Crystal structure of the solid solution Ba$_{8.35}$Pb$_{0.65}$(B$_3$O$_6$)$_6$

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Single crystals of lead barium borate, Ba$_{8.35}$Pb$_{0.65}$(B$_3$O$_6$)$_6$, octabarium lead(II) hexakis(triborate), have been obtained by spontaneous nucleation from a high-temperature melt. Its three-dimensional structure is constructed on the basis of a BaO$_9$ polyhedron, a (Pb/Ba)O$_6$ octahedron (occupancy ratio Pb:Ba = 0.216:0.784) and a condensed B$_3$O$_6$ ring anion. In the crystal, the planar B$_3$O$_6$ anions are stacked in an alternating fashion with Ba and (Pb/Ba) atoms along [001]. A comparison is made with the structures of related solid solutions in the system Ba/Pb/B/O.

1. Chemical context

The study of inorganic borates is motivated by their possible non-linear optical properties, transparency in a wide range of wavelengths, high laser-damage tolerance, piezoelectricity and luminescent and other useful properties for technical applications of the respective compounds. For example, β-BaB$_2$O$_4$ (Chen *et al.*, 1985), LiB$_3$O$_5$ (Chen *et al.*, 1989), CsB$_3$O$_5$ (Sasaki *et al.*, 2000), Sr$_2$Be$_2$B$_2$O$_7$ (Chen *et al.*, 1995), K$_5$Ba$_{10}$(BO$_3$)$_8$F (Liu *et al.*, 2016), PbB$_4$O$_7$ (Bartwal *et al.*, 2001), Pb$_2$B$_5$O$_9$$X$ (X = Cl, Br, I) (Huang *et al.*, 2010) or Ba$_3$Sr$_4$(BO$_3$)$_3$F$_5$ (Zhang *et al.*, 2009) have been studied because of their second-order
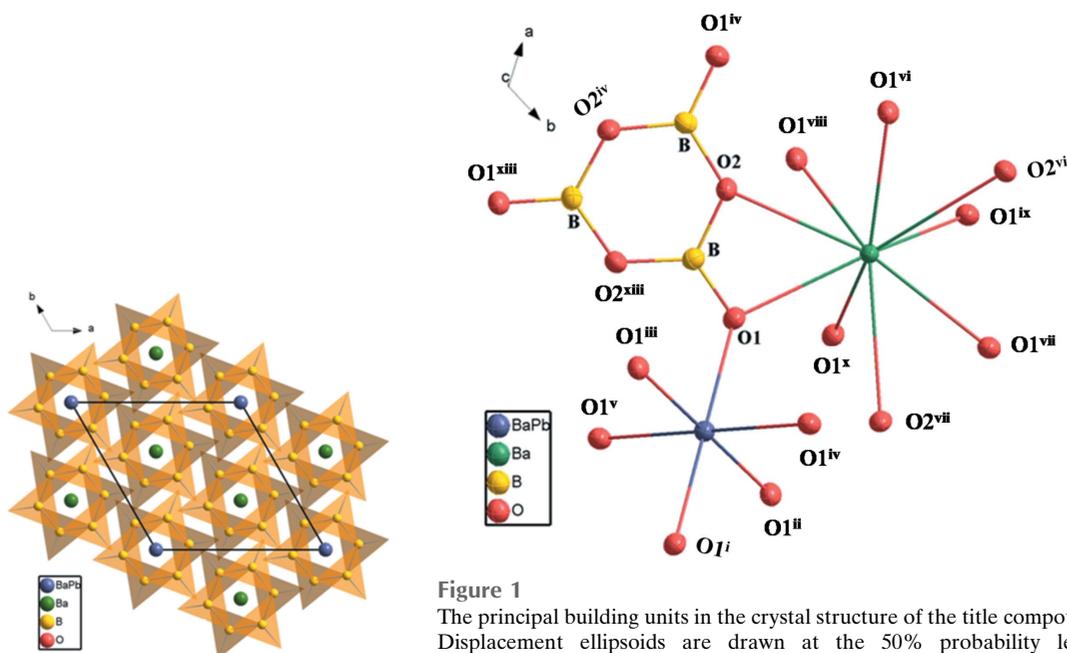

Figure 1
The principal building units in the crystal structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i) $-x$, $-y$, $-z$; (ii) $-y$, $x - y$, z; (iii) y, $-x + y$, $-z$; (iv) $x - y$, x, $-z$; (v) $-x + y$, $-x$, z; (vi) $-y + 1$, $x - y$, z; (vii) $-x + y + 1$, $-x + 1$, z; (viii) $y + \frac{2}{3}$, $-x + y + \frac{1}{3}$, $-z + \frac{1}{3}$; (ix) $x - y + \frac{2}{3}$, $x + \frac{1}{3}$, $-z + \frac{1}{3}$; (x) $-x + \frac{2}{3}$, $-y + \frac{1}{3}$, $-z + \frac{1}{3}$; (xiii) $-y$, $x - y - 1$, z; (xiv) $-x + y + 1$, $-x$, z.]

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non-linear optical behavior. Among inorganic borates synthesized and characterized over the past decades, some lead(II) borates show comprehensive applications. These features are associated with the highly asymmetric stereochemistry typical for a lead(II) atom due to the stereoactivity of the $6s^2$ lone pair (Zhang *et al.*, 2016; Mutailipu *et al.*, 2016). Accordingly, numerous studies have been devoted to this family of compounds. Some lead borates are particularly attractive because of their high second-harmonic generation (SHG) response (Wu *et al.*, 2012; Dong *et al.*, 2015; Jing *et al.*, 2015) or large birefringence (Liu *et al.*, 2015).

In this communication, we report on the synthesis and crystal structure of the solid solution $Ba_{8.35}Pb_{0.65}(B_3O_6)_6$.

2. Structural commentary

The crystal structure of $Ba_{8.35}Pb_{0.65}(B_3O_6)_6$ is based on a $Ba2O_9$ polyhedron, a $(Pb/Ba1)O_6$ polyhedron and a condensed B_3O_6 anion, as shown in Fig. 1. The planar B_3O_6 anions (point group symmetry 3.) are isolated from each other and distributed layer upon layer perpendicular to [001]. The occupationally disordered (Pb/Ba)1 site (occupancy ratio Pb:Ba = 0.216:0.784) and the Ba2 site are located alternately between the B_3O_6 sheets in (Pb/Ba)1 and Ba2 layers, as shown in Fig. 2a. The B atom is bound to one O1 atom and two O2 atoms to from a BO_3 triangle. Three BO_3 triangles are condensed through vertex-sharing to build a planar and cyclic B_3O_6 unit. The B—O bond lengths vary from 1.318 (5) to
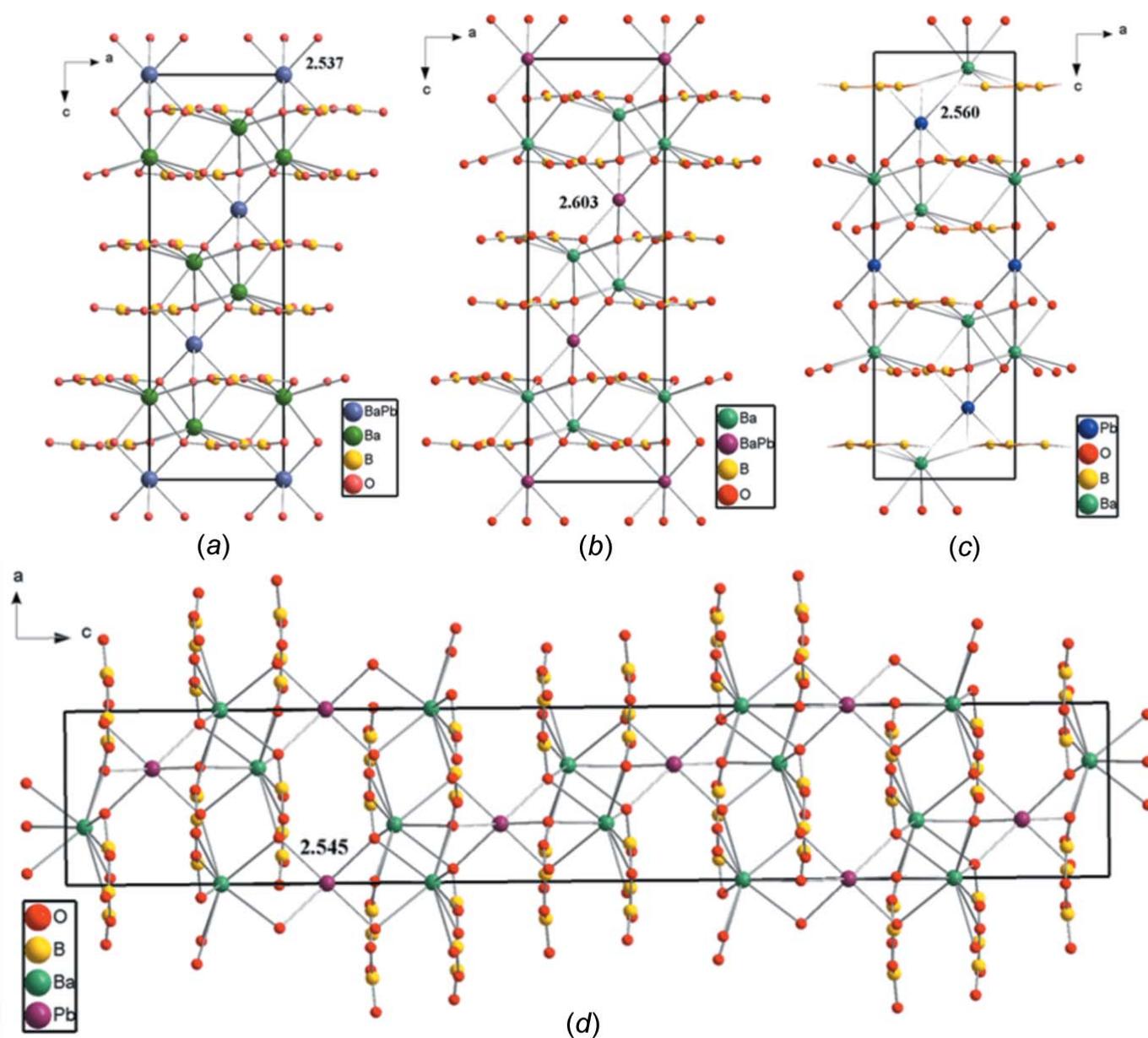

Figure 2
The crystal structures of related solid solutions in the system Ba/Pb/B/O viewed down [010]: (*a*) $Ba_{8.35}Pb_{0.65}(B_3O_6)_6$; (*b*) $Ba_{7.87}Pb_{1.13}(B_3O_6)_6$ (Wu *et al.*, 2012); (*c*) $Ba_2Pb(B_3O_6)_2$ (Li *et al.*, 2014); (*d*) $Ba_2Pb(B_3O_6)_2$ (Tang *et al.*, 2015). The numbers indicate the bond lengths (Å) of the PbO_6 or $(Ba/Pb)O_6$ octahedra.
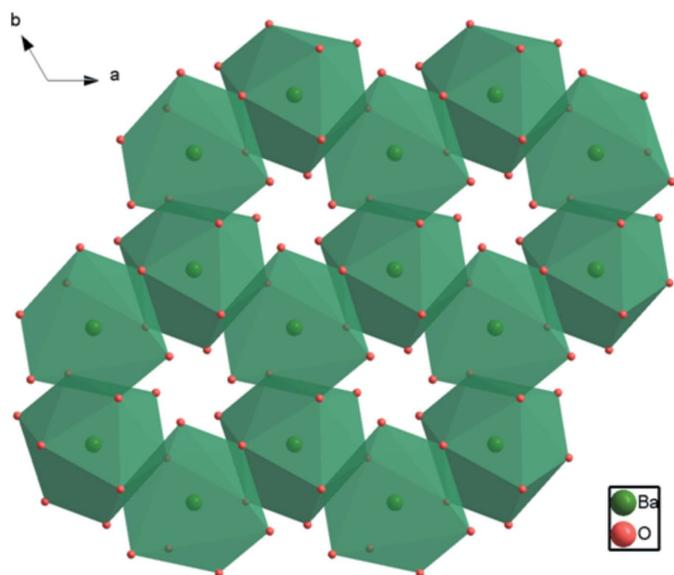
Figure 3
The formation of a corrugated layer of Ba2O$_9$ polyhedra in the crystal structure of Ba$_{8.35}$Pb$_{0.65}$(B$_3$O$_6$)$_6$ viewed down [001].

1.406 (5) Å (Table 1), and the O—B—O angles are between 116.8 (4) and 122.6 (4)°.

Table 1
Selected geometric parameters (Å, °).

(Pb/Ba)1—O1	2.537 (3)	B—O1	1.318 (5)
Ba2—O1	2.766 (3)	B—O2	1.397 (5)
Ba2—O1^i	2.810 (3)	B—O2^{ii}	1.406 (5)
Ba2—O2	3.030 (3)		
O1—B—O2	120.6 (4)	O2—B—O2^{ii}	116.8 (4)
O1—B—O2^{ii}	122.6 (4)		

Symmetry codes: (i) $-x + \frac{2}{3}, -y + \frac{1}{3}, -z + \frac{1}{3}$; (ii) $-y, x - y - 1, z$.

The Ba2 atom (site symmetry 3.) is coordinated by nine O atoms. The Ba—O bond lengths of the Ba2O$_9$ polyhedron range from 2.766 (3) to 3.030 (3) Å, with a mean distance of 2.869 Å (Table 1). A similar environment for Ba is observed in the crystal structures of Na$_3$Ba$_2$(B$_3$O$_6$)$_2$F (Zhang *et al.*, 2015), PbBa$_2$(B$_3$O$_6$)$_2$ (Li *et al.*, 2014) and α-BBO (Wu *et al.*, 2002). Each of the Ba2O$_9$ polyhedra shares edges with adjacent Ba2O$_9$ polyhedra to form six-membered rings that are arranged in corrugated layers extending parallel to (001) (Fig. 3). The (Pb/Ba)1 site (site symmetry $\overline{3}$.) is surrounded by six O atoms; the corresponding (Pb/Ba)1O$_6$ octahedra are isolated from each other. The six (Pb/Ba)1—O bonds have an identical length of 2.537 (3) Å (Table 1, Fig. 2a). In comparison with the M2 site, the M1 site has a more narrow
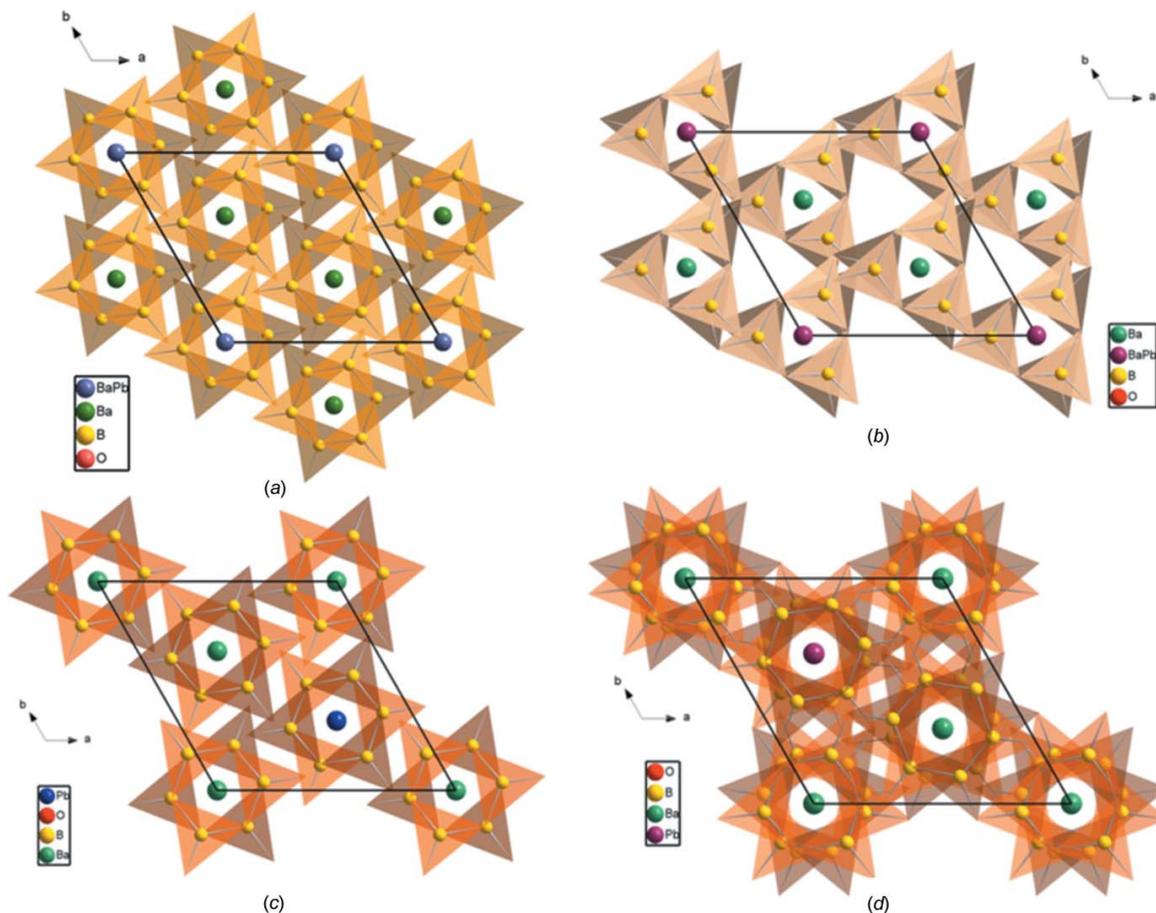

Figure 4
The arrangement of B$_3$O$_6$ groups along the [001] direction in the different solid solutions: (a) Ba$_{8.35}$Pb$_{0.65}$(B$_3$O$_6$)$_6$; (b) Ba$_{7.87}$Pb$_{1.13}$(B$_3$O$_6$)$_6$ (Wu *et al.*, 2012); (c) Ba$_2$Pb(B$_3$O$_6$)$_2$ (Li *et al.*, 2014); (d) Ba$_2$Pb(B$_3$O$_6$)$_2$ (Tang *et al.*, 2015).

coordination environment which seems to be the reason why Pb atoms exclusively substitute Ba atoms at the latter position due to their smaller ionic radius.

3. Comparison with the structures of related solid solutions

It is interesting to compare the structure of $Ba_{8.35}Pb_{0.65}(B_3O_6)_6$ with those of the related solid solutions $Ba_{7.87}Pb_{1.13}(B_3O_6)_6$ (Wu *et al.*, 2012) and $Ba_2Pb(B_3O_6)_2$ (Li *et al.*, 2014; Tang *et al.*, 2015). Whereas the title compound $Ba_{8.35}Pb_{0.65}(B_3O_6)_6$ crystallizes in space group $R\bar{3}$, $Ba_{7.87}Pb_{1.13}(B_3O_6)_6$ was solved and refined in space group $R32$ on the basis of single crystal X-ray diffraction data (Wu *et al.*, 2012); the lattice parameters of both compounds are very similar. $Ba_2Pb(B_3O_6)_2$ on the other hand was reported to crystallize either in space group $R\bar{3}$ with lattice parameters in the same range as the previous two structures (single crystal X-ray diffraction data; Li *et al.*, 2014) or in space group $R\bar{3}c$ with a doubled c axis in comparison with the other structures (powder X-ray diffraction data using the Rietveld method; Tang *et al.*, 2015). All four crystal structures are characterized by an alternating stacking of cationic and anionic (001) layers along [001], as shown in Fig. 2. In each case, the Ba site is coordinated by nine O atoms to form BaO_9 polyhedra, and the Pb or the (Pb/Ba) site is coordinated by six O atoms to form distorted PbO_6 octahedra [in $Ba_2Pb(B_3O_6)_2$] or (Pb/Ba)O_6 octahedra [in $Ba_{8.35}Pb_{0.65}(B_3O_6)_6$ and $Ba_{7.87}Pb_{1.13}(B_3O_6)_6$].

The arrangement of the planar B_3O_6 rings in the crystal structures is a determining factor in whether a non-centrosymmetric or a centrosymmetric structure is obtained. In $Ba_{7.87}Pb_{1.13}(B_3O_6)_6$ (Wu *et al.*, 2012), the rings are aligned in a chiral arrangement (Fig. 4b), responsible for the SHG effect. In $Ba_2Pb(B_3O_6)_2$ (Li *et al.*, 2014), the B_3O_6 rings are parallel to each other, distributed layer upon layer along [001], and the B_3O_6 rings in neighbouring layers point in exactly opposite directions (Fig. 4c), just like in the title compound (Fig. 4a). In the $Ba_2Pb(B_3O_6)_2$ structure with doubled volume (Tang *et al.*, 2015), all of the B_3O_6 rings are parallel to (001), and the B_3O_6 rings in two neighbouring layers are rotated slightly relative to each other (Fig. 4d).

4. Synthesis and crystallization

Suitable crystals of the solid solution $Ba_{8.35}Pb_{0.65}(B_3O_6)_6$ were obtained by spontaneous nucleation from a high-temperature melt mixture originating from PbO, H_3BO_3 and BaF_2 in molar ratios of 4:5:1. The starting materials were weighed and melted in a platinum crucible in several batches. The crucible position was fixed at the centre of a resistance-heated furnace. The temperature of the furnace was controlled within 0.1–1 K by an Al-708P controller and a Pt/Pt–Rh thermocouple. The temperature was raised by about 50 K h^{-1} to 50 K above the melting point and held for 15 h to ensure a homogenous mixture of the solution. After cooling down the furnace to 1073 K, a slow cooling rate of 5 K d^{-1}, was applied, followed

Table 2
Experimental details.

Crystal data	
Chemical formula	$Ba_{8.35}Pb_{0.65}(B_3O_6)_6$
M_r	2051.83
Crystal system, space group	Trigonal, $R\bar{3}$
Temperature (K)	296
a, c (Å)	7.206 (2), 18.653 (11)
V (Å^3)	838.7 (6)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	13.00
Crystal size (mm)	$0.16 \times 0.08 \times 0.02$
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Numerical (face-indexed using *SADABS*; Bruker, 2000)
T_{min}, T_{max}	0.141, 0.547
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	1745, 441, 430
R_{int}	0.024
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.652
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.019, 0.048, 1.23
No. of reflections	441
No. of parameters	35
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.64, −0.74

Computer programs: *APEX2* and *SAINT* (Bruker, 2000), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 2006).

by cooling to room temperature at 20 K h^{-1}. Colorless crystals in the millimetre range were obtained.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. From the two large cation positions in the structure (Wyckoff positions 3*a* and 6*c*), only those of *M*1 at 3*a* are occupationally disordered by Ba and Pb atoms. Refinement of the occupancy of Ba:Pb at this site under consideration of EXYZ and EADP commands (Sheldrick, 2008) resulted in a 21.6 (7)% occupancy of Pb. The highest peak and the deepest hole are located 0.98 and 2.06 Å from the Ba2 and B atoms, respectively.

References

Bartwal, K. S., Bhatt, R., Kar, S. & Wadhawan, V. K. (2001). *Mater. Sci. Eng. B*, **85**, 76–79.

Brandenburg, K. (2006). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.

Bruker (2000). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Chen, C., Wang, Y., Wu, B., Wu, K., Zeng, W. & Yu, L. (1995). *Nature*, **373**, 322–324.

Chen, C., Wu, Y., Jiang, A., Wu, B., You, G., Li, R. & Lin, S. (1989). *J. Opt. Soc. Am. B*, **6**, 616–621.

Chen, C., Wu, B., Jiang, A. & You, G. (1985). *Sci. Sin.* B**28**, 235–241.

Dong, X. Y., Jing, Q., Shi, Y. J., Yang, Z. H., Pan, S. L., Poeppelmeier, K. R., Young, J. & Rondinelli, J. M. (2015). *J. Am. Chem. Soc.* **137**, 9417–9422.

Huang, Y., Wu, L., Wu, X., Li, L., Chen, L. & Zhang, Y. (2010). *J. Am. Chem. Soc.* **132**, 12788–12789.

Jing, Q., Dong, X. Y., Yang, Z. H. & Pan, S. L. (2015). *Dalton Trans.* **44**, 16818–16823.

Li, H. Y., Dong, L., Lu, Y., Pan, S. L., Lu, X., Yu, H. W., Wu, H. P., Su, X. & Yang, Z. H. (2014). *J. Alloys Compd.* **615**, 561–565.

Liu, L. L., Yang, Y., Jing, Q., Dong, X. Y., Yang, Z. H., Pan, S. L. & Wu, K. (2016). *J. Phys. Chem. C*, **120**, 18763–18770.

Liu, L., Zhang, B. B., Zhang, F. F., Pan, S. L., Zhang, F. Y., Zhang, X. W., Dong, X. Y. & Yang, Z. H. (2015). *Dalton Trans.* **44**, 7041–7047.

Mutailipu, M., Hou, D. W., Zhang, M., Yang, Z. H. & Pan, S. L. (2016). *New J. Chem.* **40**, 6120–6126.

Sasaki, T., Mori, Y., Yoshimura, M., Yap, Y. K. & Kamimura, T. (2000). *Mater. Sci. Eng. Rep.* **30**, 1–54.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Tang, X. L., Feng, D. X., Wan, S. M., Kang, L., Zhang, B. & Lin, Z. S. (2015). *Mater. Chem. Phys.* **163**, 501–506.

Wu, H. P., Pan, S. L., Jia, D. Z., Chen, Z. H. & Yu, H. W. (2012). *Chem. Lett.* **41**, 812–813.

Wu, S., Wang, G., Xie, J., Wu, X., Zhang, Y. & Lin, X. (2002). *J. Cryst. Growth*, **245**, 84–86.

Zhang, G., Liu, Z., Zhang, J., Fan, F., Liu, Y. & Fu, P. (2009). *Cryst. Growth Des.* **9**, 3137–3141.

Zhang, F. F., Zhang, F. Y., Lei, B. H., Yang, Z. H. & Pan, S. L. (2016). *J. Phys. Chem. C*, **120**, 12757–12764.

Zhang, H., Zhang, M., Pan, S. L., Yang, Z., Wang, Z., Bian, Q., Hou, X., Yu, H., Zhang, F., Wu, K., Yang, F., Peng, Q., Xu, Z., Chang, K. B. & Poeppelmeier, K. R. (2015). *Cryst. Growth Des.* **15**, 523–529.

Crystal structure of the solid solution $Ba_{8.35}Pb_{0.65}(B_3O_6)_6$

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Computing details

Data collection: *APEX2* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* (Bruker, 2000); 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: *SHELXTL* (Sheldrick, 2008).

Octabarium lead(II) hexakis(triborate)

Crystal data

$Ba_{8.35}Pb_{0.65}(B_3O_6)_6$	$D_x = 4.062$ Mg m^{-3}
$M_r = 2051.83$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Trigonal, $R\bar{3}$	Cell parameters from 1161 reflections
Hall symbol: -R 3	$\theta = 3.3–27.6°$
$a = 7.206$ (2) Å	$\mu = 13.00$ mm^{-1}
$c = 18.653$ (11) Å	$T = 296$ K
$V = 838.7$ (6) Å^3	Plate, colourless
$Z = 1$	$0.16 \times 0.08 \times 0.02$ mm
$F(000) = 899$	

Data collection

Bruker APEXII CCD diffractometer	1745 measured reflections
Radiation source: fine-focus sealed tube	441 independent reflections
Graphite monochromator	430 reflections with $I > 2\sigma(I)$
phi and ω scans	$R_{int} = 0.024$
Absorption correction: numerical (face-indexed using *SADABS*; Bruker, 2000)	$\theta_{max} = 27.6°$, $\theta_{min} = 3.3°$
	$h = -8{\rightarrow}9$
	$k = -9{\rightarrow}9$
$T_{min} = 0.141$, $T_{max} = 0.547$	$l = -14{\rightarrow}23$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.019$	$w = 1/[\sigma^2(F_o^2) + (0.0178P)^2 + 5.852P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.048$	
$S = 1.23$	$(\Delta/\sigma)_{max} < 0.001$
441 reflections	$\Delta\rho_{max} = 0.64$ e Å^{-3}
35 parameters	$\Delta\rho_{min} = -0.74$ e Å^{-3}
0 restraints	Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00125 (17)

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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	$U_{iso}*/U_{eq}$	Occ. (<1)
Pb1	0.0000	0.0000	0.0000	0.0147 (2)	0.216 (7)
Ba1	0.0000	0.0000	0.0000	0.0147 (2)	0.784 (7)
Ba2	0.6667	0.3333	0.12947 (2)	0.01537 (18)	
B	0.2953 (7)	−0.1579 (7)	0.0864 (3)	0.0175 (9)	
O1	0.2633 (5)	0.0063 (4)	0.09165 (18)	0.0218 (6)	
O2	0.5029 (5)	−0.1261 (5)	0.08345 (18)	0.0234 (7)	

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Pb1	0.0136 (2)	0.0136 (2)	0.0169 (3)	0.00680 (12)	0.000	0.000
Ba1	0.0136 (2)	0.0136 (2)	0.0169 (3)	0.00680 (12)	0.000	0.000
Ba2	0.01176 (19)	0.01176 (19)	0.0226 (3)	0.00588 (9)	0.000	0.000
B	0.019 (2)	0.017 (2)	0.018 (2)	0.0103 (18)	−0.0009 (18)	−0.0002 (17)
O1	0.0185 (14)	0.0159 (13)	0.0320 (17)	0.0093 (12)	−0.0011 (12)	−0.0022 (12)
O2	0.0162 (14)	0.0142 (13)	0.0384 (18)	0.0066 (11)	0.0012 (13)	0.0017 (13)

Geometric parameters (Å, º)

(Pb/Ba)1—O1^i	2.537 (3)	Ba2—O1^{vii}	2.810 (3)
(Pb/Ba)1—O1^{ii}	2.537 (3)	Ba2—O2	3.030 (3)
(Pb/Ba)1—O1	2.537 (3)	Ba2—O2^{viii}	3.030 (3)
(Pb/Ba)1—O1^{iii}	2.537 (3)	Ba2—O2^{ix}	3.030 (3)
(Pb/Ba)1—O1^{iv}	2.537 (3)	Ba2—B^{viii}	3.296 (5)
(Pb/Ba)1—O1^{v}	2.537 (3)	Ba2—B^{ix}	3.296 (5)
Pb1—Ba2^{vi}	3.803 (2)	Ba2—Pb1^{xii}	3.803 (2)
Pb1—Ba2^{vii}	3.803 (2)	B—O1	1.318 (5)
Ba2—O1^{viii}	2.766 (3)	B—O2	1.397 (5)
Ba2—O1	2.766 (3)	B—O2^{xiii}	1.406 (5)
Ba2—O1^{ix}	2.766 (3)	O1—Ba2^{vii}	2.810 (3)
Ba2—O1^{x}	2.810 (3)	O2—B^{xiv}	1.406 (5)
Ba2—O1^{xi}	2.810 (3)		
O1^i—Pb1—O1^{ii}	100.43 (11)	O1^{xi}—Ba2—O2^{viii}	67.48 (9)
O1^i—Pb1—O1	180.00 (17)	O1^{vii}—Ba2—O2^{viii}	135.55 (8)
O1^{ii}—Pb1—O1	79.57 (11)	O2—Ba2—O2^{viii}	112.31 (6)

Atoms	Angle (°)	Atoms	Angle (°)
O1^{i}—Pb1—O1^{iii}	79.57 (11)	O1^{viii}—Ba2—O2^{ix}	147.14 (9)
O1^{ii}—Pb1—O1^{iii}	180.00 (11)	O1—Ba2—O2^{ix}	67.39 (8)
O1—Pb1—O1^{iii}	100.43 (11)	O1^{ix}—Ba2—O2^{ix}	47.75 (8)
O1^{i}—Pb1—O1^{iv}	79.57 (11)	O1^{x}—Ba2—O2^{ix}	135.55 (8)
O1^{ii}—Pb1—O1^{iv}	100.43 (11)	O1^{xi}—Ba2—O2^{ix}	107.59 (8)
O1—Pb1—O1^{iv}	100.43 (11)	O1^{vii}—Ba2—O2^{ix}	67.48 (9)
O1^{iii}—Pb1—O1^{iv}	79.57 (11)	O2—Ba2—O2^{ix}	112.31 (6)
O1^{i}—Pb1—O1^{v}	100.43 (11)	O2^{viii}—Ba2—O2^{ix}	112.31 (6)
O1^{ii}—Pb1—O1^{v}	79.57 (11)	O1^{viii}—Ba2—B^{viii}	23.05 (10)
O1—Pb1—O1^{v}	79.57 (11)	O1—Ba2—B^{viii}	134.00 (10)
O1^{iii}—Pb1—O1^{v}	100.43 (11)	O1^{ix}—Ba2—B^{viii}	92.24 (10)
O1^{iv}—Pb1—O1^{v}	180.00 (17)	O1^{x}—Ba2—B^{viii}	89.14 (10)
O1^{i}—Pb1—Ba2^{vi}	47.64 (7)	O1^{xi}—Ba2—B^{viii}	75.27 (10)
O1^{ii}—Pb1—Ba2^{vi}	132.36 (7)	O1^{vii}—Ba2—B^{viii}	144.45 (11)
O1—Pb1—Ba2^{vi}	132.36 (7)	O2—Ba2—B^{viii}	89.88 (9)
O1^{iii}—Pb1—Ba2^{vi}	47.64 (7)	O2^{viii}—Ba2—B^{viii}	25.06 (9)
O1^{iv}—Pb1—Ba2^{vi}	47.64 (7)	O2^{ix}—Ba2—B^{viii}	134.51 (10)
O1^{v}—Pb1—Ba2^{vi}	132.36 (7)	O1^{viii}—Ba2—B^{ix}	134.00 (10)
O1^{i}—Pb1—Ba2^{vii}	132.36 (7)	O1—Ba2—B^{ix}	92.24 (10)
O1^{ii}—Pb1—Ba2^{vii}	47.64 (7)	O1^{ix}—Ba2—B^{ix}	23.05 (10)
O1—Pb1—Ba2^{vii}	47.64 (7)	O1^{x}—Ba2—B^{ix}	144.45 (11)
O1^{iii}—Pb1—Ba2^{vii}	132.36 (7)	O1^{xi}—Ba2—B^{ix}	89.14 (10)
O1^{iv}—Pb1—Ba2^{vii}	132.36 (7)	O1^{vii}—Ba2—B^{ix}	75.27 (10)
O1^{v}—Pb1—Ba2^{vii}	47.64 (7)	O2—Ba2—B^{ix}	134.51 (10)
Ba2^{vi}—Pb1—Ba2^{vii}	180.0	O2^{viii}—Ba2—B^{ix}	89.88 (10)
O1^{viii}—Ba2—O1	113.73 (6)	O2^{ix}—Ba2—B^{ix}	25.06 (9)
O1^{viii}—Ba2—O1^{ix}	113.73 (6)	B^{viii}—Ba2—B^{ix}	114.27 (7)
O1—Ba2—O1^{ix}	113.73 (6)	O1^{viii}—Ba2—Pb1^{xii}	104.78 (7)
O1^{viii}—Ba2—O1^{x}	76.27 (10)	O1—Ba2—Pb1^{xii}	104.78 (7)
O1—Ba2—O1^{x}	89.15 (12)	O1^{ix}—Ba2—Pb1^{xii}	104.78 (7)
O1^{ix}—Ba2—O1^{x}	145.30 (7)	O1^{x}—Ba2—Pb1^{xii}	41.85 (7)
O1^{viii}—Ba2—O1^{xi}	89.15 (12)	O1^{xi}—Ba2—Pb1^{xii}	41.85 (7)
O1—Ba2—O1^{xi}	145.30 (7)	O1^{vii}—Ba2—Pb1^{xii}	41.85 (7)
O1^{ix}—Ba2—O1^{xi}	76.27 (10)	O2—Ba2—Pb1^{xii}	106.46 (7)
O1^{x}—Ba2—O1^{xi}	70.59 (10)	O2^{viii}—Ba2—Pb1^{xii}	106.46 (7)
O1^{viii}—Ba2—O1^{vii}	145.31 (7)	O2^{ix}—Ba2—Pb1^{xii}	106.46 (7)
O1—Ba2—O1^{vii}	76.27 (10)	B^{viii}—Ba2—Pb1^{xii}	104.10 (8)
O1^{ix}—Ba2—O1^{vii}	89.15 (12)	B^{ix}—Ba2—Pb1^{xii}	104.10 (8)
O1^{x}—Ba2—O1^{vii}	70.59 (10)	O1—B—O2	120.6 (4)
O1^{xi}—Ba2—O1^{vii}	70.59 (10)	O1—B—O2^{xiii}	122.6 (4)
O1^{viii}—Ba2—O2	67.39 (8)	O2—B—O2^{xiii}	116.8 (4)
O1—Ba2—O2	47.75 (8)	B—O1—Pb1	113.5 (3)
O1^{ix}—Ba2—O2	147.14 (9)	B—O1—Ba2	101.7 (3)
O1^{x}—Ba2—O2	67.48 (9)	Pb1—O1—Ba2	130.17 (12)
O1^{xi}—Ba2—O2	135.55 (8)	B—O1—Ba2^{vii}	117.4 (3)
O1^{vii}—Ba2—O2	107.59 (8)	Pb1—O1—Ba2^{vii}	90.51 (10)
O1^{viii}—Ba2—O2^{viii}	47.75 (8)	Ba2—O1—Ba2^{vii}	103.73 (10)
O1—Ba2—O2^{viii}	147.14 (9)	B—O2—B^{xiv}	122.9 (4)

O1^{ix}—Ba2—O2^{viii}	67.39 (8)	B—O2—Ba2	88.2 (2)
O1^x—Ba2—O2^{viii}	107.59 (8)	B^{xiv}—O2—Ba2	143.4 (3)

Symmetry codes: (i) −x, −y, −z; (ii) −y, x−y, z; (iii) y, −x+y, −z; (iv) x−y, x, −z; (v) −x+y, −x, z; (vi) x−2/3, y−1/3, z−1/3; (vii) −x+2/3, −y+1/3, −z+1/3; (viii) −y+1, x−y, z; (ix) −x+y+1, −x+1, z; (x) y+2/3, −x+y+1/3, −z+1/3; (xi) x−y+2/3, x+1/3, −z+1/3; (xii) x+2/3, y+1/3, z+1/3; (xiii) −y, x−y−1, z; (xiv) −x+y+1, −x, z.