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Redetermination of  $\beta$ -Ba(PO<sub>3</sub>)<sub>2</sub>

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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{P}-\text{O}) = 0.003$  Å;  $R$  factor = 0.020;  $wR$  factor = 0.047; data-to-parameter ratio = 19.4.

In comparison with the previous structure determination of the  $\beta$ -modification of barium *catena*-polyphosphate that was based on Weissenberg film data [Grenier *et al.* (1967). *Bull. Soc. Fr. Minéral. Cristallogr.* **90**, 24–31], the current CCD-data-based redetermination reveals all atoms with anisotropic displacement parameters, standard uncertainties for the atomic coordinates, and the determination of the absolute structure. Moreover, a much higher accuracy in terms of the bond-length distribution for the polyphosphate chain, with two shorter and two longer P–O distances, was achieved. The structure consists of polyphosphate chains extending parallel to [100] with a periodicity of two PO<sub>4</sub> tetrahedra. The Ba<sup>2+</sup> cations are located between the chains and are surrounded by ten O atoms in the form of a distorted coordination polyhedron, with Ba–O distances ranging from 2.765 (3) to 3.143 (3) Å, also reflecting the higher precision of the current redetermination.

## Related literature

For polymorphism of Ba(PO<sub>3</sub>)<sub>2</sub>, see: Grenier & Martin (1975). For the previous structure refinement of  $\beta$ -Ba(PO<sub>3</sub>)<sub>2</sub>, see: Grenier *et al.* (1967). For the structure refinement of  $\gamma$ -Ba(PO<sub>3</sub>)<sub>2</sub>, see: Coing-Boyat *et al.* (1978). For the crystal chemistry of condensed phosphates, see: Durif (1995). For standardization of structure data, see: Gelato & Parthé (1987).

## Experimental

## Crystal data

Ba(PO <sub>3</sub> ) <sub>2</sub>	$V = 502.19$ (4) Å <sup>3</sup>
$M_r = 295.28$	$Z = 4$
Orthorhombic, $P2_12_1$	Mo $K\alpha$ radiation
$a = 4.4979$ (2) Å	$\mu = 8.50$ mm <sup>-1</sup>
$b = 8.3377$ (4) Å	$T = 293$ K
$c = 13.3911$ (6) Å	$0.15 \times 0.08 \times 0.05$ mm

## Data collection

Bruker SMART CCD diffractometer	5836 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2007)	1587 independent reflections
$T_{\min} = 0.362$ , $T_{\max} = 0.676$	1560 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.016$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.020$	$\Delta\rho_{\min} = -0.75$ e Å <sup>-3</sup>
$wR(F^2) = 0.047$	Absolute structure: Flack (1983), 624 Friedel pairs
$S = 1.13$	Absolute structure parameter: 0.04 (2)
1587 reflections	
82 parameters	
$\Delta\rho_{\max} = 1.09$ e Å <sup>-3</sup>	

Table 1

Comparison of the P–O bond lengths (Å) of the two related PO<sub>4</sub> tetrahedra in the current and the previous (Grenier *et al.*, 1967) refinement of  $\beta$ -Ba(PO<sub>3</sub>)<sub>2</sub>.

current refinement	previous refinement
P1–O3 1.475 (2) <sup>viii</sup>	P2–O6 1.427
P1–O1 1.480 (2) <sup>viii</sup>	P2–O5 1.540
P1–O6 1.607 (2) <sup>ix</sup>	P2–O2 1.590
P1–O4 1.625 (2) <sup>viii</sup>	P2–O1 1.652
P2–O2 1.481 (2)	P1–O3 1.476
P2–O5 1.486 (2) <sup>vii</sup>	P1–O4 1.540
P2–O6 1.604 (3) <sup>vi</sup>	P1–O2 1.559
P2–O4 1.607 (3) <sup>vi</sup>	P1–O1 1.621

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

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ATOMS (Dowty, 2006); software used to prepare material for publication: publCIF (Westrip, 2010).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: PJ2008).

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## supporting information

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Redetermination of  $\beta$ -Ba(PO<sub>3</sub>)<sub>2</sub>

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## S1. Comment

Polymorphism of Ba(PO<sub>3</sub>)<sub>2</sub> with three modifications has been reported by Grenier & Martin (1975): The stable  $\beta$ -form transforms to the high-temperature  $\alpha$ -form at 1058 K, and the  $\gamma$ -form transforms at 978 K to the  $\beta$ -form. Structure determinations were carried out for the  $\gamma$ -form (Coing-Boyat *et al.*, 1978) and for the  $\beta$ -form (Grenier *et al.*, 1967). The crystal structure of  $\alpha$ -Ba(PO<sub>3</sub>)<sub>2</sub> is yet unknown. Comparative discussions of the structural set-up of the  $\beta$ - and  $\gamma$ -form of Ba(PO<sub>3</sub>)<sub>2</sub> and of other divalent long-chain polyphosphates were given by Durif (1995).

During experiments intended to isolate crystals of  $\alpha$ -Ba(PO<sub>3</sub>)<sub>2</sub> by quenching the reaction product from the re-crystallized melt at temperatures above the indicated transition point, high-quality crystals of  $\beta$ -Ba(PO<sub>3</sub>)<sub>2</sub> were obtained instead. Since the first structure refinement of this modification was based on Weissenberg film data and converged with a relatively high residual  $R = 0.1$ , with atoms refined only with isotropic displacement factors and without indication of standard uncertainties for the fractional atomic coordinates, a re-refinement of the structure with modern CCD-based data seemed appropriate. The results of this re-refinement are reported here, confirming in principle the results of Grenier *et al.* (1967), however, achieving bond lengths and angles with much higher accuracy and precision, as exemplified by a comparison of the P—O bond length (Table 1).

The *catena*-polyphosphate chain has a periodicity of two PO<sub>4</sub> tetrahedra and extends parallel to [100] (Fig. 1). In comparison with the previous structure refinement (Grenier *et al.*, 1967), the determined bond lengths of the present refinement are in much better agreement with the usually observed bond length distribution in such long-chain polyphosphates (Durif, 1995), with two shorter and two longer P—O distances, each with similar values (Table 1).

The Ba<sup>2+</sup> cation is located between the chains and is surrounded by ten oxygen atoms in an irregular coordination sphere with Ba—O distances in the range from 2.765 (3) to 3.143 (3) Å (Fig. 2).

## S2. Experimental

Stoichiometric amounts of BaCO<sub>3</sub> and (NH<sub>4</sub>)<sub>2</sub>HPO<sub>4</sub> (molar ratio 1:2) with a 3% excess of the phosphate precursor were finely ground, heated in a platinum crucible to 1173 K and slowly cooled to 1073 K at a rate of 2 K h<sup>-1</sup>. Then the crucible was quenched in a cold water bath. Colourless fragments of the title compound were cut from the clear, transparent reaction product.

## S3. Refinement

In contrast to the previous structure refinement (Grenier *et al.*, 1967) with  $a = 4.510$  (2),  $b = 13.44$  (2)  $c = 8.36$  (5) Å, the reduced cell setting was chosen for the current refinement. Structure data were finally standardized with *STRUCTURE-TIDY* (Gelato & Parthé, 1987). The highest and lowest remaining electron densities are located 0.75 Å from Ba and 1.19 Å from O6, respectively.

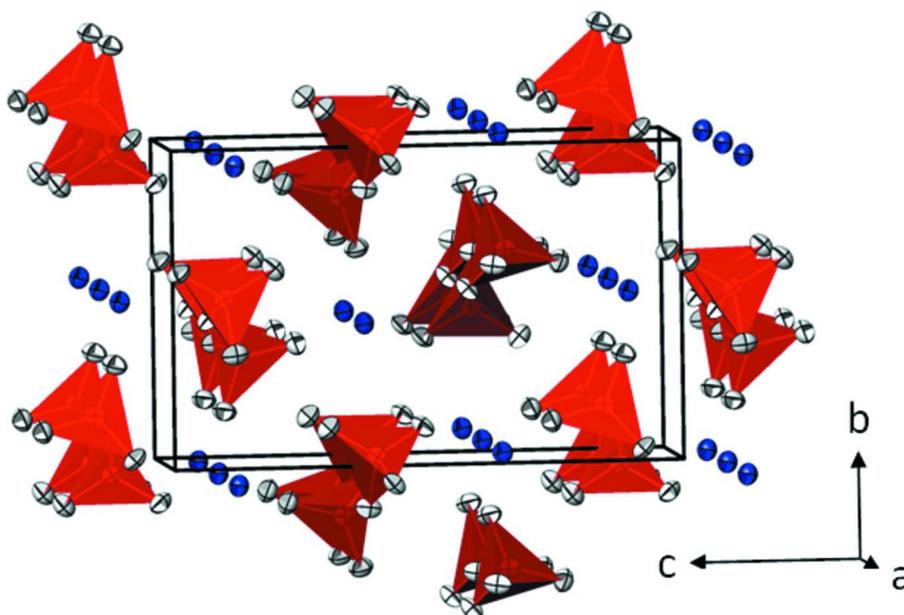
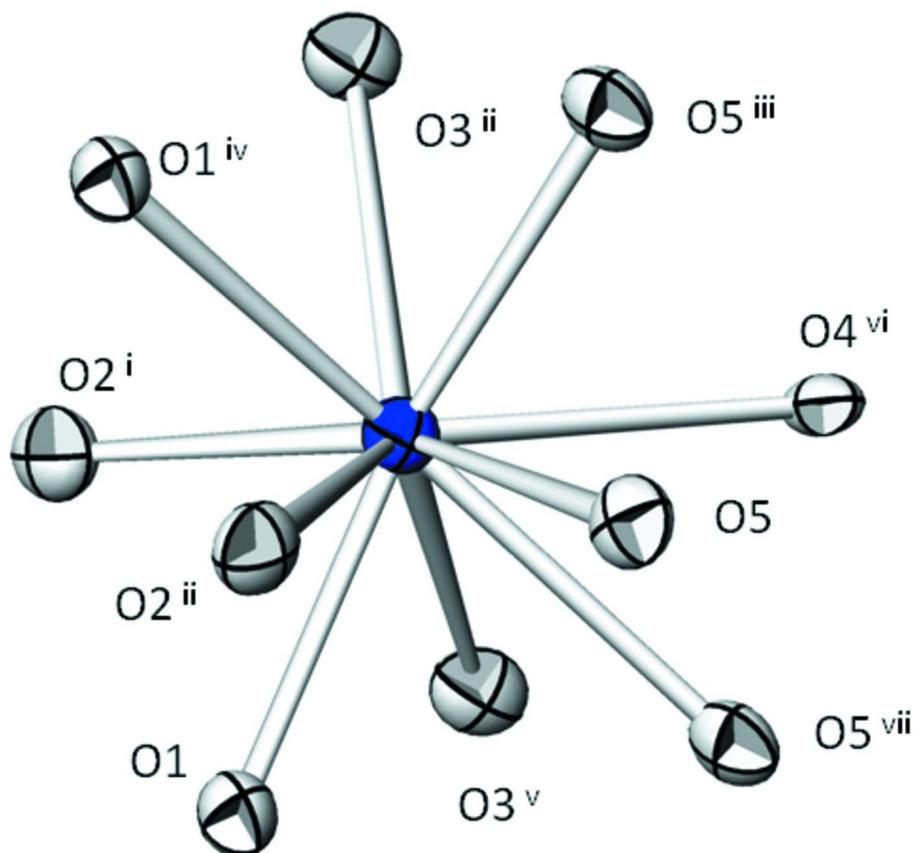


Figure 1

The crystal structure of  $\beta$ -Ba(PO<sub>3</sub>)<sub>2</sub> in a projection approximately along [100]. Ba<sup>2+</sup> cations are shown in blue, PO<sub>4</sub> tetrahedra in red with O atoms in white. Displacement ellipsoids are drawn at the 90% probability level. For clarity, no Ba—O bonds are shown.



**Figure 2**

The irregular  $\text{BaO}_{10}$  coordination polyhedron in the structure of  $\beta\text{-Ba}(\text{PO}_3)_2$ . Displacement ellipsoids are drawn at the 90% probability level. [Symmetry codes: (i)  $-x + 1/2, -y, z - 1/2$ ; (ii)  $-x + 1, y - 1/2, -z + 1/2$ ; (iii)  $x + 1/2, -y + 1/2, -z + 1$ ; (iv)  $x + 1, y, z$ ; (v)  $-x, y - 1/2, -z + 1/2$ ; (vi)  $-x + 1/2, -y, z + 1/2$ ; (vii)  $x - 1/2, -y + 1/2, -z + 1$ .]

### Barium *catena*-polyphosphate

#### Crystal data

$\text{Ba}(\text{PO}_3)_2$   
 $M_r = 295.28$   
 Orthorhombic,  $P2_12_12_1$   
 Hall symbol:  $P\ 2ac\ 2ab$   
 $a = 4.4979\ (2)\ \text{\AA}$   
 $b = 8.3377\ (4)\ \text{\AA}$   
 $c = 13.3911\ (6)\ \text{\AA}$   
 $V = 502.19\ (4)\ \text{\AA}^3$   
 $Z = 4$

$F(000) = 536$   
 $D_x = 3.905\ \text{Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$   
 Cell parameters from 4713 reflections  
 $\theta = 2.4\text{--}31.0^\circ$   
 $\mu = 8.50\ \text{mm}^{-1}$   
 $T = 293\ \text{K}$   
 Fragment, colourless  
 $0.15 \times 0.08 \times 0.05\ \text{mm}$

#### Data collection

Bruker SMART CCD  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 $\omega$  scan

Absorption correction: multi-scan  
 (*SADABS*; Bruker, 2007)  
 $T_{\min} = 0.362, T_{\max} = 0.676$   
 5836 measured reflections  
 1587 independent reflections  
 1560 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.016$   
 $\theta_{\text{max}} = 31.0^\circ$ ,  $\theta_{\text{min}} = 2.9^\circ$   
 $h = -6 \rightarrow 6$

$k = -12 \rightarrow 11$   
 $l = -19 \rightarrow 19$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.020$   
 $wR(F^2) = 0.047$   
 $S = 1.13$   
 1587 reflections  
 82 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 $w = 1/[\sigma^2(F_o^2) + (0.0223P)^2 + 0.9553P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 1.09 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.75 \text{ e } \text{\AA}^{-3}$   
 Absolute structure: Flack (1983), 624 Friedel  
 pairs  
 Absolute structure parameter: 0.04 (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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Ba	0.49023 (4)	0.05203 (2)	0.375501 (12)	0.01202 (6)
P1	0.03622 (19)	0.67382 (10)	0.34674 (6)	0.00958 (15)
P2	0.04126 (18)	0.03118 (10)	0.60393 (6)	0.01002 (15)
O1	0.0024 (8)	0.1293 (3)	0.25946 (16)	0.0142 (4)
O2	0.0272 (6)	0.1222 (3)	0.69880 (17)	0.0153 (4)
O3	0.0307 (6)	0.3369 (3)	0.11686 (17)	0.0149 (4)
O4	0.1343 (5)	0.0429 (3)	0.08393 (18)	0.0116 (4)
O5	0.4603 (6)	0.3816 (3)	0.48895 (17)	0.0142 (5)
O6	0.6315 (5)	0.1360 (3)	0.11585 (19)	0.0131 (4)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ba	0.01116 (8)	0.01345 (9)	0.01147 (8)	-0.00007 (7)	-0.00044 (8)	0.00042 (6)
P1	0.0082 (3)	0.0093 (3)	0.0113 (3)	0.0002 (3)	-0.0007 (3)	-0.0001 (3)
P2	0.0087 (3)	0.0103 (3)	0.0111 (3)	0.0000 (3)	-0.0001 (3)	0.0008 (3)
O1	0.0152 (9)	0.0156 (10)	0.0118 (9)	0.0018 (12)	0.0002 (11)	0.0016 (8)
O2	0.0163 (11)	0.0151 (10)	0.0145 (10)	-0.0008 (11)	-0.0010 (10)	-0.0037 (8)
O3	0.0167 (11)	0.0110 (10)	0.0171 (10)	-0.0020 (10)	-0.0019 (12)	0.0017 (8)
O4	0.0076 (9)	0.0135 (11)	0.0137 (11)	0.0021 (9)	-0.0010 (8)	-0.0047 (9)
O5	0.0156 (13)	0.0129 (10)	0.0140 (10)	-0.0012 (10)	0.0022 (10)	0.0041 (8)
O6	0.0072 (9)	0.0118 (10)	0.0203 (12)	-0.0004 (8)	-0.0031 (9)	-0.0014 (10)

## Geometric parameters (Å, °)

Ba—O1	2.765 (3)	Ba—O5	3.143 (3)
Ba—O2 <sup>i</sup>	2.778 (2)	P1—O3 <sup>viii</sup>	1.475 (2)
Ba—O3 <sup>ii</sup>	2.806 (2)	P1—O1 <sup>viii</sup>	1.480 (2)
Ba—O5 <sup>iii</sup>	2.841 (3)	P1—O6 <sup>ix</sup>	1.607 (2)
Ba—O1 <sup>iv</sup>	2.852 (3)	P1—O4 <sup>viii</sup>	1.625 (2)
Ba—O2 <sup>iii</sup>	2.897 (2)	P2—O2	1.481 (2)
Ba—O3 <sup>v</sup>	2.952 (2)	P2—O5 <sup>vii</sup>	1.486 (2)
Ba—O4 <sup>vi</sup>	2.955 (2)	P2—O6 <sup>vi</sup>	1.604 (3)
Ba—O5 <sup>vii</sup>	3.047 (3)	P2—O4 <sup>vi</sup>	1.607 (3)
O1—Ba—O2 <sup>i</sup>	67.71 (8)	O3 <sup>ii</sup> —Ba—O5	125.05 (7)
O1—Ba—O3 <sup>ii</sup>	141.17 (7)	O5 <sup>iii</sup> —Ba—O5	63.43 (6)
O2 <sup>i</sup> —Ba—O3 <sup>ii</sup>	73.64 (7)	O1 <sup>iv</sup> —Ba—O5	95.77 (7)
O1—Ba—O5 <sup>iii</sup>	154.74 (7)	O2 <sup>iii</sup> —Ba—O5	49.37 (6)
O2 <sup>i</sup> —Ba—O5 <sup>iii</sup>	131.84 (8)	O3 <sup>v</sup> —Ba—O5	118.72 (7)
O3 <sup>ii</sup> —Ba—O5 <sup>iii</sup>	61.94 (7)	O4 <sup>vi</sup> —Ba—O5	76.68 (7)
O1—Ba—O1 <sup>iv</sup>	106.39 (7)	O5 <sup>vii</sup> —Ba—O5	61.30 (6)
O2 <sup>i</sup> —Ba—O1 <sup>iv</sup>	71.14 (7)	O3 <sup>viii</sup> —P1—O1 <sup>viii</sup>	121.65 (14)
O3 <sup>ii</sup> —Ba—O1 <sup>iv</sup>	62.86 (7)	O3 <sup>viii</sup> —P1—O6 <sup>ix</sup>	105.50 (14)
O5 <sup>iii</sup> —Ba—O1 <sup>iv</sup>	72.72 (7)	O1 <sup>viii</sup> —P1—O6 <sup>ix</sup>	111.06 (17)
O1—Ba—O2 <sup>iii</sup>	68.54 (8)	O3 <sup>viii</sup> —P1—O4 <sup>viii</sup>	109.50 (15)
O2 <sup>i</sup> —Ba—O2 <sup>iii</sup>	101.50 (3)	O1 <sup>viii</sup> —P1—O4 <sup>viii</sup>	108.97 (15)
O3 <sup>ii</sup> —Ba—O2 <sup>iii</sup>	124.60 (7)	O6 <sup>ix</sup> —P1—O4 <sup>viii</sup>	97.43 (13)
O5 <sup>iii</sup> —Ba—O2 <sup>iii</sup>	89.67 (7)	O2—P2—O5 <sup>vii</sup>	117.17 (15)
O1 <sup>iv</sup> —Ba—O2 <sup>iii</sup>	63.57 (7)	O2—P2—O6 <sup>vi</sup>	109.83 (14)
O1—Ba—O3 <sup>v</sup>	62.04 (7)	O5 <sup>vii</sup> —P2—O6 <sup>vi</sup>	112.95 (15)
O2 <sup>i</sup> —Ba—O3 <sup>v</sup>	71.91 (7)	O2—P2—O4 <sup>vi</sup>	112.26 (15)
O3 <sup>ii</sup> —Ba—O3 <sup>v</sup>	102.70 (7)	O5 <sup>vii</sup> —P2—O4 <sup>vi</sup>	105.74 (15)
O5 <sup>iii</sup> —Ba—O3 <sup>v</sup>	133.37 (7)	O6 <sup>vi</sup> —P2—O4 <sup>vi</sup>	97.02 (13)
O1 <sup>iv</sup> —Ba—O3 <sup>v</sup>	142.84 (6)	P1 <sup>v</sup> —O1—Ba	133.76 (18)
O2 <sup>iii</sup> —Ba—O3 <sup>v</sup>	128.82 (7)	P1 <sup>v</sup> —O1—Ba <sup>x</sup>	119.03 (18)
O1—Ba—O4 <sup>vi</sup>	116.29 (7)	Ba—O1—Ba <sup>x</sup>	106.39 (7)
O2 <sup>i</sup> —Ba—O4 <sup>vi</sup>	131.24 (7)	P2—O2—Ba <sup>vi</sup>	117.64 (13)
O3 <sup>ii</sup> —Ba—O4 <sup>vi</sup>	86.55 (7)	P2—O2—Ba <sup>vii</sup>	100.85 (12)
O5 <sup>iii</sup> —Ba—O4 <sup>vi</sup>	65.78 (7)	Ba <sup>vi</sup> —O2—Ba <sup>vii</sup>	141.37 (9)
O1 <sup>iv</sup> —Ba—O4 <sup>vi</sup>	136.74 (7)	P1 <sup>v</sup> —O3—Ba <sup>ix</sup>	137.20 (14)
O2 <sup>iii</sup> —Ba—O4 <sup>vi</sup>	125.91 (7)	P1 <sup>v</sup> —O3—Ba <sup>viii</sup>	112.75 (13)
O3 <sup>v</sup> —Ba—O4 <sup>vi</sup>	69.76 (7)	Ba <sup>ix</sup> —O3—Ba <sup>viii</sup>	102.70 (7)
O1—Ba—O5 <sup>vii</sup>	70.83 (6)	P2 <sup>i</sup> —O4—P1 <sup>v</sup>	126.27 (15)
O2 <sup>i</sup> —Ba—O5 <sup>vii</sup>	125.48 (8)	P2 <sup>i</sup> —O4—Ba <sup>i</sup>	103.09 (11)
O3 <sup>ii</sup> —Ba—O5 <sup>vii</sup>	134.05 (7)	P1 <sup>v</sup> —O4—Ba <sup>i</sup>	129.06 (12)
O5 <sup>iii</sup> —Ba—O5 <sup>vii</sup>	99.57 (7)	P2 <sup>iii</sup> —O5—Ba <sup>vii</sup>	128.45 (15)
O1 <sup>iv</sup> —Ba—O5 <sup>vii</sup>	156.26 (7)	P2 <sup>iii</sup> —O5—Ba <sup>iii</sup>	102.60 (13)
O2 <sup>iii</sup> —Ba—O5 <sup>vii</sup>	94.54 (7)	Ba <sup>vii</sup> —O5—Ba <sup>iii</sup>	99.57 (7)
O3 <sup>v</sup> —Ba—O5 <sup>vii</sup>	57.92 (7)	P2 <sup>iii</sup> —O5—Ba	90.73 (11)
O4 <sup>vi</sup> —Ba—O5 <sup>vii</sup>	48.51 (6)	Ba <sup>vii</sup> —O5—Ba	120.73 (9)

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O1—Ba—O5	91.95 (7)	Ba <sup>iii</sup> —O5—Ba	114.41 (9)
O2 <sup>i</sup> —Ba—O5	150.21 (7)	P2 <sup>i</sup> —O6—P1 <sup>ii</sup>	130.68 (17)

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