Poly[aqua(μ_{11}-4,6-dihydroxybenzene-1,3-disulfonato)dipotassium]

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In the title salt, $[K_2(C_6H_4O_8S_2)(H_2O)]_n$, both K^+ ions exhibit a seven-coordination with K—O bond lengths in the range 2.6600 (14) to 3.0522 (16) Å. One K^+ ion is coordinated by seven O atoms from the sulfonate and phenolic hydroxy groups of six 4,6-dihydroxybenzene-1,3-disulfonate (L^{2-}) anions while the other K^+ ion is coordinated by six O atoms from the sulfonate and phenolic hydroxy groups of five L^{2-} anions and one water O atom. The L^{2-} anion exhibits chelating–bridging multidentate coordination to potassium, resulting in the formation of a cross-linked three-dimensional network.

Related literature

For K—O bond lengths of potassium complexes, see: Hatano *et al.* (2008); Xie *et al.* (2006); Zhang *et al.* (2006). For other complexes with seven-coordinate potassium atoms, see: Deacon *et al.* (1999).
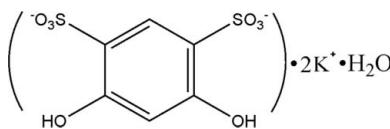
Experimental

Crystal data

$[K_2(C_6H_4O_8S_2)(H_2O)]$
M_r = 364.43

Monoclinic, $P2_1/c$
a = 7.3427 (3) Å
b = 11.5194 (5) Å
c = 14.6331 (6) Å
β = 100.495 (1)°
V = 1217.01 (9) Å^3
Z = 4

Mo $K\alpha$ radiation
μ = 1.16 mm^{-1}
T = 292 K
$0.33 \times 0.20 \times 0.17$ mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.753, T_{max} = 0.816

6519 measured reflections
2365 independent reflections
2164 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.071
S = 1.08
2365 reflections

173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O8—H8$A\cdots$O4	0.82	1.88	2.625 (2)	151
O7—H7$A\cdots$O1	0.82	1.86	2.613 (2)	152
O9—H9$A\cdots$O6^i	0.85	2.29	2.916 (2)	130
O9—H9$B\cdots$O2^{ii}	0.85	2.26	2.913 (3)	134

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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supporting information

Poly[aqua(μ_{11}-4,6-dihydroxybenzene-1,3-disulfonato)dipotassium]

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S1. Comment

The title compound, (I), consists of a three dimensional framework of K^+ ions coordinated to 4, 6-dihydroxybenzene-1, 3-disulfonate anions. The K^+ ion is typically seven-coordinated (Deacon *et al.*, 1999), in which the coordination environment around the K^+ center in (I) is a distorted pentangular dipyramid. As shown in Fig.1, the K1 ion is coordinated by seven O atoms from six 4, 6-dihydroxybenzene-1, 3-disulfonate anions, in which the K—O bond distances range from 2.7160 (14) to 3.0206 (16) Å, with an average bond distance of 2.8460 Å, and the K2 ion is also coordinated by five 4, 6-dihydroxybenzene-1, 3-disulfonate anions and one water molecule, in which the K—O bond distances range from 2.6606 (14) to 3.0518 (16) Å, with an average bond distance of 2.791 Å. The K—O bond distances are similar to the values in other potassium complexes (Hatano *et al.*, 2008; Xie *et al.*, 2006; Zhang *et al.*, 2006). The two sulfonate groups of the 4, 6-dihydroxybenzene-1, 3-disulfonate anions in (I) exhibit a chelating-bridging pentadentate or tetradentate coordination. The O1/O2 atoms and O5/O6 atoms bridge two different K^+ ions, the other O atoms including those of the hydroxide groups chelate to one type of K^+ ion (Fig. 2) giving a three dimensional structure (Fig. 3).

S2. Experimental

KOH (0.14 g, 2.5 mmol) and 4, 6-dihydroxybenzene-1, 3-disulfonate acid (0.91 g, 2.5 mmol) were dissolved in 10 ml of distilled water by vigorous stirring. Filtering solution was evaporated slowly at room temperature. Colorless block crystals of the tilted compound suitable for X-ray analysis were collected in 55% yield (based on potassium) after one week.

S3. Refinement

H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$. Water H atoms were initially located in a difference Fourier map, but they were treated as riding on their parent atoms with O—H = 0.85 Å, and with $U_{iso}(H) = 1.2U_{eq}(O)$. Hydroxy H atoms were placed in calculated positions and treated as riding on their parent atoms, with O—H = 0.82Å, and with $U_{iso}(H) = 1.5U_{eq}(O)$.
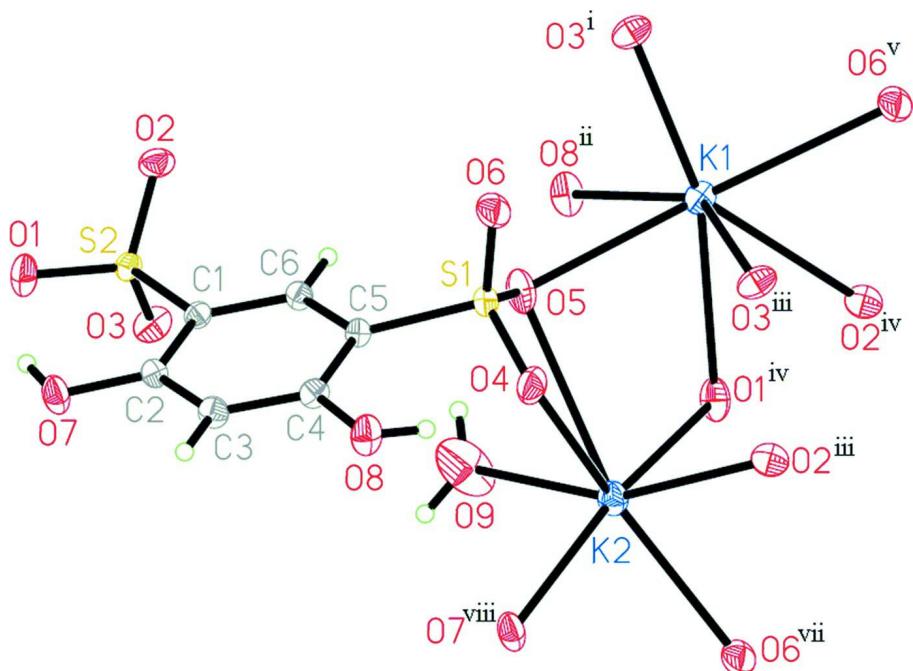
Figure 1

The coordination environment of the K⁺ ions showing displacement ellipsoids drawn at the 30% probability level. [Symmetry codes: (i) x, $-y + 1/2$, $z + 1/2$; (ii) $-x + 1$, $y + 1/2$, $-z + 1/2$; (iii) $-x + 1$, $y - 1/2$, $-z + 1/2$; (iv) $x + 1$, $-y + 1/2$, $z + 1/2$; (v) $-x + 1$, $-y$, $-z + 1$; (vii) $x + 1$, y, z; (viii) $-x + 1$, $-y$, $-z$].
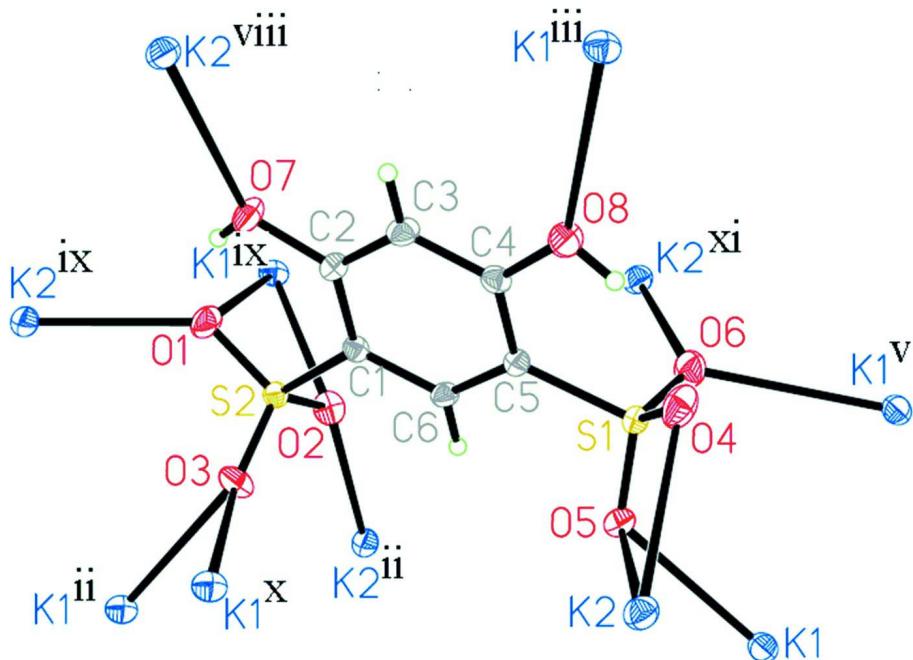
Figure 2

View of chelating/bridging to K⁺ ions by the sulfonic and phenolic hydroxy groups in the L^{2-} anion, displacement ellipsoids are drawn at 30% probability level. [Symmetry codes: (ii) $-x + 1$, $y + 1/2$, $-z + 1/2$; (iii) $-x + 1$, $y - 1/2$, $-z + 1/2$; (v) $-x + 1$, $-y$, $-z + 1$; (viii) $-x + 1$, $-y$, $-z$ (ix) $x - 1$, $-y + 1/2$, $z - 1/2$; (x) x, $-y + 1/2$, $z - 1/2$; (xi) $x - 1$, y, z].
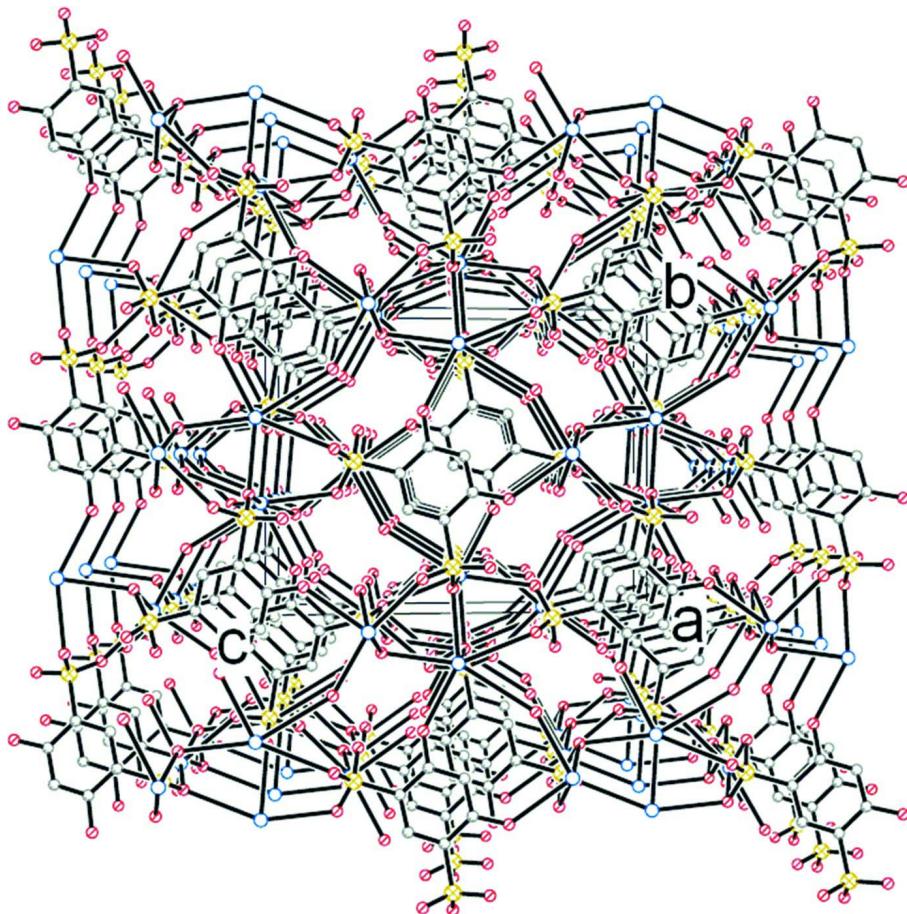
Figure 3

Perspective view of crystal packing along the *a* axis. Hydrogen atoms are omitted for clarity.

Poly[aqua(*μ*₁₁-4,6-dihydroxybenzene-1,3-disulfonato)dipotassium]

Crystal data
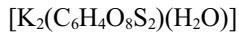
[K₂(C₆H₄O₈S₂)(H₂O)]	$F(000) = 736$
$M_r = 364.43$	$D_x = 1.989$ Mg m⁻³
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2637 reflections
$a = 7.3427$ (3) Å	$\theta = 2.3–27.4°$
$b = 11.5194$ (5) Å	$\mu = 1.16$ mm⁻¹
$c = 14.6331$ (6) Å	$T = 292$ K
$\beta = 100.495$ (1)°	Block, colorless
$V = 1217.01$ (9) Å³	$0.33 \times 0.20 \times 0.17$ mm
$Z = 4$	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
Radiation source: fine-focus sealed tube	$T_{min} = 0.753$, $T_{max} = 0.816$
Graphite monochromator	6519 measured reflections
φ and ω scans	2365 independent reflections
	2164 reflections with $I > 2\sigma(I)$

$R_{int} = 0.013$

$\theta_{max} = 26.0°$, $\theta_{min} = 2.3°$

$h = -9\rightarrow8$

$k = -14\rightarrow14$

$l = -13\rightarrow18$

Refinement

Refinement on F^2	Hydrogen site location: inferred from
Least-squares matrix: full	neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.024$	H-atom parameters constrained
$wR(F^2) = 0.071$	$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 0.4024P]$
$S = 1.08$	where $P = (F_o^2 + 2F_c^2)/3$
2365 reflections	$(\Delta/\sigma)_{max} < 0.001$
173 parameters	$\Delta\rho_{max} = 0.38$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.33$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.0022 (7)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
K1	0.65409 (5)	0.13314 (3)	0.49915 (3)	0.03113 (13)
K2	0.92404 (6)	0.02144 (4)	0.28049 (3)	0.03374 (13)
S1	0.44515 (6)	0.00084 (4)	0.26286 (3)	0.02489 (13)
S2	0.13059 (5)	0.32694 (3)	0.01439 (3)	0.02338 (13)
O1	0.0057 (2)	0.32564 (11)	−0.07575 (9)	0.0390 (3)
O2	0.03127 (18)	0.35943 (11)	0.08772 (10)	0.0349 (3)
O3	0.29405 (18)	0.39641 (11)	0.01473 (10)	0.0372 (3)
O4	0.5722 (2)	−0.09468 (13)	0.25379 (10)	0.0431 (4)
O5	0.5404 (2)	0.10174 (12)	0.30606 (9)	0.0401 (3)
O6	0.29385 (19)	−0.03620 (13)	0.30678 (9)	0.0410 (3)
O7	0.0959 (2)	0.11766 (12)	−0.12326 (9)	0.0381 (3)
H7A	0.0522	0.1834	−0.1271	0.046*
O8	0.3915 (2)	−0.15510 (11)	0.08903 (10)	0.0383 (3)
H8A	0.4576	−0.1604	0.1404	0.046*
O9	0.8087 (4)	0.21939 (16)	0.19154 (15)	0.0948 (8)
H9A	0.7450	0.2678	0.2163	0.114*
H9B	0.8358	0.2336	0.1386	0.114*
C1	0.2023 (2)	0.18131 (14)	0.03585 (11)	0.0225 (3)
C2	0.1799 (2)	0.09683 (15)	−0.03415 (11)	0.0254 (4)
C3	0.2454 (2)	−0.01451 (15)	−0.01379 (12)	0.0292 (4)

H3A	0.2321	−0.0700	−0.0607	0.035*
C4	0.3303 (2)	−0.04435 (14)	0.07530 (12)	0.0258 (3)
C5	0.3490 (2)	0.03891 (14)	0.14670 (11)	0.0233 (3)
C6	0.2866 (2)	0.15100 (14)	0.12554 (12)	0.0241 (3)
H6A	0.3015	0.2069	0.1722	0.029*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.0284 (2)	0.0278 (2)	0.0368 (2)	−0.00127 (15)	0.00475 (16)	0.00329 (15)
K2	0.0373 (2)	0.0326 (2)	0.0297 (2)	0.00037 (16)	0.00155 (17)	−0.00276 (16)
S1	0.0255 (2)	0.0254 (2)	0.0225 (2)	0.00017 (16)	0.00132 (16)	0.00241 (15)
S2	0.0237 (2)	0.0199 (2)	0.0257 (2)	0.00147 (15)	0.00221 (16)	0.00099 (15)
O1	0.0470 (8)	0.0309 (7)	0.0329 (7)	0.0074 (6)	−0.0093 (6)	0.0026 (6)
O2	0.0364 (7)	0.0305 (7)	0.0402 (8)	0.0088 (5)	0.0131 (6)	−0.0009 (5)
O3	0.0319 (7)	0.0263 (7)	0.0538 (9)	−0.0039 (5)	0.0092 (6)	0.0049 (6)
O4	0.0458 (8)	0.0437 (8)	0.0363 (7)	0.0193 (7)	−0.0020 (6)	0.0016 (6)
O5	0.0492 (8)	0.0366 (7)	0.0291 (7)	−0.0113 (6)	−0.0071 (6)	0.0010 (6)
O6	0.0364 (7)	0.0531 (9)	0.0349 (7)	−0.0057 (6)	0.0100 (6)	0.0096 (6)
O7	0.0549 (9)	0.0336 (7)	0.0219 (6)	0.0099 (6)	−0.0029 (6)	−0.0033 (5)
O8	0.0521 (8)	0.0218 (6)	0.0366 (7)	0.0081 (6)	−0.0033 (6)	−0.0020 (5)
O9	0.178 (3)	0.0389 (10)	0.0766 (14)	0.0139 (13)	0.0474 (15)	0.0119 (9)
C1	0.0222 (8)	0.0205 (8)	0.0249 (8)	0.0014 (6)	0.0041 (6)	0.0008 (6)
C2	0.0259 (8)	0.0279 (9)	0.0220 (8)	0.0002 (7)	0.0029 (6)	−0.0012 (7)
C3	0.0343 (10)	0.0250 (9)	0.0269 (9)	0.0011 (7)	0.0023 (7)	−0.0073 (7)
C4	0.0270 (8)	0.0202 (8)	0.0300 (9)	0.0001 (7)	0.0046 (7)	−0.0015 (7)
C5	0.0233 (8)	0.0236 (8)	0.0223 (8)	0.0002 (6)	0.0019 (6)	0.0007 (6)
C6	0.0256 (8)	0.0224 (8)	0.0234 (8)	−0.0004 (6)	0.0019 (6)	−0.0036 (6)

Geometric parameters (Å, º)

K1—O3[i]	2.7160 (14)	O1—K2[viii]	2.7256 (13)
K1—O8[ii]	2.7514 (13)	O1—K1[viii]	3.0207 (16)
K1—O3[iii]	2.7660 (14)	O2—K2[ii]	2.6607 (14)
K1—O5	2.8200 (14)	O2—K1[viii]	2.8372 (14)
K1—O2[iv]	2.8372 (14)	O3—K1[ix]	2.7160 (14)
K1—O6[v]	3.0104 (14)	O3—K1[ii]	2.7660 (14)
K1—O1[iv]	3.0207 (16)	O6—K2[x]	2.7535 (15)
K1—O9[i]	3.307 (2)	O6—K1[v]	3.0104 (14)
K1—S2[iv]	3.4954 (6)	O7—C2	1.359 (2)
K2—O2[iii]	2.6607 (14)	O7—K2[vii]	2.7856 (13)
K2—O9	2.6851 (19)	O7—H7A	0.8204
K2—O1[iv]	2.7256 (13)	O8—C4	1.356 (2)
K2—O6[vi]	2.7535 (15)	O8—K1[iii]	2.7514 (13)
K2—O7[vii]	2.7856 (13)	O8—H8A	0.8194
K2—O4	2.8720 (16)	O9—K1[ix]	3.307 (2)
K2—O5	3.0521 (16)	O9—H9A	0.8500
K2—S1	3.4867 (6)	O9—H9B	0.8502

S1—O5	1.4417 (13)	C1—C6	1.390 (2)
S1—O6	1.4455 (14)	C1—C2	1.401 (2)
S1—O4	1.4641 (14)	C2—C3	1.383 (2)
S1—C5	1.7729 (16)	C3—C4	1.382 (2)
S2—O3	1.4418 (13)	C3—H3A	0.9300
S2—O2	1.4519 (13)	C4—C5	1.406 (2)
S2—O1	1.4628 (13)	C5—C6	1.386 (2)
S2—C1	1.7691 (16)	C6—H6A	0.9300
S2—K1^{viii}	3.4954 (6)		
O3^i—K1—O8^{ii}	96.50 (4)	O1^{iv}—K2—S1	100.27 (3)
O3^i—K1—O3^{iii}	91.82 (4)	O6^{vi}—K2—S1	161.72 (4)
O8^{ii}—K1—O3^{iii}	147.81 (5)	O7^{vii}—K2—S1	89.95 (3)
O3^i—K1—O5	87.31 (5)	O4—K2—S1	24.24 (3)
O8^{ii}—K1—O5	69.84 (4)	O5—K2—S1	24.33 (3)
O3^{iii}—K1—O5	79.60 (4)	O2^{iii}—K2—K1	71.35 (3)
O3^i—K1—O2^{iv}	148.16 (4)	O9—K2—K1	87.63 (5)
O8^{ii}—K1—O2^{iv}	102.29 (4)	O1^{iv}—K2—K1	44.92 (3)
O3^{iii}—K1—O2^{iv}	85.83 (4)	O6^{vi}—K2—K1	123.37 (3)
O5—K1—O2^{iv}	123.22 (4)	O7^{vii}—K2—K1	146.39 (3)
O3^i—K1—O6^v	80.36 (4)	O4—K2—K1	73.30 (3)
O8^{ii}—K1—O6^v	139.02 (4)	O5—K2—K1	41.41 (3)
O3^{iii}—K1—O6^v	73.03 (4)	S1—K2—K1	58.329 (11)
O5—K1—O6^v	149.45 (4)	O2^{iii}—K2—K1^{xi}	37.90 (3)
O2^{iv}—K1—O6^v	68.57 (4)	O9—K2—K1^{xi}	144.42 (6)
O3^i—K1—O1^{iv}	163.66 (4)	O1^{iv}—K2—K1^{xi}	70.77 (3)
O8^{ii}—K1—O1^{iv}	74.31 (4)	O6^{vi}—K2—K1^{xi}	42.14 (3)
O3^{iii}—K1—O1^{iv}	89.44 (4)	O7^{vii}—K2—K1^{xi}	107.18 (3)
O5—K1—O1^{iv}	76.90 (4)	O4—K2—K1^{xi}	113.91 (3)
O2^{iv}—K1—O1^{iv}	48.18 (4)	O5—K2—K1^{xi}	124.94 (3)
O6^v—K1—O1^{iv}	115.50 (4)	S1—K2—K1^{xi}	126.161 (14)
O3^i—K1—O9^i	100.44 (5)	K1—K2—K1^{xi}	86.205 (11)
O8^{ii}—K1—O9^i	86.41 (5)	O5—S1—O6	113.19 (9)
O3^{iii}—K1—O9^i	122.58 (5)	O5—S1—O4	112.30 (9)
O5—K1—O9^i	155.78 (5)	O6—S1—O4	111.87 (9)
O2^{iv}—K1—O9^i	55.98 (6)	O5—S1—C5	107.31 (8)
O6^v—K1—O9^i	54.73 (5)	O6—S1—C5	107.16 (8)
O1^{iv}—K1—O9^i	92.56 (5)	O4—S1—C5	104.37 (8)
O3^i—K1—S2^{iv}	171.66 (4)	O5—S1—K2	60.70 (6)
O8^{ii}—K1—S2^{iv}	87.03 (3)	O6—S1—K2	146.47 (6)
O3^{iii}—K1—S2^{iv}	89.13 (3)	O4—S1—K2	53.65 (6)
O5—K1—S2^{iv}	101.01 (3)	C5—S1—K2	105.92 (6)
O2^{iv}—K1—S2^{iv}	23.71 (3)	O3—S2—O2	112.60 (8)
O6^v—K1—S2^{iv}	92.00 (3)	O3—S2—O1	113.16 (9)
O1^{iv}—K1—S2^{iv}	24.59 (2)	O2—S2—O1	110.63 (8)
O9^i—K1—S2^{iv}	72.17 (5)	O3—S2—C1	107.76 (8)
O3^i—K1—K1^v	46.45 (3)	O2—S2—C1	106.66 (8)
O8^{ii}—K1—K1^v	133.97 (3)	O1—S2—C1	105.53 (8)

$O3^{iii}$—$K1$—$K1^{v}$	45.37 (3)	$O3$—$S2$—$K1^{viii}$	138.60 (6)
$O5$—$K1$—$K1^{v}$	80.54 (3)	$O2$—$S2$—$K1^{viii}$	51.80 (6)
$O2^{iv}$—$K1$—$K1^{v}$	123.52 (3)	$O1$—$S2$—$K1^{viii}$	59.22 (6)
$O6^{v}$—$K1$—$K1^{v}$	70.68 (3)	$C1$—$S2$—$K1^{viii}$	113.46 (6)
$O1^{iv}$—$K1$—$K1^{v}$	132.54 (3)	$S2$—$O1$—$K2^{viii}$	134.67 (8)
$O9^{i}$—$K1$—$K1^{v}$	121.30 (4)	$S2$—$O1$—$K1^{viii}$	96.20 (7)
$S2^{iv}$—$K1$—$K1^{v}$	133.906 (18)	$K2^{viii}$—$O1$—$K1^{viii}$	95.50 (4)
$O3^{i}$—$K1$—$K2$	128.22 (3)	$S2$—$O2$—$K2^{ii}$	134.76 (8)
$O8^{ii}$—$K1$—$K2$	87.08 (3)	$S2$—$O2$—$K1^{viii}$	104.48 (7)
$O3^{iii}$—$K1$—$K2$	63.75 (3)	$K2^{ii}$—$O2$—$K1^{viii}$	106.93 (4)
$O5$—$K1$—$K2$	45.71 (3)	$S2$—$O3$—$K1^{ix}$	138.81 (8)
$O2^{iv}$—$K1$—$K2$	78.64 (3)	$S2$—$O3$—$K1^{ii}$	132.27 (8)
$O6^{v}$—$K1$—$K2$	126.89 (3)	$K1^{ix}$—$O3$—$K1^{ii}$	88.18 (4)
$O1^{iv}$—$K1$—$K2$	39.58 (2)	$S1$—$O4$—$K2$	102.11 (8)
$O9^{i}$—$K1$—$K2$	131.33 (5)	$S1$—$O5$—$K1$	125.04 (8)
$S2^{iv}$—$K1$—$K2$	59.350 (11)	$S1$—$O5$—$K2$	94.98 (7)
$K1^{v}$—$K1$—$K2$	96.882 (15)	$K1$—$O5$—$K2$	92.88 (4)
$O3^{i}$—$K1$—$K2^{xi}$	116.87 (3)	$S1$—$O6$—$K2^{x}$	133.23 (8)
$O8^{ii}$—$K1$—$K2^{xi}$	135.14 (3)	$S1$—$O6$—$K1^{v}$	123.58 (7)
$O3^{iii}$—$K1$—$K2^{xi}$	64.45 (3)	$K2^{x}$—$O6$—$K1^{v}$	100.01 (4)
$O5$—$K1$—$K2^{xi}$	136.03 (3)	$C2$—$O7$—$K2^{vii}$	129.60 (11)
$O2^{iv}$—$K1$—$K2^{xi}$	35.17 (3)	$C2$—$O7$—$H7A$	109.4
$O6^{v}$—$K1$—$K2^{xi}$	37.85 (3)	$K2^{vii}$—$O7$—$H7A$	120.9
$O1^{iv}$—$K1$—$K2^{xi}$	78.24 (3)	$C4$—$O8$—$K1^{iii}$	139.13 (11)
$O9^{i}$—$K1$—$K2^{xi}$	59.97 (4)	$C4$—$O8$—$H8A$	109.4
$S2^{iv}$—$K1$—$K2^{xi}$	56.355 (10)	$K1^{iii}$—$O8$—$H8A$	111.4
$K1^{v}$—$K1$—$K2^{xi}$	90.518 (14)	$K2$—$O9$—$K1^{ix}$	151.40 (8)
$K2$—$K1$—$K2^{xi}$	93.795 (11)	$K2$—$O9$—$H9A$	120.0
$O2^{iii}$—$K2$—$O9$	158.97 (6)	$K1^{ix}$—$O9$—$H9A$	84.0
$O2^{iii}$—$K2$—$O1^{iv}$	85.02 (4)	$K2$—$O9$—$H9B$	120.0
$O9$—$K2$—$O1^{iv}$	80.27 (6)	$K1^{ix}$—$O9$—$H9B$	39.3
$O2^{iii}$—$K2$—$O6^{vi}$	75.01 (4)	$H9A$—$O9$—$H9B$	120.0
$O9$—$K2$—$O6^{vi}$	119.25 (7)	$C6$—$C1$—$C2$	119.26 (15)
$O1^{iv}$—$K2$—$O6^{vi}$	88.58 (5)	$C6$—$C1$—$S2$	118.21 (12)
$O2^{iii}$—$K2$—$O7^{vii}$	100.15 (4)	$C2$—$C1$—$S2$	122.52 (13)
$O9$—$K2$—$O7^{vii}$	97.10 (5)	$O7$—$C2$—$C3$	116.73 (15)
$O1^{iv}$—$K2$—$O7^{vii}$	168.61 (5)	$O7$—$C2$—$C1$	123.46 (15)
$O6^{vi}$—$K2$—$O7^{vii}$	83.04 (4)	$C3$—$C2$—$C1$	119.80 (15)
$O2^{iii}$—$K2$—$O4$	76.18 (4)	$C4$—$C3$—$C2$	120.87 (16)
$O9$—$K2$—$O4$	97.64 (7)	$C4$—$C3$—$H3A$	119.6
$O1^{iv}$—$K2$—$O4$	118.17 (5)	$C2$—$C3$—$H3A$	119.6
$O6^{vi}$—$K2$—$O4$	138.28 (4)	$O8$—$C4$—$C3$	117.02 (15)
$O7^{vii}$—$K2$—$O4$	73.09 (4)	$O8$—$C4$—$C5$	123.15 (15)
$O2^{iii}$—$K2$—$O5$	96.80 (4)	$C3$—$C4$—$C5$	119.83 (15)
$O9$—$K2$—$O5$	65.50 (6)	$C6$—$C5$—$C4$	119.06 (15)
$O1^{iv}$—$K2$—$O5$	77.75 (4)	$C6$—$C5$—$S1$	120.16 (13)
$O6^{vi}$—$K2$—$O5$	164.73 (4)	$C4$—$C5$—$S1$	120.76 (13)
$O7^{vii}$—$K2$—$O5$	111.39 (4)	$C5$—$C6$—$C1$	121.14 (15)

O4—K2—O5	47.96 (4)	C5—C6—H6A	119.4
O2^{iii}—K2—S1	89.74 (3)	C1—C6—H6A	119.4
O9—K2—S1	78.29 (6)		

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

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O8—H8*A*⋯O4	0.82	1.88	2.625 (2)	151
O7—H7*A*⋯O1	0.82	1.86	2.613 (2)	152
O9—H9*A*⋯O6^{ii}	0.85	2.29	2.916 (2)	130
O9—H9*B*⋯O2^{vi}	0.85	2.26	2.913 (3)	134

Symmetry codes: (ii) $-x+1$, $y+1/2$, $-z+1/2$; (vi) $x+1$, y, z.