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Dipotassium biphenyl-4,4'-disulfonate dihydrate: a coordination polymer

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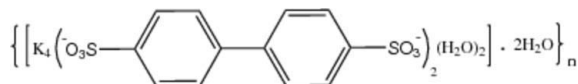
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Key indicators: single-crystal X-ray study; $T = 297$ K; mean $\sigma(\text{C}-\text{C}) = 0.006$ Å; R factor = 0.031; wR factor = 0.083; data-to-parameter ratio = 10.1.

The polymeric structure of the title compound, poly-[[diaquabis(μ -biphenyl-4,4'-disulfonato)tetrapotassium(I)] dihydrate], $\{[\text{K}_2(\text{C}_{12}\text{H}_8\text{O}_6\text{S}_2)(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}\}_n$, is based on an asymmetric unit comprising three independent and different potassium centres, one six-coordinate [$\text{K}-\text{O} = 2.657$ (3)– 2.866 (5) Å], one seven-coordinate [$\text{K}-\text{O} = 2.703$ (3)– 3.040 (4) Å], and the third ten-coordinate [$\text{K}-\text{O} = 2.751$ (3)– 3.079 (4) Å], with two of these lying on crystallographic mirror planes. The four half-occupancy water molecules also lie on the mirror planes with two coordinated (one monodentate, the other bidentate bridging) and two as molecules of solvation. The interlinked coordination polyhedra form chains which are joined laterally through the biphenyl residues as well as through head-to-tail water hydrogen-bonding interactions, giving a two-dimensional structure.

Related literature

For other 4,4'-biphenyldisulfonate crystal structures, see: Swift *et al.* (1998); Liao *et al.* (2001); Cai *et al.* (2001); Usuki *et al.* (2002). For related literature, see: Pivovarov *et al.* (2002). For synthesis, see: Feldmann (1931).



Experimental

Crystal data

$[\text{K}_2(\text{C}_{12}\text{H}_8\text{O}_6\text{S}_2)(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}$
 $M_r = 426.56$
 Monoclinic, Cm
 $a = 5.8316$ (10) Å
 $b = 19.691$ (7) Å
 $c = 14.623$ (2) Å
 $\beta = 98.953$ (13)°
 $V = 1658.7$ (7) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.86$ mm⁻¹
 $T = 297$ (2) K
 $0.32 \times 0.25 \times 0.20$ mm

Data collection

Rigaku AFC 7R diffractometer
 Absorption correction: ψ scan
 (TEXSAN for Windows; Molecular Structure Corporation, 1999)
 $T_{\min} = 0.774$, $T_{\max} = 0.849$
 2295 measured reflections
 2295 independent reflections
 2196 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.016$
 3 standard reflections
 frequency: 150 min
 intensity decay: 0.6%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.031$
 $wR(F^2) = 0.083$
 $S = 0.88$
 2295 reflections
 227 parameters
 2 restraints
 H-atom parameters not refined
 $\Delta\rho_{\text{max}} = 0.40$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.39$ e Å⁻³
 Absolute structure: Flack (1983),
 322 Friedel pairs
 Flack parameter: 0.02 (8)

Table 1

Selected bond lengths (Å).

K1—O43B	2.850 (4)	K2—O42A ^{vii}	2.741 (3)
K1—O41B ⁱ	2.703 (3)	K3—O2W	3.079 (4)
K1—O41A ⁱⁱ	3.040 (4)	K3—O41B	2.751 (3)
K1—O43A ⁱⁱⁱ	3.058 (3)	K3—O42B	3.076 (4)
K1—O42A ⁱⁱⁱ	2.866 (3)	K3—O42A ⁱⁱⁱ	2.938 (3)
K1—O43B ^{iv}	2.739 (3)	K3—O43A ⁱⁱⁱ	3.027 (3)
K1—O41A ^v	2.681 (3)	K3—O2W ^{viii}	2.793 (4)
K2—O1W	2.703 (6)	K3—O41B ^{ix}	2.751 (3)
K2—O2W	2.866 (5)	K3—O42B ^{ix}	3.076 (4)
K2—O43A ⁱⁱ	2.657 (3)	K3—O42A ^{vii}	2.938 (3)
K2—O42A ⁱⁱⁱ	2.741 (3)	K3—O43A ^{vii}	3.027 (3)
K2—O43A ^{vi}	2.657 (3)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H11W \cdots O4W ⁱⁱⁱ	0.97	2.18	2.778 (9)	119
O2W—H2W \cdots O42B	0.96	1.91	2.840 (5)	162
O3W—H3W \cdots O42B	0.96	1.95	2.884 (5)	162
O4W—H41W \cdots O3W	0.90	1.82	2.715 (9)	180
O4W—H41W \cdots O3W	0.90	1.82	2.715 (9)	180
C5A—H5A \cdots O43A	0.95	2.50	2.916 (5)	106
C5B—H5B \cdots O41B	0.94	2.47	2.873 (5)	106

Symmetry code: (iii) $x, y, z + 1$.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1999); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN for Windows* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2210).

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supplementary materials

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Dipotassium biphenyl-4,4'-disulfonate dihydrate: a coordination polymer

G. Smith, U. D. Wermuth and P. C. Healy

Comment

Compounds of 4,4'-biphenyldisulfonic acid (BPDS) are not numerous in the crystallographic literature. The guanidinium salts have been used for the generation of 2-D structures for the formation of crystalline clathrates with aromatic hydrocarbons (Swift *et al.*, 1998; Pivovar *et al.*, 2002). The bis(alaninium) salt is also known (Liao *et al.*, 2001). With coordination compounds, BDPDS is generally found as a dianionic counter ion (Cai *et al.*, 2001; Usuki *et al.*, 2002). We obtained X-ray diffraction quality crystals of the hydrated dipotassium salt of BPDS as an intermediate in the synthesis of BPDS, when recrystallized from water. The structure of this compound, $K_2^{2+} \cdot C_{12}H_8O_6S_2^{2-} \cdot 2H_2O$ (I) is reported here.

The structure of (I) is based on an asymmetric unit comprising three independent and different potassium centres, one six-coordinate (K2) [K–O range, 2.657 (3)–2.866 (5) Å], one seven-coordinate (K1) [K–O range, 2.703 (3)–3.040 (4) Å] and the third ten-coordinate (K3) [K–O range, 2.751 (3)–3.079 (4) Å], with two of these (K2 and K3) lying on crystallographic mirror planes (Fig. 1). The four half-occupancy water molecules also lie on the mirror planes with two coordinated [one monodentate (O1W on K2), and one bidentate (O2W, bridging K2 and K3)], and the other two (OW3, OW4) as molecules of solvation. The structure has pseudo $2/m$ symmetry, the 2-fold rotational symmetry along the b axis being upset largely by the differing roles of the water molecules in the structure. This was also consistent with the failure to obtain a solution of the structure in the space group $C2/m$.

The interlinked potassium coordination polyhedra form chains which extend down the b axis and are linked laterally across the c cell direction through the biphenyl residues of the BPDS ligands, giving a 2-D structure (Fig. 2). This is somewhat analogous to the 2-D but hydrogen-bonded guanidinium-BPDS open framework structures (Swift *et al.*, 1998; Pivovar *et al.*, 2002) which accommodate interstitial inert aromatic molecules. With (I), the water molecules are similarly accommodated in the interstitial spaces along the crystallographic mirror planes in linear head-to-tail interactions (Table 1) and also link the coordination polymer chains. In addition, the coordinated water molecules give lateral $O-H \cdots O_{\text{sulfonate}}$ interactions within the polymer chains.

Within the BPDS anion, the two phenyl rings (A and B) are close to co-planar [torsion angle C2A–C1A–C1B–C6B, -178.3 (5) °], which is similar to that found in the alaninium salt where the two residues are inversion related (Liao *et al.*, 2001).

Experimental

The title compound was obtained as colourless crystals from the room temperature evaporation of an aqueous solution of dipotassium 4,4'-biphenyldisulfonate, an intermediate product in the synthesis of 4,4'-biphenyldisulfonic acid by the sulfonation of biphenyl using the procedure of Feldmann (1931).

supplementary materials

Refinement

Hydrogen atoms on the water molecules were located by difference methods but their positional and isotropic displacement parameters were fixed as located and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$, respectively; see Table 1 for distances. The aromatic H atoms were included in the refinement in their calculated positions ($\text{C-H} = 0.94\text{--}0.95 \text{ \AA}$) using a riding model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

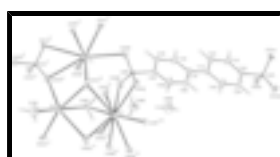


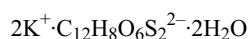
Fig. 1. Molecular configuration and atom naming scheme for the BPDS ligand, the three independent potassium coordination polyhedra and the water molecules in the asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level. Dashed lines indicate hydrogen-bonding interactions associated with the water molecules. The two potassium ions (K2, K3) and the four water molecules (O1W–O4W) lie on a crystallographic mirror plane. Symmetry codes: (i) $x - 1, y, z$; (ii) $x - 1, y, z + 1$; (iii) $x, y, z + 1$; (iv) $x - 1/2, -y + 1/2, z$; (v) $x - 1/2, -y + 1/2, z + 1$; (vi) $x - 1, -y, z + 1$; (vii) $x, -y, z + 1$; (viii) $x + 1, y, z$; (ix) $x, -y, z$.



Fig. 2. The 2-D hydrogen-bonded structure of (I) viewed down the a axis, showing $\text{K-O}_{\text{sulfonate}}$ coordination-polymer chains with the biphenyl step linkages, together with the water mediated hydrogen-bonding associations lying on the mirror planes at $y = 0, 1/2$.

dipotassium biphenyl-4,4'-disulfonate dihydrate

Crystal data



$$M_r = 426.56$$

Monoclinic, Cm

Hall symbol: $C -2y$

$$a = 5.8316 (10) \text{ \AA}$$

$$b = 19.691 (7) \text{ \AA}$$

$$c = 14.623 (2) \text{ \AA}$$

$$\beta = 98.953 (13)^\circ$$

$$V = 1658.7 (7) \text{ \AA}^3$$

$$Z = 4$$

$$F_{000} = 872$$

$$D_x = 1.708 \text{ Mg m}^{-3}$$

Mo $K\alpha$ radiation

$$\lambda = 0.71073 \text{ \AA}$$

Cell parameters from 25 reflections

$$\theta = 12.9\text{--}17.1^\circ$$

$$\mu = 0.86 \text{ mm}^{-1}$$

$$T = 297 (2) \text{ K}$$

Block, colourless

$$0.32 \times 0.25 \times 0.20 \text{ mm}$$

Data collection

Rigaku AFC 7R
diffractometer

Radiation source: rotating anode

Monochromator: graphite

$$T = 297(2) \text{ K}$$

ω - 2θ scans

Absorption correction: ψ scan

$$R_{\text{int}} = 0.016$$

$$\theta_{\text{max}} = 27.5^\circ$$

$$\theta_{\text{min}} = 2.5^\circ$$

$$h = -3 \rightarrow 7$$

$$k = 0 \rightarrow 25$$

$$l = -18 \rightarrow 18$$

supplementary materials

O43A	1.0527 (5)	0.09479 (17)	-0.3630 (2)	0.0403 (10)
O43B	0.6088 (6)	0.21186 (17)	0.3865 (2)	0.0389 (9)
C1A	0.7952 (7)	0.15078 (19)	-0.0464 (3)	0.0274 (10)
C1B	0.7699 (7)	0.1525 (2)	0.0539 (3)	0.0285 (10)
C2A	0.6400 (8)	0.1846 (3)	-0.1132 (3)	0.0459 (15)
C2B	0.5868 (9)	0.1849 (2)	0.0848 (3)	0.0427 (14)
C3A	0.6591 (9)	0.1809 (2)	-0.2069 (3)	0.0424 (15)
C3B	0.5603 (8)	0.1853 (2)	0.1778 (3)	0.0429 (15)
C4A	0.8342 (7)	0.14383 (19)	-0.2346 (2)	0.0253 (10)
C4B	0.7182 (7)	0.1511 (2)	0.2407 (3)	0.0273 (10)
C5A	0.9927 (8)	0.1114 (3)	-0.1700 (3)	0.0497 (16)
C5B	0.9036 (10)	0.1196 (4)	0.2123 (3)	0.065 (2)
C6A	0.9716 (9)	0.1150 (3)	-0.0765 (3)	0.0533 (18)
C6B	0.9281 (9)	0.1203 (4)	0.1193 (3)	0.066 (2)
O3W	0.3491 (11)	0.00000	0.2133 (3)	0.0608 (19)
O4W	0.4275 (14)	0.00000	0.0351 (5)	0.083 (2)
H2A	0.51870	0.20980	-0.09300	0.0550*
H2B	0.47780	0.20740	0.04090	0.0510*
H2W	0.34800	0.03900	0.44000	0.0420*
H3A	0.55160	0.20360	-0.25180	0.0500*
H3B	0.43380	0.20770	0.19790	0.0510*
H5A	1.11400	0.08620	-0.19020	0.0600*
H5B	1.01260	0.09710	0.25620	0.0780*
H6A	1.07910	0.09230	-0.03160	0.0640*
H6B	1.05460	0.09790	0.09920	0.0790*
H11W	0.35600	0.00000	0.88400	0.0960*
H12W	0.61400	0.00000	0.88400	0.0960*
H3W	0.39700	0.03850	0.25200	0.0730*
H41W	0.40200	0.00000	0.09400	0.0970*
H42W	0.57940	0.00000	0.03750	0.0970*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.0334 (4)	0.0286 (4)	0.0307 (3)	-0.0007 (4)	0.0082 (3)	0.0001 (4)
K2	0.0286 (6)	0.0346 (6)	0.0344 (6)	0.0000	0.0083 (5)	0.0000
K3	0.0357 (6)	0.0317 (5)	0.0325 (6)	0.0000	0.0076 (5)	0.0000
S4A	0.0243 (4)	0.0239 (4)	0.0174 (4)	0.0011 (3)	0.0058 (3)	0.0000 (3)
S4B	0.0310 (4)	0.0297 (4)	0.0166 (4)	-0.0042 (4)	0.0062 (3)	-0.0006 (3)
O1W	0.073 (4)	0.116 (6)	0.045 (3)	0.0000	-0.005 (3)	0.0000
O2W	0.038 (2)	0.036 (2)	0.035 (2)	0.0000	0.0147 (17)	0.0000
O41A	0.076 (2)	0.0276 (14)	0.0285 (14)	-0.0031 (16)	0.0174 (15)	0.0044 (11)
O41B	0.0383 (16)	0.0489 (17)	0.0230 (13)	0.0000 (14)	0.0020 (11)	0.0051 (12)
O42A	0.0328 (14)	0.0533 (18)	0.0267 (14)	-0.0133 (14)	0.0063 (11)	-0.0078 (12)
O42B	0.0453 (17)	0.0468 (19)	0.0302 (14)	-0.0183 (15)	0.0095 (13)	0.0004 (13)
O43A	0.0370 (16)	0.057 (2)	0.0279 (14)	0.0217 (15)	0.0085 (12)	0.0012 (13)
O43B	0.0518 (17)	0.0391 (16)	0.0277 (14)	0.0023 (14)	0.0120 (13)	-0.0056 (12)
C1A	0.0342 (19)	0.0320 (18)	0.0168 (15)	0.0031 (16)	0.0068 (14)	0.0009 (13)

supplementary materials

C1B	0.0317 (19)	0.0359 (19)	0.0181 (16)	0.0004 (16)	0.0041 (14)	-0.0003 (14)
C2A	0.051 (3)	0.069 (3)	0.0196 (17)	0.030 (2)	0.0114 (18)	0.0024 (18)
C2B	0.049 (2)	0.058 (3)	0.0222 (19)	0.024 (2)	0.0086 (17)	0.0073 (19)
C3A	0.049 (3)	0.059 (3)	0.0196 (18)	0.025 (2)	0.0071 (17)	0.0072 (17)
C3B	0.050 (3)	0.056 (3)	0.0252 (19)	0.025 (2)	0.0140 (18)	0.0019 (17)
C4A	0.0306 (18)	0.0305 (17)	0.0154 (15)	-0.0001 (15)	0.0057 (14)	-0.0018 (13)
C4B	0.0318 (19)	0.0332 (19)	0.0170 (16)	-0.0034 (15)	0.0041 (14)	-0.0016 (13)
C5A	0.044 (2)	0.084 (4)	0.0220 (18)	0.036 (3)	0.0079 (17)	0.001 (2)
C5B	0.061 (3)	0.116 (5)	0.0188 (19)	0.048 (3)	0.012 (2)	0.016 (2)
C6A	0.052 (3)	0.085 (4)	0.0229 (18)	0.037 (3)	0.0059 (18)	0.006 (2)
C6B	0.054 (3)	0.122 (5)	0.023 (2)	0.053 (3)	0.014 (2)	0.016 (3)
O3W	0.080 (4)	0.057 (3)	0.040 (3)	0.0000	-0.008 (3)	0.0000
O4W	0.091 (5)	0.104 (6)	0.055 (4)	0.0000	0.003 (4)	0.0000

Geometric parameters (\AA , $^\circ$)

K1—O43B	2.850 (4)	S4B—C4B	1.775 (4)
K1—O41B ⁱ	2.703 (3)	O1W—H12W	0.8300
K1—O41A ⁱⁱ	3.040 (4)	O1W—H11W	0.9700
K1—O43A ⁱⁱ	3.058 (3)	O2W—H2W ^{ix}	0.9600
K1—O42A ⁱⁱⁱ	2.866 (3)	O2W—H2W	0.9600
K1—O43B ^{iv}	2.739 (3)	O3W—H3W	0.9600
K1—O41A ^v	2.681 (3)	O3W—H3W ^{ix}	0.9600
K2—O1W	2.703 (6)	O4W—H41W	0.9000
K2—O2W	2.866 (5)	O4W—H42W	0.8800
K2—O43A ⁱⁱ	2.657 (3)	C1A—C6A	1.375 (7)
K2—O42A ⁱⁱⁱ	2.741 (3)	C1A—C2A	1.393 (6)
K2—O43A ^{vi}	2.657 (3)	C1A—C1B	1.497 (6)
K2—O42A ^{vii}	2.741 (3)	C1B—C2B	1.379 (6)
K3—O2W	3.079 (4)	C1B—C6B	1.376 (7)
K3—O41B	2.751 (3)	C2A—C3A	1.394 (6)
K3—O42B	3.076 (4)	C2B—C3B	1.392 (6)
K3—O42A ⁱⁱⁱ	2.938 (3)	C3A—C4A	1.367 (6)
K3—O43A ⁱⁱⁱ	3.027 (3)	C3B—C4B	1.373 (6)
K3—O2W ^{viii}	2.793 (4)	C4A—C5A	1.372 (6)
K3—O41B ^{ix}	2.751 (3)	C4B—C5B	1.366 (7)
K3—O42B ^{ix}	3.076 (4)	C5A—C6A	1.394 (6)
K3—O42A ^{vii}	2.938 (3)	C5B—C6B	1.389 (6)
K3—O43A ^{vii}	3.027 (3)	C2A—H2A	0.9500
S4A—O41A	1.450 (3)	C2B—H2B	0.9400
S4A—O42A	1.453 (3)	C3A—H3A	0.9500
S4A—O43A	1.455 (3)	C3B—H3B	0.9400
S4A—C4A	1.784 (3)	C5A—H5A	0.9500
S4B—O41B	1.454 (3)	C5B—H5B	0.9400
S4B—O42B	1.465 (4)	C6A—H6A	0.9500
S4B—O43B	1.446 (4)	C6B—H6B	0.9400

supplementary materials

O41B ⁱ —K1—O43B	110.25 (9)	O41B ^{ix} —K3—O42B ^{ix}	48.53 (9)
O41A ⁱⁱ —K1—O43B	160.66 (9)	O41B ^{ix} —K3—O42A ^{vii}	75.26 (9)
O43A ⁱⁱ —K1—O43B	152.59 (10)	O41B ^{ix} —K3—O43A ^{vii}	71.01 (8)
O42A ⁱⁱⁱ —K1—O43B	83.81 (9)	O42A ^{vii} —K3—O42B ^{ix}	72.09 (8)
O43B—K1—O43B ^{iv}	71.84 (10)	O42B ^{ix} —K3—O43A ^{vii}	103.14 (9)
O41A ^v —K1—O43B	95.63 (10)	O42A ^{vii} —K3—O43A ^{vii}	47.64 (8)
O41A ⁱⁱ —K1—O41B ⁱ	72.70 (9)	O41A—S4A—O42A	112.82 (19)
O41B ⁱ —K1—O43A ⁱⁱ	71.13 (9)	O41A—S4A—O43A	112.72 (19)
O41B ⁱ —K1—O42A ⁱⁱⁱ	118.54 (10)	O41A—S4A—C4A	106.33 (17)
O41B ⁱ —K1—O43B ^{iv}	80.84 (10)	O42A—S4A—O43A	111.95 (18)
O41A ^v —K1—O41B ⁱ	139.11 (11)	O42A—S4A—C4A	105.28 (17)
O41A ⁱⁱ —K1—O43A ⁱⁱ	46.73 (8)	O43A—S4A—C4A	107.12 (18)
O41A ⁱⁱ —K1—O42A ⁱⁱⁱ	112.09 (9)	K3—S4B—O41B	49.33 (13)
O41A ⁱⁱ —K1—O43B ^{iv}	90.23 (10)	K3—S4B—O42B	62.39 (13)
O41A ⁱⁱ —K1—O41A ^v	72.92 (10)	K3—S4B—O43B	129.77 (13)
O42A ⁱⁱⁱ —K1—O43A ⁱⁱ	72.58 (9)	K3—S4B—C4B	122.20 (14)
O43A ⁱⁱ —K1—O43B ^{iv}	133.53 (10)	O41B—S4B—O42B	111.53 (19)
O41A ^v —K1—O43A ⁱⁱ	99.88 (9)	O41B—S4B—O43B	114.83 (19)
O42A ⁱⁱⁱ —K1—O43B ^{iv}	153.45 (10)	O41B—S4B—C4B	105.87 (18)
O41A ^v —K1—O42A ⁱⁱⁱ	94.61 (10)	O42B—S4B—O43B	111.0 (2)
O41A ^v —K1—O43B ^{iv}	77.83 (9)	O42B—S4B—C4B	105.19 (18)
O1W—K2—O2W	178.76 (17)	O43B—S4B—C4B	107.79 (18)
O1W—K2—O43A ⁱⁱ	101.02 (12)	K2—O2W—K3	80.85 (11)
O1W—K2—O42A ⁱⁱⁱ	105.61 (11)	K2—O2W—K3 ⁱ	85.61 (12)
O1W—K2—O43A ^{vi}	101.02 (12)	K3—O2W—K3 ⁱ	166.45 (17)
O1W—K2—O42A ^{vii}	105.61 (11)	K1 ^x —O41A—S4A	99.57 (16)
O2W—K2—O43A ⁱⁱ	79.84 (9)	K1 ^{xi} —O41A—S4A	158.5 (2)
O2W—K2—O42A ⁱⁱⁱ	73.61 (8)	K1 ^x —O41A—K1 ^{xi}	85.21 (9)
O2W—K2—O43A ^{vi}	79.84 (9)	K3—O41B—S4B	107.04 (16)
O2W—K2—O42A ^{vii}	73.61 (8)	K1 ^{viii} —O41B—K3	111.44 (10)
O42A ⁱⁱⁱ —K2—O43A ⁱⁱ	81.09 (9)	K1 ^{viii} —O41B—S4B	133.48 (19)
O43A ⁱⁱ —K2—O43A ^{vi}	89.26 (10)	K1 ^{xii} —O42A—S4A	118.71 (18)
O42A ^{vii} —K2—O43A ⁱⁱ	152.93 (10)	K2 ^{xii} —O42A—S4A	132.77 (17)
O42A ⁱⁱⁱ —K2—O43A ^{vi}	152.93 (10)	K3 ^{xiii} —O42A—S4A	100.58 (15)
O42A ⁱⁱⁱ —K2—O42A ^{vii}	96.15 (10)	K1 ^{xii} —O42A—K2 ^{xii}	100.58 (10)
O42A ^{vii} —K2—O43A ^{vi}	81.09 (9)	K1 ^{xiii} —O42A—K3 ^{xii}	113.15 (10)
S4B—K3—O2W	78.47 (5)	K2 ^{xii} —O42A—K3 ^{xii}	85.52 (10)
S4B—K3—O41B	23.63 (6)	K3—O42B—S4B	92.65 (15)
S4B—K3—O42B	24.96 (7)	K3 ^{xiii} —O43A—S4A	96.74 (14)
S4B—K3—O42A ⁱⁱⁱ	70.87 (6)	K1 ^x —O43A—S4A	98.62 (15)
S4B—K3—O43A ⁱⁱⁱ	85.56 (6)	K2 ^x —O43A—S4A	163.26 (19)

supplementary materials

S4B—K3—O2W ^{viii}	94.10 (6)	K1 ^x —O43A—K3 ^{xii}	95.55 (9)
S4B—K3—S4B ^{ix}	111.64 (4)	K2 ^x —O43A—K3 ^{xii}	84.90 (9)
S4B—K3—O41B ^{ix}	121.69 (7)	K1 ^x —O43A—K2 ^x	97.79 (9)
S4B—K3—O42B ^{ix}	96.07 (7)	K1—O43B—S4B	104.92 (17)
S4B—K3—O42A ^{vii}	145.18 (7)	K1—O43B—K1 ^{xiii}	87.96 (9)
S4B—K3—O43A ^{vii}	160.55 (7)	K1 ^{xiii} —O43B—S4B	139.4 (2)
O2W—K3—O41B	101.53 (8)	H11W—O1W—H12W	113.00
O2W—K3—O42B	54.96 (9)	K2—O1W—H11W	117.00
O2W—K3—O42A ⁱⁱⁱ	67.86 (8)	K2—O1W—H12W	130.00
O2W—K3—O43A ⁱⁱⁱ	115.20 (9)	K2—O2W—H2W	111.00
O2W—K3—O2W ^{vii}	166.45 (13)	K3—O2W—H2W ^{ix}	65.00
S4B ^{ix} —K3—O2W	78.47 (5)	K2—O2W—H2W ^{ix}	111.00
O2W—K3—O41B ^{ix}	101.53 (8)	K3—O2W—H2W	65.00
O2W—K3—O42B ^{ix}	54.96 (9)	K3 ⁱ —O2W—H2W ^{ix}	121.00
O2W—K3—O42A ^{vii}	67.86 (8)	K3 ⁱ —O2W—H2W	121.00
O2W—K3—O43A ^{vii}	115.20 (9)	H2W—O2W—H2W ^{ix}	106.00
O41B—K3—O42B	48.53 (9)	H3W—O3W—H3W ^{ix}	104.00
O41B—K3—O42A ⁱⁱⁱ	75.26 (9)	H41W—O4W—H42W	106.00
O41B—K3—O43A ⁱⁱⁱ	71.01 (8)	C2A—C1A—C6A	117.2 (4)
O2W ^{viii} —K3—O41B	72.58 (8)	C1B—C1A—C6A	121.2 (4)
S4B ^{ix} —K3—O41B	121.69 (7)	C1B—C1A—C2A	121.6 (4)
O41B—K3—O41B ^{ix}	121.19 (10)	C1A—C1B—C6B	120.9 (4)
O41B—K3—O42B ^{ix}	113.82 (9)	C1A—C1B—C2B	122.1 (4)
O41B—K3—O42A ^{vii}	162.77 (10)	C2B—C1B—C6B	117.1 (4)
O41B—K3—O43A ^{vii}	138.51 (9)	C1A—C2A—C3A	121.4 (4)
O42A ⁱⁱⁱ —K3—O42B	72.09 (8)	C1B—C2B—C3B	122.1 (4)
O42B—K3—O43A ⁱⁱⁱ	103.14 (9)	C2A—C3A—C4A	119.8 (4)
O2W ^{viii} —K3—O42B	115.52 (10)	C2B—C3B—C4B	119.1 (4)
S4B ^{ix} —K3—O42B	96.07 (7)	S4A—C4A—C3A	119.6 (3)
O41B ^{ix} —K3—O42B	113.82 (9)	S4A—C4A—C5A	120.5 (3)
O42B—K3—O42B ^{ix}	75.45 (9)	C3A—C4A—C5A	119.9 (3)
O42A ^{vii} —K3—O42B	122.82 (10)	S4B—C4B—C3B	120.5 (3)
O42B—K3—O43A ^{vii}	169.11 (9)	S4B—C4B—C5B	119.5 (3)
O42A ⁱⁱⁱ —K3—O43A ⁱⁱⁱ	47.64 (8)	C3B—C4B—C5B	120.0 (4)
O2W ^{viii} —K3—O42A ⁱⁱⁱ	120.66 (8)	C4A—C5A—C6A	119.9 (4)
S4B ^{ix} —K3—O42A ⁱⁱⁱ	145.18 (7)	C4B—C5B—C6B	120.0 (5)
O41B ^{ix} —K3—O42A ⁱⁱⁱ	162.77 (10)	C1A—C6A—C5A	121.7 (5)
O42A ⁱⁱⁱ —K3—O42B ^{ix}	122.82 (10)	C1B—C6B—C5B	121.7 (5)
O42A ⁱⁱⁱ —K3—O42A ^{vii}	87.93 (9)	C1A—C2A—H2A	118.00
O42A ⁱⁱⁱ —K3—O43A ^{vii}	100.51 (9)	C3A—C2A—H2A	121.00
O2W ^{viii} —K3—O43A ⁱⁱⁱ	75.00 (9)	C1B—C2B—H2B	118.00

supplementary materials

S4B ^{ix} —K3—O43A ⁱⁱⁱ	160.55 (7)	C3B—C2B—H2B	120.00
O41B ^{ix} —K3—O43A ⁱⁱⁱ	138.51 (9)	C4A—C3A—H3A	119.00
O42B ^{ix} —K3—O43A ⁱⁱⁱ	169.11 (9)	C2A—C3A—H3A	121.00
O42A ^{vii} —K3—O43A ⁱⁱⁱ	100.51 (9)	C2B—C3B—H3B	121.00
O43A ⁱⁱⁱ —K3—O43A ^{vii}	76.15 (9)	C4B—C3B—H3B	120.00
S4B ^{ix} —K3—O2W ^{viii}	94.10 (6)	C4A—C5A—H5A	119.00
O2W ^{viii} —K3—O41B ^{ix}	72.58 (8)	C6A—C5A—H5A	121.00
O2W ^{viii} —K3—O42B ^{ix}	115.52 (10)	C6B—C5B—H5B	121.00
O2W ^{viii} —K3—O42A ^{vii}	120.66 (8)	C4B—C5B—H5B	119.00
O2W ^{viii} —K3—O43A ^{vii}	75.00 (9)	C1A—C6A—H6A	118.00
S4B ^{ix} —K3—O41B ^{ix}	23.63 (6)	C5A—C6A—H6A	120.00
S4B ^{ix} —K3—O42B ^{ix}	24.96 (7)	C5B—C6B—H6B	120.00
S4B ^{ix} —K3—O42A ^{vii}	70.87 (6)	C1B—C6B—H6B	118.00
S4B ^{ix} —K3—O43A ^{vii}	85.56 (6)		
O41B ⁱ —K1—O43B—S4B	-63.28 (18)	S4B—K3—O42A ⁱⁱⁱ —K1	36.28 (8)
O41B ⁱ —K1—O43B—K1 ^{xiii}	155.80 (9)	S4B—K3—O42A ⁱⁱⁱ —K2	135.88 (8)
O43A ⁱⁱ —K1—O43B—S4B	24.6 (3)	O2W—K3—O42A ⁱⁱⁱ —K1	-48.71 (11)
O43A ⁱⁱ —K1—O43B—K1 ^{xiii}	-116.35 (19)	O41B—K3—O42A ⁱⁱⁱ —K1	60.57 (11)
O42A ⁱⁱⁱ —K1—O43B—S4B	54.89 (16)	O41B—K3—O42A ⁱⁱⁱ —K2	160.18 (10)
O42A ⁱⁱⁱ —K1—O43B—K1 ^{xiii}	-86.03 (10)	O42B—K3—O42A ⁱⁱⁱ —K1	9.96 (11)
O43B ^{iv} —K1—O43B—S4B	-135.85 (18)	O42B—K3—O42A ⁱⁱⁱ —K2	109.57 (10)
O43B ^{iv} —K1—O43B—K1 ^{xiii}	83.23 (10)	S4B—K3—O42A ^{vii} —K2	-35.22 (15)
O41A ^v —K1—O43B—S4B	148.94 (16)	O42B—K3—O42A ^{vii} —K2	-51.07 (12)
O41A ^v —K1—O43B—K1 ^{xiii}	8.02 (10)	O42A—S4A—O41A—K1 ^x	-112.87 (16)
O43B—K1—O41B ⁱ —S4B ⁱ	-92.7 (2)	O42A—S4A—O41A—K1 ^{xi}	-11.5 (6)
O43B—K1—O43A ⁱⁱ —K2	10.8 (2)	O43A—S4A—O41A—K1 ^x	15.15 (19)
O43B—K1—O43A ⁱⁱ —S4A ⁱⁱ	-172.48 (16)	O43A—S4A—O41A—K1 ^{xi}	116.5 (5)
O43B—K1—O42A ⁱⁱⁱ —K2	-145.49 (11)	C4A—S4A—O41A—K1 ^x	132.23 (15)
O43B—K1—O42A ⁱⁱⁱ —K3	-55.87 (11)	C4A—S4A—O41A—K1 ^{xi}	-126.4 (5)
O43B—K1—O42A ⁱⁱⁱ —S4A ⁱⁱⁱ	61.65 (17)	O41A—S4A—O42A—K1 ^{xii}	-13.0 (2)
O43B—K1—O43B ^{iv} —K1 ^{iv}	-165.58 (11)	O41A—S4A—O42A—K2 ^{xii}	-155.4 (2)
O43B—K1—O43B ^{iv} —S4B ^{iv}	-54.9 (3)	O41A—S4A—O42A—K3 ^{xii}	110.94 (17)
O43B—K1—O41A ^v —S4A ^v	96.8 (5)	O43A—S4A—O42A—K1 ^{xii}	-141.42 (17)
O43B—K1—O41A ^v —K1 ^{xiii}	-7.24 (9)	O43A—S4A—O42A—K2 ^{xii}	76.2 (3)
O1W—K2—O43A ⁱⁱ —K1	125.43 (12)	O43A—S4A—O42A—K3 ^{xii}	-17.47 (19)
O2W—K2—O43A ⁱⁱ —K1	-53.67 (9)	C4A—S4A—O42A—K1 ^{xii}	102.53 (18)
O1W—K2—O42A ⁱⁱⁱ —K1	-121.86 (13)	C4A—S4A—O42A—K2 ^{xii}	-39.8 (3)
O2W—K2—O42A ⁱⁱⁱ —K1	59.14 (10)	C4A—S4A—O42A—K3 ^{xii}	-133.52 (14)
O2W—K3—S4B—O41B	167.29 (17)	O41A—S4A—O43A—K3 ^{xii}	-111.70 (15)
O2W—K3—S4B—O42B	-18.15 (16)	O41A—S4A—O43A—K1 ^x	-15.01 (18)

supplementary materials

O2W—K3—S4B—O43B	77.0 (2)	O42A—S4A—O43A—K3 ^{xii}	16.77 (18)
O2W—K3—S4B—C4B	-109.31 (18)	O42A—S4A—O43A—K1 ^x	113.45 (15)
O41B—K3—S4B—O42B	174.6 (2)	C4A—S4A—O43A—K3 ^{xii}	131.69 (15)
O41B—K3—S4B—O43B	-90.3 (2)	C4A—S4A—O43A—K1 ^x	-131.62 (15)
O41B—K3—S4B—C4B	83.4 (2)	O41A—S4A—C4A—C3A	59.0 (4)
O42B—K3—S4B—O41B	-174.6 (2)	O41A—S4A—C4A—C5A	-122.4 (4)
O42B—K3—S4B—O43B	95.2 (2)	O42A—S4A—C4A—C3A	-60.9 (4)
O42B—K3—S4B—C4B	-91.2 (2)	O42A—S4A—C4A—C5A	117.7 (4)
O42A ⁱⁱⁱ —K3—S4B—O41B	96.94 (16)	O43A—S4A—C4A—C3A	179.8 (3)
O42A ⁱⁱⁱ —K3—S4B—O42B	-88.50 (16)	O43A—S4A—C4A—C5A	-1.6 (4)
O42A ⁱⁱⁱ —K3—S4B—O43B	6.6 (2)	K3—S4B—O41B—K1 ^{viii}	-144.8 (3)
O42A ⁱⁱⁱ —K3—S4B—C4B	-179.66 (18)	O42B—S4B—O41B—K3	-5.2 (2)
O43A ⁱⁱⁱ —K3—S4B—O41B	50.45 (16)	O42B—S4B—O41B—K1 ^{viii}	-150.0 (2)
O43A ⁱⁱⁱ —K3—S4B—O42B	-135.00 (15)	O43B—S4B—O41B—K3	122.13 (18)
O43A ⁱⁱⁱ —K3—S4B—O43B	-39.9 (2)	O43B—S4B—O41B—K1 ^{viii}	-22.7 (3)
O43A ⁱⁱⁱ —K3—S4B—C4B	133.85 (17)	C4B—S4B—O41B—K3	-119.08 (16)
O2W ^{viii} —K3—S4B—O41B	-24.14 (17)	C4B—S4B—O41B—K1 ^{viii}	96.1 (2)
O2W ^{viii} —K3—S4B—O42B	150.41 (16)	O41B—S4B—O42B—K3	4.44 (17)
O2W ^{viii} —K3—S4B—O43B	-114.4 (2)	O43B—S4B—O42B—K3	-124.95 (15)
O2W ^{viii} —K3—S4B—C4B	59.26 (18)	C4B—S4B—O42B—K3	118.76 (15)
S4B ^{ix} —K3—S4B—O41B	-120.20 (16)	K3—S4B—O43B—K1	-44.0 (2)
S4B ^{ix} —K3—S4B—O42B	54.36 (14)	K3—S4B—O43B—K1 ^{xiii}	60.7 (3)
S4B ^{ix} —K3—S4B—O43B	149.50 (19)	O41B—S4B—O43B—K1	-100.68 (18)
S4B ^{ix} —K3—S4B—C4B	-36.80 (17)	O41B—S4B—O43B—K1 ^{xiii}	4.0 (3)
O41B ^{ix} —K3—S4B—O41B	-96.17 (17)	O42B—S4B—O43B—K1	26.9 (2)
O41B ^{ix} —K3—S4B—O42B	78.38 (16)	O42B—S4B—O43B—K1 ^{xiii}	131.6 (3)
O41B ^{ix} —K3—S4B—O43B	173.5 (2)	C4B—S4B—O43B—K1	141.61 (16)
O41B ^{ix} —K3—S4B—C4B	-12.77 (19)	C4B—S4B—O43B—K1 ^{xiii}	-113.7 (3)
O42B ^{ix} —K3—S4B—O41B	-140.37 (17)	K3—S4B—C4B—C3B	142.0 (3)
O42B ^{ix} —K3—S4B—O42B	34.19 (16)	K3—S4B—C4B—C5B	-36.5 (5)
O42B ^{ix} —K3—S4B—O43B	129.3 (2)	O41B—S4B—C4B—C3B	-166.4 (3)
O42B ^{ix} —K3—S4B—C4B	-56.97 (18)	O41B—S4B—C4B—C5B	15.1 (5)
O42A ^{vii} —K3—S4B—O41B	152.50 (19)	O42B—S4B—C4B—C3B	75.4 (4)
O42A ^{vii} —K3—S4B—O42B	-32.95 (18)	O42B—S4B—C4B—C5B	-103.1 (5)
O42A ^{vii} —K3—S4B—O43B	62.2 (2)	O43B—S4B—C4B—C3B	-43.0 (4)
O42A ^{vii} —K3—S4B—C4B	-124.1 (2)	O43B—S4B—C4B—C5B	138.5 (4)
S4B—K3—O2W—K2	-122.40 (3)	C2A—C1A—C1B—C2B	3.0 (6)
O41B—K3—O2W—K2	-117.24 (7)	C2A—C1A—C1B—C6B	-178.3 (5)
O42B—K3—O2W—K2	-131.64 (8)	C6A—C1A—C1B—C2B	-176.3 (4)
S4B—K3—O41B—K1 ^{viii}	153.3 (2)	C6A—C1A—C1B—C6B	2.5 (7)
O2W—K3—O41B—S4B	-12.71 (17)	C1B—C1A—C2A—C3A	-177.7 (4)
O2W—K3—O41B—K1 ^{viii}	140.62 (11)	C6A—C1A—C2A—C3A	1.6 (7)

supplementary materials

O42B—K3—O41B—S4B	3.06 (12)	C1B—C1A—C6A—C5A	178.1 (5)
O42B—K3—O41B—K1 ^{viii}	156.39 (16)	C2A—C1A—C6A—C5A	-1.2 (8)
O42A ⁱⁱⁱ —K3—O41B—S4B	-75.87 (15)	C1A—C1B—C2B—C3B	178.6 (4)
O43A ⁱⁱⁱ —K3—O41B—S4B	-125.62 (17)	C6B—C1B—C2B—C3B	-0.2 (7)
O2W ^{viii} —K3—O41B—S4B	154.69 (18)	C1A—C1B—C6B—C5B	-178.0 (6)
S4B ^{ix} —K3—O41B—S4B	70.76 (16)	C2B—C1B—C6B—C5B	0.8 (9)
O41B ^{ix} —K3—O41B—S4B	98.52 (16)	C1A—C2A—C3A—C4A	-0.5 (7)
O42B ^{ix} —K3—O41B—S4B	43.89 (18)	C1B—C2B—C3B—C4B	-1.5 (6)
O43A ^{vii} —K3—O41B—S4B	-165.15 (13)	C2A—C3A—C4A—S4A	177.5 (4)
O2W—K3—O42B—S4B	158.11 (18)	C2A—C3A—C4A—C5A	-1.1 (7)
O41B—K3—O42B—S4B	-2.91 (11)	C2B—C3B—C4B—S4B	-175.8 (3)
O42A ⁱⁱⁱ —K3—O42B—S4B	83.00 (14)	C2B—C3B—C4B—C5B	2.7 (7)
O43A ⁱⁱⁱ —K3—O42B—S4B	46.38 (15)	S4A—C4A—C5A—C6A	-177.1 (4)
O2W ^{viii} —K3—O42B—S4B	-33.08 (17)	C3A—C4A—C5A—C6A	1.5 (7)
S4B ^{ix} —K3—O42B—S4B	-130.57 (13)	S4B—C4B—C5B—C6B	176.4 (5)
O41B ^{ix} —K3—O42B—S4B	-114.34 (14)	C3B—C4B—C5B—C6B	-2.1 (9)
O42B ^{ix} —K3—O42B—S4B	-144.75 (16)	C4A—C5A—C6A—C1A	-0.3 (8)
O42A ^{vii} —K3—O42B—S4B	158.31 (12)	C4B—C5B—C6B—C1B	0.4 (10)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H11W \cdots O4W ⁱⁱⁱ	0.97	2.18	2.778 (9)	119
O2W—H2W \cdots O42B	0.96	1.91	2.840 (5)	162
O3W—H3W \cdots O42B	0.96	1.95	2.884 (5)	162
O4W—H41W \cdots O3W	0.90	1.82	2.715 (9)	180
O4W—H41W \cdots O3W	0.90	1.82	2.715 (9)	180
C5A—H5A \cdots O43A	0.95	2.50	2.916 (5)	106
C5B—H5B \cdots O41B	0.94	2.47	2.873 (5)	106

Symmetry codes: (iii) $x, y, z+1$.

Fig. 1

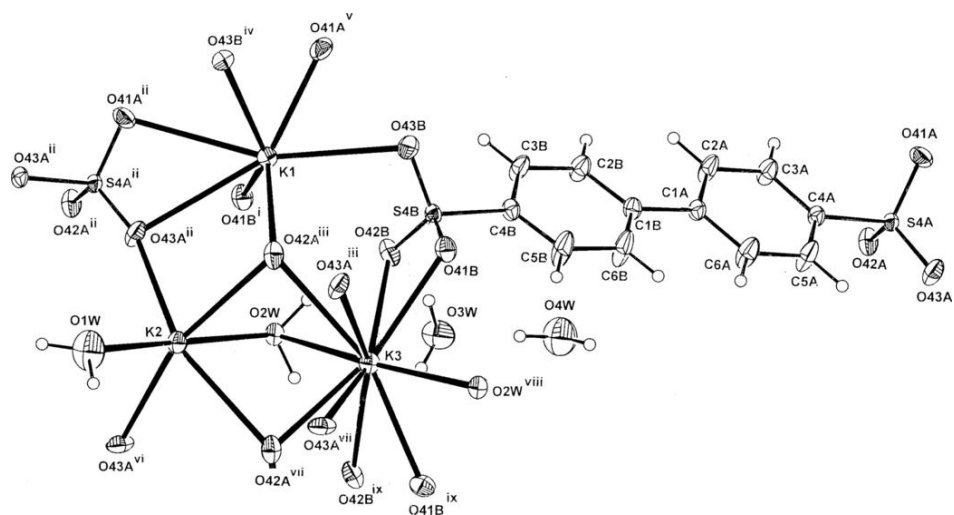


Fig. 2

