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Potassium decaborate monohydrate

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Key indicators: single-crystal X-ray study; T = 100 K; mean σ(B–O) = 0.004 Å; R factor = 0.045; wR factor = 0.113; data-to-parameter ratio = 10.6.

In the crystal structure of the title compound, $K_2[B_{10}O_{14}(OH)_4]\cdot H_2O$, the polyborate $[B_{10}O_{14}(OH)_4]^{2-}$ anions are linked together through their common O atoms, forming a helical chain-like structure. Adjacent chains are further connected into a three-dimensional structure by O—H···O hydrogen bonds. The water molecules and potassium cations are located between these chains. Further O—H···O hydrogen bonds occur between the anions and the water molecules

Related literature

For phases previously obtained in the $K_2O-B_2O_3-H_2O$ system, see: Marezio (1969); Marezio *et al.* (1963); Dewey *et al.* (1975); Salentine (1987); Touboul *et al.* (2003); Zhang *et al.* (2005); Wang *et al.* (2006); Li *et al.* (2007). For a closely related structure, $(NH_4)_2[B_{10}O_{14}(OH)_4]\cdot H_2O$, see: Li *et al.* (2003). For the non-linear optical properties of alkali metal borates, see: Mori *et al.* (1995).

Experimental

Crystal data

$K_2[B_{10}O_{14}(OH)_4]\cdot H_2O$
M_r = 496.35
Triclinic, $P\overline{1}$
a = 7.5612 (7) Å
b = 9.2236 (10) Å
c = 11.7298 (13) Å
α = 99.038 (6)°
β = 106.595 (6)°
γ = 91.314 (6)°
V = 772.26 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.72 mm^{-1}
T = 100 K
0.16 × 0.08 × 0.05 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: numerical (*SADABS*, Sheldrick, 2008*a*)
T_{min} = 0.895, T_{max} = 0.962
11219 measured reflections
3148 independent reflections
2141 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.113
S = 1.00
3148 reflections
298 parameters
5 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O11^{i}	0.88 (2)	1.76 (2)	2.599 (3)	159 (3)
O9—H9···O18^{ii}	0.87 (2)	1.98 (2)	2.797 (3)	157 (3)
O11—H11···O19^{iii}	0.92 (2)	1.65 (2)	2.553 (3)	167 (3)
O18—H18···O5^{iv}	0.89 (2)	2.10 (2)	2.940 (3)	157 (3)
O18—H18···O12^{iv}	0.89 (2)	2.66 (3)	3.193 (3)	119 (3)
O19—H19*A*···O6^{v}	0.90 (2)	1.79 (3)	2.678 (3)	169 (3)
O19—H19*B*···O16^{vi}	0.91 (2)	1.79 (3)	2.696 (3)	173 (3)

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008*b*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008*b*); molecular graphics: *SHELXTL* (Sheldrick, 2008*b*); 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: RU2014).

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supporting information

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S1. Comment

Boron can form many compounds because of the complexity of the structures involved. In the past several decades, much interest has focused on studies of alkali metals borates because some of these compounds show interesting physical properties, such as nonlinear optical behavior for $CsLiB_6O_{10}$ (Mori *et al.*, 1995). So far, several phases had been obtained in the K_2O—B_2O_3—H_2O system (Marezio *et al.*, 1963; Marezio, 1969; Dewey *et al.*, 1975; Salentine,1987; Touboul *et al.*, 2003; Zhang *et al.*, 2005; Wang *et al.*, 2006; Li *et al.*, 2007). In this paper, we describe the synthesis and the crystal structure of a new potassium borate of $K_2[B_{10}O_{14}(OH)_4]\cdot H_2O$.

Single crystal diffraction has revealed that the title compound crystallizes in the triclinic space group P-1. It is composed of two K_+ cation and polyborate anion $[B_{10}O_{14}(OH)_4]_{2-}$ (Fig.1), which is closely related to the reported compound of $(NH_4)_2[B_{10}O_{14}(OH)_4]\cdot H_2O$ (Li *et al.*, 2003).

The $[B_{10}O_{14}(OH)_4]_{2-}$ anion could be considered as two $[B_5O_7(OH)_2]_-$ cluster linked by the common oxygen atom (O3). Each of the $[B_5O_7(OH)_2]_-$ cluster consists of two six-membered rings linked by a common BO_4 tetrahedron. Each six-membered ring consists of one BO_3 triangle, one $BO_2(OH)$ triangle and a common BO_4 tetrahedron. The $[B_{10}O_{14}(OH)_4]_{2-}$ units are linked together through common oxygen atoms (O17) to neighboring units, forming a 1-D helical chainlike structure (Fig. 2). Adjacent chains are further connected into a three-dimensional structure by O—H···O hydrogen bonds interactions (Fig.3). Water molecules and potassium ions are located among these chains. In addition, there exist O—H···O hydrogen bonds between the oxygen atoms in polyborate anions and Water molecules (Table 1).

S2. Experimental

All reagents used in the synthesis were of analytic grade and were used without further purification. A mixture of K_2TeO_4 (0.216 g) and H_3BO_3 (0.992 g) was sealed in a teflon-lined bomb and heated at 473 K for 5 days and then cooled to room temperature. The resulting colorless and transparent crystals were recovered by washed with deionized water and dried at room temperature.

S3. Refinement

Hydroxyl and water H atoms were identified from a difference Fourier map and were included in with refined positional parameters.

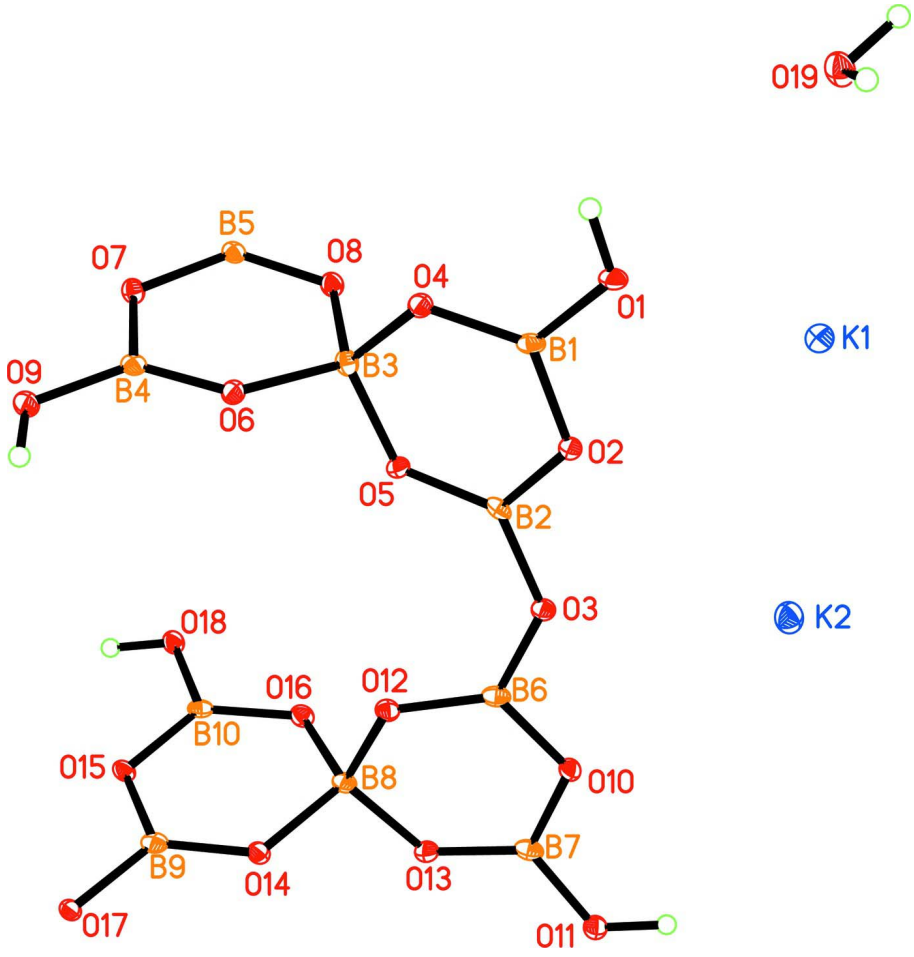

Figure 1

The asymmetric unit structure of title compound. Displacement ellipsoids are drawn at the 30% probability level.

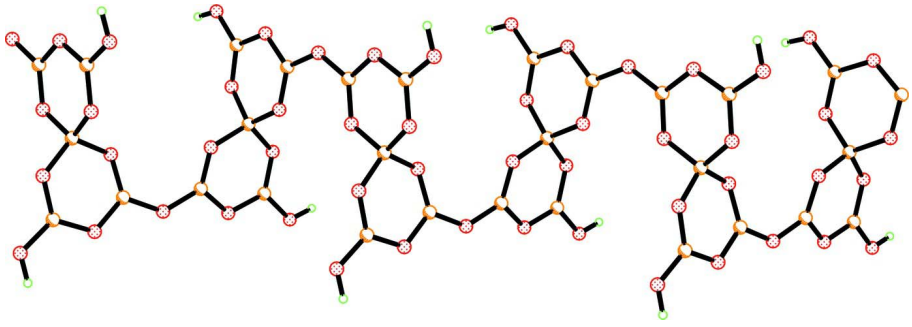

Figure 2

The one-dimensional chain structure constructed by $[B_{10}O_{14}(OH)_4]_{2-}$ units. B, O and H atoms are shown as yellow, red and green, respectively.

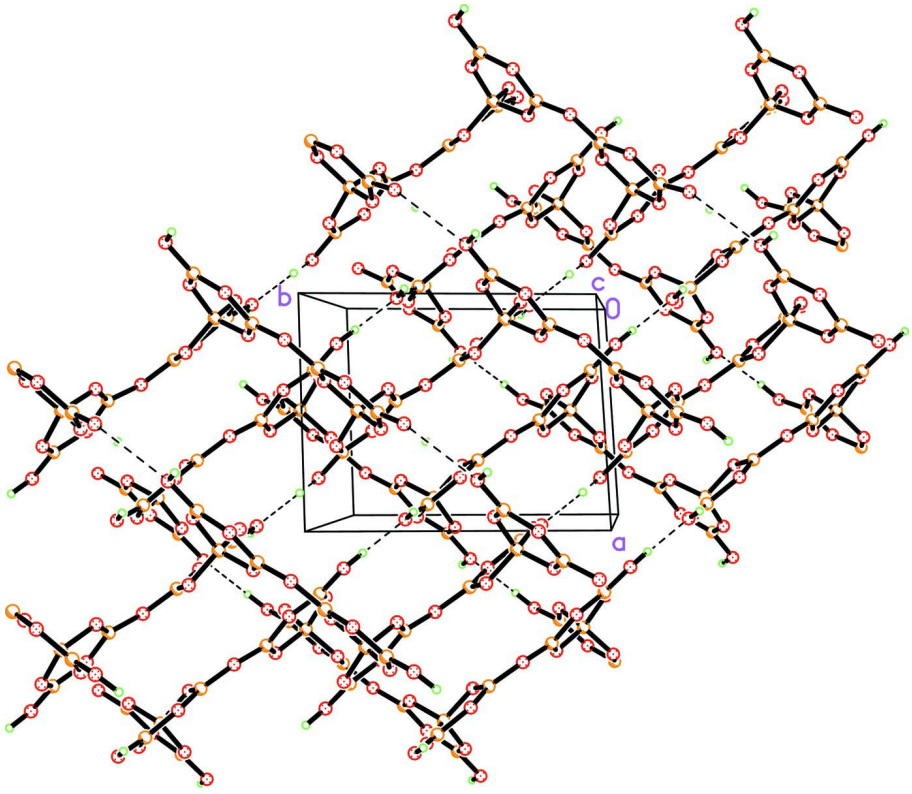

Figure 3

Packing View along the *c* axis of title compound, showing three-dimensional structure constructed by O—H···O hydrogen bonds, where all potassium cations are omitted for clarity. B, O and H atoms are shown as yellow, red and green, respectively.

(I)

Crystal data

$H_6B_{10}K_2O_{19}$
$M_r = 496.35$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.5612\ (7)$ Å
$b = 9.2236\ (10)$ Å
$c = 11.7298\ (13)$ Å
$\alpha = 99.038\ (6)°$
$\beta = 106.595\ (6)°$
$\gamma = 91.314\ (6)°$
$V = 772.26\ (14)$ Å^3
$Z = 2$
$F(000) = 492$
$D_x = 2.135$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1883 reflections
$\theta = 2.6–23.1°$
$\mu = 0.72$ mm^{-1}
$T = 100$ K
Rod, colorless
0.16 × 0.08 × 0.05 mm

Data collection

Bruker APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 83.33 pixels mm^{-1}
combination of ω and φ–scans
Absorption correction: numerical (*SADABS*, Sheldrick, 2008*a*)
$T_{min} = 0.895$, $T_{max} = 0.962$
11219 measured reflections
3148 independent reflections
2141 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$

θ_{max} = 26.5°, θ_{min} = 1.8°
h = −9→7
k = −11→11
l = −13→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.113
S = 1.00
3148 reflections
298 parameters
5 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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.
Hydroxyl and water H atoms were identified from a difference Fourier map and were included in with refined positional parameters. The thermal parameters of these H atoms were tied to that of the oxygen to which they are bonded. Mild O—H distances restraints were applied. All of the H atoms form good H-bonds to nearby O atoms.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
K1	0.02003 (11)	−0.04398 (8)	0.24158 (6)	0.0193 (2)
K2	0.57020 (11)	0.25524 (8)	0.28774 (7)	0.0228 (2)
O1	0.1964 (3)	−0.0442 (2)	0.46853 (19)	0.0157 (5)
H1	0.132 (4)	−0.108 (3)	0.492 (3)	0.019*
O2	0.4077 (3)	0.1569 (2)	0.51318 (18)	0.0135 (5)
O3	0.6155 (3)	0.3561 (2)	0.54323 (18)	0.0133 (5)
O4	0.3447 (3)	0.0566 (2)	0.67480 (18)	0.0137 (5)
O5	0.5940 (3)	0.2474 (2)	0.71450 (18)	0.0129 (5)
O6	0.4224 (3)	0.2380 (2)	0.85610 (18)	0.0135 (5)
O7	0.6184 (3)	0.1485 (2)	1.02546 (18)	0.0133 (5)
O8	0.6280 (3)	0.0473 (2)	0.82680 (18)	0.0137 (5)
O9	0.4452 (3)	0.3433 (2)	1.06130 (19)	0.0158 (5)
H9	0.372 (4)	0.410 (3)	1.037 (3)	0.019*
O10	0.8021 (3)	0.5425 (2)	0.51410 (18)	0.0142 (5)
O11	0.9851 (3)	0.7373 (2)	0.48289 (19)	0.0162 (5)
H11	0.948 (4)	0.698 (3)	0.4022 (17)	0.019*
O12	0.7542 (3)	0.5525 (2)	0.70700 (18)	0.0134 (5)
O13	0.9867 (3)	0.7205 (2)	0.67953 (18)	0.0148 (5)
O14	0.8285 (3)	0.7940 (2)	0.82488 (18)	0.0129 (5)
O15	0.9989 (3)	0.7625 (2)	1.02361 (18)	0.0131 (5)

O16	1.0478 (3)	0.6058 (2)	0.85501 (19)	0.0144 (5)
O17	0.7994 (3)	0.9505 (2)	1.00052 (18)	0.0122 (5)
O18	1.2111 (3)	0.5743 (2)	1.04997 (19)	0.0149 (5)
H18	1.247 (4)	0.615 (3)	1.1280 (17)	0.018*
O19	−0.0980 (4)	−0.3366 (3)	0.2539 (2)	0.0208 (6)
H19A	−0.213 (4)	−0.315 (4)	0.214 (3)	0.025*
H19B	−0.079 (5)	−0.424 (3)	0.213 (3)	0.025*
B1	0.3158 (5)	0.0559 (4)	0.5553 (3)	0.0130 (8)
B2	0.5436 (5)	0.2550 (4)	0.5960 (3)	0.0114 (8)
B3	0.4978 (5)	0.1472 (4)	0.7673 (3)	0.0133 (8)
B4	0.4912 (5)	0.2461 (4)	0.9766 (3)	0.0130 (8)
B5	0.6787 (5)	0.0482 (4)	0.9462 (3)	0.0126 (8)
B6	0.7263 (5)	0.4844 (4)	0.5928 (3)	0.0144 (8)
B7	0.9241 (5)	0.6669 (4)	0.5601 (3)	0.0145 (8)
B8	0.9041 (5)	0.6680 (4)	0.7659 (3)	0.0125 (8)
B9	0.8708 (5)	0.8327 (4)	0.9451 (3)	0.0139 (8)
B10	1.0838 (5)	0.6471 (4)	0.9752 (3)	0.0131 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K1	0.0252 (5)	0.0164 (4)	0.0155 (4)	−0.0002 (3)	0.0045 (3)	0.0032 (3)
K2	0.0245 (5)	0.0231 (4)	0.0189 (4)	0.0053 (3)	0.0034 (3)	0.0028 (3)
O1	0.0177 (14)	0.0115 (12)	0.0170 (12)	−0.0047 (10)	0.0038 (10)	0.0028 (9)
O2	0.0161 (13)	0.0119 (12)	0.0119 (11)	−0.0017 (10)	0.0038 (10)	0.0015 (9)
O3	0.0137 (13)	0.0117 (12)	0.0138 (11)	−0.0025 (10)	0.0036 (10)	0.0017 (9)
O4	0.0138 (13)	0.0139 (12)	0.0123 (12)	−0.0025 (10)	0.0025 (10)	0.0020 (9)
O5	0.0150 (13)	0.0118 (12)	0.0123 (11)	−0.0014 (10)	0.0044 (10)	0.0029 (9)
O6	0.0152 (13)	0.0134 (12)	0.0129 (12)	0.0023 (10)	0.0050 (10)	0.0031 (9)
O7	0.0124 (13)	0.0140 (12)	0.0136 (12)	0.0031 (10)	0.0040 (10)	0.0015 (9)
O8	0.0143 (13)	0.0132 (12)	0.0132 (12)	0.0028 (10)	0.0038 (10)	0.0016 (9)
O9	0.0181 (14)	0.0137 (12)	0.0169 (12)	0.0052 (10)	0.0065 (10)	0.0030 (10)
O10	0.0174 (14)	0.0122 (12)	0.0134 (12)	−0.0025 (10)	0.0065 (10)	0.0000 (9)
O11	0.0186 (14)	0.0148 (12)	0.0155 (12)	−0.0012 (10)	0.0061 (11)	0.0016 (10)
O12	0.0131 (13)	0.0116 (12)	0.0150 (12)	−0.0032 (9)	0.0045 (10)	0.0010 (9)
O13	0.0171 (14)	0.0125 (12)	0.0150 (12)	−0.0008 (10)	0.0048 (10)	0.0031 (9)
O14	0.0136 (13)	0.0116 (12)	0.0132 (12)	0.0015 (9)	0.0039 (10)	0.0014 (9)
O15	0.0136 (13)	0.0108 (12)	0.0141 (12)	0.0041 (10)	0.0028 (10)	0.0015 (9)
O16	0.0141 (13)	0.0128 (12)	0.0146 (12)	0.0021 (10)	0.0019 (10)	0.0017 (9)
O17	0.0135 (13)	0.0101 (11)	0.0126 (11)	0.0015 (9)	0.0037 (9)	0.0010 (9)
O18	0.0161 (14)	0.0143 (12)	0.0128 (12)	0.0027 (10)	0.0023 (10)	0.0013 (10)
O19	0.0255 (16)	0.0176 (13)	0.0182 (13)	0.0077 (12)	0.0048 (11)	0.0015 (10)
B1	0.012 (2)	0.0091 (18)	0.020 (2)	0.0032 (16)	0.0077 (17)	0.0047 (15)
B2	0.008 (2)	0.0087 (18)	0.018 (2)	0.0039 (15)	0.0052 (16)	−0.0012 (15)
B3	0.012 (2)	0.014 (2)	0.014 (2)	0.0037 (16)	0.0050 (16)	0.0009 (15)
B4	0.012 (2)	0.0109 (19)	0.017 (2)	−0.0034 (16)	0.0061 (16)	0.0010 (15)
B5	0.011 (2)	0.0112 (19)	0.016 (2)	−0.0019 (16)	0.0053 (16)	0.0002 (15)
B6	0.012 (2)	0.0109 (19)	0.020 (2)	0.0038 (16)	0.0038 (17)	0.0052 (16)

B7	0.010 (2)	0.0108 (19)	0.023 (2)	0.0028 (15)	0.0047 (17)	0.0036 (16)
B8	0.011 (2)	0.0099 (19)	0.016 (2)	−0.0008 (15)	0.0042 (16)	0.0014 (15)
B9	0.012 (2)	0.0108 (19)	0.020 (2)	−0.0033 (15)	0.0054 (16)	0.0030 (16)
B10	0.012 (2)	0.0094 (19)	0.017 (2)	−0.0020 (16)	0.0031 (16)	0.0034 (15)

Geometric parameters (Å, º)

K1—O1	2.615 (2)	O8—B5	1.341 (4)
K1—O17^{i}	2.835 (2)	O8—B3	1.469 (4)
K1—O15^{i}	2.841 (2)	O8—K1^{iii}	2.990 (2)
K1—O19	2.861 (3)	O8—K2^{iii}	3.052 (2)
K1—O14^{ii}	2.862 (2)	O9—B4	1.358 (4)
K1—O13^{ii}	2.988 (2)	O9—K2^{viii}	2.808 (2)
K1—O8^{iii}	2.990 (2)	O9—H9	0.865 (18)
K1—O4^{iv}	3.185 (2)	O10—B6	1.383 (4)
K1—B9^{i}	3.335 (4)	O10—B7	1.390 (4)
K1—B9^{ii}	3.402 (4)	O11—B7	1.366 (4)
K1—B8^{ii}	3.521 (4)	O11—H11	0.918 (18)
K1—B5^{iii}	3.589 (4)	O12—B6	1.342 (4)
K1—H1	2.97 (3)	O12—B8	1.472 (4)
K1—H19A	2.95 (4)	O12—K2^{ii}	3.069 (2)
K2—O9^{v}	2.808 (2)	O13—B7	1.350 (4)
K2—O3	2.913 (2)	O13—B8	1.468 (4)
K2—O14^{ii}	2.918 (2)	O13—K1^{ii}	2.988 (2)
K2—O4^{iii}	3.033 (2)	O13—K2^{vi}	3.260 (2)
K2—O8^{iii}	3.052 (2)	O14—B9	1.340 (4)
K2—O12^{ii}	3.069 (2)	O14—B8	1.469 (4)
K2—O7^{v}	3.205 (2)	O14—K1^{ii}	2.862 (2)
K2—O13^{vi}	3.260 (2)	O14—K2^{ii}	2.918 (2)
K2—B4^{v}	3.513 (4)	O15—B9	1.383 (4)
K2—B8^{ii}	3.568 (4)	O15—B10	1.385 (4)
K2—K1^{vii}	4.5268 (12)	O15—K1^{ix}	2.840 (2)
O1—B1	1.358 (4)	O16—B10	1.347 (4)
O1—H1	0.881 (18)	O16—B8	1.473 (4)
O2—B1	1.380 (4)	O17—B9	1.379 (4)
O2—B2	1.389 (4)	O17—B5^{x}	1.392 (4)
O3—B6	1.378 (4)	O17—K1^{ix}	2.835 (2)
O3—B2	1.378 (4)	O18—B10	1.370 (4)
O4—B1	1.355 (4)	O18—H18	0.892 (18)
O4—B3	1.473 (4)	O19—H19A	0.90 (2)
O4—K2^{iii}	3.033 (2)	O19—H19B	0.91 (2)
O4—K1^{iv}	3.185 (2)	B4—K2^{viii}	3.513 (4)
O5—B2	1.346 (4)	B5—O17^{xi}	1.392 (4)
O5—B3	1.474 (4)	B5—K1^{iii}	3.589 (4)
O6—B4	1.349 (4)	B8—K1^{ii}	3.521 (4)
O6—B3	1.483 (4)	B8—K2^{ii}	3.567 (4)
O7—B5	1.386 (4)	B9—K1^{ix}	3.335 (4)
O7—B4	1.396 (4)	B9—K1^{ii}	3.402 (4)

O7—K2^{viii}	3.205 (2)		
O1—K1—O17^{i}	174.90 (7)	B4^{v}—K2—B8^{ii}	85.73 (9)
O1—K1—O15^{i}	133.58 (7)	O9^{v}—K2—K1^{vii}	102.67 (5)
O17^{i}—K1—O15^{i}	48.29 (6)	O3—K2—K1^{vii}	110.21 (5)
O1—K1—O19	82.07 (7)	O14^{ii}—K2—K1^{vii}	128.57 (5)
O17^{i}—K1—O19	95.19 (7)	O4^{iii}—K2—K1^{vii}	44.62 (4)
O15^{i}—K1—O19	69.42 (7)	O8^{iii}—K2—K1^{vii}	74.44 (4)
O1—K1—O14^{ii}	106.78 (7)	O12^{ii}—K2—K1^{vii}	174.44 (5)
O17^{i}—K1—O14^{ii}	76.92 (6)	O7^{v}—K2—K1^{vii}	59.57 (4)
O15^{i}—K1—O14^{ii}	95.24 (6)	O13^{vi}—K2—K1^{vii}	41.24 (4)
O19—K1—O14^{ii}	163.93 (7)	B4^{v}—K2—K1^{vii}	82.73 (7)
O1—K1—O13^{ii}	84.58 (7)	B8^{ii}—K2—K1^{vii}	151.92 (6)
O17^{i}—K1—O13^{ii}	95.68 (6)	O9^{v}—K2—K1	95.28 (5)
O15^{i}—K1—O13^{ii}	137.05 (6)	O3—K2—K1	92.11 (5)
O19—K1—O13^{ii}	148.03 (7)	O14^{ii}—K2—K1	33.68 (4)
O14^{ii}—K1—O13^{ii}	47.83 (6)	O4^{iii}—K2—K1	68.36 (5)
O1—K1—O8^{iii}	92.13 (7)	O8^{iii}—K2—K1	37.13 (4)
O17^{i}—K1—O8^{iii}	92.85 (6)	O12^{ii}—K2—K1	69.44 (4)
O15^{i}—K1—O8^{iii}	65.98 (6)	O7^{v}—K2—K1	98.32 (4)
O19—K1—O8^{iii}	109.80 (7)	O13^{vi}—K2—K1	148.91 (4)
O14^{ii}—K1—O8^{iii}	57.44 (6)	B4^{v}—K2—K1	94.67 (6)
O13^{ii}—K1—O8^{iii}	99.57 (6)	B8^{ii}—K2—K1	47.09 (6)
O1—K1—O4^{iv}	85.11 (7)	K1^{vii}—K2—K1	108.49 (2)
O17^{i}—K1—O4^{iv}	89.86 (6)	B1—O1—K1	133.0 (2)
O15^{i}—K1—O4^{iv}	114.24 (6)	B1—O1—H1	118 (2)
O19—K1—O4^{iv}	67.25 (6)	K1—O1—H1	105 (2)
O14^{ii}—K1—O4^{iv}	125.91 (6)	B1—O2—B2	118.7 (3)
O13^{ii}—K1—O4^{iv}	82.81 (6)	B6—O3—B2	131.3 (3)
O8^{iii}—K1—O4^{iv}	176.19 (6)	B6—O3—K2	114.9 (2)
O1—K1—B9^{i}	157.71 (9)	B2—O3—K2	113.08 (18)
O17^{i}—K1—B9^{i}	24.12 (8)	B1—O4—B3	122.0 (3)
O15^{i}—K1—B9^{i}	24.22 (8)	B1—O4—K2^{iii}	105.55 (18)
O19—K1—B9^{i}	82.81 (8)	B3—O4—K2^{iii}	103.33 (17)
O14^{ii}—K1—B9^{i}	84.64 (8)	B1—O4—K1^{iv}	115.2 (2)
O13^{ii}—K1—B9^{i}	116.44 (8)	B3—O4—K1^{iv}	111.89 (18)
O8^{iii}—K1—B9^{i}	77.75 (8)	K2^{iii}—O4—K1^{iv}	93.40 (6)
O4^{iv}—K1—B9^{i}	103.92 (8)	B2—O5—B3	123.1 (3)
O1—K1—B9^{ii}	127.37 (8)	B4—O6—B3	123.6 (3)
O17^{i}—K1—B9^{ii}	56.94 (8)	B5—O7—B4	117.8 (3)
O15^{i}—K1—B9^{ii}	73.78 (8)	B5—O7—K2^{viii}	150.4 (2)
O19—K1—B9^{ii}	143.12 (8)	B4—O7—K2^{viii}	90.76 (18)
O14^{ii}—K1—B9^{ii}	22.67 (7)	B5—O8—B3	123.5 (3)
O13^{ii}—K1—B9^{ii}	65.68 (8)	B5—O8—K1^{iii}	105.5 (2)
O8^{iii}—K1—B9^{ii}	54.80 (8)	B3—O8—K1^{iii}	113.16 (19)
O4^{iv}—K1—B9^{ii}	129.01 (8)	B5—O8—K2^{iii}	105.48 (19)
B9^{i}—K1—B9^{ii}	62.00 (11)	B3—O8—K2^{iii}	102.58 (18)
O1—K1—B8^{ii}	98.97 (8)	K1^{iii}—O8—K2^{iii}	104.84 (6)

O17^{i}—K1—B8^{ii}	83.04 (7)	B4—O9—K2^{viii}	110.0 (2)
O15^{i}—K1—B8^{ii}	115.06 (8)	B4—O9—H9	118 (2)
O19—K1—B8^{ii}	170.63 (8)	K2^{viii}—O9—H9	131 (2)
O14^{ii}—K1—B8^{ii}	23.88 (7)	B6—O10—B7	117.7 (3)
O13^{ii}—K1—B8^{ii}	24.34 (7)	B7—O11—H11	118 (2)
O8^{iii}—K1—B8^{ii}	79.52 (8)	B6—O12—B8	122.0 (3)
O4^{iv}—K1—B8^{ii}	103.49 (7)	B6—O12—K2^{ii}	107.8 (2)
B9^{i}—K1—B8^{ii}	98.62 (9)	B8—O12—K2^{ii}	97.29 (18)
B9^{ii}—K1—B8^{ii}	41.76 (8)	B7—O13—B8	121.6 (3)
O1—K1—B5^{iii}	113.22 (8)	B7—O13—K1^{ii}	117.81 (19)
O17^{i}—K1—B5^{iii}	71.76 (7)	B8—O13—K1^{ii}	98.63 (17)
O15^{i}—K1—B5^{iii}	51.42 (7)	B7—O13—K2^{vi}	99.5 (2)
O19—K1—B5^{iii}	111.08 (8)	B8—O13—K2^{vi}	124.05 (19)
O14^{ii}—K1—B5^{iii}	53.30 (7)	K1^{ii}—O13—K2^{vi}	92.77 (6)
O13^{ii}—K1—B5^{iii}	100.87 (7)	B9—O14—B8	123.0 (3)
O8^{iii}—K1—B5^{iii}	21.09 (7)	B9—O14—K1^{ii}	101.92 (19)
O4^{iv}—K1—B5^{iii}	161.47 (7)	B8—O14—K1^{ii}	104.07 (18)
B9^{i}—K1—B5^{iii}	58.07 (9)	B9—O14—K2^{ii}	111.8 (2)
B9^{ii}—K1—B5^{iii}	41.61 (9)	B8—O14—K2^{ii}	103.88 (18)
B8^{ii}—K1—B5^{iii}	77.18 (8)	K1^{ii}—O14—K2^{ii}	111.90 (7)
O1—K1—H1	16.6 (4)	B9—O15—B10	118.2 (3)
O17^{i}—K1—H1	158.9 (5)	B9—O15—K1^{ix}	98.35 (19)
O15^{i}—K1—H1	128.2 (6)	B10—O15—K1^{ix}	142.67 (19)
O19—K1—H1	67.4 (5)	B10—O16—B8	123.4 (3)
O14^{ii}—K1—H1	122.9 (5)	B9—O17—B5^{x}	127.9 (3)
O13^{ii}—K1—H1	94.0 (6)	B9—O17—K1^{ix}	98.70 (19)
O8^{iii}—K1—H1	104.0 (6)	B5^{x}—O17—K1^{ix}	132.52 (19)
O4^{iv}—K1—H1	72.8 (6)	B10—O18—H18	116 (2)
B9^{i}—K1—H1	149.0 (5)	K1—O19—H19A	87 (2)
B9^{ii}—K1—H1	143.9 (5)	K1—O19—H19B	129 (2)
B8^{ii}—K1—H1	112.2 (5)	H19A—O19—H19B	106 (3)
B5^{iii}—K1—H1	124.6 (6)	O4—B1—O1	122.8 (3)
O1—K1—H19A	94.6 (6)	O4—B1—O2	122.0 (3)
O17^{i}—K1—H19A	81.8 (6)	O1—B1—O2	115.2 (3)
O15^{i}—K1—H19A	68.3 (7)	O5—B2—O3	125.8 (3)
O19—K1—H19A	17.8 (5)	O5—B2—O2	121.4 (3)
O14^{ii}—K1—H19A	158.6 (6)	O3—B2—O2	112.9 (3)
O13^{ii}—K1—H19A	138.3 (6)	O8—B3—O4	107.8 (3)
O8^{iii}—K1—H19A	122.1 (6)	O8—B3—O5	109.8 (3)
O4^{iv}—K1—H19A	55.7 (6)	O4—B3—O5	111.9 (3)
B9^{i}—K1—H19A	74.9 (6)	O8—B3—O6	110.3 (3)
B9^{ii}—K1—H19A	136.6 (6)	O4—B3—O6	109.0 (3)
B8^{ii}—K1—H19A	154.1 (5)	O5—B3—O6	108.0 (3)
B5^{iii}—K1—H19A	117.3 (7)	O6—B4—O9	125.4 (3)
H1—K1—H19A	78.5 (7)	O6—B4—O7	121.1 (3)
O9^{v}—K2—O3	141.92 (7)	O9—B4—O7	113.5 (3)
O9^{v}—K2—O14^{ii}	65.70 (6)	O6—B4—K2^{viii}	167.7 (2)
O3—K2—O14^{ii}	105.21 (6)	O9—B4—K2^{viii}	48.70 (16)

O9^{v}—K2—O4^{iii}	124.58 (6)	O7—B4—K2^{viii}	65.83 (16)
O3—K2—O4^{iii}	92.81 (6)	O8—B5—O7	122.7 (3)
O14^{ii}—K2—O4^{iii}	98.79 (6)	O8—B5—O17^{xi}	122.6 (3)
O9^{v}—K2—O8^{iii}	88.70 (6)	O7—B5—O17^{xi}	114.7 (3)
O3—K2—O8^{iii}	117.87 (6)	O8—B5—K1^{iii}	53.38 (16)
O14^{ii}—K2—O8^{iii}	56.20 (6)	O7—B5—K1^{iii}	138.7 (2)
O4^{iii}—K2—O8^{iii}	45.99 (6)	O17^{xi}—B5—K1^{iii}	83.00 (19)
O9^{v}—K2—O12^{ii}	72.67 (6)	O12—B6—O3	123.4 (3)
O3—K2—O12^{ii}	75.21 (6)	O12—B6—O10	121.7 (3)
O14^{ii}—K2—O12^{ii}	47.02 (6)	O3—B6—O10	114.8 (3)
O4^{iii}—K2—O12^{ii}	135.50 (6)	O13—B7—O11	118.4 (3)
O8^{iii}—K2—O12^{ii}	102.11 (6)	O13—B7—O10	122.2 (3)
O9^{v}—K2—O7^{v}	44.43 (6)	O11—B7—O10	119.4 (3)
O3—K2—O7^{v}	167.31 (6)	O13—B8—O14	107.9 (3)
O14^{ii}—K2—O7^{v}	87.46 (6)	O13—B8—O12	112.3 (3)
O4^{iii}—K2—O7^{v}	84.39 (6)	O14—B8—O12	108.8 (3)
O8^{iii}—K2—O7^{v}	68.47 (6)	O13—B8—O16	109.0 (3)
O12^{ii}—K2—O7^{v}	115.24 (6)	O14—B8—O16	111.0 (3)
O9^{v}—K2—O13^{vi}	98.63 (7)	O12—B8—O16	107.9 (3)
O3—K2—O13^{vi}	93.83 (6)	O13—B8—K1^{ii}	57.03 (15)
O14^{ii}—K2—O13^{vi}	160.94 (6)	O14—B8—K1^{ii}	52.05 (14)
O4^{iii}—K2—O13^{vi}	80.88 (6)	O12—B8—K1^{ii}	136.1 (2)
O8^{iii}—K2—O13^{vi}	115.44 (6)	O16—B8—K1^{ii}	115.82 (19)
O12^{ii}—K2—O13^{vi}	141.42 (6)	O13—B8—K2^{ii}	112.4 (2)
O7^{v}—K2—O13^{vi}	73.52 (6)	O14—B8—K2^{ii}	52.56 (15)
O9^{v}—K2—B4^{v}	21.30 (7)	O12—B8—K2^{ii}	58.56 (15)
O3—K2—B4^{v}	162.61 (8)	O16—B8—K2^{ii}	138.4 (2)
O14^{ii}—K2—B4^{v}	72.97 (8)	K1^{ii}—B8—K2^{ii}	85.00 (8)
O4^{iii}—K2—B4^{v}	104.57 (7)	O14—B9—O17	123.1 (3)
O8^{iii}—K2—B4^{v}	76.05 (7)	O14—B9—O15	122.4 (3)
O12^{ii}—K2—B4^{v}	92.23 (8)	O17—B9—O15	114.4 (3)
O7^{v}—K2—B4^{v}	23.41 (7)	O14—B9—K1^{ix}	172.8 (2)
O13^{vi}—K2—B4^{v}	88.60 (8)	O17—B9—K1^{ix}	57.17 (16)
O9^{v}—K2—B8^{ii}	71.35 (8)	O15—B9—K1^{ix}	57.43 (16)
O3—K2—B8^{ii}	87.22 (7)	O14—B9—K1^{ii}	55.40 (16)
O14^{ii}—K2—B8^{ii}	23.57 (7)	O17—B9—K1^{ii}	90.79 (19)
O4^{iii}—K2—B8^{ii}	115.36 (8)	O15—B9—K1^{ii}	123.9 (2)
O8^{iii}—K2—B8^{ii}	77.97 (7)	K1^{ix}—B9—K1^{ii}	118.00 (11)
O12^{ii}—K2—B8^{ii}	24.15 (7)	O16—B10—O18	118.4 (3)
O7^{v}—K2—B8^{ii}	105.18 (7)	O16—B10—O15	121.5 (3)
O13^{vi}—K2—B8^{ii}	163.68 (7)	O18—B10—O15	120.0 (3)
O1—K1—K2—O9^{v}	−171.23 (7)	B8^{ii}—K2—O3—B2	75.7 (2)
O17^{i}—K1—K2—O9^{v}	6.68 (7)	K1^{vii}—K2—O3—B2	−81.7 (2)
O15^{i}—K1—K2—O9^{v}	56.06 (7)	K1—K2—O3—B2	28.9 (2)
O19—K1—K2—O9^{v}	126.23 (9)	B3—O4—B1—O1	168.5 (3)
O14^{ii}—K1—K2—O9^{v}	−27.88 (9)	K2^{iii}—O4—B1—O1	51.4 (4)
O13^{ii}—K1—K2—O9^{v}	−81.77 (7)	K1^{iv}—O4—B1—O1	−50.1 (4)

O8^{iii}—K1—K2—O9^{v}	80.80 (8)	B3—O4—B1—O2	−10.9 (5)
O4^{iv}—K1—K2—O9^{v}	−105.08 (9)	K2^{iii}—O4—B1—O2	−128.0 (3)
B9^{i}—K1—K2—O9^{v}	31.46 (8)	K1^{iv}—O4—B1—O2	130.5 (3)
B9^{ii}—K1—K2—O9^{v}	−1.60 (10)	K1—O1—B1—O4	157.5 (2)
B8^{ii}—K1—K2—O9^{v}	−58.36 (9)	K1—O1—B1—O2	−23.0 (4)
B5^{iii}—K1—K2—O9^{v}	54.42 (9)	B2—O2—B1—O4	4.9 (5)
O1—K1—K2—O3	−28.62 (7)	B2—O2—B1—O1	−174.6 (3)
O17^{i}—K1—K2—O3	149.28 (6)	B3—O5—B2—O3	173.0 (3)
O15^{i}—K1—K2—O3	−161.33 (6)	B3—O5—B2—O2	−6.7 (5)
O19—K1—K2—O3	−91.17 (9)	B6—O3—B2—O5	−12.3 (6)
O14^{ii}—K1—K2—O3	114.72 (9)	K2—O3—B2—O5	156.9 (3)
O13^{ii}—K1—K2—O3	60.83 (6)	B6—O3—B2—O2	167.4 (3)
O8^{iii}—K1—K2—O3	−136.60 (8)	K2—O3—B2—O2	−23.3 (3)
O4^{iv}—K1—K2—O3	37.52 (9)	B1—O2—B2—O5	3.9 (4)
B9^{i}—K1—K2—O3	174.06 (8)	B1—O2—B2—O3	−175.8 (3)
B9^{ii}—K1—K2—O3	141.00 (10)	B5—O8—B3—O4	−123.3 (3)
B8^{ii}—K1—K2—O3	84.24 (9)	K1^{iii}—O8—B3—O4	107.5 (2)
B5^{iii}—K1—K2—O3	−162.98 (9)	K2^{iii}—O8—B3—O4	−4.9 (3)
O1—K1—K2—O14^{ii}	−143.35 (9)	B5—O8—B3—O5	114.5 (3)
O17^{i}—K1—K2—O14^{ii}	34.55 (9)	K1^{iii}—O8—B3—O5	−14.7 (3)
O15^{i}—K1—K2—O14^{ii}	83.94 (9)	K2^{iii}—O8—B3—O5	−127.1 (2)
O19—K1—K2—O14^{ii}	154.10 (11)	B5—O8—B3—O6	−4.4 (4)
O13^{ii}—K1—K2—O14^{ii}	−53.89 (9)	K1^{iii}—O8—B3—O6	−133.6 (2)
O8^{iii}—K1—K2—O14^{ii}	108.68 (10)	K2^{iii}—O8—B3—O6	114.0 (2)
O4^{iv}—K1—K2—O14^{ii}	−77.20 (10)	B1—O4—B3—O8	−113.3 (3)
B9^{i}—K1—K2—O14^{ii}	59.34 (10)	K2^{iii}—O4—B3—O8	5.0 (3)
B9^{ii}—K1—K2—O14^{ii}	26.28 (11)	K1^{iv}—O4—B3—O8	104.2 (2)
B8^{ii}—K1—K2—O14^{ii}	−30.49 (10)	B1—O4—B3—O5	7.6 (4)
B5^{iii}—K1—K2—O14^{ii}	82.30 (11)	K2^{iii}—O4—B3—O5	125.8 (2)
O1—K1—K2—O4^{iii}	63.57 (7)	K1^{iv}—O4—B3—O5	−134.9 (2)
O17^{i}—K1—K2—O4^{iii}	−118.53 (6)	B1—O4—B3—O6	126.9 (3)
O15^{i}—K1—K2—O4^{iii}	−69.14 (6)	K2^{iii}—O4—B3—O6	−114.8 (2)
O19—K1—K2—O4^{iii}	1.02 (9)	K1^{iv}—O4—B3—O6	−15.6 (3)
O14^{ii}—K1—K2—O4^{iii}	−153.08 (9)	B2—O5—B3—O8	120.7 (3)
O13^{ii}—K1—K2—O4^{iii}	153.02 (6)	B2—O5—B3—O4	1.0 (4)
O8^{iii}—K1—K2—O4^{iii}	−44.41 (8)	B2—O5—B3—O6	−118.9 (3)
O4^{iv}—K1—K2—O4^{iii}	129.71 (10)	B4—O6—B3—O8	11.5 (4)
B9^{i}—K1—K2—O4^{iii}	−93.75 (8)	B4—O6—B3—O4	129.8 (3)
B9^{ii}—K1—K2—O4^{iii}	−126.81 (10)	B4—O6—B3—O5	−108.5 (3)
B8^{ii}—K1—K2—O4^{iii}	176.43 (9)	B3—O6—B4—O9	169.7 (3)
B5^{iii}—K1—K2—O4^{iii}	−70.79 (9)	B3—O6—B4—O7	−11.6 (5)
O1—K1—K2—O8^{iii}	107.97 (9)	B3—O6—B4—K2^{viii}	−132.9 (10)
O17^{i}—K1—K2—O8^{iii}	−74.12 (8)	K2^{viii}—O9—B4—O6	166.1 (3)
O15^{i}—K1—K2—O8^{iii}	−24.74 (8)	K2^{viii}—O9—B4—O7	−12.7 (3)
O19—K1—K2—O8^{iii}	45.42 (10)	B5—O7—B4—O6	3.3 (5)
O14^{ii}—K1—K2—O8^{iii}	−108.68 (10)	K2^{viii}—O7—B4—O6	−168.5 (3)
O13^{ii}—K1—K2—O8^{iii}	−162.57 (8)	B5—O7—B4—O9	−177.9 (3)
O4^{iv}—K1—K2—O8^{iii}	174.12 (10)	K2^{viii}—O7—B4—O9	10.4 (3)

B9^{i}—K1—K2—O8^{iii}	−49.34 (9)	B5—O7—B4—K2^{viii}	171.7 (3)
B9^{ii}—K1—K2—O8^{iii}	−82.40 (11)	B3—O8—B5—O7	−2.9 (5)
B8^{ii}—K1—K2—O8^{iii}	−139.17 (10)	K1^{iii}—O8—B5—O7	129.4 (3)
B5^{iii}—K1—K2—O8^{iii}	−26.38 (10)	K2^{iii}—O8—B5—O7	−119.9 (3)
O1—K1—K2—O12^{ii}	−101.97 (7)	B3—O8—B5—O17^{xi}	178.6 (3)
O17^{i}—K1—K2—O12^{ii}	75.94 (6)	K1^{iii}—O8—B5—O17^{xi}	−49.1 (4)
O15^{i}—K1—K2—O12^{ii}	125.32 (6)	K2^{iii}—O8—B5—O17^{xi}	61.6 (3)
O19—K1—K2—O12^{ii}	−164.51 (9)	B3—O8—B5—K1^{iii}	−132.3 (3)
O14^{ii}—K1—K2—O12^{ii}	41.38 (8)	K2^{iii}—O8—B5—K1^{iii}	110.65 (13)
O13^{ii}—K1—K2—O12^{ii}	−12.51 (6)	B4—O7—B5—O8	3.9 (5)
O8^{iii}—K1—K2—O12^{ii}	150.06 (8)	K2^{viii}—O7—B5—O8	166.9 (2)
O4^{iv}—K1—K2—O12^{ii}	−35.82 (8)	B4—O7—B5—O17^{xi}	−177.5 (3)
B9^{i}—K1—K2—O12^{ii}	100.72 (8)	K2^{viii}—O7—B5—O17^{xi}	−14.5 (6)
B9^{ii}—K1—K2—O12^{ii}	67.66 (9)	B4—O7—B5—K1^{iii}	73.8 (4)
B8^{ii}—K1—K2—O12^{ii}	10.89 (9)	K2^{viii}—O7—B5—K1^{iii}	−123.2 (3)
B5^{iii}—K1—K2—O12^{ii}	123.68 (9)	B8—O12—B6—O3	165.6 (3)
O1—K1—K2—O7^{v}	144.12 (7)	K2^{ii}—O12—B6—O3	−83.5 (3)
O17^{i}—K1—K2—O7^{v}	−37.98 (6)	B8—O12—B6—O10	−17.2 (5)
O15^{i}—K1—K2—O7^{v}	11.41 (6)	K2^{ii}—O12—B6—O10	93.8 (3)
O19—K1—K2—O7^{v}	81.57 (9)	B2—O3—B6—O12	−15.1 (6)
O14^{ii}—K1—K2—O7^{v}	−72.53 (8)	K2—O3—B6—O12	175.8 (2)
O13^{ii}—K1—K2—O7^{v}	−126.43 (6)	B2—O3—B6—O10	167.5 (3)
O8^{iii}—K1—K2—O7^{v}	36.14 (8)	K2—O3—B6—O10	−1.6 (4)
O4^{iv}—K1—K2—O7^{v}	−149.74 (8)	B7—O10—B6—O12	6.3 (5)
B9^{i}—K1—K2—O7^{v}	−13.20 (8)	B7—O10—B6—O3	−176.2 (3)
B9^{ii}—K1—K2—O7^{v}	−46.26 (9)	B8—O13—B7—O11	169.1 (3)
B8^{ii}—K1—K2—O7^{v}	−103.02 (9)	K1^{ii}—O13—B7—O11	47.5 (4)
B5^{iii}—K1—K2—O7^{v}	9.76 (9)	K2^{vi}—O13—B7—O11	−50.7 (3)
O1—K1—K2—O13^{vi}	72.35 (10)	B8—O13—B7—O10	−11.6 (5)
O17^{i}—K1—K2—O13^{vi}	−109.75 (9)	K1^{ii}—O13—B7—O10	−133.2 (3)
O15^{i}—K1—K2—O13^{vi}	−60.36 (9)	K2^{vi}—O13—B7—O10	128.6 (3)
O19—K1—K2—O13^{vi}	9.80 (12)	B6—O10—B7—O13	8.2 (5)
O14^{ii}—K1—K2—O13^{vi}	−144.30 (11)	B6—O10—B7—O11	−172.5 (3)
O13^{ii}—K1—K2—O13^{vi}	161.81 (12)	B7—O13—B8—O14	−118.7 (3)
O8^{iii}—K1—K2—O13^{vi}	−35.62 (10)	K1^{ii}—O13—B8—O14	11.6 (3)
O4^{iv}—K1—K2—O13^{vi}	138.49 (10)	K2^{vi}—O13—B8—O14	110.9 (2)
B9^{i}—K1—K2—O13^{vi}	−84.97 (11)	B7—O13—B8—O12	1.2 (4)
B9^{ii}—K1—K2—O13^{vi}	−118.03 (12)	K1^{ii}—O13—B8—O12	131.5 (2)
B8^{ii}—K1—K2—O13^{vi}	−174.79 (12)	K2^{vi}—O13—B8—O12	−129.2 (2)
B5^{iii}—K1—K2—O13^{vi}	−62.00 (11)	B7—O13—B8—O16	120.7 (3)
O1—K1—K2—B4^{v}	167.40 (8)	K1^{ii}—O13—B8—O16	−109.0 (2)
O17^{i}—K1—K2—B4^{v}	−14.70 (8)	K2^{vi}—O13—B8—O16	−9.7 (3)
O15^{i}—K1—K2—B4^{v}	34.69 (8)	B7—O13—B8—K1^{ii}	−130.3 (3)
O19—K1—K2—B4^{v}	104.85 (10)	K2^{vi}—O13—B8—K1^{ii}	99.29 (16)
O14^{ii}—K1—K2—B4^{v}	−49.25 (10)	B7—O13—B8—K2^{ii}	−62.6 (3)
O13^{ii}—K1—K2—B4^{v}	−103.14 (8)	K1^{ii}—O13—B8—K2^{ii}	67.70 (15)
O8^{iii}—K1—K2—B4^{v}	59.43 (9)	K2^{vi}—O13—B8—K2^{ii}	166.99 (8)
O4^{iv}—K1—K2—B4^{v}	−126.46 (9)	B9—O14—B8—O13	−127.0 (3)

B9^{i}—K1—K2—B4^{v}	10.08 (9)	K1^{ii}—O14—B8—O13	−12.4 (3)
B9^{ii}—K1—K2—B4^{v}	−22.97 (11)	K2^{ii}—O14—B8—O13	104.9 (2)
B8^{ii}—K1—K2—B4^{v}	−79.74 (10)	B9—O14—B8—O12	110.9 (3)
B5^{iii}—K1—K2—B4^{v}	33.05 (10)	K1^{ii}—O14—B8—O12	−134.4 (2)
O1—K1—K2—B8^{ii}	−112.86 (10)	K2^{ii}—O14—B8—O12	−17.1 (3)
O17^{i}—K1—K2—B8^{ii}	65.04 (9)	B9—O14—B8—O16	−7.6 (4)
O15^{i}—K1—K2—B8^{ii}	114.43 (9)	K1^{ii}—O14—B8—O16	107.0 (2)
O19—K1—K2—B8^{ii}	−175.41 (11)	K2^{ii}—O14—B8—O16	−135.7 (2)
O14^{ii}—K1—K2—B8^{ii}	30.49 (10)	B9—O14—B8—K1^{ii}	−114.6 (3)
O13^{ii}—K1—K2—B8^{ii}	−23.40 (9)	K2^{ii}—O14—B8—K1^{ii}	117.26 (12)
O8^{iii}—K1—K2—B8^{ii}	139.17 (10)	B9—O14—B8—K2^{ii}	128.1 (3)
O4^{iv}—K1—K2—B8^{ii}	−46.71 (11)	K1^{ii}—O14—B8—K2^{ii}	−117.26 (12)
B9^{i}—K1—K2—B8^{ii}	89.82 (11)	B6—O12—B8—O13	12.9 (4)
B9^{ii}—K1—K2—B8^{ii}	56.77 (11)	K2^{ii}—O12—B8—O13	−103.4 (2)
B5^{iii}—K1—K2—B8^{ii}	112.79 (11)	B6—O12—B8—O14	132.3 (3)
O1—K1—K2—K1^{vii}	83.51 (6)	K2^{ii}—O12—B8—O14	15.9 (2)
O17^{i}—K1—K2—K1^{vii}	−98.58 (5)	B6—O12—B8—O16	−107.2 (3)
O15^{i}—K1—K2—K1^{vii}	−49.20 (5)	K2^{ii}—O12—B8—O16	136.4 (2)
O19—K1—K2—K1^{vii}	20.96 (9)	B6—O12—B8—K1^{ii}	77.9 (4)
O14^{ii}—K1—K2—K1^{vii}	−133.14 (8)	K2^{ii}—O12—B8—K1^{ii}	−38.4 (3)
O13^{ii}—K1—K2—K1^{vii}	172.97 (5)	B6—O12—B8—K2^{ii}	116.4 (3)
O8^{iii}—K1—K2—K1^{vii}	−24.46 (7)	B10—O16—B8—O13	127.4 (3)
O4^{iv}—K1—K2—K1^{vii}	149.66 (7)	B10—O16—B8—O14	8.7 (4)
B9^{i}—K1—K2—K1^{vii}	−73.80 (7)	B10—O16—B8—O12	−110.5 (3)
B9^{ii}—K1—K2—K1^{vii}	−106.86 (9)	B10—O16—B8—K1^{ii}	65.6 (3)
B8^{ii}—K1—K2—K1^{vii}	−163.63 (8)	B10—O16—B8—K2^{ii}	−48.0 (4)
B5^{iii}—K1—K2—K1^{vii}	−50.84 (8)	B8—O14—B9—O17	−179.7 (3)
O17^{i}—K1—O1—B1	−125.6 (7)	K1^{ii}—O14—B9—O17	64.6 (3)
O15^{i}—K1—O1—B1	125.2 (3)	K2^{ii}—O14—B9—O17	−55.1 (4)
O19—K1—O1—B1	176.7 (3)	B8—O14—B9—O15	4.2 (5)
O14^{ii}—K1—O1—B1	10.5 (3)	K1^{ii}—O14—B9—O15	−111.5 (3)
O13^{ii}—K1—O1—B1	−32.4 (3)	K2^{ii}—O14—B9—O15	128.9 (3)
O8^{iii}—K1—O1—B1	67.0 (3)	B8—O14—B9—K1^{ix}	90.4 (19)
O4^{iv}—K1—O1—B1	−115.6 (3)	K1^{ii}—O14—B9—K1^{ix}	−25 (2)
B9^{i}—K1—O1—B1	129.0 (3)	K2^{ii}—O14—B9—K1^{ix}	−145.0 (19)
B9^{ii}—K1—O1—B1	21.2 (3)	B8—O14—B9—K1^{ii}	115.7 (3)
B8^{ii}—K1—O1—B1	−12.7 (3)	K2^{ii}—O14—B9—K1^{ii}	−119.68 (15)
B5^{iii}—K1—O1—B1	67.1 (3)	B5^{x}—O17—B9—O14	−1.0 (5)
O9^{v}—K2—O3—B6	−58.7 (2)	K1^{ix}—O17—B9—O14	−171.4 (3)
O14^{ii}—K2—O3—B6	−128.5 (2)	B5^{x}—O17—B9—O15	175.3 (3)
O4^{iii}—K2—O3—B6	131.6 (2)	K1^{ix}—O17—B9—O15	4.9 (3)
O8^{iii}—K2—O3—B6	172.0 (2)	B5^{x}—O17—B9—K1^{ix}	170.3 (3)
O12^{ii}—K2—O3—B6	−91.9 (2)	B5^{x}—O17—B9—K1^{ii}	47.0 (3)
O7^{v}—K2—O3—B6	54.7 (4)	K1^{ix}—O17—B9—K1^{ii}	−123.35 (8)
O13^{vi}—K2—O3—B6	50.5 (2)	B10—O15—B9—O14	−0.8 (5)
B4^{v}—K2—O3—B6	−47.0 (4)	K1^{ix}—O15—B9—O14	171.4 (3)
B8^{ii}—K2—O3—B6	−113.1 (2)	B10—O15—B9—O17	−177.1 (3)
K1^{vii}—K2—O3—B6	89.4 (2)	K1^{ix}—O15—B9—O17	−4.9 (3)

K1—K2—O3—B6	−160.0 (2)	B10—O15—B9—K1^{ix}	−172.2 (3)
O9^{v}—K2—O3—B2	130.2 (2)	B10—O15—B9—K1^{ii}	−68.3 (3)
O14^{ii}—K2—O3—B2	60.3 (2)	K1^{ix}—O15—B9—K1^{ii}	103.98 (19)
O4^{iii}—K2—O3—B2	−39.5 (2)	B8—O16—B10—O18	175.3 (3)
O8^{iii}—K2—O3—B2	0.9 (2)	B8—O16—B10—O15	−6.3 (5)
O12^{ii}—K2—O3—B2	97.0 (2)	B9—O15—B10—O16	1.8 (5)
O7^{v}—K2—O3—B2	−116.4 (3)	K1^{ix}—O15—B10—O16	−165.4 (2)
O13^{vi}—K2—O3—B2	−120.6 (2)	B9—O15—B10—O18	−179.8 (3)
B4^{v}—K2—O3—B2	141.9 (3)	K1^{ix}—O15—B10—O18	13.0 (5)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O11^{xii}	0.88 (2)	1.76 (2)	2.599 (3)	159 (3)
O9—H9···O18^{xiii}	0.87 (2)	1.98 (2)	2.797 (3)	157 (3)
O11—H11···O19^{xiv}	0.92 (2)	1.65 (2)	2.553 (3)	167 (3)
O18—H18···O5^{xv}	0.89 (2)	2.10 (2)	2.940 (3)	157 (3)
O18—H18···O12^{xv}	0.89 (2)	2.66 (3)	3.193 (3)	119 (3)
O19—H19*A*···O6^{iv}	0.90 (2)	1.79 (3)	2.678 (3)	169 (3)
O19—H19*B*···O16^{iii}	0.91 (2)	1.79 (3)	2.696 (3)	173 (3)

Symmetry codes: (iii) −*x*+1, −*y*, −*z*+1; (iv) −*x*, −*y*, −*z*+1; (xii) *x*−1, *y*−1, *z*; (xiii) *x*−1, *y*, *z*; (xiv) *x*+1, *y*+1, *z*; (xv) −*x*+2, −*y*+1, −*z*+2.