

Ba₂VO₄Br

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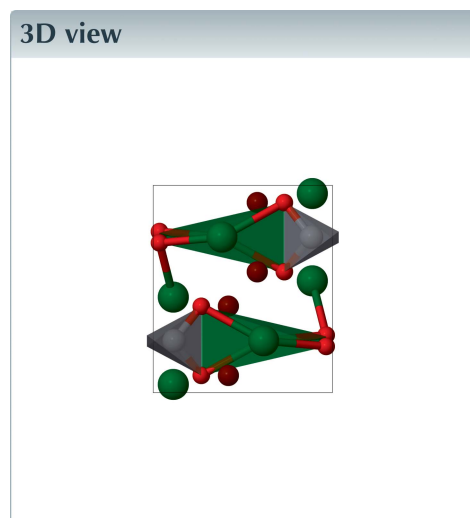
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Structural data: full structural data are available from iucrdata.iucr.org

Single crystals of dibarium vanadate(V) bromide, Ba₂VO₄Br, were grown from a melt of Ba₃(VO₄)₂ and BaBr₂. Ba₂VO₄Br crystallizes in the space group *Pbcm* and is isotypic with the structure of chlorspodiosite, Ca₂PO₄Cl. Although the ionic radii in chlorspodiosite are different from those in dibarium vanadate bromide, the structures are very similar to one another. The V atom is coordinated by four O atoms, forming a slightly distorted tetrahedron. The Ba atoms occupy two different sites and are coordinated by six O atoms and three or four Br atoms, depending on the site occupied.



Structure description

This work is part of investigations or reinvestigations of compounds with the general formula A_2BO_4X (A = alkaline earth metal; B = P, As, V or other pentavalent atoms; X = halogen atom). The intention behind the current work is to understand conditions of the stability of the different structure types and to search for new structure types with this general formula.

The title compound Ba₂VO₄Br crystallizes isotypically with chlorspodiosite, Ca₂PO₄Cl (Mackay, 1953), despite of different ionic radii and the existence of other structure types with the same general formula (Haberkorn *et al.*, 2014). The crystal structure of Ca₂PO₄Cl was published by Greenblatt *et al.* (1967). For an easier comparison of both structures, the atomic sites were normalized and sorted in the same manner as for the title compound (*cf. Refinement* section). The normalized atomic positions of Ca₂PO₄Cl and Ba₂VO₄Br are given within the *Supporting information*. The relative distances d/d_{Shannon} between the cations and the surrounding anions of both compounds are given in Tables 1 and 2, respectively. There are also ‘ideal’ distances d_{Shannon} provided, calculated from the sum of the corresponding ionic radii (Shannon, 1976) using $r_{\text{Ca}^{2+},[8]} = 1.12 \text{ \AA}$, $r_{\text{Ba}^{2+},[8]} = 1.42 \text{ \AA}$, $r_{\text{P}^{5+},[4]} = 0.29 \text{ \AA}$, $r_{\text{V}^{5+},[4]} = 0.355 \text{ \AA}$, $r_{\text{O}^{2-},[3-4]} = 1.37 \text{ \AA}$, $r_{\text{Cl}^{1-},[6]} = 1.81 \text{ \AA}$, and $r_{\text{Br}^{1-},[6]} = 1.96 \text{ \AA}$.

Table 1
Selected relative interatomic distances in Ca₂PO₄Cl.

Central atom	ligand	d_1/d_{Shannon}	d_2/d_{Shannon}	d_3/d_{Shannon}	d_4/d_{Shannon}	d_{Shannon} (Å)
Ca1	O ²⁻	2 × 0.943	2 × 1.001	2 × 1.016	2 × 1.677	2.49
	Cl ¹⁻	2 × 0.957	2 × 1.482	2 × 1.602		2.93
Ca2	O ²⁻	2 × 0.967	2 × 0.973	2 × 1.066	2 × 1.595	2.49
	Cl ¹⁻	1 × 0.947	1 × 1.023	1 × 1.424	1 × 1.486	2.93
P	O ²⁻	2 × 0.923	2 × 0.934	2 × 2.083		1.66

Values of d_{Shannon} were calculated from the sum of the corresponding ionic radii (Shannon, 1976).

Table 2
Selected relative interatomic distances in Ba₂VO₄Br.

Central atom	ligand	d_1/d_{Shannon}	d_2/d_{Shannon}	d_3/d_{Shannon}	d_4/d_{Shannon}	d_{Shannon} (Å)
Ba1	O ²⁻	2 × 0.981	2 × 0.983	2 × 0.993	2 × 1.665	2.79
	Br ¹⁻	2 × 1.048	2 × 1.182	2 × 1.794		3.38
Ba2	O ²⁻	2 × 0.964	2 × 0.965	2 × 1.022	2 × 1.566	2.79
	Br ¹⁻	1 × 0.986	1 × 1.078	1 × 1.108	1 × 1.578	3.38
V	O ²⁻	2 × 0.992	2 × 0.999	2 × 2.165		1.73

Values of d_{Shannon} were calculated from the sum of the corresponding ionic radii (Shannon, 1976).

Four O atoms form in a similar manner marginally distorted tetrahedra around B for both compounds (Fig. 1).

The cation A occupies two different sites, one at Wyckoff position 4c (site symmetry 2.; Ca1 and Ba1), the other at Wyckoff position 4d (.m; Ca2 and Ba2). For Ca at the 4d sites (Ca2) in Ca₂PO₄Cl six O atoms form a distorted trigonal prism capped by two Cl atoms. Ca at the 4c site (Ca1) is also coordinated by two Cl atoms and six O atoms. The eight atoms form an irregular polyhedron. Additional Cl atoms are much more distant and do not belong to the coordination polyhedra of Ca1 and Ca2.

Ba²⁺ requires more than twice the volume in comparison with Ca²⁺. Hence, the coordination numbers of the A-sites

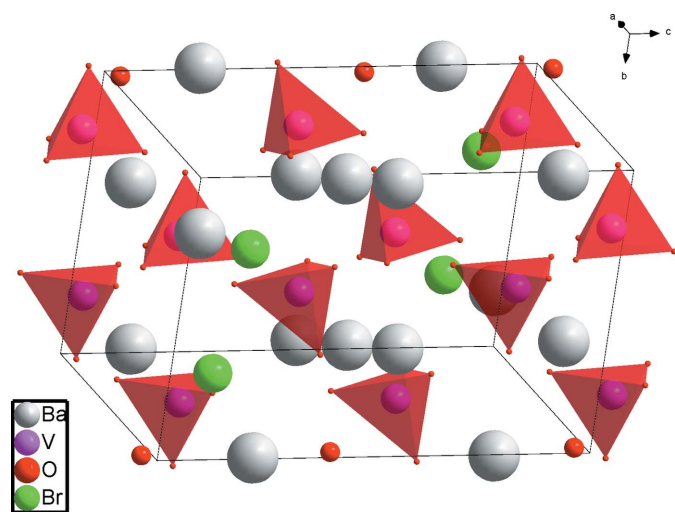


Figure 1
The crystal structure of Ba₂VO₄Br with VO₄ anions displayed as coordination polyhedra.

Table 3
Similarity of Ca₂PO₄Cl to some isotopic compounds.

Compound	Ca ₂ CrO ₄ Cl	Ca ₂ VO ₄ Cl	Ba ₂ VO ₄ Br
S	0.0092	0.0121	0.0561
d_{max} (Å)	0.3665	0.2445	1.1214
d_{av} (Å)	0.1575	0.1278	0.2607
Δ	0.045	0.030	0.092

increase in Ba₂VO₄Br compared to Ca₂PO₄Cl. The Ba2 site is ninefold coordinated by six O atoms and three Br atoms, forming a distorted tricapped trigonal prism (Fig. 2). The distortion of the trigonal prism is very similar to that of Ca2 in Ca₂PO₄Cl. Ba1 has an irregular shaped coordination polyhedron consisting of six O atoms and four Br atoms (Fig. 3). As can be seen in the Voronoi polyhedron, two of these bromine ligands belong to the coordination sphere; nevertheless they are more distant than the other bromine ligands and their Ba—Br distance is 118% of the sum of the ionic radii.

The compounds Ca₂CrO₄Cl (Greenblatt *et al.*, 1967), Ca₂VO₄Cl (Banks *et al.*, 1970), and Ba₂VO₄Br crystallize in

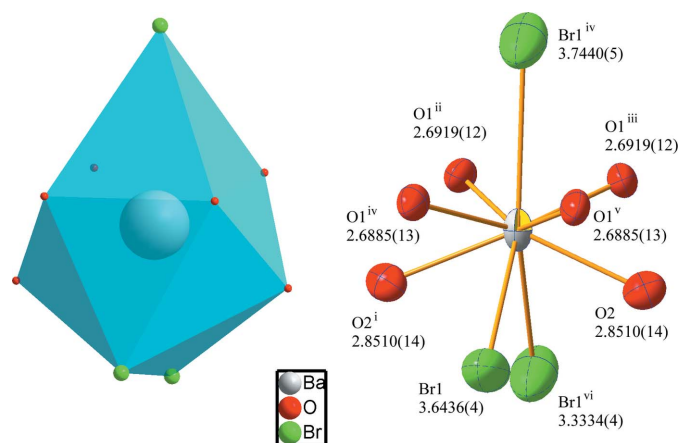


Figure 2
The coordination polyhedron of Ba at the 4d site (Ba2) in Ba₂VO₄Br with interatomic distances. Displacement ellipsoids are drawn at the 99.8% probability level. [Symmetry codes: (i) $x, y, -z + \frac{1}{2}$; (ii) $x, y - 1, -z + \frac{1}{2}$; (iii) $x, y - 1, z$; (iv) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$; (v) $-x, y - \frac{1}{2}, z$; (vi) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$.]

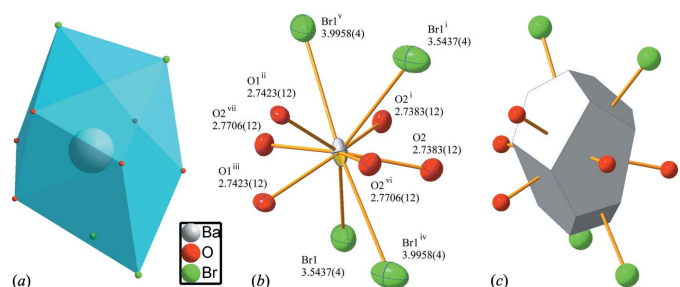


Figure 3
(a) The coordination polyhedron of Ba at the 4c site (Ba1) in Ba₂VO₄Br, (b) displacement ellipsoid plot (99.8% probability level) with interatomic distances and (c) Voronoi polyhedron. [Symmetry codes: (i) $x, -y + \frac{1}{2}, -z$; (ii) $-x + 1, -y + 1, -z$; (iii) $-x + 1, y - \frac{1}{2}, z$; (iv) $-x + 1, y - \frac{1}{2}, -z + \frac{1}{2}$; (v) $-x + 1, -y + 1, z - \frac{1}{2}$; (vi) $-x + 1, -y, -z$; (vii) $-x + 1, y + \frac{1}{2}, z$.]

the same space group type *Pbcm* as $\text{Ca}_2\text{PO}_4\text{Cl}$ and are isopointal. The similarity of $\text{Ca}_2\text{PO}_4\text{Cl}$ to these compounds was numerically determined using the program *COMPSTRU* (de la Flor *et al.*, 2016). The results are given in Table 3, where S is the degree of lattice distortion, d_{max} and d_{av} are the maximum and mean displacements of equivalent atoms and Δ is the measure of similarity taking atomic positions and lattice parameters into account. The structure of $\text{Ba}_2\text{VO}_4\text{Br}$ is less similar to $\text{Ca}_2\text{PO}_4\text{Cl}$ than the structures of the other compounds due to a larger difference of the ionic radii. The large volume of the unit cell of $\text{Ba}_2\text{VO}_4\text{Br}$ ($V_{\text{Ba}_2\text{VO}_4\text{Br}}/V_{\text{Ca}_2\text{PO}_4\text{Cl}} = 138\%$) causes high values of S and Δ . The displacement of the X atom of more than 1 \AA enables higher coordination numbers of the A atoms for $\text{Ba}_2\text{VO}_4\text{Br}$. The mean displacement d_{av} is less than twice the value for $\text{Ca}_2\text{CrO}_4\text{Cl}$ and demonstrates rather small displacements of the other sites. Despite different ionic radii and different coordination numbers of the A atoms, the structures of all these compounds are very similar and can be regarded as isotypic (Lima-de-Faria *et al.*, 1990).

Synthesis and crystallization

$\text{Ba}_2\text{VO}_4\text{Br}$ may be synthesized either *via* a solid-state reaction (ssr) of $\text{Ba}_3(\text{VO}_4)_2$ with BaBr_2 or *via* a melt of $\text{Ba}_3(\text{VO}_4)_2$ and an excess of BaBr_2 . While the ssr supports the preparation of a polycrystalline mass, the melt enables the yield of single crystals. Both methods were used, but the synthesis of single crystals will be focused on here.

Single crystals of $\text{Ba}_2\text{VO}_4\text{Br}$ were grown from a melt of BaBr_2 using as flux and as reacting agent. 0.4 mmol of $\text{Ba}_3(\text{VO}_4)_2$, 1.6 mmol $\text{BaBr}_2 \cdot 2\text{H}_2\text{O}$, and 1.6 mmol NH_4Br were mixed and filled into a platinum crucible. NH_4Br was added to minimize the formation of hydroxides. After an initial step of slowly heating to 523 K allowing water to evaporate, the mixture was heated to 1173 K. This temperature was held for 2 h. Then the melt was allowed to cool down to 1053 K within 10 h, followed by cooling to room temperature with a higher cooling rate. The excess BaBr_2 was leached out with distilled water.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. The atomic coordinates were standardized by the program *STRUCTURE TIDY* (Gelato & Parthé 1987) as implemented in the program *PLATON* (Spek, 2009), though with a different sequence of the sites. The sites were sorted in the same order as the chemical symbols in the chemical formula. For sites with the same atom type these sites were arranged in alphabetical order of their Wyckoff letters.

Table 4
Experimental details.

Crystal data	
Chemical formula	$\text{Ba}_2\text{VO}_4\text{Br}$
M_r	469.52
Crystal system, space group	Orthorhombic, <i>Pbcm</i>
Temperature (K)	200
a, b, c (Å)	6.8103 (7), 7.8855 (9), 12.0131 (14)
V (Å ³)	645.14 (12)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	19.61
Crystal size (mm)	0.04 × 0.04 × 0.03
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
$T_{\text{min}}, T_{\text{max}}$	0.663, 0.749
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	32756, 2741, 2132
R_{int}	0.062
($\sin \theta/\lambda$) _{max} (Å ⁻¹)	0.994
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.023, 0.042, 1.05
No. of reflections	2741
No. of parameters	42
$\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ (e Å ⁻³)	1.63, -1.14

Computer programs: *APEX2*, *SAINT* (Bruker, 2012), *SHELXT2014* (Sheldrick, 2015a), *SHELXL2015* (Sheldrick, 2015b), *DIAMOND* (Brandenburg *et al.*, 1999) and *publCIF* (Westrip, 2010).

For sites with the same atom type and the same Wyckoff letter the sites were arranged according to increasing x .

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full crystallographic data

IUCrData (2017). **2**, x170219 [https://doi.org/10.1107/S241431461700219X]

Ba₂VO₄Br

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Dibarium vanadate(V) bromide

Crystal data

Ba ₂ VO ₄ Br	$D_x = 4.834 \text{ Mg m}^{-3}$
$M_r = 469.52$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Orthorhombic, <i>Pbcm</i>	Cell parameters from 5232 reflections
$a = 6.8103 (7) \text{ \AA}$	$\theta = 4.3\text{--}40.6^\circ$
$b = 7.8855 (9) \text{ \AA}$	$\mu = 19.61 \text{ mm}^{-1}$
$c = 12.0131 (14) \text{ \AA}$	$T = 200 \text{ K}$
$V = 645.14 (12) \text{ \AA}^3$	Cuboid, colorless
$Z = 4$	$0.04 \times 0.04 \times 0.03 \text{ mm}$
$F(000) = 808$	

Data collection

Bruker APEXII CCD diffractometer	2741 independent reflections
Radiation source: sealed X-ray tube	2132 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.062$
Absorption correction: multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)	$\theta_{\text{max}} = 44.9^\circ$, $\theta_{\text{min}} = 3.0^\circ$
$T_{\text{min}} = 0.663$, $T_{\text{max}} = 0.749$	$h = -13 \rightarrow 13$
32756 measured reflections	$k = -15 \rightarrow 15$
	$l = -20 \rightarrow 23$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0146P)^2]$
Least-squares matrix: full	where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.023$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$wR(F^2) = 0.042$	$\Delta\rho_{\text{max}} = 1.63 \text{ e \AA}^{-3}$
$S = 1.05$	$\Delta\rho_{\text{min}} = -1.14 \text{ e \AA}^{-3}$
2741 reflections	Extinction correction: SHELXL2015
42 parameters	(Sheldrick, 2015 <i>b</i>),
0 restraints	$F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
	Extinction coefficient: 0.00114 (12)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ba1	0.61644 (2)	0.2500	0.0000	0.00879 (3)
Ba2	0.11189 (2)	0.03912 (2)	0.2500	0.00733 (3)
V1	0.11728 (5)	0.2500	0.0000	0.00469 (6)
O1	0.03522 (17)	0.77707 (15)	0.11312 (11)	0.0074 (2)
O2	0.26812 (17)	0.08342 (15)	0.03175 (11)	0.0085 (2)
Br1	0.41944 (4)	0.41720 (4)	0.2500	0.01897 (6)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ba1	0.00453 (5)	0.00797 (5)	0.01389 (7)	0.000	0.000	-0.00337 (4)
Ba2	0.01093 (5)	0.00591 (5)	0.00515 (6)	0.00088 (4)	0.000	0.000
V1	0.00453 (12)	0.00486 (12)	0.00467 (15)	0.000	0.000	0.00036 (10)
O1	0.0071 (4)	0.0097 (5)	0.0054 (5)	-0.0011 (3)	-0.0005 (4)	-0.0014 (4)
O2	0.0079 (4)	0.0073 (4)	0.0104 (6)	0.0013 (3)	0.0006 (4)	0.0012 (4)
Br1	0.01411 (11)	0.02987 (15)	0.01293 (13)	-0.00761 (10)	0.000	0.000

Geometric parameters (\AA , $^\circ$)

Ba1—O2 ⁱ	2.7383 (12)	Ba2—O1 ^x	2.6919 (12)
Ba1—O2	2.7383 (12)	Ba2—O1 ^{xi}	2.6919 (12)
Ba1—O1 ⁱⁱ	2.7423 (12)	Ba2—O2	2.8510 (14)
Ba1—O1 ⁱⁱⁱ	2.7423 (12)	Ba2—O2 ^{xii}	2.8510 (14)
Ba1—O2 ^{iv}	2.7706 (12)	Ba2—Br1 ^{vii}	3.3334 (4)
Ba1—O2 ^v	2.7706 (12)	Ba2—Br1	3.6436 (4)
Ba1—Br1 ^{vi}	3.5437 (4)	Ba2—Br1 ^{viii}	3.7440 (5)
Ba1—Br1	3.5437 (4)	V1—O2	1.7107 (12)
Ba1—Br1 ⁱⁱⁱ	3.9958 (4)	V1—O2 ⁱ	1.7107 (12)
Ba1—Br1 ^{vii}	3.9958 (4)	V1—O1 ^{xiii}	1.7236 (13)
Ba2—O1 ^{viii}	2.6885 (13)	V1—O1 ^{ix}	1.7236 (13)
Ba2—O1 ^{ix}	2.6885 (13)		
O2 ⁱ —Ba1—O2	59.94 (5)	Br1 ⁱⁱⁱ —Ba1—Br1 ^{vii}	172.988 (9)
O2 ⁱ —Ba1—O1 ⁱⁱ	141.36 (4)	O1 ^{viii} —Ba2—O1 ^{ix}	75.41 (5)
O2—Ba1—O1 ⁱⁱ	135.87 (4)	O1 ^{viii} —Ba2—O1 ^x	146.830 (14)
O2 ⁱ —Ba1—O1 ⁱⁱⁱ	135.87 (4)	O1 ^{ix} —Ba2—O1 ^x	95.16 (4)
O2—Ba1—O1 ⁱⁱⁱ	141.36 (4)	O1 ^{viii} —Ba2—O1 ^{xi}	95.16 (4)
O1 ⁱⁱ —Ba1—O1 ⁱⁱⁱ	60.21 (5)	O1 ^{ix} —Ba2—O1 ^{xi}	146.830 (14)
O2 ⁱ —Ba1—O2 ^{iv}	79.03 (4)	O1 ^x —Ba2—O1 ^{xi}	75.30 (6)
O2—Ba1—O2 ^{iv}	132.99 (4)	O1 ^{viii} —Ba2—O2	128.03 (4)
O1 ⁱⁱ —Ba1—O2 ^{iv}	67.20 (4)	O1 ^{ix} —Ba2—O2	59.41 (3)
O1 ⁱⁱⁱ —Ba1—O2 ^{iv}	84.07 (4)	O1 ^x —Ba2—O2	66.72 (4)
O2 ⁱ —Ba1—O2 ^v	132.99 (4)	O1 ^{xi} —Ba2—O2	136.73 (4)
O2—Ba1—O2 ^v	79.03 (4)	O1 ^{viii} —Ba2—O2 ^{xii}	59.41 (3)
O1 ⁱⁱ —Ba1—O2 ^v	84.07 (4)	O1 ^{ix} —Ba2—O2 ^{xii}	128.03 (4)

O1 ⁱⁱⁱ —Ba1—O2 ^v	67.20 (4)	O1 ^x —Ba2—O2 ^{xii}	136.73 (4)
O2 ^{iv} —Ba1—O2 ^v	147.03 (5)	O1 ^{xi} —Ba2—O2 ^{xii}	66.72 (4)
O2 ⁱ —Ba1—Br1 ^{vi}	74.48 (3)	O2—Ba2—O2 ^{xii}	133.74 (5)
O2—Ba1—Br1 ^{vi}	67.15 (3)	O1 ^{viii} —Ba2—Br1 ^{vii}	123.92 (3)
O1 ⁱⁱ —Ba1—Br1 ^{vi}	140.94 (3)	O1 ^{ix} —Ba2—Br1 ^{vii}	123.92 (3)
O1 ⁱⁱⁱ —Ba1—Br1 ^{vi}	83.03 (3)	O1 ^x —Ba2—Br1 ^{vii}	87.96 (3)
O2 ^{iv} —Ba1—Br1 ^{vi}	125.25 (3)	O1 ^{xi} —Ba2—Br1 ^{vii}	87.96 (3)
O2 ^v —Ba1—Br1 ^{vi}	68.76 (3)	O2—Ba2—Br1 ^{vii}	71.22 (2)
O2 ⁱ —Ba1—Br1	67.15 (3)	O2 ^{xii} —Ba2—Br1 ^{vii}	71.21 (2)
O2—Ba1—Br1	74.48 (3)	O1 ^{viii} —Ba2—Br1	69.09 (3)
O1 ⁱⁱ —Ba1—Br1	83.03 (3)	O1 ^{ix} —Ba2—Br1	69.09 (3)
O1 ⁱⁱⁱ —Ba1—Br1	140.94 (3)	O1 ^x —Ba2—Br1	137.70 (3)
O2 ^{iv} —Ba1—Br1	68.76 (3)	O1 ^{xi} —Ba2—Br1	137.70 (3)
O2 ^v —Ba1—Br1	125.25 (3)	O2—Ba2—Br1	71.65 (2)
Br1 ^{vi} —Ba1—Br1	135.507 (11)	O2 ^{xii} —Ba2—Br1	71.65 (2)
O2 ⁱ —Ba1—Br1 ⁱⁱⁱ	61.79 (3)	Br1 ^{vii} —Ba2—Br1	71.673 (8)
O2—Ba1—Br1 ⁱⁱⁱ	111.52 (3)	O1 ^{viii} —Ba2—Br1 ^{viii}	79.58 (3)
O1 ⁱⁱ —Ba1—Br1 ⁱⁱⁱ	111.98 (3)	O1 ^{ix} —Ba2—Br1 ^{viii}	79.58 (3)
O1 ⁱⁱⁱ —Ba1—Br1 ⁱⁱⁱ	74.43 (3)	O1 ^x —Ba2—Br1 ^{viii}	67.38 (3)
O2 ^{iv} —Ba1—Br1 ⁱⁱⁱ	59.84 (3)	O1 ^{xi} —Ba2—Br1 ^{viii}	67.38 (3)
O2 ^v —Ba1—Br1 ⁱⁱⁱ	122.49 (3)	O2—Ba2—Br1 ^{viii}	113.09 (3)
Br1 ^{vi} —Ba1—Br1 ⁱⁱⁱ	65.431 (8)	O2 ^{xii} —Ba2—Br1 ^{viii}	113.09 (2)
Br1—Ba1—Br1 ⁱⁱⁱ	111.683 (8)	Br1 ^{vii} —Ba2—Br1 ^{viii}	148.359 (12)
O2 ⁱ —Ba1—Br1 ^{vii}	111.52 (3)	Br1—Ba2—Br1 ^{viii}	139.968 (10)
O2—Ba1—Br1 ^{vii}	61.79 (3)	O2—V1—O2 ⁱ	106.18 (8)
O1 ⁱⁱ —Ba1—Br1 ^{vii}	74.43 (3)	O2—V1—O1 ^{xiii}	116.27 (6)
O1 ⁱⁱⁱ —Ba1—Br1 ^{vii}	111.98 (3)	O2 ⁱ —V1—O1 ^{xiii}	106.33 (6)
O2 ^{iv} —Ba1—Br1 ^{vii}	122.49 (3)	O2—V1—O1 ^{ix}	106.33 (6)
O2 ^v —Ba1—Br1 ^{vii}	59.84 (3)	O2 ⁱ —V1—O1 ^{ix}	116.27 (6)
Br1 ^{vi} —Ba1—Br1 ^{vii}	111.683 (8)	O1 ^{xiii} —V1—O1 ^{ix}	105.90 (8)
Br1—Ba1—Br1 ^{vii}	65.431 (8)		

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