.3273 (9) Å.

Each $-SO_3$ group in the ssa⁻ anion acts as a tridentate ligand linked with three different potassium ions through two sulfonate oxygen atoms, in which one binds to two potassium ions from the dinuclear unit while the other binds to only a single potassium ion. The $-CO_2H$ group monodentately coordinate to one potassium ion from the dinuclear unit. Thus, each ssa⁻ anion acting as tetradentate ligand binding to four potassium ions.

As shown in Figs. 2 and 3, the network structure of (I) may be described in terms of a three-dimensional open framework which consists of dinuclear $\{K_2O_{10}\}$ fragments linked by sulfonate(carboxylic) oxygen atoms from the ssa⁻ ligands. The most unusual feature is that in the 3-D network of (I), there exist different types of channels along the *a*, *b* and *c* axes. In fact, there are intercrossing three-dimensional channels in the open framework of compound (I).

In the crystal structure, classical intermolecular O—H…O hydrogen bonds are observed (Table 2),which link –OH, –CO₂H and –SO₃H in the ssa⁻ ligand and coordinated water molecules and also stabilize the 3-D structure.

Experimental

An aqueous solution (10 cm^3) of 5-sulfosalicylic acid(0.219 g, 1.0 mmol) was added dropwise to a stirred solution (10 cm^3) of KCl(0.091 g, 1.2 mmol) at 70°C for 20 min. Then the solution was adjusted to pH=2.8 by the addition of dilute HCl solution. The resulting colerless solution was allowed to stand in air at room temperature for a week, yielding block colorless crystals(65%). Elemental analysis found(calculated): C 24.01(23.99),H 3.46(3.50), S 3.39(3.36).

Refinement

The water and hydroxyl H atoms were found in a difference Fourier map and were refined with distance restraints O—H=0.85 (1)Å and H···H=1.39 (1) Å. H atoms bonded to C atoms were treated as riding, with $U_{iso}(H)$ values equal to $1.2U_{eq}(C)$ and C—H distances of 0.93 Å.

Figures



Fig. 1. View of the asymmetric unit of (I) with the atom labeling scheme. Displacement ellipsoids are drawn at the 35% probability level and H atoms are drawn as spheres of arbitrary radii. The symmetry codes are those used in Table 1.



Fig. 2. Ball-stick views of compound (I) showing different channels along the *a* axis. The H atoms of the coordinated water are omitted for clarity.



Fig. 3. Ball-stick views of compound (I) showing different channels along the *b* axis. The H atoms of the coordinated water are omitted for clarity.

poly[triaqua(µ4-5-sulfosalicylato)potassium(l)]

Crystal data

$[K(C_7H_5O_6S)(H_2O)_3]$	V = 594.44 (3) Å ³
$M_r = 310.32$	Z = 2
Triclinic, <i>P</i> T	$F_{000} = 320$
Hall symbol: -P 1	$D_{\rm x} = 1.734 {\rm ~Mg~m}^{-3}$
a = 7.2648 (2) Å	Mo $K\alpha$ radiation $\lambda = 0.71070$ Å
b = 7.2760 (2) Å	$\mu = 0.66 \text{ mm}^{-1}$
c = 11.9225 (4) Å	T = 223 (2) K
$\alpha = 87.394 \ (2)^{\circ}$	Block, colourless
$\beta = 81.907 \ (2)^{\circ}$	$0.60 \times 0.38 \times 0.30 \text{ mm}$
$\gamma = 72.313 \ (2)^{\circ}$	

Data collection

Siemens SMART CCD area-detector diffractometer	2149 independent reflections
Radiation source: fine-focus sealed tube	2002 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\rm int} = 0.017$
T = 223(2) K	$\theta_{\text{max}} = 25.4^{\circ}$
ϕ and ω scans	$\theta_{\min} = 3.2^{\circ}$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 8$
$T_{\min} = 0.693, T_{\max} = 0.827$	$k = -8 \rightarrow 8$
5725 measured reflections	$l = -13 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.129$	$w = 1/[\sigma^2(F_o^2) + (0.112P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
<i>S</i> = 1.01	$(\Delta/\sigma)_{\text{max}} = 0.014$
2149 reflections	$\Delta \rho_{max} = 0.57 \text{ e } \text{\AA}^{-3}$
188 parameters	$\Delta \rho_{min} = -0.66 \text{ e } \text{\AA}^{-3}$
11 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct	

Primary atom site location: structure-invariant direct methods

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2 , conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	У	Ζ	$U_{\rm iso}*/U_{\rm eq}$
K1	-0.21738 (6)	-0.07091 (6)	0.89768 (4)	0.0259 (2)
S1	-0.00136 (7)	0.35575 (6)	0.84164 (4)	0.0204 (2)
01	-0.2733 (2)	0.2594 (3)	0.41097 (13)	0.0375 (4)
H1B	-0.178 (3)	0.218 (4)	0.3606 (17)	0.045*
O2	0.0876 (2)	0.1545 (2)	0.32035 (12)	0.0336 (4)
O3	0.3188 (2)	0.1565 (2)	0.42516 (13)	0.0344 (4)
H3A	0.388 (3)	0.135 (3)	0.3612 (12)	0.041*
O4	0.2022 (2)	0.3544 (2)	0.81377 (12)	0.0277 (4)
O5	-0.1288 (2)	0.5369 (2)	0.88906 (12)	0.0303 (4)
O6	-0.0158 (2)	0.1913 (2)	0.91284 (12)	0.0286 (4)
O7	0.2490 (3)	-0.2851 (2)	0.86574 (14)	0.0408 (4)
H7B	0.244 (5)	-0.390 (3)	0.8412 (19)	0.061*
H7A	0.201 (4)	-0.271 (4)	0.9349 (11)	0.061*
O8	-0.5126 (2)	0.2531 (2)	0.96902 (14)	0.0377 (4)
H8A	-0.519 (4)	0.341 (3)	1.0167 (18)	0.045*
H8B	-0.613 (3)	0.301 (3)	0.933 (2)	0.045*
O9	-0.5442 (2)	-0.0411 (2)	0.77160 (13)	0.0309 (4)
H9B	-0.614 (3)	-0.108 (3)	0.8055 (16)	0.037*
H9A	-0.523 (4)	-0.071 (3)	0.7020 (9)	0.037*
C1	-0.2767 (3)	0.3642 (3)	0.70429 (18)	0.0281 (5)
H1A	-0.3683	0.4060	0.7690	0.034*
C2	-0.3391 (3)	0.3402 (3)	0.60464 (18)	0.0311 (5)
H2A	-0.4729	0.3647	0.6013	0.037*
C3	-0.2040 (3)	0.2791 (3)	0.50731 (17)	0.0264 (5)
C4	-0.0053 (3)	0.2436 (3)	0.51325 (16)	0.0222 (4)
C5	0.0560 (3)	0.2686 (3)	0.61575 (16)	0.0209 (4)
H5A	0.1894	0.2453	0.6200	0.025*
C6	-0.0788 (3)	0.3274 (3)	0.71112 (16)	0.0210 (4)
C7	0.1370 (3)	0.1813 (3)	0.41096 (17)	0.0240 (4)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.0292 (3)	0.0247 (3)	0.0241 (3)	-0.0091 (2)	-0.0019 (2)	-0.0032 (2)
S1	0.0232 (3)	0.0198 (3)	0.0183 (3)	-0.0071 (2)	-0.0006 (2)	-0.0029 (2)
01	0.0273 (9)	0.0596 (11)	0.0249 (8)	-0.0089 (8)	-0.0084 (6)	-0.0059 (7)
O2	0.0330 (9)	0.0487 (9)	0.0183 (8)	-0.0118 (7)	-0.0009 (6)	-0.0043 (7)
O3	0.0260 (9)	0.0536 (10)	0.0241 (8)	-0.0148 (8)	0.0033 (6)	-0.0075 (7)
O4	0.0246 (8)	0.0335 (8)	0.0270 (8)	-0.0116 (6)	-0.0023 (6)	-0.0065 (6)
O5	0.0364 (9)	0.0249 (7)	0.0257 (8)	-0.0039 (6)	-0.0005 (6)	-0.0083 (6)
O6	0.0372 (9)	0.0274 (7)	0.0241 (8)	-0.0137 (6)	-0.0057 (6)	0.0012 (6)
O7	0.0563 (11)	0.0404 (9)	0.0337 (9)	-0.0304 (8)	0.0058 (8)	-0.0100 (7)
O8	0.0310 (9)	0.0449 (9)	0.0326 (9)	-0.0036 (7)	-0.0041 (7)	-0.0067 (7)
O9	0.0297 (8)	0.0392 (9)	0.0249 (8)	-0.0140 (7)	0.0028 (6)	-0.0047 (7)
C1	0.0237 (11)	0.0316 (11)	0.0245 (11)	-0.0045 (9)	0.0032 (8)	-0.0017 (9)
C2	0.0195 (10)	0.0409 (12)	0.0297 (11)	-0.0052 (9)	-0.0017 (8)	0.0001 (9)
C3	0.0290 (11)	0.0275 (10)	0.0224 (10)	-0.0069 (9)	-0.0066 (8)	0.0010 (8)
C4	0.0245 (10)	0.0212 (9)	0.0190 (10)	-0.0054 (8)	0.0008 (8)	-0.0008 (8)
C5	0.0190 (10)	0.0221 (9)	0.0218 (10)	-0.0070 (8)	-0.0018 (7)	-0.0007 (7)
C6	0.0258 (10)	0.0182 (9)	0.0189 (10)	-0.0065 (8)	-0.0026 (8)	-0.0027 (7)
C7	0.0262 (10)	0.0244 (10)	0.0205 (10)	-0.0077 (8)	0.0001 (8)	-0.0001 (8)

Atomic displacement parameters $(Å^2)$

Geometric parameters (Å, °)

$K1 - O2^{i}$	2.6686 (15)	ОЗ—НЗА	0.845 (10)
K1—O5 ⁱⁱ	2.7315 (14)	O5—K1 ^v	2.7315 (14)
K1—O8	2.7345 (16)	O6—K1 ^{iv}	2.9556 (14)
K1—O6	2.7604 (15)	O7—H7B	0.843 (10)
K1—O9	2.9338 (16)	O7—H7A	0.847 (10)
K1—O8 ⁱⁱⁱ	2.9394 (18)	O8—K1 ⁱⁱⁱ	2.9394 (18)
K1—O6 ^{iv}	2.9556 (14)	O8—H8A	0.862 (10)
K1—O7	3.2456 (19)	O8—H8B	0.870 (10)
K1—K1 ⁱⁱⁱ	4.3258 (9)	O9—H9B	0.859 (10)
K1—K1 ^{iv}	4.6230 (9)	О9—Н9А	0.847 (9)
K1—H7A	3.03 (3)	C1—C2	1.366 (3)
S1—O5	1.4465 (14)	C1—C6	1.394 (3)
S1—O6	1.4569 (14)	C1—H1A	0.9400
S1—O4	1.4662 (15)	C2—C3	1.403 (3)
S1—C6	1.7683 (19)	C2—H2A	0.9400
O1—C3	1.347 (3)	C3—C4	1.398 (3)
O1—H1B	0.840 (10)	C4—C5	1.395 (3)
O2—C7	1.227 (3)	C4—C7	1.474 (3)
O2—K1 ⁱ	2.6686 (15)	C5—C6	1.382 (3)
O3—C7	1.311 (3)	C5—H5A	0.9400
02 ⁱ —K1—O5 ⁱⁱ	75.99 (5)	O6 ^{iv} —K1—H7A	40.9 (2)
O2 ⁱ —K1—O8	123.24 (5)	O7—K1—H7A	15.0 (2)

$02^{j}-k1-06$ $95.58(5)$ $k1^{jk}-k1-H7A$ $45.4(4)$ $03^{j}-k1-06$ $153.33(5)$ $05-81-06$ $112.4(9)$ $08-k1-06$ $78.32(5)$ $05-81-04$ $110.93(9)$ $03^{ij}-k1-09$ $69.64(4)$ $06-81-04$ $110.93(9)$ $03^{ij}-k1-09$ $88.56(5)$ $05-81-C6$ $106.78(9)$ $08-k1-09$ $129.16(4)$ $04-81-C6$ $105.0(8)$ $02^{ij}-k1-08^{iii}$ $61.99(5)$ $C7-02-k1^{i}$ $143.75(14)$ $08-k1-08^{iii}$ $80.71(5)$ $C7-03-H3A$ $108.3(18)$ $06-k1-08^{iii}$ $122.55(5)$ $S1-05-k1^{i}$ $143.05(9)$ $09-k1-06^{iii}$ $125.55(5)$ $S1-06-k1$ $13.10(8)$ $02^{ij}-k1-06^{iii}$ $125.55(5)$ $K1-07-H7B$ $97(2)$ $06-k1-06^{iii}$ $106.27(5)$ $K1-07-H7B$ $97(2)$ $06-k1-06^{iii}$ $155.59(5)$ $H7B-07-H7A$ $103.1(6)$ $08^{iiii}-k1-06^{iii}$ $155.59(5)$ $H7B-07-H7A$ $103.2(6)$ $09-k1-06^{iiiii}$ $155.59(5)$ $H7B-07-H7A$	O5 ⁱⁱ —K1—O8	142.02 (5)	K1 ⁱⁱⁱ —K1—H7A	136.3 (2)
$0S^{ii}-K1-06$ 156.33 (5) $05-S1-06$ 112.44 (9) $08-K1-06$ 78.32 (5) $05-S1-04$ 113.18 (9) $02^{ii}-K1-09$ 69.64 (4) $06-S1-04$ 110.93 (9) $03^{ii}-K1-09$ 88.56 (5) $05-S1-C6$ 106.78 (9) $08-K1-09$ 129.16 (4) $04-S1-C6$ 105.60 (8) $02^{ii}-K1-08^{iii}$ 12.94 (5) $C3-01-H1B$ 108.01 (9) $02^{ii}-K1-08^{iii}$ 61.99 (5) $C7-02-K1^{i}$ 143.75 (14) $08-K1-08^{iii}$ 61.99 (5) $C7-03-H3A$ 108.3 (18) $06-K1-08^{iii}$ 142.48 (5) $81-06-K1^{iv}$ 120.92 (8) $09-K1-08^{iii}$ 71.07 (4) $81-06-K1^{iv}$ 120.92 (8) $05^{ii}-K1-06^{iv}$ 78.51 (4) $K1-06-K1^{iv}$ 120.92 (8) $05^{ii}-K1-06^{iv}$ 78.51 (4) $K1-07-H7B$ 97.22 $06-K1-06^{iv}$ 72.10 (4) $K1-07-H7A$ 86 (2) $09-K1-06^{iv}$ 75.51 (5) $R1-07-H7A$ 110.3 (16) $08^{iii}-K1-06^{iv}$ 84.56 (4) $K1-08-H18A$ 131.3 (16) $08^{iii}-K1-06^{iv}$ 84.56 (4) $K1-08-H18A$ 23.19 $09-K1-06^{iv}$ 84.56 (4) $K1-08-H18A$ 23.19 $09-K1-06^{iv}$ 84.56 (4) $K1-08-H18A$ 23.19 $09-K1-07$ $65.47.40$ $K1-08-H18A$ 23.19 $09-K1-07$ $65.49.40$ $K1-09-H9A$ 107.3 (14) $08^{iii}-K1-07$ $69.99.(4)$ $K1-09-H9A$ $102.11(7)$ $08-K1-07$ $69.49.(4)$ $K1-09-H9A$	O2 ⁱ —K1—O6	95.58 (5)	K1 ^{iv} —K1—H7A	45.4 (4)
$08-K1-06$ $78.32 (5)$ $05-S1-04$ $113.18 (9)$ $02^{L}-K1-09$ $69.64 (4)$ $06-S1-04$ $110.93 (9)$ $05^{L}-K1-09$ $88.56 (5)$ $05-S1-C6$ $107.43 (8)$ $06-K1-09$ $12.15 (5)$ $06-S1-C6$ $107.43 (8)$ $06-K1-09$ $12.91.6 (4)$ $04-S1-C6$ $107.43 (8)$ $0c^{2L}-K1-08^{iii}$ $12.194 (5)$ $C7-02-K1^{1}$ $143.75 (14)$ $08-K1-08^{iii}$ $80.71 (5)$ $C7-03-H3A$ $108.3 (18)$ $06-K1-08^{iii}$ $80.71 (5)$ $C7-03-H3A$ $108.3 (18)$ $06-K1-08^{iii}$ $122.55 (5)$ $S1-06-K1^{17}$ $120.92 (8)$ $07-K1-06^{iv}$ $78.51 (4)$ $K1-06-K1^{10}$ $17.90 (4)$ $08-K1-06^{iv}$ $78.51 (4)$ $K1-07-H7A$ $68 (2)$ $09-K1-06^{iv}$ $75.59 (5)$ $H7B-07-H7A$ $103 (16)$ $08^{ii}-K1-06^{iv}$ $84.56 (4)$ $K1-08-K1^{iii}$ $92.29 (5)$ $02^{ii}-K1-07$ $69.99 (4)$ $K1-08-H8B$ $81.3 (19)$ $08^{iii}-K1-07$ $69.40 (4)$	O5 ⁱⁱ —K1—O6	136.33 (5)	O5—S1—O6	112.44 (9)
$02^{1}-K1-09$ 69.64 (4) $06-S1-04$ 110.93 (9) $03^{ii}-K1-09$ 88.56 (5) $05-S1-C6$ 106.78 (9) $08-K1-09$ 71.83 (5) $06-S1-C6$ 105.06 (8) $02^{1}-K1-09$ 12.16 (4) $04-S1-C6$ 105.06 (8) $02^{1}-K1-08^{iii}$ 12.194 (5) $C3-01-H1B$ 108.0 (19) $08^{ii}-K1-08^{iii}$ 80.71 (5) $C7-02-K1^{1}$ 143.75 (14) $08-K1-08^{iii}$ 80.71 (5) $C7-03-H3A$ 108.3 (18) $06-K1-08^{iii}$ 71.07 (4) $S1-06-K1$ 131.03 (8) $09-K1-08^{iii}$ 71.07 (4) $S1-06-K1^{1v}$ 120.92 (8) $03^{ii}-K1-06^{iv}$ 78.51 (4) $K1-06-K1^{1v}$ 109.29 (8) $03^{ii}-K1-06^{iv}$ 78.51 (4) $K1-07-H7A$ 68 (2) $09-K1-06^{iv}$ 72.10 (4) $K1-07-H7A$ 68 (2) $09-K1-06^{iv}$ 72.10 (4) $K1-07-H7A$ 88 (2) $09^{ii}-K1-07$ 67.47 (4) $K1^{1ii}-08-H8A$ 131.3 (16) $05^{ii}-K1-07$ 67.47 (4) $K1^{1ii}-08-H8A$ 131.3 (16) $05^{ii}-K1-07$ 67.47 (4) $K1^{1ii}-08-H8B$ 122.5 (15) $06-K1-07$ 69.40 (4) $K1^{1ii}-08-H8B$ 104.8 (14) $08^{ii}-K1-07$ 120.54 (4) $K1-09-H9A$ 107.3 (14) $08^{ii}-K1-07$ 120.54 (4) $K1-09-H9A$ 107.3 (14) $09^{ii}-K1-07$ 58.7 (4) $K1-09-H9A$ 107.3 (14) $08^{ii}-K1-07$ 120.54 (4) $K1-09-H9A$ 107.3 (14) $08^{ii}-K1-07$ <	O8—K1—O6	78.32 (5)	O5—S1—O4	113.18 (9)
$OS^{ii}_{ii} - K1 - O9$ $88.56 (5)$ $OS - S1 - C6$ $106.78 (9)$ $OS - K1 - O9$ $71.83 (5)$ $O6 - S1 - C6$ $107.43 (8)$ $OG - K1 - O9$ $129.16 (4)$ $O4 - S1 - C6$ $105.60 (8)$ $OS^{ii}_{ii} - K1 - O8^{iii}$ $121.94 (5)$ $C3 - O1 - H1B$ $108.0 (19)$ $OS^{ii}_{ii} - K1 - O8^{iii}$ $61.99 (5)$ $C7 - O2 - K1^{i}$ $143.75 (14)$ $O8 - K1 - O8^{iii}$ $102.94 (8)$ $S1 - O5 - K1^{v}$ $148.50 (9)$ $O9 - K1 - O8^{iii}$ $122.55 (5)$ $S1 - O6 - K1$ $131.03 (8)$ $O2^{ii} - K1 - O6^{iv}$ $125.55 (5)$ $S1 - O6 - K1$ $120.92 (8)$ $O3^{ii} - K1 - O6^{iv}$ $78.51 (4)$ $K1 - O6 - K1^{iv}$ $120.92 (8)$ $O3^{ii} - K1 - O6^{iv}$ $72.10 (4)$ $K1 - O7 - H7B$ $97 (2)$ $O - K1 - O6^{iv}$ $72.10 (4)$ $K1 - O7 - H7A$ $68 (2)$ $O9 - K1 - O6^{iv}$ $72.10 (4)$ $K1 - O8 - K1^{iu}$ $110.3 (16)$ $O3^{ii} - K1 - O7$ $69.99 (4)$ $K1 - O8 - K1^{iui}$ $99.29 (5)$ $O2^{i} - K1 - O7$ $69.99 (4)$ $K1^{ii} - O8 - H8A$ $98 (2)$ $O8 - K1 - O7$ $69.40 (4)$ $K1^{iii} - O8 - H8A$ $98 (2)$ $O8 - K1 - O7$ $69.40 (4)$ $K1^{iii} - O8 - H8B$ $104.8 (14)$ $O8^{iii} - K1 - O7$ $55.87 (4)$ $K1 - O9 - H9A$ $120.1 (7)$ $O9 - K1 - O7$ $55.87 (4)$ $K1 - O9 - H9A$ $120.1 (7)$ $O9^{iii} - K1 - K1^{iii}$ $132.6 (3)$ $C1 - C2 - C1 - C6$ $120.72 (19)$ $O8^{iii} - K1 - K1^{iii}$ $132.6 ($	O2 ⁱ —K1—O9	69.64 (4)	O6—S1—O4	110.93 (9)
$08-K1-09$ 71.83 (5) $06-K1-C6$ 107.43 (8) $06-K1-09$ 129.16 (4) $04-S1-C6$ 105.60 (8) $02^{1-}K1-08^{iii}$ 121.94 (5) $C3-01-H1B$ 108.0 (19) $0S^{ii}-K1-08^{iii}$ 61.99 (5) $C7-02-K1^{i}$ 143.75 (14) $08-K1-08^{iii}$ 142.48 (5) $S1-05-K1^{v}$ 148.50 (9) $09-K1-08^{iii}$ 71.07 (4) $S1-06-K1$ 131.03 (8) $02^{1-}K1-06^{iv}$ 125.55 (5) $S1-06-K1^{1v}$ 120.92 (8) $05^{ii}-K1-06^{iv}$ 78.51 (4) $K1-06-K1^{1v}$ 107.90 (4) $08-K1-06^{iv}$ 78.51 (4) $K1-07-H7B$ 97 (2) $06-K1-06^{iv}$ 72.10 (4) $K1-07-H7A$ (8) (2) $09-K1-06^{iv}$ 155.59 (5) H7B-07-H7A 110.3 (16) $08^{iii}-K1-07$ 69.99 (4) $K1-08-H8A$ 131.3 (16) $05^{iii}-K1-07$ 69.40 (4) $K1^{iii}-08-H8A$ 131.3 (16) $05^{iii}-K1-07$ 146.52 (5) $K1-09-H9B$ 109.1 (16) $06^{iii}-K1-07$ 59.87 (4) $K1-09-H9B$ <	O5 ⁱⁱ —K1—O9	88.56 (5)	O5—S1—C6	106.78 (9)
$06 = K_1 = 09$ 129.16 (4) $04 = S_1 = C6$ 105.60 (8) $02^1 = K_1 = 08^{iii}$ 121.94 (5) $C3 = 01 = H1B$ 108.0 (19) $08^{ii} = K_1 = 08^{iii}$ 80.71 (5) $C7 = 02 = K1^i$ 143.75 (14) $08 = K1 = 08^{iii}$ 142.48 (5) $S1 = 06 = K1$ 131.03 (8) $09 = K_1 = 08^{iii}$ 71.07 (4) $S1 = 06 = K1$ 131.03 (8) $02^1 = K1 = 06^{iv}$ 125.55 (5) $S1 = 06 = K1$ 131.03 (8) $02^1 = K1 = 06^{iv}$ 125.55 (5) $S1 = 06 = K1^{1v}$ 120.92 (8) $03^{ii} = K1 = 06^{iv}$ 72.10 (4) $K1 = 07 = H7A$ 103.3 (16) $08^{iii} = K1 = 06^{iv}$ 72.10 (4) $K1 = 08 = K1$ 131.3 (16) $08^{iii} = K1 = 06^{iv}$ 72.10 (4) $K1 = 08 = H8A$ 93.13 (16) $08^{iii} = K1 = 06^{iv}$ 72.10 (4) $K1 = 08 = H8A$ 98.22 $02^1 = K1 = 07^i$ 69.99 (4) $K1 = 08 = H8B$ 131.3 (16) $08^{iii} = K1 = 07^i$ 64.64 $K1 = 08 = H8B$ 132.5 (15) $06 = K1 = 07$ 69.49 (4) $K^{1ii} = 08 = H8B$ 104.8 (14)	08—K1—09	71.83 (5)	O6—S1—C6	107.43 (8)
$O2^{i}$ —K1— $O8^{iii}$ 121.94 (5) $C3$ — $O1$ —H1B 108.0 (19) $O5^{ii}$ —K1— $O8^{iii}$ 61.99 (5) $C7$ — $O2$ —K1 ⁱ 143.75 (14) $O8$ —K1— $O8^{iii}$ 80.71 (5) $C7$ — $O3$ —H3A 108.3 (18) $O6$ —K1— $O8^{iii}$ 142.48 (5) $S1$ — $O5$ —K1 V 148.50 (9) $O9$ —K1— $O6^{iii}$ 125.55 (5) $S1$ — $O6$ —K1 iii 120.92 (8) $O5^{ii}$ —K1— $O6^{iv}$ 125.55 (5) $K1$ — $O7$ —H7B 97 (2) $O6$ —K1— $O6^{iv}$ 72.10 (4) $K1$ — $O7$ —H7B 97 (2) $O6$ —K1— $O6^{iv}$ 72.10 (4) $K1$ — $O7$ —H7A 68 (2) $O9$ —K1— $O6^{iv}$ 72.10 (4) $K1$ — $O7$ —H7A 103.16) $O8^{ii}$ —K1— $O6^{iv}$ 84.56 (4) $K1$ — $O8$ — $K1^{iii}$ 99.29 (5) $O2^{i}$ —K1— $O7$ 69.99 (4) $K1$ — $O8$ —H8A 31.3 (16) $O8^{iii}$ —K1— $O7$ 146.52 (5) $K1$ — $O8$ —H8B 122.5 (15) $O6$ —K1— $O7$ 136.88 (4) $H8$ — $O8$ —H8B 104.8 (4) $O8^{iii}$ —K1— $O7$ 55.87 (4) $K1$ — $O9$ —H9A 107.3 (14)	O6—K1—O9	129.16 (4)	O4—S1—C6	105.60 (8)
$0S^{ii}-K1-08^{iii}$ $61.99(5)$ $C7-02-K1^{i}$ $143.75(14)$ $08-K1-08^{iii}$ $80.71(5)$ $C7-03-H3A$ $108.3(18)$ $06-K1-08^{iii}$ $142.48(5)$ $S1-05-K1^{v}$ $148.50(9)$ $09-K1-08^{iii}$ $71.07(4)$ $S1-06-K1^{v}$ $120.92(8)$ $02^{i}-K1-06^{iv}$ $125.55(5)$ $S1-06-K1^{iv}$ $120.92(8)$ $05^{iii}-K1-06^{iv}$ $78.51(4)$ $K1-07-H7B$ $97(2)$ $06-K1-06^{iv}$ $72.10(4)$ $K1-07-H7B$ $97(2)$ $06-K1-06^{iv}$ $72.10(4)$ $K1-07-H7A$ $68(2)$ $09-K1-06^{iv}$ $155.59(5)$ $H7B-07-H7A$ $110.3(16)$ $08^{iii}-K1-06^{iv}$ $84.56(4)$ $K1-08-H8A$ $31.3(16)$ $08^{iii}-K1-07$ $67.47(4)$ $K1^{iii}-08-H8A$ $98(2)$ $08-K1-07$ $69.99(4)$ $K1-08-H8B$ $122.5(15)$ $06-K1-07$ $69.40(4)$ $K1^{iii}-08-H8B$ $122.5(15)$ $06-K1-07$ $136.88(4)$ $H8A-08-H8B$ $109.1(16)$ $09^{iii}-K1-07$ $120.54(4)$ $K1-09-H9B$ $109.1(16)$ $06^{iv}-K1-07$ $55.87(4)$ $K1-09-H9A$ $120.1(17)$ $02^{i}-K1-K1^{iiii}$ $134.91(4)$ $49B-09-H9A$ $107.3(14)$ $09-K1-K1^{iiii}$ $120.54(3)$ $C1-C2-H2A$ 19.9 $06^{iv}-K1-K1^{iiii}$ $120.53(3)$ $C1-C2-H2A$ 19.9 $06^{iv}-K1-K1^{iiii}$ $134.91(4)$ $49B-09-H9A$ $107.3(14)$ $09-K1-K1^{iiii}$ $136.86(3)$ $C1-C2-H2A$ 19.9 $07-K1-K1^{iiii}$ $114.26(4)$ $C6-C1-$	O2 ⁱ —K1—O8 ⁱⁱⁱ	121.94 (5)	C3—O1—H1B	108.0 (19)
$08-K1-08^{iii}$ 80.71 (5) $C7-03-H3A$ 108.3 (18) $06-K1-08^{iii}$ 142.48 (5) $S1-05-K1^{V}$ 148.50 (9) $09-K1-08^{iii}$ 1107 (4) $S1-06-K1$ 131.03 (8) $02^{i}-K1-06^{iv}$ 125.55 (5) $S1-06-K1^{iv}$ 120.92 (8) $05^{ii}-K1-06^{iv}$ 125.57 (5) $K1-07-H7B$ 97 (2) $06-K1-06^{iv}$ 125.59 (5) $H7B-07-H7A$ 68 (2) $09-K1-06^{iv}$ 155.59 (5) $H7B-07-H7A$ 68 (2) $09-K1-06^{iv}$ 155.59 (5) $H7B-07-H7A$ 103.3 (16) $08^{iii}-K1-06^{iv}$ 84.56 (4) $K1-08-H8A$ 131.3 (16) $09^{ii}-K1-07$ 69.99 (4) $K1-08-H8A$ 98 (2) $08-K1-07$ 146.52 (5) $K1-08-H8B$ 122.5 (15) $06-K1-07$ 69.40 (4) $K1^{iii}-08-H8B$ 104.8 (14) $08^{iii}-K1-07$ 136.88 (4) $H8-08-H8B$ 102.1 (17) $09-K1-07$ 136.88 (4) $H8-09-H9B$ 107.3 (14) $08^{iii}-K1-07$ 120.54 (4)	O5 ⁱⁱ —K1—O8 ⁱⁱⁱ	61.99 (5)	C7—O2—K1 ⁱ	143.75 (14)
$06-K1-08^{iii}$ $142.48 (5)$ $S1-05-K1^{v}$ $148.50 (9)$ $09-K1-08^{iii}$ $71.07 (4)$ $S1-06-K1$ $131.03 (8)$ $02^{i}-K1-06^{iv}$ $125.55 (5)$ $S1-06-K1^{iv}$ $120.92 (8)$ $05^{ii}-K1-06^{iv}$ $78.51 (4)$ $K1-06-K1^{iv}$ $107.90 (4)$ $08-K1-06^{iv}$ $70.21 (4)$ $K1-07-H7B$ $97 (2)$ $06-K1-06^{iv}$ $72.10 (4)$ $K1-07-H7A$ $68 (2)$ $09-K1-06^{iv}$ $155.59 (5)$ $H7B-07-H7A$ $110.3 (16)$ $08^{iii}-K1-06^{iv}$ $84.56 (4)$ $K1-08-K1^{iii}$ $99.29 (5)$ $02^{i}-K1-06^{iv}$ $84.56 (4)$ $K1-08-H8A$ $131.3 (16)$ $08^{iii}-K1-07$ $69.99 (4)$ $K1-08-H8A$ $98 (2)$ $08-K1-07$ $67.47 (4)$ $K1^{iii}-08-H8A$ $98 (2)$ $08-K1-07$ $69.40 (4)$ $K1^{iii}-08-H8B$ $122.5 (15)$ $06-K1-07$ $69.40 (4)$ $K1^{iii}-08-H8B$ $104.8 (14)$ $08^{iii}-K1-07$ $120.54 (4)$ $K1-09-H9B$ $109.1 (16)$ $06^{iv}-K1-K1^{iii}$ $134.91 (4)$ $H9B-09-H9A$ $107.3 (14)$ $08^{ii}-K1-K1^{iii}$ $100.32 (4)$ $C2-C1-C6$ $120.72 (19)$ $08-K1-K1^{iii}$ $114.26 (4)$ $C6-C1-H1A$ 119.6 $06-K1-K1^{iii}$ $114.26 (4)$ $C6-C1-H1A$ 119.9 $07-K1-K1^{iii}$ $150.75 (3)$ $01-C3-C2$ $117.81 (18)$ $09^{ii}-K1-K1^{iii}$ $150.75 (3)$ $01-C3-C2$ $117.81 (18)$ $06^{iv}-K1-K1^{iii}$ $153.63 (3)$ $C3-C4-C7$ $120.71 (17)$	08—K1—08 ⁱⁱⁱ	80.71 (5)	С7—О3—НЗА	108.3 (18)
$09-K1-08^{iii}$ $71.07 (4)$ $S1-06-K1$ $131.03 (8)$ $02^{i}-K1-06^{iv}$ $125.55 (5)$ $S1-06-K1^{iv}$ $120.92 (8)$ $03^{ii}-K1-06^{iv}$ $78.51 (4)$ $K1-06-K1^{iv}$ $107.90 (4)$ $08-K1-06^{iv}$ $106.27 (5)$ $K1-07-H7B$ $97 (2)$ $06-K1-06^{iv}$ $72.10 (4)$ $K1-07-H7A$ $68 (2)$ $09-K1-06^{iv}$ $155.59 (5)$ $H7B-07-H7A$ $110.3 (16)$ $08^{iii}-K1-06^{iv}$ $84.56 (4)$ $K1-08-K1^{iii}$ $9929 (5)$ $02^{i}-K1-07$ $69.99 (4)$ $K1-08-H8A$ $98 (2)$ $08-K1-07$ $67.47 (4)$ $K1^{iii}-08-H8A$ $98 (2)$ $08-K1-07$ $69.40 (4)$ $K1^{iii}-08-H8B$ $122.5 (15)$ $06-K1-07$ $69.40 (4)$ $K1^{iii}-08-H8B$ $104.8 (14)$ $08^{iii}-K1-07$ $136.88 (4)$ $H8A-08-H8B$ $104.8 (14)$ $08^{iii}-K1-07$ $136.88 (4)$ $H8A-08-H8B$ $104.5 (14)$ $08^{iii}-K1-07$ $55.87 (4)$ $K1-09-H9A$ $107.3 (14)$ $09^{ii}-K1-K1^{iii}$ $100.32 (4)$ $C2-C1-C6$ $120.72 (19)$ $08-K1-K1^{iii}$ $114.26 (4)$ $C6-C1-H1A$ 119.6 $09-K1-K1^{iii}$ 186.03 $C1-C2-H2A$ 119.9 $06^{iv}-K1-K1^{iii}$ $150.75 (3)$ $01-C3-C2$ $117.81 (18)$ $09^{ii}-K1-K1^{iii}$ $150.75 (3)$ $01-C3-C2$ $117.81 (18)$ $09^{ii}-K1-K1^{iii}$ $150.75 (3)$ $01-C3-C2$ $119.40 (18)$ $08^{ii}-K1-K1^{iii}$ $107.73 (4)$ $C4-C3-C2$ $119.94 (18)$ 08^{ii	06—K1—08 ⁱⁱⁱ	142.48 (5)	S1—O5—K1 ^v	148.50 (9)
$O2^{i}-K1-O6^{iv}$ 125.55 (5) $S1-O6-K1^{iv}$ 120.92 (8) $O5^{ii}-K1-O6^{iv}$ 78.51 (4) $K1-O6-K1^{iv}$ 107.90 (4) $O8-K1-O6^{iv}$ 106.27 (5) $K1-O7-H7B$ 97 (2) $O6-K1-O6^{iv}$ 72.10 (4) $K1-O7-H7A$ 68 (2) $O9-K1-O6^{iv}$ 155.59 (5) $H7B-O7-H7A$ 110.3 (16) $O8^{iii}-K1-O6^{iv}$ 84.56 (4) $K1-O8-K1^{iii}$ 99.29 (5) $O2^{i}-K1-O7$ 69.99 (4) $K1-O8-H8A$ 131.3 (16) $O5^{ii}-K1-O7$ 67.47 (4) $K1^{iii}-O8-H8A$ 98 (2) $O8-K1-O7$ 69.40 (4) $K1^{iii}-O8-H8B$ 122.5 (15) $O9-K1-O7$ 69.40 (4) $K1^{iii}-O8-H8B$ 13.3 (19) $O9-K1-O7$ 126.58 (4)H8A-O8-H8B104.8 (14) $O8^{iii}-K1-O7$ 120.54 (4) $K1-O9-H9B$ 109.1 (16) $O6^{iv}-K1-O7$ 55.87 (4) $K1-O9-H9A$ 120.1 (17) $O2^{i}-K1-K1^{iii}$ 134.91 (4)H9B-O9-H9A107.3 (14) $O5^{ii}-K1-K1^{iii}$ 100.32 (4)C2-C1-C6120.72 (19) $O8-K1-K1^{iii}$ 114.26 (4)C6-C1-H1A119.6 $O9-K1-K1^{iii}$ 38.60 (3)C1-C2-C3120.2 (2) $O8^{iii}-K1-K1^{iii}$ 150.75 (3)O1-C3-C2117.81 (18) $O2^{ii}-K1-K1^{iii}$ 150.75 (3)O1-C3-C2117.81 (18) $O5^{ii}-K1-K1^{iii}$ 153.53 (3)C3-C4-C7109.6 (17) $O-K1-K1^{iii}$ 134.91 (4)C5-C4-C3119.9 (18) $O6^{ii}-K1-K1^{iii}$ 163.58 (3)C3-C2-H2A119.6 (17) $O9-K1-$	09—K1—08 ⁱⁱⁱ	71.07 (4)	S1—O6—K1	131.03 (8)
$OS^{ii} - K1 - O6^{iv}$ 78.51 (4) $K1 - O6 - K1^{iv}$ 107.90 (4) $O8 - K1 - O6^{iv}$ 106.27 (5) $K1 - O7 - H7B$ 97 (2) $O6 - K1 - O6^{iv}$ 72.10 (4) $K1 - O7 - H7A$ 68 (2) $O9 - K1 - O6^{iv}$ 155.59 (5) $H7B - O7 - H7A$ 110.3 (16) $O8^{iii} - K1 - O6^{iv}$ 84.56 (4) $K1 - O8 - K1^{iii}$ 99.29 (5) $O2^{i} - K1 - O7$ 69.99 (4) $K1 - O8 - H8A$ 131.3 (16) $O5^{ii} - K1 - O7$ 67.47 (4) $K1^{iii} - O8 - H8A$ 98 (2) $O8 - K1 - O7$ 67.47 (4) $K1^{iii} - O8 - H8B$ 122.5 (15) $O6 - K1 - O7$ 69.40 (4) $K1^{iii} - O8 - H8B$ 104.8 (14) $O9^{iii} - K1 - O7$ 136.88 (4)H8A - O8 - H8B104.8 (14) $O9^{iii} - K1 - O7$ 120.54 (4) $K1 - O9 - H9B$ 109.1 (16) $O6^{iv} - K1 - O7$ 55.87 (4) $K1 - O9 - H9A$ 120.1 (17) $O2^{i} - K1 - K1^{iii}$ 100.32 (4)C2 - C1 - C6120.72 (19) $O8 - K1 - K1^{iii}$ 100.32 (4)C2 - C1 - H1A119.6 $O9 - K1 - K1^{iii}$ 14.26 (4)C6 - C1 - H1A119.6 $O9 - K1 - K1^{iii}$ 38.60 (3)C1 - C2 - H2A119.9 $O6^{ii} - K1 - K1^{iii}$ 150.75 (3)O1 - C3 - C2117.81 (18) $O2^{i} - K1 - K1^{iii}$ 150.75 (3)O1 - C3 - C2119.40 (18) $O2^{i} - K1 - K1^{iii}$ 33.33 (4)C5 - C4 - C3119.60 (17) $O - K1 - K1^{iii}$ 13.33 (3)C3 - C4 - C7120.71 (17) $O - K1 - K1^{iii}$ 163.58 (3)C3	O2 ⁱ —K1—O6 ^{iv}	125.55 (5)	S1—O6—K1 ^{iv}	120.92 (8)
$08-K1-06^{iv}$ $106.27 (5)$ $K1-07-H7B$ $97 (2)$ $06-K1-06^{iv}$ $72.10 (4)$ $K1-07-H7A$ $68 (2)$ $09-K1-06^{iv}$ $155.59 (5)$ $H7B-07-H7A$ $110.3 (16)$ $08^{iii}-K1-06^{iv}$ $84.56 (4)$ $K1-08-K1^{iii}$ $99.29 (5)$ $02^{i}-K1-07$ $69.99 (4)$ $K1-08-H8A$ $131.3 (16)$ $05^{ii}-K1-07$ $67.47 (4)$ $K1^{iii}-08-H8A$ $98 (2)$ $08-K1-07$ $67.47 (4)$ $K1^{iii}-08-H8B$ $122.5 (15)$ $06-K1-07$ $69.40 (4)$ $K1^{iii}-08-H8B$ $81.3 (19)$ $09-K1-07$ $136.88 (4)$ $H8A-08-H8B$ $104.8 (14)$ $08^{iii}-K1-07$ $120.54 (4)$ $K1-09-H9B$ $109.1 (16)$ $06^{iv}-K1-07$ $55.87 (4)$ $K1-09-H9A$ $120.1 (17)$ $02^{i}-K1-K1^{iii}$ $100.32 (4)$ $C2-C1-C6$ $120.72 (19)$ $08^{iii}-K1-K1^{iii}$ $100.32 (4)$ $C2-C1-H1A$ 119.6 $09-K1-K1^{iii}$ $114.26 (4)$ $C6-C1-H1A$ 119.6 $09-K1-K1^{iii}$ $38.60 (3)$ $C1-C2-C3$ $120.2 (2)$ $08^{iii}-K1-K1^{iii}$ 36.03 $C1-C2-H2A$ 119.9 $06^{iv}-K1-K1^{iii}$ $150.75 (3)$ $01-C3-C4$ $122.78 (18)$ $02^{i}-K1-K1^{iii}$ $107.73 (4)$ $C4-C3-C2$ $119.40 (18)$ $08-K1-K1^{iiv}$ $93.33 (4)$ $C5-C4-C7$ $120.71 (17)$ $09-K1-K1^{iv}$ $37.47 (3)$ $C5-C4-C7$ $120.71 (17)$ $09-K1-K1^{iv}$ $134.92 (4)$ $C6-C5-C4$ $120.24 (18)$ $06^{iv}-K1-K1^{iv}$ 1	O5 ⁱⁱ —K1—O6 ^{iv}	78.51 (4)	K1—O6—K1 ^{iv}	107.90 (4)
$06-K1-06^{i\nu}$ 72.10 (4) $K1-07-H7A$ 68 (2) $09-K1-06^{i\nu}$ 155.59 (5) $H7B-07-H7A$ 110.3 (16) $08^{iii}-K1-06^{i\nu}$ 84.56 (4) $K1-08-K1^{iii}$ 99.29 (5) $02^{i}-K1-07$ 69.99 (4) $K1-08-H8A$ 131.3 (16) $08^{ii}-K1-07$ 67.47 (4) $K1^{iii}-08-H8A$ 98 (2) $08-K1-07$ 146.52 (5) $K1-08-H8B$ 122.5 (15) $06-K1-07$ 69.40 (4) $K1^{iii}-08-H8B$ 122.5 (15) $06-K1-07$ 69.40 (4) $K1^{iii}-08-H8B$ 104.8 (14) $08^{iii}-K1-07$ 126.54 (4) $K1-09-H9B$ 109.1 (16) $06^{i\nu}-K1-07$ 55.87 (4) $K1-09-H9A$ 120.1 (17) $02^{i}-K1-K1^{iii}$ 103.2 (4) $C2-C1-C6$ 120.72 (19) $08-K1-K1^{iii}$ 103.2 (4) $C2-C1-H1A$ 119.6 $09-K1-K1^{iii}$ 103.2 (4) $C2-C1-H1A$ 119.6 $09-K1-K1^{iii}$ 114.26 (4) $C6-C1-H1A$ 119.6 $09-K1-K1^{iii}$ 38.60 (3) $C1-C2-H2A$ 119.9 $06^{i\nu}-K1-K1^{iii}$ 150.75 (3) $01-C3-C2$ 117.81 (18) $02^{i}-K1-K1^{iii}$ 107.3 (4) $C4-C3-C2$ 119.40 (18) $08-K1-K1^{iii}$ 107.3 (4) $C5-C4-C7$ 120.71 (17) $09-K1-K1^{i\nu}$ 37.47 (3) $C5-C4-C7$ 120.71 (17) $09-K1-K1^{i\nu}$ 163.58 (3) $C3-C2-H2A$ 119.68 (17) $06^{ii}-K1-K1^{i\nu}$ 114.39 (4) $C5-C4-C7$ 120.71 (17) $09-K1-K1^{i\nu}$ 37.47 (3)	08—K1—O6 ^{iv}	106.27 (5)	К1—О7—Н7В	97 (2)
$O9-K1-O6^{iv}$ 155.59 (5)H7B-O7-H7A110.3 (16) $O8^{iii}-K1-O6^{iv}$ 84.56 (4) $K1-O8-K1^{iii}$ 99.29 (5) $O2^{1}-K1-O7$ 69.99 (4) $K1-O8-H8A$ 131.3 (16) $O8^{ii}-K1-O7$ 67.47 (4) $K1^{iii}-O8-H8A$ 98 (2) $O8-K1-O7$ 146.52 (5) $K1-O8-H8B$ 122.5 (15) $O6-K1-O7$ 69.40 (4) $K1^{iii}-O8-H8B$ 81.3 (19) $O9-K1-O7$ 136.88 (4)H8A-O8-H8B104.8 (14) $O8^{iii}-K1-O7$ 120.54 (4) $K1-O9-H9B$ 109.1 (16) $O6^{iv}-K1-O7$ 55.87 (4) $K1-O9-H9A$ 120.1 (17) $O2^{1}-K1-K1^{iii}$ 134.91 (4)H9B-O9-H9A107.3 (14) $O5^{ii}-K1-K1^{iii}$ 100.32 (4)C2-C1-H1A119.6 $O6-K1-K1^{iii}$ 114.26 (4)C6-C1-H1A119.6 $O9-K1-K1^{iii}$ 38.60 (3)C1-C2-C3120.2 (2) $O8^{iii}-K1-K1^{iii}$ 96.46 (3)C3-C2119.9 $O7-K1-K1^{iii}$ 150.75 (3)O1-C3-C4122.78 (18) $O2^{1}-K1-K1^{iii}$ 107.73 (4)C4-C3-C2119.40 (18) $O8-K1-K1^{iiv}$ 37.47 (3)C5-C4-C7120.71 (17) $O9-K1-K1^{iv}$ 163.58 (3)C3-C4-C7120.71 (17) $O9-K1-K1^{iv}$ 143.94 (4)C6-C5-C4120.27 (17) $O8^{iii}-K1-K1^{iv}$ 37.47 (3)C5-C4-C7120.71 (17) $O9-K1-K1^{iv}$ 143.94 (4)C6-C5-C4120.24 (18) $O6^{iv}-K1-K1^{iv}$ 37.47 (3)C5-C4-C7120.71 (17) $O9-K1-K1^{iv}$ 143.94 (4)C6	O6—K1—O6 ^{iv}	72.10 (4)	К1—О7—Н7А	68 (2)
08^{iii} —K1— 06^{iv} 84.56 (4) $K1$ — 08 — $K1^{iii}$ 99.29 (5) 02^{i} —K1— 07 69.99 (4) $K1$ — 08 — $H8A$ 131.3 (16) 05^{ii} —K1— 07 67.47 (4) $K1^{iii}$ — 08 — $H8A$ 98 (2) 08 — $K1$ — 07 146.52 (5) $K1$ — 08 — $H8B$ 122.5 (15) 06 — $K1$ — 07 69.40 (4) $K1^{iii}$ — 08 — $H8B$ 131.3 (19) 09 — $K1$ — 07 136.88 (4) $H8A$ — 08 — $H8B$ 104.8 (14) 08^{iii} — $K1$ — 07 120.54 (4) $K1$ — 09 — $H9B$ 109.1 (16) 06^{iv} — $K1$ — 07 55.87 (4) $K1$ — 09 — $H9A$ 120.1 (17) 02^{i} — $K1$ — $K1^{iii}$ 134.91 (4) $H9B$ — 09 — $H9A$ 107.3 (14) 05^{ii} — $K1$ — $K1^{iii}$ 100.32 (4) $C2$ — $C1$ — $C6$ 120.72 (19) 08 — $K1$ — $K1^{iii}$ 100.32 (4) $C2$ — $C1$ — $C6$ 120.22 (2) 08^{iii} — $K1$ — $K1^{iii}$ 103.2 (3) $C1$ — $C2$ — $C3$ 120.2 (2) 08^{iii} — $K1$ — $K1^{iii}$ 38.60 (3) $C1$ — $C2$ — $C1$ — $C4$ 122.78 (18) 02^{i} — $K1$ — $K1^{iii}$ 96.46 (3) $C3$ — $C2$ — $H2A$ 119.9 06^{iv} — $K1$ — $K1^{iii}$ 150.75 (3) 01 — $C3$ — $C4$ 122.78 (18) 02^{i} — $K1$ — $K1^{iii}$ 107.3 (4) $C4$ — $C3$ — $C2$ 119.40 (18) 08 — $K1$ — $K1^{iv}$ 93.33 (4) $C5$ — $C4$ — $C7$ 120.71 (17) 09 — $K1$ — $K1^{iv}$ 143.9 (4) $C6$ — $C5$ — $C4$ 120.27 (17) 08 — $K1$ — $K1^{iv}$ 143.9 (4) $C6$ — $C5$ — $C4$ — $C7$ 120.71 (17) 09 — $K1$ — $K1^{iv}$ 134.91	09—K1—O6 ^{iv}	155.59 (5)	H7B—O7—H7A	110.3 (16)
$O2^{i}-K1-O7$ $69.99(4)$ $K1-O8-H8A$ $131.3(16)$ $OS^{ii}-K1-O7$ $67.47(4)$ $K1^{iii}-O8-H8A$ $98(2)$ $O8-K1-O7$ $146.52(5)$ $K1-O8-H8B$ $122.5(15)$ $O6-K1-O7$ $69.40(4)$ $K1^{iii}-O8-H8B$ $81.3(19)$ $O9-K1-O7$ $136.88(4)$ $H8A-O8-H8B$ $104.8(14)$ $O8^{iii}-K1-O7$ $120.54(4)$ $K1-O9-H9B$ $109.1(16)$ $O6^{iv}-K1-O7$ $55.87(4)$ $K1-O9-H9A$ $120.1(17)$ $O2^{i}-K1-K1^{iii}$ $134.91(4)$ $H9B-O9-H9A$ $120.72(19)$ $O8-K1-K1^{iii}$ $100.32(4)$ $C2-C1-C6$ $120.72(19)$ $O8-K1-K1^{iii}$ $114.26(4)$ $C6-C1-H1A$ 119.6 $O9-K1-K1^{iii}$ $36.60(3)$ $C1-C2-C3$ $120.2(2)$ $O8^{iii}-K1-K1^{iii}$ $96.46(3)$ $C3-C2-H2A$ 119.9 $O7-K1-K1^{iii}$ $150.75(3)$ $O1-C3-C4$ $122.78(18)$ $O2^{i}-K1-K1^{iii}$ $107.73(4)$ $C4-C3-C2$ $119.40(18)$ $O8-K1-K1^{iii}$ $107.73(4)$ $C4-C7$ $120.71(17)$ $O9-K1-K1^{iii}$ $37.47(3)$ $C5-C4-C7$ $120.71(17)$ $O9-K1-K1^{iiv}$ $37.47(3)$ $C5-C4-C7$ $120.71(17)$ $O9-K1-K1^{iiv}$ $163.58(3)$ $C3-C4-C7$ $119.62(17)$ $O8^{iii}-K1-K1^{iv}$ $37.47(3)$ $C5-C4-C7$ $120.24(18)$ $O6^{iv}-K1-K1^{iv}$ $34.62(3)$ $C6-C5-H5A$ 119.9	08 ⁱⁱⁱ —K1—O6 ^{iv}	84.56 (4)	K1—O8—K1 ⁱⁱⁱ	99.29 (5)
OS^{ii} —K1—O7 $67.47 (4)$ $K1^{iii}$ —O8—H8A $98 (2)$ $O8$ —K1—O7146.52 (5) $K1$ —O8—H8B122.5 (15) $O6$ —K1—O7 $69.40 (4)$ $K1^{iii}$ —O8—H8B $81.3 (19)$ $O9$ —K1—O7136.88 (4)H8A—O8—H8B104.8 (14) $O8^{iii}$ —K1—O7120.54 (4) $K1$ —O9—H9B109.1 (16) $O6^{iv}$ —K1—O755.87 (4) $K1$ —O9—H9A120.1 (17) $O2^{i}$ —K1—K1 ⁱⁱⁱ 134.91 (4)H9B—O9—H9A107.3 (14) $O5^{ii}$ —K1—K1 ⁱⁱⁱ 100.32 (4)C2—C1—C6120.72 (19) $O8$ —K1—K1 ⁱⁱⁱ 114.26 (4)C6—C1—H1A119.6 $O9$ —K1—K1 ⁱⁱⁱ 114.26 (4)C6—C1—H1A119.6 $O9$ —K1—K1 ⁱⁱⁱ 114.26 (4)C3—C2—H2A119.9 $O7$ —K1—K1 ⁱⁱⁱ 96.46 (3)C3—C2—H2A119.9 $O7$ —K1—K1 ⁱⁱⁱ 150.75 (3)O1—C3—C4122.78 (18) $O2^{i}$ —K1—K1 ⁱⁱⁱ 107.73 (4)C4—C3—C2119.40 (18) $O8$ —K1—K1 ^{iv} 33.3 (4)C5—C4—C7120.71 (17) $O9$ —K1—K1 ^{iv} 163.58 (3)C3—C4—C7119.62 (17) $O6$ —K1—K1 ^{iv} 114.39 (4)C5—C4—C7120.271 (17) $O9$ —K1—K1 ^{iv} 114.39 (4)C6—C5—H5A119.9	02 ⁱ —K1—07	69.99 (4)	K1—O8—H8A	131.3 (16)
$08-K1-07$ 146.52 (5) $K1-08-H8B$ 122.5 (15) $06-K1-07$ 69.40 (4) $K1^{1ii}-08-H8B$ 81.3 (19) $09-K1-07$ 136.88 (4) $H8A-08-H8B$ 104.8 (14) $08^{1ii}-K1-07$ 120.54 (4) $K1-09-H9B$ 109.1 (16) $06^{1v}-K1-07$ 55.87 (4) $K1-09-H9A$ 120.1 (17) $02^{1}-K1-K1^{1ii}$ 134.91 (4) $H9B-09-H9A$ 107.3 (14) $05^{1i}-K1-K1^{1ii}$ 100.32 (4) $C2-C1-C6$ 120.72 (19) $08-K1-K1^{1ii}$ 100.32 (4) $C2-C1-H1A$ 119.6 $06-K1-K1^{1ii}$ 114.26 (4) $C6-C1-H1A$ 119.6 $09-K1-K1^{1ii}$ 65.32 (3) $C1-C2-C3$ 120.2 (2) $08^{1ii}-K1-K1^{1ii}$ 38.60 (3) $C1-C2-H2A$ 119.9 $06^{1v}-K1-K1^{1ii}$ 150.75 (3) $01-C3-C4$ 122.78 (18) $02^{1}-K1-K1^{1ii}$ 107.73 (4) $C4-C3-C2$ 117.81 (18) $05^{1i}-K1-K1^{1iv}$ 93.33 (4) $C5-C4-C7$ 120.71 (17) $09-K1-K1^{1iv}$ 37.47 (3) $C5-C4-C7$ 120.71 (17) $09-K1-K1^{1iv}$ 143.9 (4) $C6-C5-C4$ 120.71 (17) $09-K1-K1^{1iv}$ 143.9 (4) $C6-C5-C4$ 120.24 (18) $06^{1v}-K1-K1^{1iv}$ 114.39 (4) $C6-C5-C4$ 120.24 (18) $06^{1i}-K1-K1^{1iv}$ 114.39 (4) $C6-C5-H5A$ 119.9	O5 ⁱⁱ —K1—O7	67.47 (4)	K1 ⁱⁱⁱ —O8—H8A	98 (2)
$06-K1-07$ 69.40 (4) $K1^{iii}-08-H8B$ 81.3 (19) $09-K1-07$ 136.88 (4) $H8A-08-H8B$ 104.8 (14) $08^{iii}-K1-07$ 120.54 (4) $K1-09-H9B$ 109.1 (16) $06^{iv}-K1-07$ 55.87 (4) $K1-09-H9B$ 120.1 (17) $02^{i}-K1-K1^{iii}$ 134.91 (4) $H9B-09-H9A$ 107.3 (14) $05^{ii}-K1-K1^{iii}$ 100.32 (4) $C2-C1-C6$ 120.72 (19) $08-K1-K1^{iii}$ 42.11 (4) $C2-C1-H1A$ 119.6 $06-K1-K1^{iii}$ 114.26 (4) $C6-C1-H1A$ 119.6 $09-K1-K1^{iii}$ 65.32 (3) $C1-C2-C3$ 120.2 (2) $08^{iii}-K1-K1^{iii}$ 38.60 (3) $C1-C2-H2A$ 119.9 $06^{iv}-K1-K1^{iii}$ 96.46 (3) $C3-C2-H2A$ 119.9 $07-K1-K1^{iii}$ 150.75 (3) $01-C3-C2$ 117.81 (18) $02^{i}-K1-K1^{iii}$ 107.73 (4) $C4-C3-C2$ 119.40 (18) $08-K1-K1^{iv}$ 93.33 (4) $C5-C4-C7$ 120.71 (17) $09-K1-K1^{iv}$ 37.47 (3) $C5-C4-C7$ 120.71 (17) $09-K1-K1^{iv}$ 114.39 (4) $C6-C5-C4$ 120.24 (18) $06^{iv}-K1-K1^{iv}$ 114.39 (4) $C6-C5-H5A$ 119.9	08—K1—07	146.52 (5)	K1—O8—H8B	122.5 (15)
$O9-K1-O7$ 136.88 (4)H8A-O8-H8B104.8 (14) $O8^{iii}-K1-O7$ 120.54 (4) $K1-O9-H9B$ 109.1 (16) $O6^{iv}-K1-O7$ 55.87 (4) $K1-O9-H9A$ 120.1 (17) $O2^{i}-K1-K1^{iii}$ 134.91 (4)H9B-O9-H9A107.3 (14) $O5^{ii}-K1-K1^{iii}$ 100.32 (4)C2-C1-C6120.72 (19) $O8-K1-K1^{iii}$ 42.11 (4)C2-C1-H1A119.6 $O6-K1-K1^{iii}$ 114.26 (4)C6-C1-H1A119.6 $O9-K1-K1^{iii}$ 65.32 (3)C1-C2-C3120.2 (2) $O8^{iii}-K1-K1^{iii}$ 38.60 (3)C1-C2-H2A119.9 $O7-K1-K1^{iii}$ 96.46 (3)C3-C2-H2A119.9 $O2^{i}-K1-K1^{iii}$ 150.75 (3)O1-C3-C2117.81 (18) $O5^{ii}-K1-K1^{iii}$ 107.73 (4)C4-C3-C2119.40 (18) $O8-K1-K1^{iiv}$ 37.47 (3)C5-C4-C7120.71 (17) $O9-K1-K1^{iiv}$ 163.58 (3)C3-C2-H2A119.68 (17) $O6^{iv}-K1-K1^{iv}$ 37.47 (3)C5-C4-C7120.71 (17) $O9-K1-K1^{iv}$ 163.58 (3)C3-C4-C7120.24 (18) $O6^{iv}-K1-K1^{iv}$ 14.39 (4)C6-C5-C4120.24 (18)	O6—K1—O7	69.40 (4)	K1 ⁱⁱⁱ —O8—H8B	81.3 (19)
08^{iii} —K1—O7120.54 (4)K1—O9—H9B109.1 (16) 06^{iv} —K1—O755.87 (4)K1—O9—H9A120.1 (17) 02^{i} —K1—K1 ⁱⁱⁱ 134.91 (4)H9B—O9—H9A107.3 (14) 05^{ii} —K1—K1 ⁱⁱⁱ 100.32 (4)C2—C1—C6120.72 (19) 08 —K1—K1 ⁱⁱⁱ 42.11 (4)C2—C1—H1A119.6 06 —K1—K1 ⁱⁱⁱ 114.26 (4)C6—C1—H1A119.6 09 —K1—K1 ⁱⁱⁱ 65.32 (3)C1—C2—C3120.2 (2) 08^{iii} —K1—K1 ⁱⁱⁱ 38.60 (3)C1—C2—H2A119.9 06^{iv} —K1—K1 ⁱⁱⁱ 96.46 (3)C3—C2—H2A119.9 07 —K1—K1 ⁱⁱⁱ 150.75 (3)01—C3—C4122.78 (18) 02^{i} —K1—K1 ⁱⁱⁱ 107.73 (4)C4—C3—C2119.40 (18) 08 —K1—K1 ^{iv} 93.33 (4)C5—C4—C3119.68 (17) 06 —K1—K1 ^{iv} 163.58 (3)C3—C4—C7120.71 (17) 09 —K1—K1 ^{iv} 163.58 (3)C3—C4—C7120.21 (18) 06^{iv} —K1—K1 ^{iv} 114.39 (4)C6—C5—C4120.24 (18)	09—K1—07	136.88 (4)	H8A—O8—H8B	104.8 (14)
$O6^{iv}-K1-O7$ 55.87 (4) $K1-O9-H9A$ 120.1 (17) $O2^i-K1-K1^{iii}$ 134.91 (4)H9B-O9-H9A107.3 (14) $O5^{ii}-K1-K1^{iii}$ 100.32 (4) $C2-C1-C6$ 120.72 (19) $O8-K1-K1^{iii}$ 42.11 (4) $C2-C1-H1A$ 119.6 $O6-K1-K1^{iii}$ 114.26 (4) $C6-C1-H1A$ 119.6 $O9-K1-K1^{iii}$ 65.32 (3) $C1-C2-C3$ 120.2 (2) $O8^{iii}-K1-K1^{iii}$ 38.60 (3) $C1-C2-H2A$ 119.9 $O6^{iv}-K1-K1^{iii}$ 96.46 (3) $C3-C2-H2A$ 119.9 $O7-K1-K1^{iii}$ 150.75 (3) $O1-C3-C4$ 122.78 (18) $O2^i-K1-K1^{iii}$ 107.73 (4) $C4-C3-C2$ 117.81 (18) $O5^{ii}-K1-K1^{iv}$ 93.33 (4) $C5-C4-C7$ 120.71 (17) $O9-K1-K1^{iv}$ 37.47 (3) $C5-C4-C7$ 120.71 (17) $O9-K1-K1^{iv}$ 114.39 (4) $C6-C5-C4$ 120.24 (18) $O6^{iv}-K1-K1^{iv}$ 114.39 (4) $C6-C5-H5A$ 119.9	08 ⁱⁱⁱ —K1—O7	120.54 (4)	К1—О9—Н9В	109.1 (16)
$O2^{i}-K1-K1^{iii}$ 134.91 (4)H9B-O9-H9A107.3 (14) $O5^{ii}-K1-K1^{iii}$ 100.32 (4) $C2-C1-C6$ 120.72 (19) $O8-K1-K1^{iii}$ 42.11 (4) $C2-C1-H1A$ 119.6 $O6-K1-K1^{iii}$ 114.26 (4) $C6-C1-H1A$ 119.6 $O9-K1-K1^{iii}$ 65.32 (3) $C1-C2-C3$ 120.2 (2) $O8^{iii}-K1-K1^{iii}$ 38.60 (3) $C1-C2-H2A$ 119.9 $O6^{iv}-K1-K1^{iii}$ 96.46 (3) $C3-C2-H2A$ 119.9 $O7-K1-K1^{iii}$ 150.75 (3) $O1-C3-C4$ 122.78 (18) $O2^{i}-K1-K1^{iiv}$ 115.45 (4) $O1-C3-C2$ 117.81 (18) $O5^{ii}-K1-K1^{iv}$ 93.33 (4) $C5-C4-C3$ 119.68 (17) $O6-K1-K1^{iv}$ 37.47 (3) $C5-C4-C7$ 120.71 (17) $O9-K1-K1^{iv}$ 114.39 (4) $C6-C5-C4$ 120.24 (18) $O6^{iv}-K1-K1^{iv}$ 114.39 (4) $C6-C5-H5A$ 119.9	O6 ^{iv} —K1—O7	55.87 (4)	К1—О9—Н9А	120.1 (17)
$O5^{ii}-K1-K1^{iii}$ $100.32 (4)$ $C2-C1-C6$ $120.72 (19)$ $O8-K1-K1^{iii}$ $42.11 (4)$ $C2-C1-H1A$ 119.6 $O6-K1-K1^{iii}$ $114.26 (4)$ $C6-C1-H1A$ 119.6 $O9-K1-K1^{iii}$ $65.32 (3)$ $C1-C2-C3$ $120.2 (2)$ $O8^{iii}-K1-K1^{iii}$ $38.60 (3)$ $C1-C2-H2A$ 119.9 $O6^{iv}-K1-K1^{iii}$ $96.46 (3)$ $C3-C2-H2A$ 119.9 $O7-K1-K1^{iii}$ $150.75 (3)$ $O1-C3-C4$ $122.78 (18)$ $O2^i-K1-K1^{iii}$ $150.75 (3)$ $O1-C3-C2$ $117.81 (18)$ $O2^i-K1-K1^{iv}$ $107.73 (4)$ $C4-C3-C2$ $119.40 (18)$ $O8-K1-K1^{iv}$ $93.33 (4)$ $C5-C4-C7$ $120.71 (17)$ $O9-K1-K1^{iv}$ $37.47 (3)$ $C5-C4-C7$ $120.71 (17)$ $O9-K1-K1^{iv}$ $163.58 (3)$ $C3-C4-C7$ $119.62 (17)$ $O8^{iii}-K1-K1^{iv}$ $14.39 (4)$ $C6-C5-C4$ $120.24 (18)$ $O6^{iv}-K1-K1^{iv}$ $114.39 (4)$ $C6-C5-H5A$ 119.9	O2 ⁱ —K1—K1 ⁱⁱⁱ	134.91 (4)	H9B—O9—H9A	107.3 (14)
$O8-K1-K1^{iii}$ $42.11 (4)$ $C2-C1-H1A$ 119.6 $O6-K1-K1^{iii}$ $114.26 (4)$ $C6-C1-H1A$ 119.6 $O9-K1-K1^{iii}$ $65.32 (3)$ $C1-C2-C3$ $120.2 (2)$ $O8^{iii}-K1-K1^{iii}$ $38.60 (3)$ $C1-C2-H2A$ 119.9 $O6^{iv}-K1-K1^{iii}$ $96.46 (3)$ $C3-C2-H2A$ 119.9 $O7-K1-K1^{iii}$ $150.75 (3)$ $O1-C3-C4$ $122.78 (18)$ $O2^i-K1-K1^{iii}$ $150.75 (3)$ $O1-C3-C2$ $117.81 (18)$ $O2^i-K1-K1^{iv}$ $115.45 (4)$ $O1-C3-C2$ $119.40 (18)$ $O5^{ii}-K1-K1^{iv}$ $93.33 (4)$ $C5-C4-C3$ $119.68 (17)$ $O6-K1-K1^{iv}$ $37.47 (3)$ $C5-C4-C7$ $120.71 (17)$ $O9-K1-K1^{iv}$ $163.58 (3)$ $C3-C4-C7$ $119.62 (17)$ $O8^{iii}-K1-K1^{iv}$ $114.39 (4)$ $C6-C5-C4$ $120.24 (18)$ $O6^{iv}-K1-K1^{iv}$ $34.62 (3)$ $C6-C5-H5A$ 119.9	O5 ⁱⁱ —K1—K1 ⁱⁱⁱ	100.32 (4)	C2—C1—C6	120.72 (19)
$O6-K1-K1^{iii}$ $I14.26$ (4) $C6-C1-H1A$ $I19.6$ $O9-K1-K1^{iii}$ 65.32 (3) $C1-C2-C3$ 120.2 (2) $O8^{iii}-K1-K1^{iii}$ 38.60 (3) $C1-C2-H2A$ 119.9 $O6^{iv}-K1-K1^{iii}$ 96.46 (3) $C3-C2-H2A$ 119.9 $O7-K1-K1^{iii}$ 150.75 (3) $O1-C3-C4$ 122.78 (18) $O2^i-K1-K1^{iv}$ 115.45 (4) $O1-C3-C2$ 117.81 (18) $O5^{ii}-K1-K1^{iv}$ 107.73 (4) $C4-C3-C2$ 119.40 (18) $O8-K1-K1^{iv}$ 93.33 (4) $C5-C4-C3$ 119.68 (17) $O6-K1-K1^{iv}$ 37.47 (3) $C5-C4-C7$ 120.71 (17) $O9-K1-K1^{iv}$ 163.58 (3) $C3-C4-C7$ 119.62 (17) $O8^{iii}-K1-K1^{iv}$ 14.39 (4) $C6-C5-C4$ 120.24 (18) $O6^{iv}-K1-K1^{iv}$ 34.62 (3) $C6-C5-H5A$ 119.9	08—K1—K1 ⁱⁱⁱ	42.11 (4)	C2C1H1A	119.6
$O9-K1-K1^{iii}$ $65.32 (3)$ $C1-C2-C3$ $120.2 (2)$ $O8^{iii}-K1-K1^{iii}$ $38.60 (3)$ $C1-C2-H2A$ 119.9 $O6^{iv}-K1-K1^{iii}$ $96.46 (3)$ $C3-C2-H2A$ 119.9 $O7-K1-K1^{iii}$ $150.75 (3)$ $O1-C3-C4$ $122.78 (18)$ $O2^i-K1-K1^{iv}$ $115.45 (4)$ $O1-C3-C2$ $117.81 (18)$ $O5^{ii}-K1-K1^{iv}$ $107.73 (4)$ $C4-C3-C2$ $119.40 (18)$ $O8-K1-K1^{iv}$ $93.33 (4)$ $C5-C4-C3$ $119.68 (17)$ $O6-K1-K1^{iv}$ $37.47 (3)$ $C5-C4-C7$ $120.71 (17)$ $O9-K1-K1^{iv}$ $163.58 (3)$ $C3-C4-C7$ $119.62 (17)$ $O8^{iii}-K1-K1^{iv}$ $114.39 (4)$ $C6-C5-C4$ $120.24 (18)$ $O6^{iv}-K1-K1^{iv}$ $34.62 (3)$ $C6-C5-H5A$ 119.9	06—K1—K1 ⁱⁱⁱ	114.26 (4)	C6—C1—H1A	119.6
$O8^{iii}$ —K1—K1 ⁱⁱⁱ 38.60 (3)C1—C2—H2A119.9 $O6^{iv}$ —K1—K1 ⁱⁱⁱ 96.46 (3)C3—C2—H2A119.9 $O7$ —K1—K1 ⁱⁱⁱ 150.75 (3)O1—C3—C4122.78 (18) $O2^i$ —K1—K1 ^{iiv} 115.45 (4)O1—C3—C2117.81 (18) $O5^{ii}$ —K1—K1 ^{iv} 107.73 (4)C4—C3—C2119.40 (18) $O8$ —K1—K1 ^{iv} 93.33 (4)C5—C4—C3119.68 (17) $O6$ —K1—K1 ^{iv} 37.47 (3)C5—C4—C7120.71 (17) $O9$ —K1—K1 ^{iv} 163.58 (3)C3—C4—C7119.62 (17) $O8^{iii}$ —K1—K1 ^{iv} 114.39 (4)C6—C5—C4120.24 (18) $O6^{iv}$ —K1—K1 ^{iv} 34.62 (3)C6—C5—H5A119.9	09—K1—K1 ⁱⁱⁱ	65.32 (3)	C1—C2—C3	120.2 (2)
$O6^{iv}$ —K1—K1 ⁱⁱⁱ 96.46 (3)C3—C2—H2A119.9 $O7$ —K1—K1 ⁱⁱⁱ 150.75 (3)O1—C3—C4122.78 (18) $O2^{i}$ —K1—K1 ^{iiv} 115.45 (4)O1—C3—C2117.81 (18) $O5^{ii}$ —K1—K1 ^{iv} 107.73 (4)C4—C3—C2119.40 (18) $O8$ —K1—K1 ^{iv} 93.33 (4)C5—C4—C3119.68 (17) $O6$ —K1—K1 ^{iv} 37.47 (3)C5—C4—C7120.71 (17) $O9$ —K1—K1 ^{iv} 163.58 (3)C3—C4—C7119.62 (17) $O8^{iii}$ —K1—K1 ^{iv} 114.39 (4)C6—C5—C4120.24 (18)	O8 ⁱⁱⁱ —K1—K1 ⁱⁱⁱ	38.60 (3)	C1—C2—H2A	119.9
$07-K1-K1^{iii}$ $150.75 (3)$ $01-C3-C4$ $122.78 (18)$ $02^{i}-K1-K1^{iv}$ $115.45 (4)$ $01-C3-C2$ $117.81 (18)$ $05^{ii}-K1-K1^{iv}$ $107.73 (4)$ $C4-C3-C2$ $119.40 (18)$ $08-K1-K1^{iv}$ $93.33 (4)$ $C5-C4-C3$ $119.68 (17)$ $06-K1-K1^{iv}$ $37.47 (3)$ $C5-C4-C7$ $120.71 (17)$ $09-K1-K1^{iv}$ $163.58 (3)$ $C3-C4-C7$ $119.62 (17)$ $08^{iii}-K1-K1^{iv}$ $114.39 (4)$ $C6-C5-C4$ $120.24 (18)$ $06^{iv}-K1-K1^{iv}$ $34.62 (3)$ $C6-C5-H5A$ 119.9	O6 ^{iv} —K1—K1 ⁱⁱⁱ	96.46 (3)	C3—C2—H2A	119.9
$O2^{i}$ —K1—K1 ^{iv} 115.45 (4)O1—C3—C2117.81 (18) $O5^{ii}$ —K1—K1 ^{iv} 107.73 (4)C4—C3—C2119.40 (18) $O8$ —K1—K1 ^{iv} 93.33 (4)C5—C4—C3119.68 (17) $O6$ —K1—K1 ^{iv} 37.47 (3)C5—C4—C7120.71 (17) $O9$ —K1—K1 ^{iv} 163.58 (3)C3—C4—C7119.62 (17) $O8^{iii}$ —K1—K1 ^{iv} 114.39 (4)C6—C5—C4120.24 (18) $O6^{iv}$ —K1—K1 ^{iv} 34.62 (3)C6—C5—H5A119.9	07—K1—K1 ⁱⁱⁱ	150.75 (3)	O1—C3—C4	122.78 (18)
$O5^{ii}$ —K1—K1 ^{iv} 107.73 (4)C4—C3—C2119.40 (18) $O8$ —K1—K1 ^{iv} 93.33 (4)C5—C4—C3119.68 (17) $O6$ —K1—K1 ^{iv} 37.47 (3)C5—C4—C7120.71 (17) $O9$ —K1—K1 ^{iv} 163.58 (3)C3—C4—C7119.62 (17) $O8^{iii}$ —K1—K1 ^{iv} 114.39 (4)C6—C5—C4120.24 (18) $O6^{iv}$ —K1—K1 ^{iv} 34.62 (3)C6—C5—H5A119.9	$O2^{i}$ —K1—K1 ^{iv}	115.45 (4)	O1—C3—C2	117.81 (18)
$O8-K1-K1^{iv}$ 93.33 (4) $C5-C4-C3$ 119.68 (17) $O6-K1-K1^{iv}$ 37.47 (3) $C5-C4-C7$ 120.71 (17) $O9-K1-K1^{iv}$ 163.58 (3) $C3-C4-C7$ 119.62 (17) $O8^{iii}-K1-K1^{iv}$ 114.39 (4) $C6-C5-C4$ 120.24 (18) $O6^{iv}-K1-K1^{iv}$ 34.62 (3) $C6-C5-H5A$ 119.9	O5 ⁱⁱ —K1—K1 ^{iv}	107.73 (4)	C4—C3—C2	119.40 (18)
$O6-K1-K1^{iv}$ 37.47 (3) $C5-C4-C7$ 120.71 (17) $O9-K1-K1^{iv}$ 163.58 (3) $C3-C4-C7$ 119.62 (17) $O8^{iii}-K1-K1^{iv}$ 114.39 (4) $C6-C5-C4$ 120.24 (18) $O6^{iv}-K1-K1^{iv}$ 34.62 (3) $C6-C5-H5A$ 119.9	08—K1—K1 ^{iv}	93.33 (4)	C5—C4—C3	119.68 (17)
O9-K1-K1 ^{iv} 163.58 (3)C3-C4-C7119.62 (17) $O8^{iii}$ -K1-K1 ^{iv} 114.39 (4)C6-C5-C4120.24 (18) $O6^{iv}$ -K1-K1 ^{iv} 34.62 (3)C6-C5-H5A119.9	O6—K1—K1 ^{iv}	37.47 (3)	C5—C4—C7	120.71 (17)
$O8^{iii}$ —K1—K1 ^{iv} 114.39 (4) C6—C5—C4 120.24 (18) $O6^{iv}$ —K1—K1 ^{iv} 34.62 (3) C6—C5—H5A 119.9	09—K1—K1 ^{iv}	163.58 (3)	C3—C4—C7	119.62 (17)
$O6^{iv}$ —K1—K1 ^{iv} 34.62 (3) C6—C5—H5A 119.9	$O8^{iii}$ —K1—K1 ^{iv}	114.39 (4)	C6—C5—C4	120.24 (18)
	$O6^{iv}$ —K1—K1 ^{iv}	34.62 (3)	C6—C5—H5A	119.9

O7—K1—K1 ^{iv}	55.33 (3)	C4—C5—H5A	119.9
K1 ⁱⁱⁱ —K1—K1 ^{iv}	108.502 (17)	C5—C6—C1	119.76 (18)
O2 ⁱ —K1—H7A	84.9 (2)	C5—C6—S1	120.37 (15)
O5 ⁱⁱ —K1—H7A	68.1 (5)	C1—C6—S1	119.87 (15)
O8—K1—H7A	138.7 (4)	O2—C7—O3	123.26 (19)
O6—K1—H7A	68.5 (5)	O2—C7—C4	122.08 (18)
O9—K1—H7A	149.2 (3)	O3—C7—C4	114.66 (17)
O8 ⁱⁱⁱ —K1—H7A	111.5 (4)		
06—S1—O5—K1 ^v	159.19 (15)	08 ⁱⁱⁱ —K1—O8—K1 ⁱⁱⁱ	0.0
O4—S1—O5—K1 ^v	32.5 (2)	06 ^{iv} —K1—O8—K1 ⁱⁱⁱ	-81.50 (5)
C6—S1—O5—K1 ^v	-83.23 (18)	O7—K1—O8—K1 ⁱⁱⁱ	-133.31 (7)
O5—S1—O6—K1	99.55 (11)	K1 ^{iv} —K1—O8—K1 ⁱⁱⁱ	-114.18 (4)
O4—S1—O6—K1	-132.59 (10)	C6—C1—C2—C3	-0.4 (3)
C6—S1—O6—K1	-17.64 (13)	C1—C2—C3—O1	-179.40 (19)
O5—S1—O6—K1 ^{iv}	-85.42 (11)	C1—C2—C3—C4	-0.2 (3)
O4—S1—O6—K1 ^{iv}	42.44 (11)	O1—C3—C4—C5	179.45 (17)
C6—S1—O6—K1 ^{iv}	157.38 (8)	C2—C3—C4—C5	0.3 (3)
O2 ⁱ —K1—O6—S1	49.90 (12)	O1—C3—C4—C7	-0.2 (3)
O5 ⁱⁱ —K1—O6—S1	125.43 (11)	C2—C3—C4—C7	-179.40 (19)
08—K1—06—S1	-72.93 (12)	C3—C4—C5—C6	0.2 (3)
O9—K1—O6—S1	-18.31 (14)	C7—C4—C5—C6	179.90 (17)
O8 ⁱⁱⁱ —K1—O6—S1	-130.24 (10)	C4—C5—C6—C1	-0.8 (3)
O6 ^{iv} —K1—O6—S1	175.52 (15)	C4—C5—C6—S1	179.07 (13)
O7—K1—O6—S1	116.07 (12)	C2—C1—C6—C5	0.9 (3)
K1 ⁱⁱⁱ —K1—O6—S1	-95.39 (11)	C2—C1—C6—S1	-178.97 (16)
K1 ^{iv} —K1—O6—S1	175.52 (15)	O5—S1—C6—C5	134.71 (15)
O2 ⁱ —K1—O6—K1 ^{iv}	-125.61 (5)	O6—S1—C6—C5	-104.47 (16)
O5 ⁱⁱ —K1—O6—K1 ^{iv}	-50.09 (8)	O4—S1—C6—C5	13.98 (18)
08—K1—O6—K1 ^{iv}	111.55 (6)	O5—S1—C6—C1	-45.39 (18)
O9—K1—O6—K1 ^{iv}	166.17 (5)	O6—S1—C6—C1	75.43 (17)
08 ⁱⁱⁱ —K1—O6—K1 ^{iv}	54.24 (9)	O4—S1—C6—C1	-166.12 (15)
O6 ^{iv} —K1—O6—K1 ^{iv}	0.0	K1 ⁱ —O2—C7—O3	-5.6 (4)
O7—K1—O6—K1 ^{iv}	-59.44 (5)	K1 ⁱ —O2—C7—C4	174.65 (14)
K1 ⁱⁱⁱ —K1—O6—K1 ^{iv}	89.09 (5)	C5—C4—C7—O2	178.52 (18)
O2 ⁱ —K1—O8—K1 ⁱⁱⁱ	122.25 (5)	C3—C4—C7—O2	-1.8 (3)
O5 ⁱⁱ —K1—O8—K1 ⁱⁱⁱ	10.60 (10)	C5—C4—C7—O3	-1.2 (3)
06—K1—08—K1 ⁱⁱⁱ	-148.71 (5)	C3—C4—C7—O3	178.45 (17)
09—K1—08—K1 ⁱⁱⁱ	73.01 (5)		
Symmetry codes: (i) $-x$, $-y$, $-z+1$; (ii) x	z, y-1, z; (iii) -x-1, -y, -z+2	2; (iv) - <i>x</i> , - <i>y</i> , - <i>z</i> +2; (v) <i>x</i> , <i>y</i> +1, <i>z</i> .	

Hydrogen-bond geometry (Å, °)

D—H···A	<i>D</i> —Н	H···A	$D \cdots A$	D—H··· A

O1—H1B…O2	0.840 (10)	1.839 (18)	2.586 (2)	147 (3)
O3—H3A…O9 ⁱ	0.845 (10)	1.838 (11)	2.674 (2)	170 (2)
O7—H7A···O6 ^{iv}	0.847 (10)	2.092 (13)	2.917 (2)	164 (3)
O7—H7B···O4 ⁱⁱ	0.843 (10)	2.021 (12)	2.852 (2)	168 (2)
O8—H8A···O5 ^{vi}	0.862 (10)	2.55 (3)	2.926 (2)	108 (2)
O8—H8A····O7 ^{iv}	0.862 (10)	2.50 (2)	2.997 (2)	117.9 (18)
O8—H8B···O4 ^{vii}	0.870 (10)	2.037 (11)	2.879 (2)	163 (2)
O9—H9A···O3 ⁱ	0.847 (9)	1.945 (16)	2.674 (2)	144 (2)
O9—H9B…O7 ^{vii}	0.859 (10)	1.910 (11)	2.763 (2)	172 (2)

Symmetry codes: (i) -*x*, -*y*, -*z*+1; (iv) -*x*, -*y*, -*z*+2; (ii) *x*, *y*-1, *z*; (vi) -*x*-1, -*y*+1, -*z*+2; (vii) *x*-1, *y*, *z*.



Fig. 1







Fig. 3