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Potassium zinc borate, $KZnB_3O_6$

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Key indicators: single-crystal X-ray study; T = 93 K; mean σ(O–B) = 0.003 Å; R factor = 0.020; wR factor = 0.050; data-to-parameter ratio = 12.2.

The title compound, $KZnB_3O_6$ contains a remarkable $[B_6O_{12}]^{6-}$ group ($\overline{1}$ symmetry) formed by two rings linked by edge-sharing BO_4 tetrahedra, a feature that has only been observed previously under high pressure conditions. These borate groups are connected through distorted ZnO_4 tetrahedra in edge-shared pairs ($\overline{1}$ symmetry), forming a three-dimensional network whose cavities are filled by K^+ cations.

Related literature

For an independent determination of the title compound, see: Chen *et al.* (2010). For related structures, see: Chen *et al.* (2005); Emme & Huppertz (2003, 2004, 2005); Huppertz (2003); Huppertz & Emme (2004); Huppertz & von der Eltz (2002); Knyrim *et al.* (2007); Smith *et al.* (1992).

Experimental

Crystal data

$KZnB_3O_6$
M_r = 232.90
Triclinic, $P\overline{1}$
a = 6.7139 (13) Å
b = 6.9301 (14) Å
c = 7.0632 (14) Å
α = 63.12 (3)°
β = 72.02 (3)°
γ = 68.99 (3)°
V = 269.37 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 5.29 mm^{-1}
T = 93 K
0.50 × 0.30 × 0.20 mm

Data collection

Rigaku Saturn 724+ diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.480, T_{max} = 1.000
2707 measured reflections
1223 independent reflections
1118 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.050
S = 0.94
1223 reflections
100 parameters
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ATOMS* (Dowty, 1998); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MG2092).

References

Chen, X. L., Cai, G. M., Wan, W. Y., He, M., Jin, S. F. & Wang, S. C. (2010). *Angew Chem. Int. Ed.* DOI:10.1002/anie.200907075.
Chen, D.-G., Cheng, W.-D., Wu, D.-S., Zhang, H., Zhang, Y.-C., Gong, Y.-J. & Kan, Z.-G. (2005). *Solid State Sci.* **7**, 179–188.
Dowty, E. (1998). *ATOMS*. Shape Software, Kingsport, Tennessee, USA.
Emme, H. & Huppertz, H. (2003). *Chem. Eur. J.* **9**, 3623–3633.
Emme, H. & Huppertz, H. (2004). *Z. Anorg. Allg. Chem.* **630**, 2450–2457.
Emme, H. & Huppertz, H. (2005). *Acta Cryst.* C**61**, i29–i31.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Huppertz, H. (2003). *Z. Naturforsch. Teil B*, **58**, 278–290.
Huppertz, H. & Emme, H. (2004). *J. Phys. Condens. Matter*, **16**, S1283–S1290.
Huppertz, H. & von der Eltz, B. (2002). *J. Am. Chem. Soc.* **124**, 9376–9377.
Knyrim, J. S., Roessner, F., Jakob, S., Johrendt, D., Kinski, I., Glaum, R. & Huppertz, H. (2007). *Angew. Chem. Int. Ed.* **46**, 9097–9100.
Rigaku (2008). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Smith, R. W., Luce, J. L. & Keszler, D. A. (1992). *Inorg. Chem.* **31**, 4679–4682.

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supplementary materials

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Potassium zinc borate, $KZnB_3O_6$

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Comment

In efforts to identify new borates as optical materials or catalysts, investigations have been carried out in the K_2O–ZnO–B_2O_3 system, where only one quaternary compound so far, $KZn_4B_3O_9$, has been structurally characterized (Smith *et al.*, 1992; Chen *et al.*, 2005). Here, we report a new compound, $KZnB_3O_6$, with an unusual anion group. It is the first example of a borate prepared at ambient conditions that contains edge-sharing BO_4 tetrahedra, a feature that has only been previously found in high-pressure phases (Huppertz & von der Eltz, 2002; Huppertz, 2003; Huppertz & Emme, 2004; Emme & Huppertz, 2003, 2004, 2005; Knyrim *et al.*, 2007).

The structure consists of BO_3 triangles, BO_4 tetrahedra, and ZnO_4 tetrahedra linked to form a three-dimensional framework whose cavities are filled with K^+ cations in nine-coordinate environments (Fig. 1). The fundamental building block is a $[B_6O_{12}]^{6-}$ anion in which two six-membered rings formed by borate polyhedra are connected through a shared edge between two BO_4 tetrahedra (Fig. 2). Within the resulting B_2O_2 ring, the transannular B–B distance [2.080 (5) Å] is similar to those in HP-NiB_2O_4 [2.088 (2) Å] and $Dy_4B_6O_{15}$ [2.072 (8) Å] (Knyrim *et al.*, 2007; Huppertz & von der Eltz, 2002). The Raman spectrum of $KZnB_3O_6$ shows bands at 1319 and 1456 cm^{-1}, which lie in the range (about 1200 to 1450 cm^{-1}) expected for the Raman-active modes of edge-sharing BO_4 tetrahedra (Knyrim *et al.*, 2007). Two distorted ZnO_4 tetrahedra also share a common edge, similar to the case of $Zn_3B_2O_6$ (Chen *et al.*, 2005).

Experimental

A mixture of 7 mmol K_2CO_3, 10 mmol ZnO, and 43 mmol H_3BO_3 (all from Beijing Chemical Reagents Company) was heated to 1173 K in a platinum crucible. The transparent melt was cooled slowly from 1173 K to 1053 K at 1 K h^{-1}. Upon further cooling to room temperature, column-shaped colorless crystals were obtained.

Refinement

(type here to add refinement details)

Figures

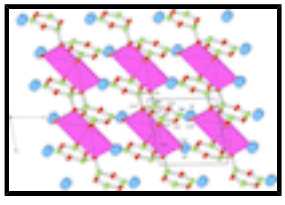

Fig. 1. $KZnB_3O_6$ viewed along b axis showing ZnO_4 tetrahedra (magenta) linked by BO_3 triangles and BO_4 tetrahedra, with K^+ cations (blue) located within the three-dimensional framework.

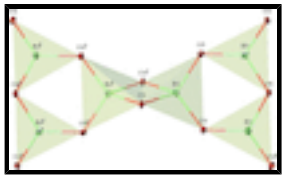

Fig. 2. $[B_6O_{12}]^{6-}$ anion, with displacement ellipsoids drawn at the 50% probability level. [Symmetry code: (i) -x, -y, -z.]

potassium zinc triborate

Crystal data

$KZnB_3O_6$	$Z = 2$
$M_r = 232.90$	$F(000) = 224$
Triclinic, $P\bar{1}$	$D_x = 2.871$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 6.7139$ (13) Å	Cell parameters from 1009 reflections
$b = 6.9301$ (14) Å	$\theta = 3.3$–$27.5°$
$c = 7.0632$ (14) Å	$\mu = 5.29$ mm^{-1}
$\alpha = 63.12$ (3)°	$T = 93$ K
$\beta = 72.02$ (3)°	Prism, colorless
$\gamma = 68.99$ (3)°	0.50 × 0.30 × 0.20 mm
$V = 269.37$ (12) Å^3	

Data collection

Rigaku Saturn 724+ diffractometer	1223 independent reflections
Radiation source: fine-focus sealed tube	1118 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.023$
ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -7 \rightarrow 8$
$T_{min} = 0.480$, $T_{max} = 1.000$	$k = -8 \rightarrow 9$
2707 measured reflections	$l = -9 \rightarrow 8$

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	Primary atom site location: structure-invariant direct methods
$R[F^2 > 2\sigma(F^2)] = 0.020$	Secondary atom site location: difference Fourier map
$wR(F^2) = 0.050$	$w = 1/[\sigma^2(F_o^2) + (0.030P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.94$	$(\Delta/\sigma)_{max} = 0.001$
1223 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
100 parameters	$\Delta\rho_{min} = -0.58$ e Å^{-3}

Special details

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

Refinement. 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}
K	0.25708 (8)	0.29494 (8)	0.57923 (7)	0.00606 (12)
Zn	0.67490 (4)	0.35335 (4)	0.12712 (4)	0.00346 (9)
B1	0.0964 (4)	0.9933 (4)	0.0944 (4)	0.0048 (5)
B2	0.2441 (4)	0.8171 (4)	0.4350 (4)	0.0050 (5)
B3	0.2977 (4)	0.1817 (4)	0.1685 (4)	0.0052 (5)
O1	0.8584 (2)	0.0829 (3)	0.0849 (2)	0.0046 (3)
O2	0.3702 (3)	0.3605 (3)	0.1211 (2)	0.0054 (3)
O3	0.1393 (3)	0.8112 (3)	0.2984 (2)	0.0055 (3)
O4	0.7213 (3)	0.3533 (3)	0.3794 (2)	0.0065 (3)
O5	0.1989 (3)	0.1716 (3)	0.0323 (2)	0.0056 (3)
O6	0.3232 (3)	0.0056 (3)	0.3678 (2)	0.0058 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
K	0.0064 (3)	0.0064 (2)	0.0060 (2)	−0.00214 (19)	−0.00063 (19)	−0.00281 (19)
Zn	0.00389 (15)	0.00353 (14)	0.00324 (14)	−0.00047 (10)	−0.00134 (10)	−0.00143 (10)
B1	0.0042 (12)	0.0045 (12)	0.0061 (11)	0.0002 (10)	−0.0021 (9)	−0.0027 (9)
B2	0.0038 (12)	0.0070 (12)	0.0047 (11)	−0.0002 (10)	−0.0002 (9)	−0.0041 (9)
B3	0.0027 (12)	0.0052 (12)	0.0061 (11)	0.0011 (10)	−0.0001 (9)	−0.0030 (9)
O1	0.0036 (8)	0.0068 (8)	0.0046 (7)	−0.0004 (6)	−0.0018 (6)	−0.0032 (6)
O2	0.0048 (8)	0.0056 (8)	0.0062 (7)	−0.0020 (6)	−0.0024 (6)	−0.0013 (6)
O3	0.0058 (8)	0.0053 (8)	0.0055 (7)	−0.0013 (6)	−0.0030 (6)	−0.0008 (6)
O4	0.0096 (9)	0.0056 (8)	0.0050 (7)	−0.0022 (7)	−0.0034 (6)	−0.0013 (6)
O5	0.0074 (8)	0.0052 (7)	0.0044 (7)	−0.0024 (6)	−0.0019 (6)	−0.0008 (6)
O6	0.0071 (8)	0.0059 (8)	0.0056 (7)	−0.0022 (7)	−0.0035 (6)	−0.0013 (6)

Geometric parameters (Å, °)

K—O4^{i}	2.6404 (16)	B1—B1^{viii}	2.080 (5)
K—O3^{ii}	2.7890 (18)	B1—K^{ii}	3.286 (3)
K—O1^{iii}	2.791 (2)	B1—K^{ix}	3.330 (3)

K—O6	2.8476 (17)	B2—O4^{i}	1.326 (3)
K—O5^{iv}	2.8491 (17)	B2—O3	1.380 (3)
K—O6^{iii}	2.856 (2)	B2—O6^{vi}	1.412 (3)
K—O2	2.9418 (17)	B2—K^{i}	3.135 (3)
K—O4	3.0888 (19)	B3—O2	1.357 (3)
K—B2^{i}	3.135 (3)	B3—O5	1.363 (3)
K—O3	3.144 (2)	B3—O6	1.395 (3)
K—B3	3.244 (3)	O1—B1^{v}	1.492 (3)
K—B2	3.261 (3)	O1—B1^{x}	1.503 (3)
Zn—O4	1.9013 (15)	O1—K^{iii}	2.791 (2)
Zn—O1	1.9347 (17)	O2—Zn^{v}	1.9628 (18)
Zn—O2^{v}	1.9628 (18)	O3—K^{ii}	2.7890 (18)
Zn—O2	2.0414 (16)	O4—B2^{i}	1.326 (3)
Zn—Zn^{v}	2.9584 (14)	O4—K^{i}	2.6404 (16)
B1—O3	1.450 (3)	O5—B1^{xi}	1.458 (3)
B1—O5^{vi}	1.458 (3)	O5—K^{xii}	2.8491 (17)
B1—O1^{v}	1.492 (3)	O6—B2^{xi}	1.412 (3)
B1—O1^{vii}	1.503 (3)	O6—K^{iii}	2.856 (2)
O4^{i}—K—O3^{ii}	119.60 (6)	O1—Zn—K^{iii}	41.67 (5)
O4^{i}—K—O1^{iii}	125.80 (5)	O2^{v}—Zn—K^{iii}	153.56 (5)
O3^{ii}—K—O1^{iii}	52.15 (6)	O2—Zn—K^{iii}	83.72 (6)
O4^{i}—K—O6	156.86 (5)	Zn^{v}—Zn—K^{iii}	121.23 (3)
O3^{ii}—K—O6	76.47 (5)	K—Zn—K^{iii}	75.71 (4)
O1^{iii}—K—O6	76.88 (5)	O4—Zn—K^{i}	32.09 (5)
O4^{i}—K—O5^{iv}	75.13 (5)	O1—Zn—K^{i}	131.51 (5)
O3^{ii}—K—O5^{iv}	81.16 (6)	O2^{v}—Zn—K^{i}	85.63 (5)
O1^{iii}—K—O5^{iv}	51.22 (5)	O2—Zn—K^{i}	118.91 (5)
O6—K—O5^{iv}	126.26 (5)	Zn^{v}—Zn—K^{i}	106.44 (3)
O4^{i}—K—O6^{iii}	103.77 (5)	K—Zn—K^{i}	75.22 (3)
O3^{ii}—K—O6^{iii}	127.90 (5)	K^{iii}—Zn—K^{i}	120.74 (2)
O1^{iii}—K—O6^{iii}	79.99 (6)	O3—B1—O5^{vi}	113.83 (19)
O6—K—O6^{iii}	73.35 (6)	O3—B1—O1^{v}	113.47 (18)
O5^{iv}—K—O6^{iii}	83.76 (6)	O5^{vi}—B1—O1^{v}	111.49 (18)
O4^{i}—K—O2	109.74 (5)	O3—B1—O1^{vii}	112.28 (18)
O3^{ii}—K—O2	101.75 (6)	O5^{vi}—B1—O1^{vii}	111.87 (19)
O1^{iii}—K—O2	124.46 (5)	O1^{v}—B1—O1^{vii}	92.02 (17)
O6—K—O2	47.88 (5)	O3—B1—B1^{viii}	124.0 (2)
O5^{iv}—K—O2	171.41 (5)	O5^{vi}—B1—B1^{viii}	122.1 (2)
O6^{iii}—K—O2	88.14 (6)	O1^{v}—B1—B1^{viii}	46.22 (12)
O4^{i}—K—O4	72.24 (6)	O1^{vii}—B1—B1^{viii}	45.79 (12)
O3^{ii}—K—O4	167.20 (5)	O3—B1—K^{ii}	57.50 (11)

O1^{iii}—K—O4	126.59 (6)	O5^{vi}—B1—K^{ii}	150.31 (15)
O6—K—O4	90.79 (5)	O1^{v}—B1—K^{ii}	97.21 (12)
O5^{iv}—K—O4	107.95 (5)	O1^{vii}—B1—K^{ii}	57.78 (10)
O6^{iii}—K—O4	46.94 (5)	B1^{viii}—B1—K^{ii}	72.83 (13)
O2—K—O4	67.96 (5)	O3—B1—K^{ix}	151.61 (16)
O4^{i}—K—B2^{i}	79.31 (7)	O5^{vi}—B1—K^{ix}	58.34 (11)
O3^{ii}—K—B2^{i}	154.09 (6)	O1^{v}—B1—K^{ix}	56.22 (10)
O1^{iii}—K—B2^{i}	103.00 (7)	O1^{vii}—B1—K^{ix}	95.19 (13)
O6—K—B2^{i}	91.80 (6)	B1^{viii}—B1—K^{ix}	70.52 (13)
O5^{iv}—K—B2^{i}	87.75 (7)	K^{ii}—B1—K^{ix}	143.35 (9)
O6^{iii}—K—B2^{i}	26.75 (5)	O4^{i}—B2—O3	121.2 (2)
O2—K—B2^{i}	86.28 (7)	O4^{i}—B2—O6^{vi}	120.5 (2)
O4—K—B2^{i}	24.59 (6)	O3—B2—O6^{vi}	118.2 (2)
O4^{i}—K—O3	47.12 (4)	O4^{i}—B2—K^{i}	75.76 (14)
O3^{ii}—K—O3	102.99 (5)	O3—B2—K^{i}	128.91 (16)
O1^{iii}—K—O3	150.43 (5)	O6^{vi}—B2—K^{i}	65.55 (12)
O6—K—O3	116.19 (5)	O4^{i}—B2—K	51.19 (11)
O5^{iv}—K—O3	116.19 (5)	O3—B2—K	72.85 (12)
O6^{iii}—K—O3	128.27 (5)	O6^{vi}—B2—K	158.31 (17)
O2—K—O3	71.27 (5)	K^{i}—B2—K	92.88 (8)
O4—K—O3	81.38 (6)	O2—B3—O5	122.7 (2)
B2^{i}—K—O3	102.92 (7)	O2—B3—O6	117.3 (2)
O4^{i}—K—B3	133.81 (6)	O5—B3—O6	119.95 (19)
O3^{ii}—K—B3	82.79 (6)	O2—B3—K	65.06 (11)
O1^{iii}—K—B3	100.12 (6)	O5—B3—K	149.00 (16)
O6—K—B3	25.42 (5)	O6—B3—K	61.19 (11)
O5^{iv}—K—B3	151.06 (6)	B1^{v}—O1—B1^{x}	87.98 (17)
O6^{iii}—K—B3	87.36 (6)	B1^{v}—O1—Zn	132.19 (14)
O2—K—B3	24.73 (5)	B1^{x}—O1—Zn	125.03 (13)
O4—K—B3	85.14 (6)	B1^{v}—O1—K^{iii}	97.40 (12)
B2^{i}—K—B3	96.54 (7)	B1^{x}—O1—K^{iii}	95.11 (12)
O3—K—B3	90.81 (6)	Zn—O1—K^{iii}	110.89 (7)
O4^{i}—K—B2	23.03 (5)	B3—O2—Zn^{v}	126.73 (15)
O3^{ii}—K—B2	117.32 (7)	B3—O2—Zn	126.50 (16)
O1^{iii}—K—B2	145.28 (6)	Zn^{v}—O2—Zn	95.24 (7)
O6—K—B2	136.67 (6)	B3—O2—K	90.21 (13)
O5^{iv}—K—B2	97.00 (6)	Zn^{v}—O2—K	126.87 (7)
O6^{iii}—K—B2	113.85 (6)	Zn—O2—K	87.73 (6)
O2—K—B2	88.87 (6)	B2—O3—B1	123.45 (18)
O4—K—B2	71.34 (6)	B2—O3—K^{ii}	124.93 (14)
B2^{i}—K—B2	87.12 (8)	B1—O3—K^{ii}	96.48 (13)

O3—K—B2	24.79 (5)	B2—O3—K	82.36 (13)
B3—K—B2	111.77 (7)	B1—O3—K	149.76 (13)
O4—Zn—O1	109.34 (7)	K^{ii}—O3—K	77.01 (5)
O4—Zn—$O2^{v}$	117.70 (7)	$B2^{i}$—O4—Zn	128.77 (15)
O1—Zn—$O2^{v}$	120.18 (7)	$B2^{i}$—O4—K^{i}	105.78 (13)
O4—Zn—O2	117.57 (7)	Zn—O4—K^{i}	125.42 (8)
O1—Zn—O2	104.70 (7)	$B2^{i}$—O4—K	79.65 (13)
$O2^{v}$—Zn—O2	84.76 (7)	Zn—O4—K	86.04 (6)
O4—Zn—Zn^{v}	128.89 (6)	K^{i}—O4—K	107.76 (6)
O1—Zn—Zn^{v}	120.57 (5)	B3—O5—$B1^{xi}$	122.58 (18)
$O2^{v}$—Zn—Zn^{v}	43.41 (5)	B3—O5—K^{xii}	136.44 (13)
O2—Zn—Zn^{v}	41.35 (5)	$B1^{xi}$—O5—K^{xii}	95.84 (12)
O4—Zn—K	61.28 (5)	B3—O6—$B2^{xi}$	121.34 (18)
O1—Zn—K	117.35 (6)	B3—O6—K	93.39 (12)
$O2^{v}$—Zn—K	116.70 (6)	$B2^{xi}$—O6—K	130.47 (13)
O2—Zn—K	56.78 (5)	B3—O6—K^{iii}	118.51 (14)
Zn^{v}—Zn—K	85.42 (3)	$B2^{xi}$—O6—K^{iii}	87.70 (14)
O4—Zn—K^{iii}	88.71 (6)	K—O6—K^{iii}	106.65 (6)
$O4^{i}$—K—Zn—O4	50.46 (9)	K^{iii}—Zn—O2—Zn^{v}	−156.16 (5)
$O3^{ii}$—K—Zn—O4	−170.08 (8)	K^{i}—Zn—O2—Zn^{v}	82.07 (6)
$O1^{iii}$—K—Zn—O4	−95.13 (8)	O4—Zn—O2—K	−8.22 (8)
O6—K—Zn—O4	−137.47 (7)	O1—Zn—O2—K	113.32 (6)
$O5^{iv}$—K—Zn—O4	−19.56 (8)	$O2^{v}$—Zn—O2—K	−126.83 (7)
$O6^{iii}$—K—Zn—O4	−53.81 (7)	Zn^{v}—Zn—O2—K	−126.83 (7)
O2—K—Zn—O4	171.69 (8)	K^{iii}—Zn—O2—K	77.02 (5)
$B2^{i}$—K—Zn—O4	−23.73 (8)	K^{i}—Zn—O2—K	−44.76 (6)
O3—K—Zn—O4	95.11 (7)	$O4^{i}$—K—O2—B3	−168.31 (13)
B3—K—Zn—O4	−163.59 (8)	$O3^{ii}$—K—O2—B3	−40.67 (14)
B2—K—Zn—O4	70.13 (8)	$O1^{iii}$—K—O2—B3	11.21 (15)
$O4^{i}$—K—Zn—O1	148.61 (6)	O6—K—O2—B3	18.64 (13)
$O3^{ii}$—K—Zn—O1	−71.93 (8)	$O6^{iii}$—K—O2—B3	87.72 (14)
$O1^{iii}$—K—Zn—O1	3.02 (9)	O4—K—O2—B3	131.35 (14)
O6—K—Zn—O1	−39.32 (6)	$B2^{i}$—K—O2—B3	114.45 (14)
$O5^{iv}$—K—Zn—O1	78.59 (8)	O3—K—O2—B3	−140.57 (14)
$O6^{iii}$—K—Zn—O1	44.34 (6)	B2—K—O2—B3	−158.37 (14)
O2—K—Zn—O1	−90.16 (8)	$O4^{i}$—K—O2—Zn^{v}	−29.68 (10)
O4—K—Zn—O1	98.15 (8)	$O3^{ii}$—K—O2—Zn^{v}	97.96 (9)
$B2^{i}$—K—Zn—O1	74.42 (8)	$O1^{iii}$—K—O2—Zn^{v}	149.85 (8)
O3—K—Zn—O1	−166.75 (6)	O6—K—O2—Zn^{v}	157.27 (11)
B3—K—Zn—O1	−65.44 (8)	$O6^{iii}$—K—O2—Zn^{v}	−133.65 (9)
B2—K—Zn—O1	168.27 (7)	O4—K—O2—Zn^{v}	−90.02 (9)

O4^{i}—K—Zn—O2^{v}	−58.07 (6)	B2^{i}—K—O2—Zn^{v}	−106.92 (10)
O3^{ii}—K—Zn—O2^{v}	81.39 (8)	O3—K—O2—Zn^{v}	−1.94 (7)
O1^{iii}—K—Zn—O2^{v}	156.34 (7)	B3—K—O2—Zn^{v}	138.63 (18)
O6—K—Zn—O2^{v}	114.00 (6)	B2—K—O2—Zn^{v}	−19.73 (9)
O5^{iv}—K—Zn—O2^{v}	−128.09 (7)	O4^{i}—K—O2—Zn	65.17 (7)
O6^{iii}—K—Zn—O2^{v}	−162.34 (6)	O3^{ii}—K—O2—Zn	−167.19 (5)
O2—K—Zn—O2^{v}	63.16 (9)	O1^{iii}—K—O2—Zn	−115.30 (6)
O4—K—Zn—O2^{v}	−108.53 (8)	O6—K—O2—Zn	−107.88 (8)
B2^{i}—K—Zn—O2^{v}	−132.26 (8)	O6^{iii}—K—O2—Zn	−38.80 (5)
O3—K—Zn—O2^{v}	−13.42 (6)	O4—K—O2—Zn	4.83 (5)
B3—K—Zn—O2^{v}	87.88 (8)	B2^{i}—K—O2—Zn	−12.07 (6)
B2—K—Zn—O2^{v}	−38.41 (7)	O3—K—O2—Zn	92.91 (6)
O4^{i}—K—Zn—O2	−121.23 (7)	B3—K—O2—Zn	−126.52 (15)
O3^{ii}—K—Zn—O2	18.23 (7)	B2—K—O2—Zn	75.12 (7)
O1^{iii}—K—Zn—O2	93.19 (8)	O4^{i}—B2—O3—B1	179.7 (2)
O6—K—Zn—O2	50.85 (7)	O6^{vi}—B2—O3—B1	−3.2 (3)
O5^{iv}—K—Zn—O2	168.75 (8)	K^{i}—B2—O3—B1	−83.4 (3)
O6^{iii}—K—Zn—O2	134.50 (6)	K—B2—O3—B1	−162.96 (19)
O4—K—Zn—O2	−171.69 (8)	O4^{i}—B2—O3—K^{ii}	50.9 (3)
B2^{i}—K—Zn—O2	164.58 (8)	O6^{vi}—B2—O3—K^{ii}	−132.00 (17)
O3—K—Zn—O2	−76.58 (7)	K^{i}—B2—O3—K^{ii}	147.80 (11)
B3—K—Zn—O2	24.72 (8)	K—B2—O3—K^{ii}	68.26 (12)
B2—K—Zn—O2	−101.56 (8)	O4^{i}—B2—O3—K	−17.4 (2)
O4^{i}—K—Zn—Zn^{v}	−89.18 (4)	O6^{vi}—B2—O3—K	159.7 (2)
O3^{ii}—K—Zn—Zn^{v}	50.27 (6)	K^{i}—B2—O3—K	79.54 (16)
O1^{iii}—K—Zn—Zn^{v}	125.23 (5)	O5^{vi}—B1—O3—B2	7.7 (3)
O6—K—Zn—Zn^{v}	82.89 (4)	O1^{v}—B1—O3—B2	136.6 (2)
O5^{iv}—K—Zn—Zn^{v}	−159.20 (5)	O1^{vii}—B1—O3—B2	−120.7 (2)
O6^{iii}—K—Zn—Zn^{v}	166.54 (4)	B1^{viii}—B1—O3—B2	−171.5 (2)
O2—K—Zn—Zn^{v}	32.04 (5)	K^{ii}—B1—O3—B2	−140.0 (2)
O4—K—Zn—Zn^{v}	−139.64 (6)	K^{ix}—B1—O3—B2	74.7 (4)
B2^{i}—K—Zn—Zn^{v}	−163.37 (6)	O5^{vi}—B1—O3—K^{ii}	147.63 (16)
O3—K—Zn—Zn^{v}	−44.54 (4)	O1^{v}—B1—O3—K^{ii}	−83.43 (18)
B3—K—Zn—Zn^{v}	56.77 (6)	O1^{vii}—B1—O3—K^{ii}	19.24 (17)
B2—K—Zn—Zn^{v}	−69.52 (6)	B1^{viii}—B1—O3—K^{ii}	−31.5 (3)
O4^{i}—K—Zn—K^{iii}	146.95 (4)	K^{ix}—B1—O3—K^{ii}	−145.3 (3)
O3^{ii}—K—Zn—K^{iii}	−73.59 (6)	O5^{vi}—B1—O3—K	−137.1 (2)
O1^{iii}—K—Zn—K^{iii}	1.37 (4)	O1^{v}—B1—O3—K	−8.2 (4)
O6—K—Zn—K^{iii}	−40.97 (4)	O1^{vii}—B1—O3—K	94.5 (3)
O5^{iv}—K—Zn—K^{iii}	76.93 (6)	B1^{viii}—B1—O3—K	43.7 (4)
O6^{iii}—K—Zn—K^{iii}	42.68 (4)	K^{ii}—B1—O3—K	75.3 (2)

O2—K—Zn—K^{iii}	−91.82 (6)	K^{ix}—B1—O3—K	−70.0 (4)
O4—K—Zn—K^{iii}	96.49 (6)	O4^{i}—K—O3—B2	10.06 (12)
B2^{i}—K—Zn—K^{iii}	72.76 (7)	O3^{ii}—K—O3—B2	128.59 (13)
O3—K—Zn—K^{iii}	−168.40 (3)	O1^{iii}—K—O3—B2	98.98 (15)
B3—K—Zn—K^{iii}	−67.10 (6)	O6—K—O3—B2	−150.28 (12)
B2—K—Zn—K^{iii}	166.62 (5)	O5^{iv}—K—O3—B2	42.17 (13)
O4^{i}—K—Zn—K^{i}	19.17 (4)	O6^{iii}—K—O3—B2	−61.35 (14)
O3^{ii}—K—Zn—K^{i}	158.63 (6)	O2—K—O3—B2	−133.21 (13)
O1^{iii}—K—Zn—K^{i}	−126.42 (5)	O4—K—O3—B2	−63.66 (13)
O6—K—Zn—K^{i}	−168.76 (4)	B2^{i}—K—O3—B2	−51.73 (16)
O5^{iv}—K—Zn—K^{i}	−50.85 (5)	B3—K—O3—B2	−148.62 (13)
O6^{iii}—K—Zn—K^{i}	−85.10 (4)	O4^{i}—K—O3—B1	161.0 (3)
O2—K—Zn—K^{i}	140.40 (6)	O3^{ii}—K—O3—B1	−80.5 (3)
O4—K—Zn—K^{i}	−31.29 (6)	O1^{iii}—K—O3—B1	−110.1 (3)
B2^{i}—K—Zn—K^{i}	−55.02 (6)	O6—K—O3—B1	0.7 (3)
O3—K—Zn—K^{i}	63.81 (4)	O5^{iv}—K—O3—B1	−166.9 (3)
B3—K—Zn—K^{i}	165.12 (6)	O6^{iii}—K—O3—B1	89.6 (3)
B2—K—Zn—K^{i}	38.83 (5)	O2—K—O3—B1	17.7 (3)
O3^{ii}—K—B2—O4^{i}	101.89 (15)	O4—K—O3—B1	87.3 (3)
O1^{iii}—K—B2—O4^{i}	39.7 (2)	B2^{i}—K—O3—B1	99.2 (3)
O6—K—B2—O4^{i}	−158.69 (12)	B3—K—O3—B1	2.3 (3)
O5^{iv}—K—B2—O4^{i}	18.26 (15)	B2—K—O3—B1	150.9 (3)
O6^{iii}—K—B2—O4^{i}	−67.98 (15)	O4^{i}—K—O3—K^{ii}	−118.53 (7)
O2—K—B2—O4^{i}	−155.45 (14)	O3^{ii}—K—O3—K^{ii}	0.0
O4—K—B2—O4^{i}	−88.37 (15)	O1^{iii}—K—O3—K^{ii}	−29.61 (10)
B2^{i}—K—B2—O4^{i}	−69.11 (14)	O6—K—O3—K^{ii}	81.13 (6)
O3—K—B2—O4^{i}	160.9 (2)	O5^{iv}—K—O3—K^{ii}	−86.42 (6)
B3—K—B2—O4^{i}	−165.01 (14)	O6^{iii}—K—O3—K^{ii}	170.06 (5)
O4^{i}—K—B2—O3	−160.9 (2)	O2—K—O3—K^{ii}	98.19 (5)
O3^{ii}—K—B2—O3	−59.00 (14)	O4—K—O3—K^{ii}	167.74 (5)
O1^{iii}—K—B2—O3	−121.16 (12)	B2^{i}—K—O3—K^{ii}	179.68 (6)
O6—K—B2—O3	40.42 (16)	B3—K—O3—K^{ii}	82.79 (6)
O5^{iv}—K—B2—O3	−142.63 (12)	B2—K—O3—K^{ii}	−128.59 (13)
O6^{iii}—K—B2—O3	131.12 (12)	O1—Zn—O4—B2^{i}	−37.9 (2)
O2—K—B2—O3	43.66 (12)	O2^{v}—Zn—O4—B2^{i}	−179.73 (18)
O4—K—B2—O3	110.73 (13)	O2—Zn—O4—B2^{i}	81.2 (2)
B2^{i}—K—B2—O3	129.99 (15)	Zn^{v}—Zn—O4—B2^{i}	129.37 (18)
B3—K—B2—O3	34.10 (14)	K—Zn—O4—B2^{i}	73.35 (19)
O4^{i}—K—B2—O6^{vi}	74.8 (4)	K^{iii}—Zn—O4—B2^{i}	−1.03 (19)
O3^{ii}—K—B2—O6^{vi}	176.7 (4)	K^{i}—Zn—O4—B2^{i}	−177.6 (3)
O1^{iii}—K—B2—O6^{vi}	114.5 (4)	O1—Zn—O4—K^{i}	139.70 (9)

O6—K—B2—O6^{vi}	−83.9 (4)	O2^{v}—Zn—O4—K^{i}	−2.11 (12)
O5^{iv}—K—B2—O6^{vi}	93.0 (4)	O2—Zn—O4—K^{i}	−101.18 (10)
O6^{iii}—K—B2—O6^{vi}	6.8 (4)	Zn^{v}—Zn—O4—K^{i}	−53.01 (11)
O2—K—B2—O6^{vi}	−80.7 (4)	K—Zn—O4—K^{i}	−109.03 (10)
O4—K—B2—O6^{vi}	−13.6 (4)	K^{iii}—Zn—O4—K^{i}	176.59 (8)
B2^{i}—K—B2—O6^{vi}	5.7 (4)	O1—Zn—O4—K	−111.28 (6)
O3—K—B2—O6^{vi}	−124.3 (5)	O2^{v}—Zn—O4—K	106.92 (7)
B3—K—B2—O6^{vi}	−90.2 (4)	O2—Zn—O4—K	7.84 (7)
O4^{i}—K—B2—K^{i}	69.11 (14)	Zn^{v}—Zn—O4—K	56.02 (6)
O3^{ii}—K—B2—K^{i}	171.01 (5)	K^{iii}—Zn—O4—K	−74.39 (5)
O1^{iii}—K—B2—K^{i}	108.85 (10)	K^{i}—Zn—O4—K	109.03 (10)
O6—K—B2—K^{i}	−89.57 (9)	O4^{i}—K—O4—B2^{i}	103.40 (14)
O5^{iv}—K—B2—K^{i}	87.38 (7)	O3^{ii}—K—O4—B2^{i}	−98.0 (2)
O6^{iii}—K—B2—K^{i}	1.13 (7)	O1^{iii}—K—O4—B2^{i}	−18.42 (14)
O2—K—B2—K^{i}	−86.33 (7)	O6—K—O4—B2^{i}	−92.60 (13)
O4—K—B2—K^{i}	−19.26 (4)	O5^{iv}—K—O4—B2^{i}	36.17 (14)
B2^{i}—K—B2—K^{i}	0.0	O6^{iii}—K—O4—B2^{i}	−26.49 (12)
O3—K—B2—K^{i}	−129.99 (15)	O2—K—O4—B2^{i}	−135.79 (14)
B3—K—B2—K^{i}	−95.89 (8)	O3—K—O4—B2^{i}	151.02 (13)
O4^{i}—K—B3—O2	15.32 (17)	B3—K—O4—B2^{i}	−117.42 (14)
O3^{ii}—K—B3—O2	139.97 (14)	B2—K—O4—B2^{i}	127.65 (12)
O1^{iii}—K—B3—O2	−170.63 (12)	O4^{i}—K—O4—Zn	−126.01 (9)
O6—K—B3—O2	−146.5 (2)	O3^{ii}—K—O4—Zn	32.6 (2)
O5^{iv}—K—B3—O2	−163.33 (11)	O1^{iii}—K—O4—Zn	112.17 (6)
O6^{iii}—K—B3—O2	−91.29 (13)	O6—K—O4—Zn	37.99 (6)
O4—K—B3—O2	−44.29 (13)	O5^{iv}—K—O4—Zn	166.76 (5)
B2^{i}—K—B3—O2	−66.12 (14)	O6^{iii}—K—O4—Zn	104.10 (8)
O3—K—B3—O2	36.98 (13)	O2—K—O4—Zn	−5.20 (5)
B2—K—B3—O2	23.39 (15)	B2^{i}—K—O4—Zn	130.59 (15)
O4^{i}—K—B3—O5	−97.2 (3)	O3—K—O4—Zn	−78.39 (6)
O3^{ii}—K—B3—O5	27.5 (3)	B3—K—O4—Zn	13.17 (6)
O1^{iii}—K—B3—O5	76.9 (3)	B2—K—O4—Zn	−101.76 (8)
O6—K—B3—O5	101.0 (3)	O4^{i}—K—O4—K^{i}	0.0
O5^{iv}—K—B3—O5	84.2 (3)	O3^{ii}—K—O4—K^{i}	158.64 (19)
O6^{iii}—K—B3—O5	156.2 (3)	O1^{iii}—K—O4—K^{i}	−121.82 (6)
O2—K—B3—O5	−112.5 (4)	O6—K—O4—K^{i}	164.00 (6)
O4—K—B3—O5	−156.8 (3)	O5^{iv}—K—O4—K^{i}	−67.23 (7)
B2^{i}—K—B3—O5	−178.6 (3)	O6^{iii}—K—O4—K^{i}	−129.90 (8)
O3—K—B3—O5	−75.5 (3)	O2—K—O4—K^{i}	120.81 (7)
B2—K—B3—O5	−89.1 (3)	B2^{i}—K—O4—K^{i}	−103.40 (14)
O4^{i}—K—B3—O6	161.80 (11)	O3—K—O4—K^{i}	47.62 (5)

O3^{ii}—K—B3—O6	−73.54 (13)	B3—K—O4—K^{i}	139.18 (7)
O1^{iii}—K—B3—O6	−24.14 (13)	B2—K—O4—K^{i}	24.25 (6)
O5^{iv}—K—B3—O6	−16.8 (2)	O2—B3—O5—B1^{xi}	−171.9 (2)
O6^{iii}—K—B3—O6	55.19 (13)	O6—B3—O5—B1^{xi}	6.6 (3)
O2—K—B3—O6	146.5 (2)	K—B3—O5—B1^{xi}	−76.4 (4)
O4—K—B3—O6	102.19 (13)	O2—B3—O5—K^{xii}	40.2 (3)
B2^{i}—K—B3—O6	80.36 (14)	O6—B3—O5—K^{xii}	−141.28 (16)
O3—K—B3—O6	−176.54 (12)	K—B3—O5—K^{xii}	135.7 (2)
B2—K—B3—O6	169.87 (12)	O2—B3—O6—B2^{xi}	177.2 (2)
O4—Zn—O1—B1^{v}	−173.34 (17)	O5—B3—O6—B2^{xi}	−1.4 (3)
O2^{v}—Zn—O1—B1^{v}	−32.6 (2)	K—B3—O6—B2^{xi}	142.9 (2)
O2—Zn—O1—B1^{v}	59.85 (19)	O2—B3—O6—K	34.3 (2)
Zn^{v}—Zn—O1—B1^{v}	18.13 (19)	O5—B3—O6—K	−144.30 (19)
K—Zn—O1—B1^{v}	119.73 (17)	O2—B3—O6—K^{iii}	−76.7 (2)
K^{iii}—Zn—O1—B1^{v}	122.1 (2)	O5—B3—O6—K^{iii}	104.7 (2)
K^{i}—Zn—O1—B1^{v}	−146.02 (16)	K—B3—O6—K^{iii}	−111.02 (10)
O4—Zn—O1—B1^{x}	−48.07 (17)	O4^{i}—K—O6—B3	−35.0 (2)
O2^{v}—Zn—O1—B1^{x}	92.65 (16)	O3^{ii}—K—O6—B3	101.87 (13)
O2—Zn—O1—B1^{x}	−174.87 (15)	O1^{iii}—K—O6—B3	155.58 (13)
Zn^{v}—Zn—O1—B1^{x}	143.40 (14)	O5^{iv}—K—O6—B3	169.98 (12)
K—Zn—O1—B1^{x}	−115.00 (15)	O6^{iii}—K—O6—B3	−121.12 (14)
K^{iii}—Zn—O1—B1^{x}	−112.59 (17)	O2—K—O6—B3	−18.14 (12)
K^{i}—Zn—O1—B1^{x}	−20.75 (18)	O4—K—O6—B3	−76.92 (13)
O4—Zn—O1—K^{iii}	64.52 (8)	B2^{i}—K—O6—B3	−101.49 (14)
O2^{v}—Zn—O1—K^{iii}	−154.77 (6)	O3—K—O6—B3	3.86 (14)
O2—Zn—O1—K^{iii}	−62.29 (8)	B2—K—O6—B3	−13.77 (16)
Zn^{v}—Zn—O1—K^{iii}	−104.01 (6)	O4^{i}—K—O6—B2^{xi}	−172.34 (18)
K—Zn—O1—K^{iii}	−2.41 (8)	O3^{ii}—K—O6—B2^{xi}	−35.48 (19)
K^{i}—Zn—O1—K^{iii}	91.84 (7)	O1^{iii}—K—O6—B2^{xi}	18.23 (19)
O5—B3—O2—Zn^{v}	6.8 (3)	O5^{iv}—K—O6—B2^{xi}	32.6 (2)
O6—B3—O2—Zn^{v}	−171.72 (14)	O6^{iii}—K—O6—B2^{xi}	101.5 (2)
K—B3—O2—Zn^{v}	−138.72 (16)	O2—K—O6—B2^{xi}	−155.5 (2)
O5—B3—O2—Zn	−127.1 (2)	O4—K—O6—B2^{xi}	145.74 (19)
O6—B3—O2—Zn	54.3 (3)	B2^{i}—K—O6—B2^{xi}	121.17 (17)
K—B3—O2—Zn	87.33 (13)	O3—K—O6—B2^{xi}	−133.48 (18)
O5—B3—O2—K	145.6 (2)	B3—K—O6—B2^{xi}	−137.3 (3)
O6—B3—O2—K	−33.0 (2)	B2—K—O6—B2^{xi}	−151.1 (2)
O4—Zn—O2—B3	−96.81 (18)	O4^{i}—K—O6—K^{iii}	86.13 (14)
O1—Zn—O2—B3	24.73 (18)	O3^{ii}—K—O6—K^{iii}	−137.01 (6)
O2^{v}—Zn—O2—B3	144.6 (2)	O1^{iii}—K—O6—K^{iii}	−83.30 (6)
Zn^{v}—Zn—O2—B3	144.6 (2)	O5^{iv}—K—O6—K^{iii}	−68.90 (8)

K—Zn—O2—B3	−88.59 (17)	O6^{iii}—K—O6—K^{iii}	0.0
K^{iii}—Zn—O2—B3	−11.57 (16)	O2—K—O6—K^{iii}	102.98 (8)
K^{i}—Zn—O2—B3	−133.34 (16)	O4—K—O6—K^{iii}	44.20 (5)
O4—Zn—O2—Zn^{v}	118.60 (7)	B2^{i}—K—O6—K^{iii}	19.63 (6)
O1—Zn—O2—Zn^{v}	−119.85 (7)	O3—K—O6—K^{iii}	124.98 (6)
O2^{v}—Zn—O2—Zn^{v}	0.0	B3—K—O6—K^{iii}	121.12 (14)
K—Zn—O2—Zn^{v}	126.83 (7)	B2—K—O6—K^{iii}	107.35 (9)

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

Fig. 1

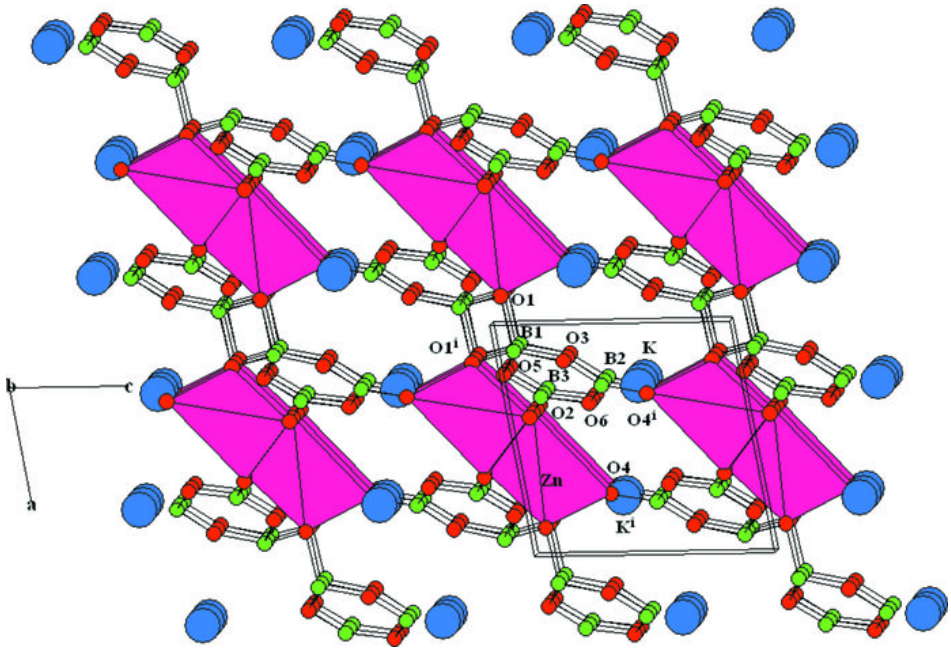

Fig. 2