

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

 $\alpha$ -Ba<sub>2</sub>P<sub>2</sub>O<sub>7</sub>Driss Zakaria,<sup>a</sup> Fatima Erragh,<sup>a</sup> Abdelghani Oudahmane,<sup>b</sup> Malika El-Ghozzi<sup>b</sup> and Daniel Avignant<sup>b\*</sup>

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Received 6 October 2010; accepted 25 October 2010

Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{P}-\text{O}) = 0.001$  Å;  $R$  factor = 0.021;  $wR$  factor = 0.046; data-to-parameter ratio = 69.4.

Single crystals of  $\alpha$ -Ba<sub>2</sub>P<sub>2</sub>O<sub>7</sub>, dibarium diphosphate, were obtained by solid-state reaction. The orthorhombic structure is isotypic with  $\alpha$ -Sr<sub>2</sub>P<sub>2</sub>O<sub>7</sub> and is the second polymorph obtained for this composition. The structure is built from two different BaO<sub>9</sub> polyhedra (both with  $m$  symmetry), with Ba—O distances in the ranges 2.7585 (10)–3.0850 (6) and 2.5794 (13)–2.9313 (4) Å. These polyhedra are further linked by sharing corners along [010] and either edges or triangular faces perpendicularly to [010] to form the three-dimensional framework. This polyhedral linkage delimits large channels parallel to [010] where the P<sub>2</sub>O<sub>7</sub> diphosphate anions are located. These groups (symmetry  $m$ ) are characterized by a P—O—P angle of 131.52 (9)° and an eclipsed conformation. They are connected to the BaO<sub>9</sub> polyhedra through edges and corners.

## Related literature

Besides crystals of the title compound, crystals of the hexagonal polymorph  $\sigma$ -Ba<sub>2</sub>P<sub>2</sub>O<sub>7</sub> were obtained (ElBelghitti *et al.* 1995). For isotypic structures, see: Hagman *et al.* (1968); Grenier & Masse (1977); Barbier & Echard (1998). For closely related structures, see: Elmarzouki *et al.* (1995). For polymorphism in Ba<sub>2</sub>P<sub>2</sub>O<sub>7</sub>, see: McCauley & Hummel (1968); Mehdi *et al.* (1977); Bian *et al.* (2004); Kokhanovskii (2004). For a review of the crystal chemistry of diphosphates, see: Durif (1995). For applications of alkaline earth diphosphates, see: Pang *et al.* (2009); Peng *et al.* (2010). For an independent refinement of the  $\alpha$ -Ba<sub>2</sub>P<sub>2</sub>O<sub>7</sub> structure based on data from a hydrothermally grown crystal, see: Heyward *et al.* (2010).

## Experimental

## Crystal data

Ba<sub>2</sub>P<sub>2</sub>O<sub>7</sub>  
 $M_r = 448.62$

Orthorhombic,  $Pnma$   
 $a = 9.2875$  (1) Å

$b = 5.6139$  (1) Å  
 $c = 13.8064$  (1) Å  
 $V = 719.85$  (2) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 11.31$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.26 \times 0.14 \times 0.14$  mm

## Data collection

Bruker APEXII CCD diffractometer  
Absorption correction: multi-scan (SADABS; Bruker, 2008)  
 $T_{\min} = 0.155$ ,  $T_{\max} = 0.205$

18034 measured reflections  
4304 independent reflections  
3726 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.028$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.021$   
 $wR(F^2) = 0.046$   
 $S = 1.07$   
4304 reflections

62 parameters  
 $\Delta\rho_{\text{max}} = 1.59$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -1.99$  e Å<sup>-3</sup>

Table 1

Selected bond lengths (Å).

Ba1—O3 <sup>i</sup>	2.7585 (10)	Ba2—O4 <sup>vi</sup>	2.9313 (4)
Ba1—O2 <sup>ii</sup>	2.7591 (10)	P1—O5	1.5067 (13)
Ba1—O4 <sup>iii</sup>	2.7978 (13)	P1—O2 <sup>vii</sup>	1.5208 (11)
Ba1—O2	2.8392 (10)	P1—O2	1.5208 (11)
Ba1—O5	3.0850 (6)	P1—O1	1.6148 (13)
Ba2—O5 <sup>iv</sup>	2.5794 (13)	P2—O4 <sup>viii</sup>	1.5175 (13)
Ba2—O3 <sup>ii</sup>	2.7377 (10)	P2—O3 <sup>vii</sup>	1.5236 (11)
Ba2—O2 <sup>iii</sup>	2.8133 (10)	P2—O3	1.5236 (11)
Ba2—O3 <sup>v</sup>	2.9094 (10)	P2—O1	1.6012 (14)

Symmetry codes: (i)  $x + \frac{1}{2}, y, -z + \frac{3}{2}$ ; (ii)  $x + \frac{1}{2}, -y + \frac{1}{2}, -z + \frac{3}{2}$ ; (iii)  $-x, -y, -z + 1$ ; (iv)  $-x + \frac{1}{2}, -y, z - \frac{1}{2}$ ; (v)  $-x - \frac{1}{2}, -y, z - \frac{1}{2}$ ; (vi)  $x + \frac{1}{2}, y + 1, -z + \frac{3}{2}$ ; (vii)  $x, -y - \frac{1}{2}, z$ ; (viii)  $x, y, z + 1$ .

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 1999) and ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

This work was supported by the French–Moroccan integrated action (grant No. MA/05/119 F).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2413).

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## supporting information

*Acta Cryst.* (2010). E66, i76–i77 [doi:10.1107/S1600536810043539]

 **$\alpha$ -Ba<sub>2</sub>P<sub>2</sub>O<sub>7</sub>**

**Driss Zakaria, Fatima Erragh, Abdelghani Oudahmane, Malika El-Ghozzi and Daniel Avignant**

**S1. Comment**

Due to their potential applications as optical materials (Pang *et al.*, 2009, Peng *et al.*, 2010), alkaline earth diphosphates exhibit at the present time a growing interest. Since the optical properties are strongly related to the crystal structure, the study of polymorphism in these materials is worth investigating. Besides the hexagonal form  $\sigma$ -Ba<sub>2</sub>P<sub>2</sub>O<sub>7</sub> described by ElBelghitti *et al.* (1995), the title compound is the second polymorph for this composition obtained in the form of single-crystals. The orthorhombic title compound  $\alpha$ -Ba<sub>2</sub>P<sub>2</sub>O<sub>7</sub> is isotypic with  $\alpha$ -Sr<sub>2</sub>P<sub>2</sub>O<sub>7</sub> (Hagman *et al.* 1968; Grenier & Masse, 1977; Barbier & Echard, 1998) and closely related to BaPbP<sub>2</sub>O<sub>7</sub> (Elmarzouki *et al.*, 1995). The existence of this polymorph has previously been mentioned by Durif (1995) and several other authors (McCauley & Hummel, 1968; Mehdi *et al.*, 1977; Bian *et al.*, 2004; Kokhanovskii, 2004).

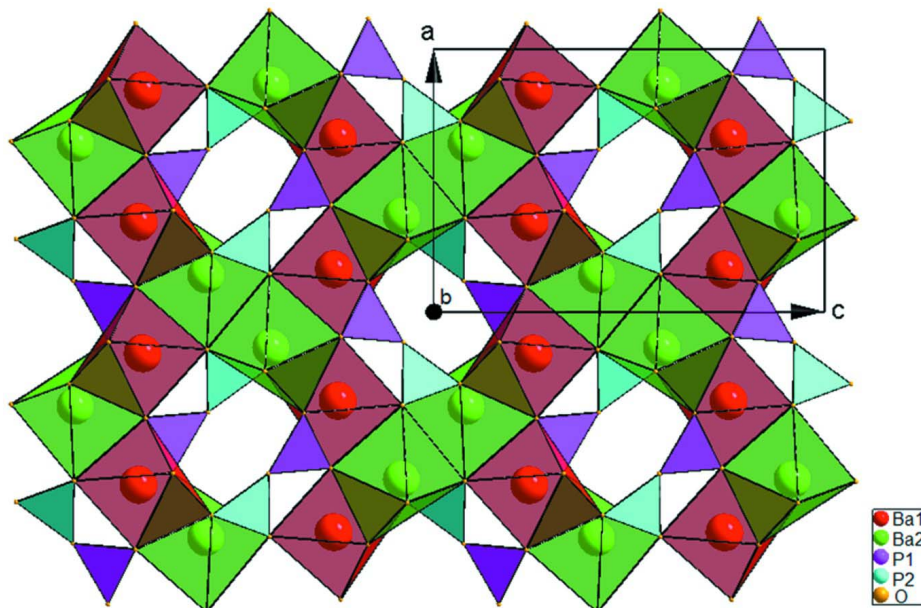
The structure of the  $\alpha$ -polymorph is built up from two different BaO<sub>9</sub> polyhedra with Ba—O distances ranging from 2.7585 (10) Å to 3.0850 (6) Å and from 2.5794 (13) Å to 2.9313 (4) Å, respectively. Figure 1 displays details of these coordination polyhedra as well as their linkage by corners, edges or triangular faces to form the three-dimensional framework. This polyhedral linkage delimits large channels parallel to [010] where the P<sub>2</sub>O<sub>7</sub> diphosphate groups are located (Fig. 2). These groups (symmetry *m*) are characterized by a P—O—P angle of 131.52 (9)° and an eclipsed conformation. They are connected to the BaO<sub>9</sub> polyhedra through edges and corners. Each oxygen atom of the P<sub>2</sub>O<sub>7</sub> groups, apart from the O1 bridging oxygen, is bonded to three Ba atoms and one phosphorus atom. During the anisotropic refinement of the displacement parameters of the isotypic  $\alpha$ -Sr<sub>2</sub>P<sub>2</sub>O<sub>7</sub> structure (Barbier & Echard, 1998), the authors observed a very strong anisotropy along the *b* direction for both O5 and O1 atoms located in the (010) mirror plane and interpreted this phenomenon as a possible atomic-scale disorder associated with the local loss of mirror symmetry resulting in a non-centrosymmetric structural arrangement. Such an outstanding feature is still present in our anisotropic structure refinement, although the amplitudes of the atomic displacement parameters are significantly lower, especially for the *U*<sub>22</sub> component of the O5 atom. If the strong anisotropy of the O1 atom is perfectly understandable because of its bridging role, that of the O5 atom strongly bonded to two Ba1 atoms at 3.0850 (6) Å, one Ba2 atom at 2.5794 (13) Å and one P1 atom at 1.5067 (13) Å is more surprising. However, due to the relative homogeneity of the values of the isotropic displacement parameters of all oxygen atoms, it does not seem necessary to envisage any atomic-scale disorder for the O5 atom in the present case.

Simultaneous with our refinement, an independent study of the  $\alpha$ -Ba<sub>2</sub>P<sub>2</sub>O<sub>7</sub> structure from a hydrothermally grown crystal was reported by Heyward *et al.* (2010). The results of both refinements in terms of geometric parameters are the same within the threefold standard deviation.

**S2. Experimental**

Single crystals of the title compound have been obtained during the study of the phase relationships in the ternary system Na<sub>2</sub>O—BaO—P<sub>2</sub>O<sub>5</sub>. They were synthesized in the solid state by reacting Na<sub>2</sub>CO<sub>3</sub>, BaCO<sub>3</sub> and (NH<sub>4</sub>)<sub>2</sub>HPO<sub>4</sub> in a platinum



**Figure 2**

Projection of the  $\alpha$ -Ba<sub>2</sub>P<sub>2</sub>O<sub>7</sub> structure along [010] showing the connections between the P<sub>2</sub>O<sub>7</sub> diphosphate groups and the three-dimensional framework of the BaO<sub>9</sub> polyhedra.

### dibarium diphosphate

#### Crystal data

Ba<sub>2</sub>P<sub>2</sub>O<sub>7</sub>

$M_r = 448.62$

Orthorhombic, *Pnma*

Hall symbol: -P 2ac 2n

$a = 9.2875$  (1) Å

$b = 5.6139$  (1) Å

$c = 13.8064$  (1) Å

$V = 719.85$  (2) Å<sup>3</sup>

$Z = 4$

$F(000) = 792$

$D_x = 4.139$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 7790 reflections

$\theta = 3.7$ – $52.2^\circ$

$\mu = 11.31$  mm<sup>-1</sup>

$T = 296$  K

Hexagonal prism, colourless

$0.26 \times 0.14 \times 0.14$  mm

#### Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 8.3333 pixels mm<sup>-1</sup>

$\omega$  and  $\varphi$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2008)

$T_{\min} = 0.155$ ,  $T_{\max} = 0.205$

18034 measured reflections

4304 independent reflections

3726 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.028$

$\theta_{\max} = 52.4^\circ$ ,  $\theta_{\min} = 4.5^\circ$

$h = -17 \rightarrow 20$

$k = -12 \rightarrow 10$

$l = -30 \rightarrow 28$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.021$

$wR(F^2) = 0.046$

$S = 1.07$

4304 reflections

62 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

$$w = 1/[\sigma^2(F_o^2) + (0.0176P)^2 + 0.4317P]$$

where  $P = (F_o^2 + 2F_c^2)/3$

$$(\Delta/\sigma)_{\max} = 0.004$$

$$\Delta\rho_{\max} = 1.59 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.99 \text{ e } \text{\AA}^{-3}$$

Extinction correction: *SHELXL97* (Sheldrick,  
2008),  $F_c^* = kFc[1 + 0.001x\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0075 (2)

*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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ba1	0.159652 (9)	0.2500	0.744870 (6)	0.00801 (2)
Ba2	0.138138 (9)	0.2500	0.417071 (6)	0.00841 (2)
P1	-0.04603 (4)	-0.2500	0.81569 (3)	0.00724 (6)
P2	-0.28072 (4)	-0.2500	0.95778 (3)	0.00722 (6)
O1	-0.11642 (14)	-0.2500	0.92264 (9)	0.0129 (2)
O2	-0.09496 (10)	-0.0264 (2)	0.76295 (7)	0.01169 (13)
O3	-0.35537 (10)	-0.0271 (2)	0.91982 (6)	0.01215 (14)
O4	-0.27382 (15)	-0.2500	0.06760 (9)	0.0130 (2)
O5	0.11429 (14)	-0.2500	0.83242 (11)	0.0160 (3)

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ba1	0.00795 (3)	0.00736 (4)	0.00873 (3)	0.000	-0.00047 (2)	0.000
Ba2	0.00856 (3)	0.00891 (4)	0.00776 (3)	0.000	0.00084 (2)	0.000
P1	0.00544 (11)	0.00757 (16)	0.00873 (13)	0.000	0.00010 (9)	0.000
P2	0.00839 (12)	0.00706 (16)	0.00622 (12)	0.000	0.00066 (9)	0.000
O1	0.0088 (4)	0.0198 (7)	0.0100 (4)	0.000	0.0012 (3)	0.000
O2	0.0126 (3)	0.0091 (4)	0.0133 (3)	0.0008 (3)	0.0005 (2)	0.0022 (3)
O3	0.0145 (3)	0.0101 (4)	0.0119 (3)	0.0029 (3)	0.0000 (2)	0.0022 (3)
O4	0.0161 (5)	0.0160 (6)	0.0069 (4)	0.000	0.0003 (3)	0.000
O5	0.0061 (3)	0.0243 (8)	0.0176 (5)	0.000	-0.0008 (3)	0.000

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

Ba1—O3 <sup>i</sup>	2.7585 (10)	P1—O2 <sup>xiii</sup>	1.5208 (11)
Ba1—O3 <sup>ii</sup>	2.7585 (10)	P1—O2	1.5208 (11)
Ba1—O2 <sup>ii</sup>	2.7591 (10)	P1—O1	1.6148 (13)
Ba1—O2 <sup>i</sup>	2.7591 (10)	P1—Ba2 <sup>iii</sup>	3.3255 (4)
Ba1—O4 <sup>iii</sup>	2.7978 (13)	P2—O4 <sup>xiv</sup>	1.5175 (13)

Ba1—O2	2.8392 (10)	P2—O3 <sup>xiii</sup>	1.5236 (11)
Ba1—O2 <sup>iv</sup>	2.8392 (10)	P2—O3	1.5236 (11)
Ba1—O5 <sup>v</sup>	3.0850 (6)	P2—O1	1.6012 (14)
Ba1—O5	3.0850 (6)	P2—Ba2 <sup>xv</sup>	3.3668 (4)
Ba2—O5 <sup>vi</sup>	2.5794 (13)	P2—Ba2 <sup>xvi</sup>	3.3812 (2)
Ba2—O3 <sup>ii</sup>	2.7377 (10)	P2—Ba2 <sup>xvii</sup>	3.3812 (2)
Ba2—O3 <sup>i</sup>	2.7377 (10)	O2—Ba1 <sup>xvi</sup>	2.7591 (10)
Ba2—O2 <sup>iii</sup>	2.8133 (10)	O2—Ba2 <sup>iii</sup>	2.8133 (10)
Ba2—O2 <sup>vii</sup>	2.8133 (10)	O3—Ba2 <sup>xvi</sup>	2.7377 (10)
Ba2—O3 <sup>viii</sup>	2.9094 (10)	O3—Ba1 <sup>xvi</sup>	2.7585 (10)
Ba2—O3 <sup>ix</sup>	2.9094 (10)	O3—Ba2 <sup>xv</sup>	2.9094 (10)
Ba2—O4 <sup>x</sup>	2.9313 (4)	O4—P2 <sup>xviii</sup>	1.5175 (13)
Ba2—O4 <sup>xi</sup>	2.9313 (4)	O4—Ba1 <sup>iii</sup>	2.7978 (13)
Ba2—P1 <sup>iii</sup>	3.3255 (4)	O4—Ba2 <sup>xix</sup>	2.9313 (4)
Ba2—P2 <sup>viii</sup>	3.3668 (4)	O4—Ba2 <sup>xx</sup>	2.9313 (4)
Ba2—P2 <sup>xii</sup>	3.3812 (2)	O5—Ba2 <sup>xxi</sup>	2.5794 (13)
P1—O5	1.5067 (13)	O5—Ba1 <sup>xxii</sup>	3.0850 (6)
O3 <sup>i</sup> —Ba1—O3 <sup>ii</sup>	68.66 (5)	O3 <sup>ii</sup> —Ba2—O3 <sup>ix</sup>	76.39 (3)
O3 <sup>i</sup> —Ba1—O2 <sup>ii</sup>	109.06 (3)	O3 <sup>i</sup> —Ba2—O3 <sup>ix</sup>	104.688 (19)
O3 <sup>ii</sup> —Ba1—O2 <sup>ii</sup>	72.09 (3)	O2 <sup>iii</sup> —Ba2—O3 <sup>ix</sup>	94.29 (3)
O3 <sup>i</sup> —Ba1—O2 <sup>i</sup>	72.09 (3)	O2 <sup>vii</sup> —Ba2—O3 <sup>ix</sup>	71.99 (3)
O3 <sup>ii</sup> —Ba1—O2 <sup>i</sup>	109.06 (3)	O3 <sup>viii</sup> —Ba2—O3 <sup>ix</sup>	50.95 (4)
O2 <sup>ii</sup> —Ba1—O2 <sup>i</sup>	68.43 (4)	O5 <sup>vi</sup> —Ba2—O4 <sup>x</sup>	77.53 (3)
O3 <sup>i</sup> —Ba1—O4 <sup>iii</sup>	141.44 (2)	O3 <sup>ii</sup> —Ba2—O4 <sup>x</sup>	52.44 (3)
O3 <sup>ii</sup> —Ba1—O4 <sup>iii</sup>	141.44 (3)	O3 <sup>i</sup> —Ba2—O4 <sup>x</sup>	118.59 (3)
O2 <sup>ii</sup> —Ba1—O4 <sup>iii</sup>	73.93 (3)	O2 <sup>iii</sup> —Ba2—O4 <sup>x</sup>	122.07 (3)
O2 <sup>i</sup> —Ba1—O4 <sup>iii</sup>	73.93 (3)	O2 <sup>vii</sup> —Ba2—O4 <sup>x</sup>	71.11 (3)
O3 <sup>i</sup> —Ba1—O2	73.87 (3)	O3 <sup>viii</sup> —Ba2—O4 <sup>x</sup>	131.51 (3)
O3 <sup>ii</sup> —Ba1—O2	109.79 (3)	O3 <sup>ix</sup> —Ba2—O4 <sup>x</sup>	80.73 (3)
O2 <sup>ii</sup> —Ba1—O2	177.035 (6)	O5 <sup>vi</sup> —Ba2—O4 <sup>xi</sup>	77.53 (3)
O2 <sup>i</sup> —Ba1—O2	112.59 (4)	O3 <sup>ii</sup> —Ba2—O4 <sup>xi</sup>	118.59 (3)
O4 <sup>iii</sup> —Ba1—O2	103.55 (3)	O3 <sup>i</sup> —Ba2—O4 <sup>xi</sup>	52.44 (3)
O3 <sup>i</sup> —Ba1—O2 <sup>iv</sup>	109.79 (3)	O2 <sup>iii</sup> —Ba2—O4 <sup>xi</sup>	71.11 (3)
O3 <sup>ii</sup> —Ba1—O2 <sup>iv</sup>	73.87 (3)	O2 <sup>vii</sup> —Ba2—O4 <sup>xi</sup>	122.07 (3)
O2 <sup>ii</sup> —Ba1—O2 <sup>iv</sup>	112.59 (4)	O3 <sup>viii</sup> —Ba2—O4 <sup>xi</sup>	80.73 (3)
O2 <sup>i</sup> —Ba1—O2 <sup>iv</sup>	177.035 (6)	O3 <sup>ix</sup> —Ba2—O4 <sup>xi</sup>	131.51 (3)
O4 <sup>iii</sup> —Ba1—O2 <sup>iv</sup>	103.55 (3)	O4 <sup>x</sup> —Ba2—O4 <sup>xi</sup>	146.51 (5)
O2—Ba1—O2 <sup>iv</sup>	66.25 (4)	O5—P1—O2 <sup>xiii</sup>	111.63 (5)
O3 <sup>i</sup> —Ba1—O5 <sup>v</sup>	146.01 (3)	O5—P1—O2	111.63 (5)
O3 <sup>ii</sup> —Ba1—O5 <sup>v</sup>	78.63 (3)	O2 <sup>xiii</sup> —P1—O2	111.29 (8)
O2 <sup>ii</sup> —Ba1—O5 <sup>v</sup>	67.45 (3)	O5—P1—O1	105.06 (8)
O2 <sup>i</sup> —Ba1—O5 <sup>v</sup>	129.77 (3)	O2 <sup>xiii</sup> —P1—O1	108.47 (5)
O4 <sup>iii</sup> —Ba1—O5 <sup>v</sup>	71.89 (3)	O2—P1—O1	108.47 (5)
O2—Ba1—O5 <sup>v</sup>	110.43 (3)	P2—O1—P1	131.52 (9)
O2 <sup>iv</sup> —Ba1—O5 <sup>v</sup>	49.81 (3)	P1—O2—Ba1 <sup>xvi</sup>	136.86 (5)
O3 <sup>i</sup> —Ba1—O5	78.63 (3)	P1—O2—Ba2 <sup>iii</sup>	95.57 (5)
O3 <sup>ii</sup> —Ba1—O5	146.01 (3)	Ba1 <sup>xvi</sup> —O2—Ba2 <sup>iii</sup>	95.66 (3)

O2 <sup>ii</sup> —Ba1—O5	129.77 (3)	P1—O2—Ba1	104.14 (5)
O2 <sup>i</sup> —Ba1—O5	67.45 (3)	Ba1 <sup>xvi</sup> —O2—Ba1	112.16 (4)
O4 <sup>iii</sup> —Ba1—O5	71.89 (3)	Ba2 <sup>iii</sup> —O2—Ba1	106.55 (3)
O2—Ba1—O5	49.81 (3)	P2—O3—Ba2 <sup>xvi</sup>	101.17 (4)
O2 <sup>iv</sup> —Ba1—O5	110.43 (3)	P2—O3—Ba1 <sup>xvi</sup>	136.36 (5)
O5 <sup>v</sup> —Ba1—O5	130.97 (5)	Ba2 <sup>xvi</sup> —O3—Ba1 <sup>xvi</sup>	111.02 (4)
O5 <sup>vi</sup> —Ba2—O3 <sup>ii</sup>	110.68 (3)	P2—O3—Ba2 <sup>xv</sup>	93.55 (5)
O5 <sup>vi</sup> —Ba2—O3 <sup>i</sup>	110.68 (3)	Ba2 <sup>xvi</sup> —O3—Ba2 <sup>xv</sup>	103.61 (3)
O3 <sup>ii</sup> —Ba2—O3 <sup>i</sup>	69.25 (4)	Ba1 <sup>xvi</sup> —O3—Ba2 <sup>xv</sup>	106.11 (3)
O5 <sup>vi</sup> —Ba2—O2 <sup>iii</sup>	74.14 (3)	P2 <sup>xviii</sup> —O4—Ba1 <sup>iii</sup>	160.15 (8)
O3 <sup>ii</sup> —Ba2—O2 <sup>iii</sup>	169.56 (3)	P2 <sup>xviii</sup> —O4—Ba2 <sup>xix</sup>	93.46 (3)
O3 <sup>i</sup> —Ba2—O2 <sup>iii</sup>	118.44 (3)	Ba1 <sup>iii</sup> —O4—Ba2 <sup>xix</sup>	92.23 (3)
O5 <sup>vi</sup> —Ba2—O2 <sup>vii</sup>	74.14 (3)	P2 <sup>xviii</sup> —O4—Ba2 <sup>xx</sup>	93.46 (3)
O3 <sup>ii</sup> —Ba2—O2 <sup>vii</sup>	118.44 (3)	Ba1 <sup>iii</sup> —O4—Ba2 <sup>xx</sup>	92.23 (3)
O3 <sup>i</sup> —Ba2—O2 <sup>vii</sup>	169.56 (3)	Ba2 <sup>xix</sup> —O4—Ba2 <sup>xx</sup>	146.51 (5)
O2 <sup>iii</sup> —Ba2—O2 <sup>vii</sup>	53.01 (4)	P1—O5—Ba2 <sup>xxi</sup>	161.87 (9)
O5 <sup>vi</sup> —Ba2—O3 <sup>viii</sup>	144.15 (3)	P1—O5—Ba1 <sup>xxii</sup>	94.30 (3)
O3 <sup>ii</sup> —Ba2—O3 <sup>viii</sup>	104.688 (19)	Ba2 <sup>xxi</sup> —O5—Ba1 <sup>xxii</sup>	93.20 (3)
O3 <sup>i</sup> —Ba2—O3 <sup>viii</sup>	76.39 (3)	P1—O5—Ba1	94.30 (3)
O2 <sup>iii</sup> —Ba2—O3 <sup>viii</sup>	71.99 (3)	Ba2 <sup>xxi</sup> —O5—Ba1	93.20 (3)
O2 <sup>vii</sup> —Ba2—O3 <sup>viii</sup>	94.29 (3)	Ba1 <sup>xxii</sup> —O5—Ba1	130.97 (5)
O5 <sup>vi</sup> —Ba2—O3 <sup>ix</sup>	144.15 (3)		

Symmetry codes: (i)  $x+1/2, y, -z+3/2$ ; (ii)  $x+1/2, -y+1/2, -z+3/2$ ; (iii)  $-x, -y, -z+1$ ; (iv)  $x, -y+1/2, z$ ; (v)  $x, y+1, z$ ; (vi)  $-x+1/2, -y, z-1/2$ ; (vii)  $-x, y+1/2, -z+1$ ; (viii)  $-x-1/2, -y, z-1/2$ ; (ix)  $-x-1/2, y+1/2, z-1/2$ ; (x)  $x+1/2, y+1, -z+1/2$ ; (xi)  $x+1/2, y, -z+1/2$ ; (xii)  $x+1/2, y+1, -z+3/2$ ; (xiii)  $x, -y-1/2, z$ ; (xiv)  $x, y, z+1$ ; (xv)  $-x-1/2, -y, z+1/2$ ; (xvi)  $x-1/2, y, -z+3/2$ ; (xvii)  $x-1/2, y-1, -z+3/2$ ; (xviii)  $x, y, z-1$ ; (xix)  $x-1/2, y-1, -z+1/2$ ; (xx)  $x-1/2, y, -z+1/2$ ; (xxi)  $-x+1/2, -y, z+1/2$ ; (xxii)  $x, y-1, z$ .