Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

The β-modification of trizinc borate phosphate, $Zn_3(BO_3)(PO_4)$

Erpan Zhang,[a,b] Sangen Zhao,[a,b] Jianxiu Zhang,[a] Peizhen Fu[a] and Jiyong Yao[a]*

[a]Key Laboratory of Functional Crystal and Laser Technology, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences, Beijing 100190, People's Republic of China, and [b]Graduate University of Chinese Academy of Sciences, Beijing 100049, People's Republic of China
Correspondence e-mail: jyao@mail.ipc.ac.cn

Received 20 October 2010; accepted 10 December 2010

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(P–O) = 0.003 Å; R factor = 0.019; wR factor = 0.039; data-to-parameter ratio = 12.3.

Crystals of β-$Zn_3(BO_3)(PO_4)$ have been grown by the Kyropoulos method. The asymmetric unit contains three Zn sites, three B-atom sites (all with symmetry 3), two P sites (both with m symmetry) and nine O-atom sites (four with m symmetry). The fundamental building units of the title structure are isolated BO_3 triangles and PO_4 tetrahedra, which are bridged by ZnO_4 tetrahedra or ZnO_5 trigonal bipyramids through common O atoms, leading to a three-dimensional framework structure. Some significant structural differences between the β-polymorph and the α-polymorph are discussed.

Related literature

For general backround to $Zn_3(BO_3)(PO_4)$, see: Liebertz & Stahr (1982). For crystal growth of β-$Zn_3(BO_3)(PO_4)$, see: Wang *et al.* (2000); Wu & Wang (2001); Liu *et al.* (2002). For structure refinement of α-$Zn_3(BO_3)(PO_4)$, see: Bluhm & Park (1997). For structurally related compounds, see: Ma *et al.* (2004); Yilmaz *et al.* (2001). Reviews on borophosphates were given by Kniep *et al.* (1998) and Ewald *et al.* (2007).

Experimental

Crystal data

$Zn_3(BO_3)(PO_4)$
M_r = 349.89
Hexagonal, $P\bar{6}$
a = 8.4624 (3) Å
c = 13.0690 (7) Å
V = 810.51 (4) Å^3
Z = 6
Mo $K\alpha$ radiation
μ = 13.49 mm^{-1}
T = 294 K
0.25 × 0.22 × 0.16 mm

Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: numerical (*NUMABS*; Rigaku, 2005)
T_{min} = 0.133, T_{max} = 0.221
10584 measured reflections
1453 independent reflections
1226 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.019
$wR(F^2)$ = 0.039
S = 0.96
1453 reflections
118 parameters
$\Delta\rho_{max}$ = 0.61 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}
Absolute structure: Flack (1983), 718 Friedel pairs
Flack parameter: 0.011 (10)

Table 1
Selected bond lengths (Å).

Zn1—O7	1.9248 (17)	Zn3—O6^{vi}	2.0748 (18)
Zn1—O2^{i}	1.9293 (19)	Zn3—O9	2.079 (2)
Zn1—O3^{ii}	2.084 (2)	B1—O7	1.3792 (18)
Zn1—O1	2.100 (2)	B2—O8	1.3880 (18)
Zn2—O7	1.9529 (17)	B3—O9	1.3775 (17)
Zn2—O9^{iii}	1.9604 (18)	P1—O3	1.541 (3)
Zn2—O8^{iv}	1.9656 (17)	P1—O1	1.542 (3)
Zn2—O4	2.2019 (18)	P1—O2	1.5484 (18)
Zn2—O2	2.3238 (18)	P2—O5	1.529 (3)
Zn3—O4^{v}	1.9958 (18)	P2—O6	1.540 (3)
Zn3—O8	2.035 (2)	P2—O4	1.5412 (18)
Zn3—O5	2.0704 (18)		

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

Data collection: *CrystalClear* (Rigaku, 2005); 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: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

This work was supported by the National Natural Science Foundation of China (grant No. 50932005).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2419).

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supporting information

Acta Cryst. (2011). E**67**, i3 [https://doi.org/10.1107/S1600536810051871]

The *β*-modification of trizinc borate phosphate, $Zn_3(BO_3)(PO_4)$

Erpan Zhang, Sangen Zhao, Jianxiu Zhang, Peizhen Fu and Jiyong Yao

S1. Comment

Liebertz & Stahr reported the existence of $Zn_3(BO_3)(PO_4)$ in 1982 (Liebertz & Stahr, 1982). $Zn_3(BO_3)(PO_4)$ (ZBP) can exist in two modifications, one low-temperature phase denoted *α* and one high-temperature phase denoted *β*. The phase transition point is 875 K. Some significant features of *β*-$Zn_3(BO_3)(PO_4)$ make it attractive as a promising NLO material. However, *β*-$Zn_3(BO_3)(PO_4)$ crystals grown from the melt frequently have a poor quality when cooling to room temperature. Hence considerable effort has been made to obtain high-quality *β*-$Zn_3(BO_3)(PO_4)$ crystals (Wang *et al.*, 2000; Wu & Wang, 2001; Liu *et al.*, 2002). In this paper, *β*-$Zn_3(BO_3)(PO_4)$ crystals were obtained through a rapid cooling method. The structural differences between *α*-$Zn_3(BO_3)(PO_4)$ and *β*-$Zn_3(BO_3)(PO_4)$ are described, and we also briefly discuss the structural differences between *β*-$Zn_3(BO_3)(PO_4)$ and the structures of other borate-phosphates and borophosphates.

The asymmetric unit of the title structure contains three Zn sites, three B sites (all with site symmetry 3), two P sites (both with *m* symmetry) and nine O sites (four of which with *m* symmetry) (Fig. 1). The fundamental structural building units are isolated BO_3 triangles and PO_4 tetrahedra. These units are alternately oriented parallel to (001) and stacked layer upon layer along [001] (Figs. 2 and 3). The isolated character of the anionic units classifies this compound as a borate-phosphate in contrast to borophosphates, where at least one BO_3 (or BO_4) group and one PO_4 tetrahedron share a common O atom. Reviews on the crystal chemistry of the latter class of compounds were given by Kniep *et al.* (1998) and Ewald *et al.* (2007).

The BO_3 triangles show an equilateral trigonal-planar configuration. The P—O distances range between 1.529 (3) Å and 1.5484 (18) Å, indicating a slight distortion of the two PO_4 tetrahedra in this structure. The Zn atoms selectively occupy the space between the anionic layers and are bonded to the terminal O atoms of the anions. The coordination environments of the three independent Zn are different from another. Zn1 is tetrahedrally surrounded by atoms O7, O2, O3 and O1, with Zn—O distances in the range 1.9248 (17) Å – 2.100 (2) Å. Zn2 and Zn3 are five-coordinate by oxygen within a trigonal bipyramid and Zn—O distances range from 1.9529 (17) Å to 2.3238 (18) Å for Zn2 and from 1.9958 (17) Å to 2.079 (2) Å for Zn3. The isolated BO_3 and PO_4 groups are linked to ZnO_5 or ZnO_4 polyhedra by sharing one corner O atom. In addition, ZnO_5 and ZnO_4 polyhedra are linked together by sharing one corner O atom. Individual ZnO_4 tetrahedra and ZnO_5 polyhedra, respectively, also share a common edge.

To the best of our knowledge, besides *β*-$Zn_3(BO_3)(PO_4)$, *α*-$Zn_3(BO_3)(PO_4)$ (Bluhm & Park, 1997), $Co_3(BO_3)(PO_4)$ (Yilmaz *et al.*, 2001) and $Ba_3(BO_3)(PO_4)$ (Ma *et al.*., 2004) are the only three other borate-phosphates. In comparison with *β*-$Zn_3(BO_3)(PO_4)$, in the structure of *α*-$Zn_3(BO_3)(PO_4)$ the BO_3 and PO_4 groups are also linked to ZnO_5 trigonal bipyramids and ZnO_4 tetrahedra by sharing O atoms. However, the symmetry of the two structures is different. During the $\alpha \rightarrow \beta$ phase transformation, the positions of the isolated BO_3 and PO_4 groups are rearranged, accompanied with a change from space group *Cm* (*α*-phase) to $P\overline{6}$ (*β*-phase). The density of low-temperature *α*-$Zn_3(BO_3)(PO_4)$ is 4.44 g/cm^3 (Bluhm & Park, 1997), while the density of high-temperature *β*-$Zn_3(BO_3)(PO_4)$ is 4.30 g/cm^3, pointing to *α*-$Zn_3(BO_3)(PO_4)$ as the thermodynamically stable phase. It should be noted that the *β*-$Zn_3(BO_3)(PO_4)$ structure type is different from $Ba_3(BO_3)(PO_4)$ (space group *P*6₃*mc*) whereas $Co_3(BO_3)(PO_4)$ is isotypic with *α*-$Zn_3(BO_3)(PO_4)$. The differences between the Ba-containing structure and the structures containing the first row-transition metals is caused by the different ionic radii of the metal cations and consequently by a different coordination environment.

S2. Experimental

$Zn_3(BO_3)(PO_4)$ was synthesized by a standard solid-state reaction of the starting components, using chemically pure ZnO, H_3BO_3 and $NH_4H_2PO_4$ in the molar ratio of 3:1:1. A platinum crucible filled with $Zn_3(BO_3)(PO_4)$ was heated to 1273 K, kept at that temperature for 12 h, and then was cooled to the saturation temperature. A seed crystal of *β*-$Zn_3(BO_3)(PO_4)$ attached to a platinum rod was inserted into the solution, and then the temperature was cooled at a rate of 0.3 K·d^{-1} until the end of the growth. The obtained crystal was pulled out of the surface of the solution, cooled to 700 K at a rate of 20 K/h, and then cooled rapidly to 620 K in 1.5 h. Finally, the crystal was removed out of the furnace and cooled to room temperature.

S3. Refinement

One B atom (B1) has been refined with an isotropic displacement parameter. Refinement with anisotropic displacement parameters for this atom resulted in physically meaningless values.

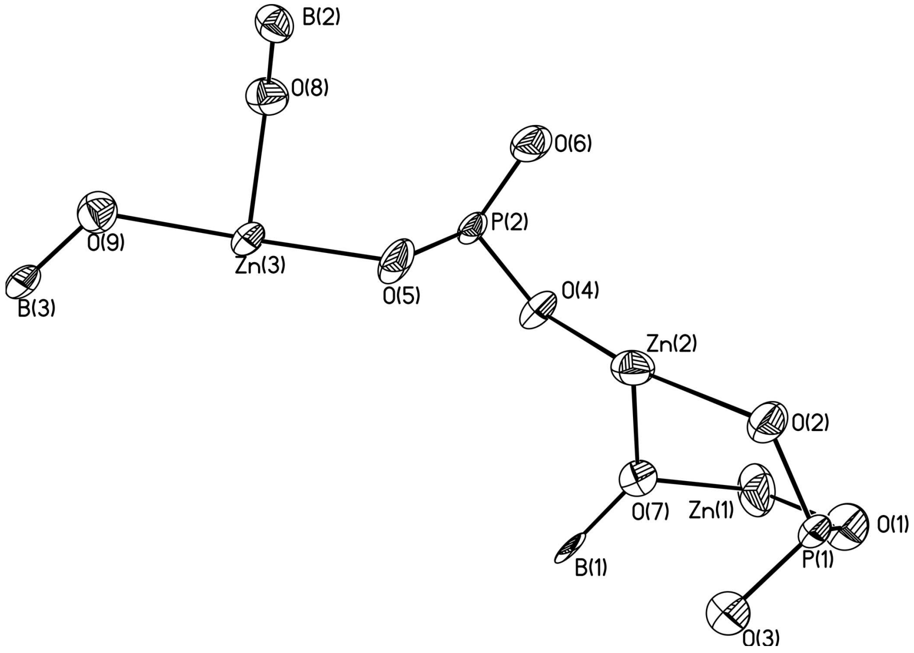

Figure 1

The asymmetric unit of *β*-$Zn_3(BO_3)(PO_4)$ with atom labelling and ellipsoids drawn at the 90% probability level.

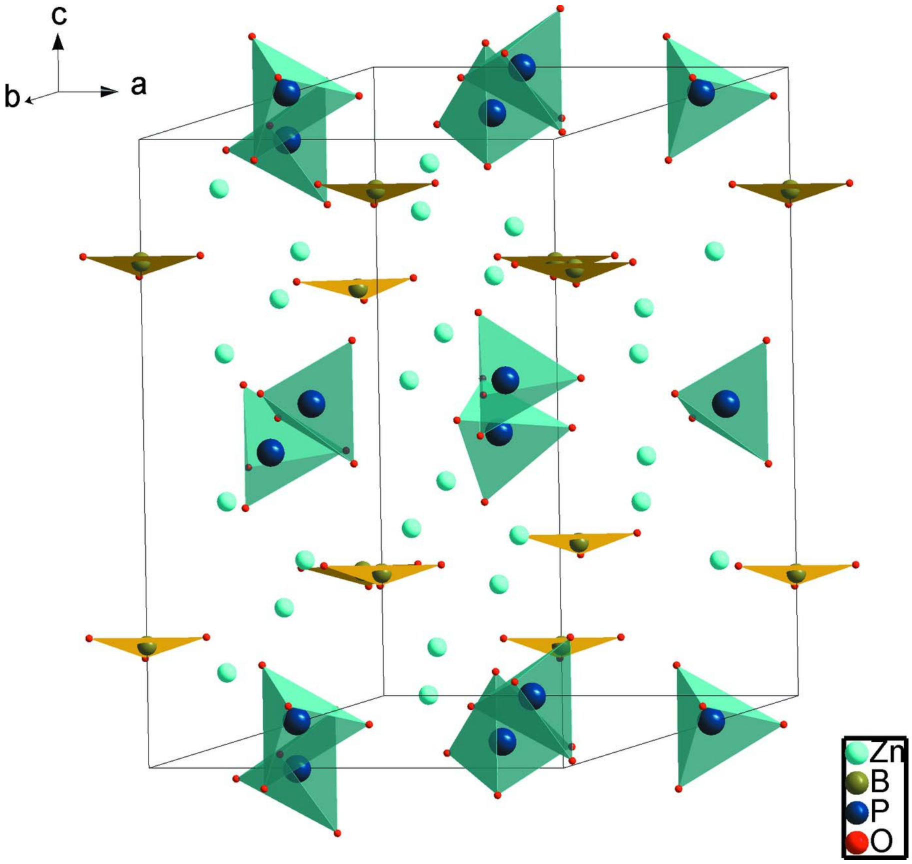

Figure 2

Crystal structure of β-$Zn_3(BO_3)(PO_4)$ illustrated with isolated BO_3 and PO_4 groups.

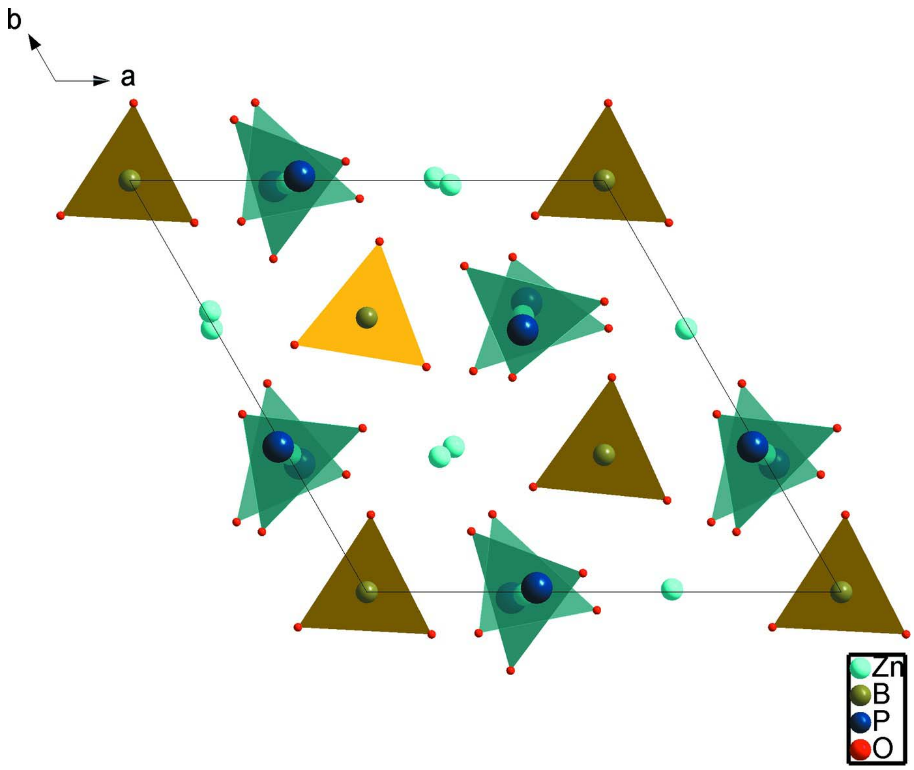

Figure 3

The structure of β-$Zn_3(BO_3)(PO_4)$ viewed along [001].

trizinc borate phosphate

Crystal data

$Zn_3(BO_3)(PO_4)$
$M_r = 349.89$
Hexagonal, $P\overline{6}$
Hall symbol: -P 6
$a = 8.4624$ (3) Å
$c = 13.0690$ (7) Å
$V = 810.51$ (4) Å^3
$Z = 6$
$F(000) = 996$

$D_x = 4.301$ Mg m^{-3}
Melting point: 1200 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2470 reflections
$\theta = 1.6–28.7°$
$\mu = 13.49$ mm^{-1}
$T = 294$ K
Prism, colorless
0.25 × 0.22 × 0.16 mm

Data collection

Rigaku Saturn CCD diffractometer
Radiation source: fine-focus sealed tube
Confocal monochromator
Detector resolution: 7.31 pixels mm^{-1}
ω scans
Absorption correction: numerical (*NUMABS*; Rigaku, 2005)
$T_{min} = 0.133$, $T_{max} = 0.221$

10584 measured reflections
1453 independent reflections
1226 reflections with $I > 2\sigma(I)$
$R_{int} = 0.062$
$\theta_{max} = 28.6°$, $\theta_{min} = 1.6°$
$h = -11\rightarrow10$
$k = -11\rightarrow11$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.019$
$wR(F^2) = 0.039$
$S = 0.96$
1453 reflections
118 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0099P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.004$
$\Delta\rho_{\max} = 0.61$ e Å^{-3}
$\Delta\rho_{\min} = -0.52$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0328 (7)
Absolute structure: Flack (1983), 718 Friedel pairs
Absolute structure parameter: 0.011 (10)

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 (Å²)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
Zn1	0.67111 (7)	0.98916 (9)	0.88495 (3)	0.01824 (11)
Zn2	0.66452 (5)	0.67089 (5)	0.74557 (2)	0.01218 (11)
Zn3	0.99324 (6)	0.64008 (5)	0.38229 (3)	0.00982 (9)
B1	1.0000	1.0000	0.8052 (5)	0.0097 (11)*
B2	0.6667	0.3333	0.2820 (5)	0.0110 (12)
B3	1.3333	0.6667	0.2751 (4)	0.0088 (11)
P1	0.64705 (15)	0.63672 (14)	1.0000	0.0085 (2)
P2	0.68800 (15)	0.70242 (14)	0.5000	0.0083 (2)
O1	0.6018 (3)	0.7921 (4)	1.0000	0.0140 (6)
O2	0.5676 (3)	0.5214 (2)	0.90172 (13)	0.0137 (4)
O3	0.8535 (3)	0.7058 (4)	1.0000	0.0146 (7)
O4	0.7144 (2)	0.8140 (2)	0.59811 (13)	0.0116 (4)
O5	0.8298 (4)	0.6407 (4)	0.5000	0.0141 (6)
O6	0.4931 (4)	0.5371 (4)	0.5000	0.0135 (6)
O7	0.8121 (2)	0.9147 (2)	0.80352 (13)	0.0116 (4)
O8	0.7773 (3)	0.5217 (2)	0.28461 (17)	0.0123 (5)
O9	1.1480 (2)	0.6008 (2)	0.27238 (16)	0.0124 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0165 (2)	0.0204 (2)	0.0210 (2)	0.01163 (17)	0.00515 (18)	−0.00218 (19)
Zn2	0.0110 (2)	0.01191 (19)	0.0137 (2)	0.00580 (16)	−0.00283 (15)	−0.00386 (13)

Zn3	0.0110 (2)	0.01235 (19)	0.00559 (17)	0.00543 (19)	−0.00002 (14)	−0.00152 (13)
B2	0.0095 (18)	0.0095 (18)	0.014 (3)	0.0048 (9)	0.000	0.000
B3	0.0120 (17)	0.0120 (17)	0.002 (3)	0.0060 (9)	0.000	0.000
P1	0.0091 (5)	0.0101 (5)	0.0051 (5)	0.0039 (5)	0.000	0.000
P2	0.0109 (6)	0.0114 (5)	0.0035 (5)	0.0064 (5)	0.000	0.000
O1	0.0167 (15)	0.0155 (15)	0.0142 (17)	0.0112 (13)	0.000	0.000
O2	0.0136 (10)	0.0141 (10)	0.0083 (10)	0.0029 (9)	0.0011 (8)	−0.0003 (8)
O3	0.0118 (14)	0.0173 (15)	0.0125 (17)	0.0058 (12)	0.000	0.000
O4	0.0175 (11)	0.0137 (10)	0.0060 (10)	0.0096 (9)	−0.0005 (8)	−0.0016 (8)
O5	0.0191 (15)	0.0243 (16)	0.0047 (16)	0.0153 (13)	0.000	0.000
O6	0.0146 (15)	0.0137 (15)	0.0075 (16)	0.0036 (12)	0.000	0.000
O7	0.0119 (9)	0.0123 (10)	0.0100 (11)	0.0056 (8)	−0.0005 (8)	−0.0012 (8)
O8	0.0122 (10)	0.0120 (10)	0.0141 (13)	0.0072 (8)	−0.0026 (9)	−0.0014 (9)
O9	0.0128 (10)	0.0109 (10)	0.0137 (11)	0.0060 (9)	0.0004 (9)	−0.0010 (9)

Geometric parameters (Å, º)

Zn1—O7	1.9248 (17)	B1—O7^{ii}	1.3792 (18)
Zn1—O2^{i}	1.9293 (19)	B1—O7	1.3792 (18)
Zn1—O3^{ii}	2.084 (2)	B1—O7^{ix}	1.3792 (18)
Zn1—O1	2.100 (2)	B2—O8^{vii}	1.3880 (18)
Zn1—Zn1^{iii}	3.0071 (9)	B2—O8	1.3880 (18)
Zn2—O7	1.9529 (17)	B2—O8^{x}	1.3880 (18)
Zn2—O9^{iv}	1.9604 (18)	B3—O9	1.3775 (17)
Zn2—O8^{v}	1.9656 (17)	B3—O9^{xi}	1.3775 (17)
Zn2—O4	2.2019 (18)	B3—O9^{xii}	1.3775 (17)
Zn2—O2	2.3238 (18)	P1—O3	1.541 (3)
Zn2—Zn3^{iv}	3.1202 (5)	P1—O1	1.542 (3)
Zn3—O4^{vi}	1.9958 (18)	P1—O2	1.5484 (18)
Zn3—O8	2.035 (2)	P1—O2^{iii}	1.5484 (18)
Zn3—O5	2.0704 (18)	P2—O5	1.529 (3)
Zn3—O6^{vii}	2.0748 (18)	P2—O6	1.540 (3)
Zn3—O9	2.079 (2)	P2—O4	1.5412 (18)
Zn3—Zn3^{v}	3.0766 (7)	P2—O4^{v}	1.5412 (18)
Zn3—Zn2^{viii}	3.1202 (5)		
O7—Zn1—O2^{i}	152.13 (8)	O1—P1—O2	108.83 (10)
O7—Zn1—O3^{ii}	103.27 (9)	O3—P1—O2^{iii}	106.96 (10)
O2^{i}—Zn1—O3^{ii}	101.65 (9)	O1—P1—O2^{iii}	108.83 (10)
O7—Zn1—O1	96.22 (8)	O2—P1—O2^{iii}	112.09 (15)
O2^{i}—Zn1—O1	100.50 (9)	O5—P2—O6	110.90 (15)
O3^{ii}—Zn1—O1	79.32 (8)	O5—P2—O4	108.15 (9)
O7—Zn2—O9^{iv}	124.56 (7)	O6—P2—O4	108.54 (9)
O7—Zn2—O8^{v}	119.80 (8)	O5—P2—O4^{v}	108.15 (9)
O9^{iv}—Zn2—O8^{v}	115.29 (7)	O6—P2—O4^{v}	108.54 (9)
O7—Zn2—O4	85.00 (7)	O4—P2—O4^{v}	112.59 (15)
O9^{iv}—Zn2—O4	92.42 (7)	P1—O1—Zn1^{iii}	125.99 (8)
O8^{v}—Zn2—O4	99.02 (8)	P1—O1—Zn1	125.99 (8)

O7—Zn2—O2	95.72 (7)	Zn1^{iii}—O1—Zn1	91.46 (11)
O9^{iv}—Zn2—O2	79.41 (8)	P1—O2—Zn1^{xiii}	124.98 (11)
O8^{v}—Zn2—O2	88.80 (8)	P1—O2—Zn2	117.49 (10)
O4—Zn2—O2	170.57 (7)	Zn1^{xiii}—O2—Zn2	107.41 (8)
O4^{vi}—Zn3—O8	131.36 (8)	P1—O3—Zn1^{xiv}	128.42 (8)
O4^{vi}—Zn3—O5	94.60 (9)	P1—O3—Zn1^{ix}	128.42 (8)
O8—Zn3—O5	91.76 (8)	Zn1^{xiv}—O3—Zn1^{ix}	92.36 (11)
O4^{vi}—Zn3—O6^{vii}	103.14 (9)	P2—O4—Zn3^{xv}	126.50 (11)
O8—Zn3—O6^{vii}	125.21 (9)	P2—O4—Zn2	117.50 (10)
O5—Zn3—O6^{vii}	76.73 (8)	Zn3^{xv}—O4—Zn2	106.43 (8)
O4^{vi}—Zn3—O9	91.86 (7)	P2—O5—Zn3^{v}	129.80 (7)
O8—Zn3—O9	88.31 (8)	P2—O5—Zn3	129.80 (7)
O5—Zn3—O9	171.33 (10)	Zn3^{v}—O5—Zn3	95.98 (11)
O6^{vii}—Zn3—O9	96.17 (8)	P2—O6—Zn3^{x}	127.95 (8)
O7^{ii}—B1—O7	119.976 (16)	P2—O6—Zn3^{iv}	127.95 (8)
O7^{ii}—B1—O7^{ix}	119.976 (16)	Zn3^{x}—O6—Zn3^{iv}	95.71 (11)
O7—B1—O7^{ix}	119.976 (16)	B1—O7—Zn1	124.1 (2)
O8^{vii}—B2—O8	119.94 (3)	B1—O7—Zn2	121.32 (16)
O8^{vii}—B2—O8^{x}	119.94 (3)	Zn1—O7—Zn2	112.75 (9)
O8—B2—O8^{x}	119.94 (3)	B2—O8—Zn2^{v}	117.88 (13)
O9—B3—O9^{xi}	119.93 (2)	B2—O8—Zn3	120.3 (2)
O9—B3—O9^{xii}	119.93 (2)	Zn2^{v}—O8—Zn3	114.50 (9)
O9^{xi}—B3—O9^{xii}	119.93 (2)	B3—O9—Zn2^{viii}	112.75 (11)
O3—P1—O1	113.22 (15)	B3—O9—Zn3	126.7 (2)
O3—P1—O2	106.96 (10)	Zn2^{viii}—O9—Zn3	101.09 (8)

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