



Orthosilicates with glaserite-type crystal structures: $\text{Na}_2\text{BaZr}[\text{SiO}_4]_2$ and $\text{Na}_2\text{BaHf}[\text{SiO}_4]_2$

Hisanori Yamane, Shiro Funahashi, Naoto Hirosaki and Takashi Takeda*

Research Center for Electronic and Optical Materials, National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan. *Correspondence e-mail: takeda.takashi@nims.go.jp

Received 28 February 2025

Accepted 2 April 2025

Edited by M. Weil, Vienna University of Technology, Austria

Keywords: crystal structure; glaserite-type structure; orthosilicate; single-crystal X-ray diffraction; twin analysis.**CCDC references:** 2440344; 2440343**Supporting information:** this article has supporting information at journals.iucr.org/e

Single crystal particles of $\text{Na}_2\text{BaZr}[\text{SiO}_4]_2$ [systematic name: disodium barium zirconium bis(orthosilicate)] and $\text{Na}_2\text{BaHf}[\text{SiO}_4]_2$ [disodium barium hafnium bis(orthosilicate)] were extracted from grain-grown polycrystals obtained by heating compacts of binary oxide mixtures at 1473 K. Single crystal X-ray diffraction analysis revealed that these are isostructural orthosilicates with a glaserite-type crystal structure, in which all sites of X , Y , M , and T in the general formula $XY_2[M(\text{TO}_4)_2]$ are fully occupied by atoms of different elements. The crystal structures of the title compounds were refined in space group $P\bar{3}$ under consideration of a two-component twin model. The SiO_4 tetrahedra are rotated approximately $\pm 10.2^\circ$ from the mirror plane of space group $P\bar{3}m$ around an axis parallel to $[001]$.

1. Chemical context

Nikolova & Kostov-Kytin (2013) described more than 100 oxides with glaserite-type crystal structures by the general formula $X_{(\square;1)}Y_{(\square;2)}[M(\text{TO}_4)_2]$ and summarized their crystal structural features: the T sites are always fully occupied by the atoms of transition metals (V, Cr, Mo, W, Re, Fe, Ru) or non-metals (Si, P, S, Se). These T atoms are fourfold coordinated by oxygen atoms to form isolated tetrahedra in the crystal structures. Silicates ($T = \text{Si}$), such as $\text{BaMg}[\text{SiO}_4]$ and $\text{Ba}(\text{Ba}, \text{Sr}, \text{Ca})_2\text{Mg}[\text{SiO}_4]_2$ doped with Eu^{2+} , have been studied for their fluorescent properties and photochromism (Yonesaki *et al.*, 2008, 2011; Yonesaki, 2013; Yonezaki *et al.*, 2018; Yonezaki, 2015, 2018, 2020; Yonezaki & Takei, 2016; Yonezaki & Yanai, 2021; Birkel *et al.*, 2015). Recently, ferroaxial transitions of compounds with glaserite-type crystal structures were investigated, in which the space-group type changes from $P\bar{3}$ to $P\bar{3}m$ (Yamagishi *et al.*, 2023). The rotation angle φ of the TO_4 tetrahedron was defined relative to the mirror plane of $P\bar{3}m$, and $\text{BaCa}_2\text{Mg}[\text{SiO}_4]_2$ with $\varphi = 12.5^\circ$ was proposed as a potential ferroaxial transition material. For the compounds with $M = \text{Zr}$, Kostov-Kytin and co-workers analysed the crystal structures of $\text{Na}_{3-x}\text{H}_{1+x}\text{Zr}(\text{SiO}_4)_4 \cdot y\text{H}_2\text{O}$ in which water molecules are located between the ZrO_6 octahedra (Kostov-Kytin *et al.*, 2012, 2013).

In the current study, we report the synthesis and crystal structure analysis of two new orthosilicate compounds with glaserite-type crystal structure, $\text{Na}_2\text{BaZr}[\text{SiO}_4]_2$ and $\text{Na}_2\text{BaHf}[\text{SiO}_4]_2$.

2. Structural commentary

According to the classification by Nikolova & Kostov-Kytin (2013) using the general formula $X_{(\square;1)}Y_{(\square;2)}[M(\text{TO}_4)_2]$ for compounds with glaserite-type crystal structures, Na_2BaZr

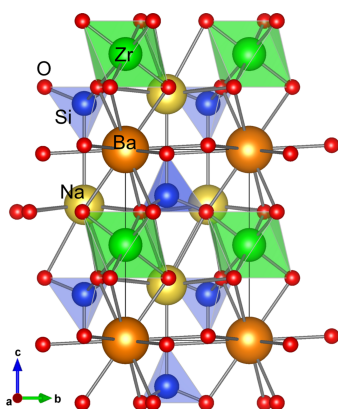


Table 1

Selected bond lengths (Å) for Na₂BaZr[SiO₄]₂.

Na1—O1 ⁱ	2.9791 (15)	Ba1—O2	3.1198 (2)
Na1—O1 ⁱⁱⁱ	2.4461 (15)	Zr1—O1	2.0667 (13)
Na1—O1	3.1545 (19)	Si1—O1	1.6373 (13)
Na1—O2 ⁱⁱⁱ	2.250 (3)	Si1—O2	1.578 (2)
Ba1—O1	2.8764 (15)		

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

[SiO₄]₂ and Na₂BaHf[SiO₄]₂ meet the condition $X \neq Y \neq M \neq T$ of $XY_2[M(TO_4)_2]$ with no vacancy. The two new orthosilicates are isostructural and crystallize in the trigonal space group $P\bar{3}$. The crystal structures of both silicates were refined under consideration of a two-component twin model in each case. Multiplicity, Wyckoff letter, and site symmetry are: 1, a and $\bar{3}$ for Ba1, 1, b and $\bar{3}$ for Zr1/Hf1, 2, d and 3 for Na1, Si1 and O2, and 6, g and 1 for O1. As shown in Fig. 1, slabs identified in the crystal structure are composed of $M = \text{Zr-}$ or Hf-centred oxygen octahedra and SiO₄ tetrahedra.

Fig. 2 shows the arrangement of oxygen atoms around each cation. Interatomic distances of Zr—O and Hf—O are 2.0667 (14) Å ($\times 6$) and 2.0600 (15) Å ($\times 6$), respectively (Tables 1 and 2), which are consistent with the sizes of Shannon's effective ionic radii [six-coordinated Zr (0.72 Å) and Hf (0.71 Å); Shannon, 1976]. The Si—O distances of 1.6373 (13) and 1.578 (2) Å for Na₂BaZr[SiO₄]₂ agree with those of 1.6354 (16) and 1.575 (2) Å for Na₂BaHf[SiO₄]₂. The Ba—O distances for the 12-coordinate X site are slightly longer for Na₂BaZr[SiO₄]₂ [2.8764 (15)–3.1198 (2) Å] than for

Table 2

Selected bond lengths (Å) for Na₂BaHf[SiO₄]₂.

Na1—O1 ⁱ	2.4423 (15)	Ba1—O2	3.1158 (2)
Na1—O1 ⁱⁱⁱ	2.9738 (15)	Hf1—O1	2.0600 (15)
Na1—O1	3.145 (2)	Si1—O1	1.6354 (16)
Na1—O2 ⁱⁱⁱ	2.258 (3)	Si1—O2	1.575 (2)
Ba1—O1	2.8687 (16)		

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

Na₂BaHf[SiO₄]₂ [2.8687 (16)–3.1158 (2) Å]. The distances between O1 and Na1 at the tenfold coordination sites are slightly longer for Na₂BaM[SiO₄]₂ $M = \text{Zr}$ [2.4461 (15)–3.1545 (19) Å] than for $M = \text{Hf}$ [2.4423 (15)–3.145 (2) Å], while the Na1—O2 distance of 2.250 (3) Å for $M = \text{Zr}$ is slightly shorter than that of 2.258 (3) Å for $M = \text{Hf}$. The bond valence sums for Na1, Ba1, Zr1, Hf1, and Si1 calculated with the bond valence parameters provided by Gagné & Hawthorne (2015) are 1.00, 1.86, 4.03, and 4.11 valence units for Na₂BaM[SiO₄]₂ $M = \text{Zr}$, and 1.01, 1.89, 4.05, and 4.09 valence units for $M = \text{Hf}$. The rotation angles φ of the [SiO₄] tetrahedra are 10.18° for $M = \text{Zr}$ and 10.15° for $M = \text{Hf}$ (Fig. 3).

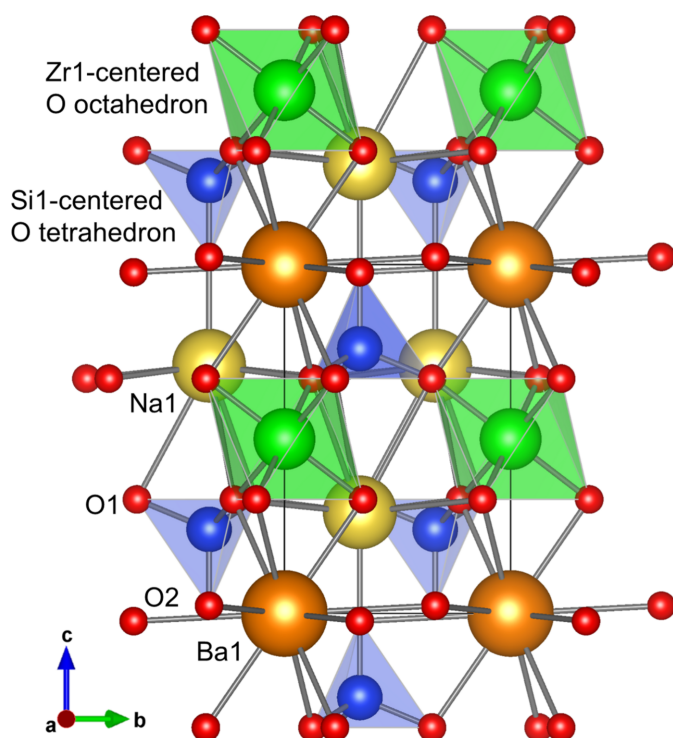


Figure 1

Crystal structure of Na₂BaZr[SiO₄]₂ in a projection along [100], drawn with Zr1-centred oxygen octahedra and Si1-centred oxygen tetrahedra.

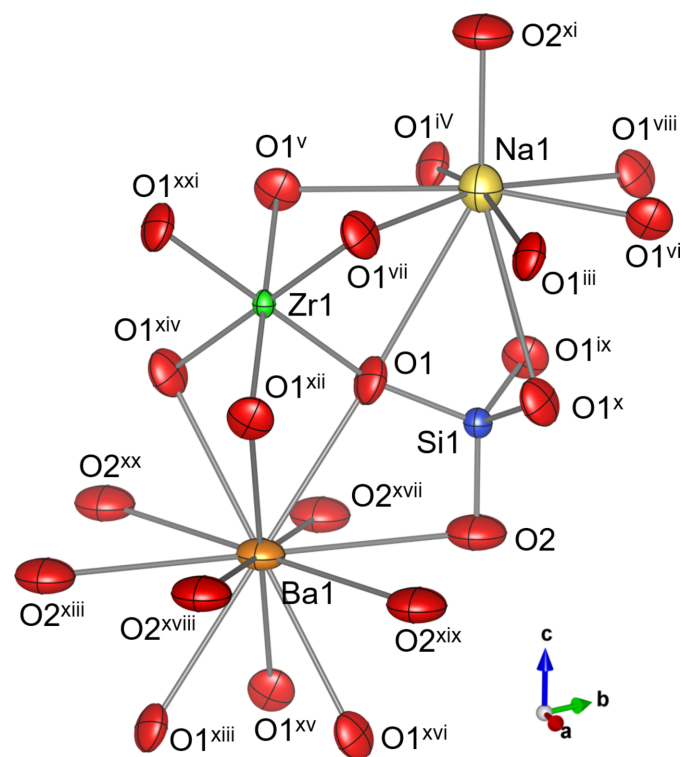


Figure 2

Atomic arrangements around Na1, Ba1, Zr1, and Si1 in the crystal structure of Na₂BaZr[SiO₄]₂. Displacement ellipsoids are depicted at the 90% probability level. [Symmetry codes: (i) $x, y + 1, z$; (ii) $-x + 1, -y + 2, -z + 1$; (iii) $-x + 1, -y + 1, -z + 1$; (iv) $-x, -y + 1, -z + 1$; (v) $x - y, x, -z + 1$; (vi) $x - y + 1, x + 1, -z + 1$; (vii) $y, -x + y, -z + 1$; (viii) $y, -x + y + 1, -z + 1$; (ix) $-x + y, -x + 1, z$; (x) $-y + 1, x - y + 1, z$; (xi) $x, y, z + 1$; (xii) $-x + y, -x, z$; (xiii) $-x, -y, -z$; (xiv) $-y, x - y, z$; (xv) $x - y, x, -z$; (xvi) $y, -x + y, -z$; (xvii) $-x, -y + 1, -z$; (xviii) $x, y - 1, z$; (xix) $-x + 1, -y + 1, -z$; (xx) $x - 1, y - 1, z$; (xxi) $-x, -y, -z + 1$; (xxii) $x + 1, y + 1, z$; (xxiii) $x, y, z - 1$.]

Table 3
Experimental details.

	Na ₂ BaZr[SiO ₄] ₂	Na ₂ BaHf[SiO ₄] ₂
Crystal data		
<i>M_r</i>	458.72	545.99
Crystal system, space group	Trigonal, <i>P</i> $\bar{3}$	Trigonal, <i>P</i> $\bar{3}$
Temperature (K)	293	293
<i>a</i> , <i>c</i> (Å)	5.3966 (2), 7.2153 (3)	5.3889 (2), 7.1996 (2)
<i>V</i> (Å ³)	181.98 (2)	181.07 (1)
<i>Z</i>	1	1
Radiation type	Mo <i>K</i> α	Mo <i>K</i> α
<i>μ</i> (mm ⁻¹)	7.27	20.19
Crystal size (mm)	0.04 × 0.03 × 0.01	0.03 × 0.03 × 0.01
Data collection		
Diffractometer	ROD, Synergy Custom system, HyPix-Arc 150	ROD, Synergy Custom system, HyPix-Arc 150
Absorption correction	Gaussian (<i>CrysAlis PRO</i> ; Rigaku OD, 2023)	Gaussian (<i>CrysAlis PRO</i> ; Rigaku OD, 2023)
<i>T_{min}</i> , <i>T_{max}</i>	0.544, 0.817	0.641, 0.883
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	9034, 587, 543	8609, 538, 532
<i>R_{int}</i>	0.043	0.045
(sin θ/λ) _{max} (Å ⁻¹)	0.832	0.806
Refinement		
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.016, 0.035, 1.11	0.010, 0.024, 1.11
No. of reflections	587	538
No. of parameters	24	24
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.52, -0.59	0.61, -0.60

Computer programs: *CrysAlis PRO* (Rigaku OD, 2023), *SHELXT* (Sheldrick, 2015a), *SHELXL* (Sheldrick, 2015b), *VESTA* (Momma & Izumi, 2011), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

The Madelung energy part of the lattice energies (*MAPLE*; Hoppe, 1995) of Na₂BaM[SiO₄]₂ calculated using *VESTA* (Momma & Izumi, 2011) are -50.170 MJ mol⁻¹ (*M* = Zr) and -50.260 MJ mol⁻¹ (*M* = Hf). These values are close to those of -49.880 MJ mol⁻¹ and -49.880 MJ mol⁻¹ with differences of 0.6% and 0.8%, respectively, as calculated from the equation BaO + MO₂ + α-Na₂Si₂O₅ = Na₂BaM[SiO₄]₂ using *MAPLE* values calculated from the crystal structure data for BaO (-3.510 MJ mol⁻¹; Zollweg, 1955), ZrO₂ (-12.740 MJ mol⁻¹; Gualtieri *et al.*, 1996), HfO₂ (-12.740 MJ mol⁻¹; Pathak *et al.*, 2020) and α-Na₂Si₂O₅ (-33.630 MJ mol⁻¹; Pant & Cruickshank, 1968).

3. Database survey

The crystal structures listed for glaserite-type silicates in the ICSD database (ICSD, 2025) are the high-temperature phase

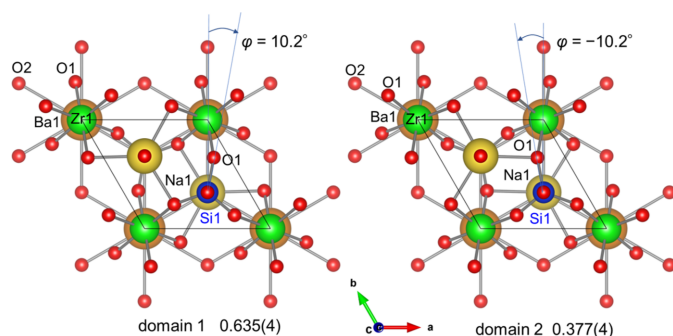


Figure 3
[001] projection of the twin domains in the crystal structure of Na₂BaZr[SiO₄]₂.

of Ca₂[SiO₄] (*P* $\bar{3}m$, *Z* = 2, *V* = 194.19 Å³; Mumme *et al.*, 1996), Ba₃Mg[SiO₄]₂ (*P* $\bar{3}m$, *Z* = 1, *V* = 198.64 Å³; Iwata *et al.*, 2009) and its superstructure (*P* $\bar{3}$, *Z* = 3, *V* = 594.71 Å³; Park *et al.*, 2009), BaCa₂Mg[SiO₄]₂ (*P* $\bar{3}$, *Z* = 1, *V* = 173.31 Å³; Park *et al.*, 2011), Ba_xSr_{3-x}Mg[SiO₄]₂ (*x* = 0.0 – 0.5, *C2*, *Z* = 4, *V* = 714.9 – 723.7 Å³; *x* = 0.625 – 2.375, *P* $\bar{3}m$, *Z* = 1, *V* = 181.81 – 193.46 Å³; *x* = 2.5 – 3.0, *P* $\bar{3}$, *Z* = 3, *V* = 583.2 – 594.72 Å³; Yonezaki, 2015), Ba(Sr_{1-x}Ca_x)₂Mg[SiO₄]₂ (*x* = 0.0 – 0.5, *P* $\bar{3}m$, *Z* = 1, *V* = 182.76 – 178.70 Å³; *x* = 0.5625 – 1.0, *P* $\bar{3}$, *Z* = 1, *V* = 177.97 – 174.00 Å³; Yonesaki *et al.*, 2008; Yonesaki, 2013), Ba₃Mn[SiO₄] (*P* $\bar{3}m$, *Z* = 1, *V* = 203.44 Å³; Avdeev *et al.*, 2018), Na₃HZr[SiO₄]₂ (*P* $\bar{1}$, *Z* = 2, *V* = 350.12 Å³; Na₃HZr[SiO₄]₂·0.4H₂O, *P* $\bar{1}$, *Z* = 2, *V* = 350.19 Å³; Na₃HZr[SiO₄]₂·H₂O, *C2/m*, *Z* = 4, *V* = 683.92 Å³; Kostov-Kytin *et al.*, 2012).

4. Synthesis and crystallization

The starting materials were powders of Na₂O (~80%, Sigma-Aldrich), SiO₂ (99.9% Kojundo Chemical Lab. Co., Ltd.), BaO (99.99%, Sigma-Aldrich), ZrO₂ (99%, Sigma-Aldrich), and HfO₂ (98%, Kojundo Chemical Lab. Co., Ltd.), which were weighed in a glove box in a nitrogen atmosphere, mixed in an agate mortar, and formed into disk-shaped compacts. The compacts were placed in a nickel boat and sealed in a stainless-steel container. The container was heated up to 1473 K for 3 h in a nitrogen gas flow to prevent oxidation of the stainless steel, and this temperature was maintained for 30 min. The temperature was subsequently lowered to 1073 K at a rate of -100 K h⁻¹. The power supply to the heater wire was stopped at this temperature, and the sample was allowed to cool in the furnace. The single crystal grains of Na₂BaZr[SiO₄]₂ used for

single crystal X-ray diffraction data measurements were isolated from fragments of polycrystals synthesised from a starting material mixture with a metal element molar ratio of Na:Ba:Zr:Si = 2:1:1:2. Single crystal grains of Na₂BaHf[SiO₄]₂ were obtained from polycrystals prepared with a starting mixture of Na:Ba:Hf:Si = 2.2:1:1:2.2.

Semi-quantitative analysis of the Na₂BaZr[SiO₄]₂ and Na₂BaHf[SiO₄]₂ grains was performed using an energy-dispersive X-ray detector (Bruker AXS, XFlash 5010) attached to a scanning electron microscope (Hitachi High-Tech SU1510) and measurement analysis software (Bruker AXS, QUANTAX2000). The atomic ratios acquired from the analysis were Na:Ba:Hf:Si = 2.0 (3):0.6 (1):0.66 (5):2.0 (3) for Na₂BaZr[SiO₄]₂ and Na:Ba:Zr:Si = 2.3 (4):1.2 (1):1.3 (1):2.0 (1) for Na₂BaHf[SiO₄]₂, both of which correspond sufficiently with the metal element ratios of the formulae.

5. Refinement

Crystal data, data collection and structural refinement details are summarised in Table 3. In the first refinement step, the ideal model of the glaserite-type structure with space group $P\bar{3}m$ was adopted and the $R1$ values were 0.032 and 0.018 for Na₂BaM[SiO₄]₂ for $M = \text{Zr}$ and Hf, respectively. However, the ratio of the mean-square displacements of the major and minor axes of the atomic displacement ellipsoid of O1 was 30.3 ($M = \text{Zr}$) and 22.4 ($M = \text{Hf}$). Subsequently, when the refinement was performed in $P\bar{3}$ removing mirror symmetry operation from $P\bar{3}m$, the $R1$ values were 0.035 and 0.020, and the displacement ratios were still large at 27.6 and 18.2, for $M = \text{Zr}$ and Hf, respectively. Further analysis in space group $P\bar{3}$ under consideration of twinning (twin matrix 010, 100, 00 $\bar{1}$) resulted in $R1$ values of 0.016 and 0.010 for $M = \text{Zr}$ and Hf, respectively, and both displacement ratios were reasonable with a value of 3.2. The twin ratios of domains 1 and 2 were refined to 0.635 (4):0.365 for $M = \text{Zr}$ and 0.623 (4):0.377 (4) for $M = \text{Hf}$.

Funding information

Funding for this research was provided by: JST, the Core Research for Evolutionary Science and Technology (grant No. JPMJCR19J2); Innovative Science and Technology Initiative for Security (grant No. JPJ004596).

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supporting information

Acta Cryst. (2025). E81, 368-371 [https://doi.org/10.1107/S2056989025002956]

Orthosilicates with glaserite-type crystal structures: Na₂BaZr[SiO₄]₂ and Na₂BaHf[SiO₄]₂

Hisanori Yamane, Shiro Funahashi, Naoto Hirosaki and Takashi Takeda

Computing details

Disodium barium zirconium bis(orthosilicate) (I)

Crystal data

Na₂BaZr[SiO₄]₂

$M_r = 458.72$

Trigonal, $P\bar{3}$

$a = 5.3966$ (2) Å

$c = 7.2153$ (3) Å

$V = 181.98$ (2) Å³

$Z = 1$

$F(000) = 210$

$D_x = 4.186$ Mg m⁻³

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

Cell parameters from 5734 reflections

$\theta = 2.8$ – 47.6°

$\mu = 7.27$ mm⁻¹

$T = 293$ K

Plate, colourless

0.04 × 0.03 × 0.01 mm

Data collection

ROD, Synergy Custom system, HyPix-Arc 150 diffractometer

Radiation source: Rotating-anode X-ray tube, Rigaku (Mo) X-ray Source

Mirror monochromator

Detector resolution: 10.0000 pixels mm⁻¹

ω scans

Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2023)

$T_{\min} = 0.544$, $T_{\max} = 0.817$

9034 measured reflections

587 independent reflections

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

$R_{\text{int}} = 0.043$

$\theta_{\max} = 36.2^\circ$, $\theta_{\min} = 2.8^\circ$

$h = -8 \rightarrow 7$

$k = -8 \rightarrow 8$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.016$

$wR(F^2) = 0.035$

$S = 1.11$

587 reflections

24 parameters

0 restraints

Primary atom site location: dual

$w = 1/[\sigma^2(F_o^2) + (0.0092P)^2 + 0.1709P]$

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

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.52$ e Å⁻³

$\Delta\rho_{\min} = -0.59$ e Å⁻³

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. Refined as a 2-component twin. 1. Twinned data refinement Scales: 0.635 (4) 0.365 (4)

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Na1	0.333333	0.666667	0.71034 (19)	0.0167 (2)
Ba1	0.000000	0.000000	0.000000	0.01522 (7)
Zr1	0.000000	0.000000	0.500000	0.00498 (6)
Si1	0.333333	0.666667	0.24086 (9)	0.00685 (12)
O1	0.1242 (3)	0.3476 (3)	0.3269 (2)	0.0144 (3)
O2	0.333333	0.666667	0.0221 (3)	0.0222 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0157 (4)	0.0157 (4)	0.0188 (6)	0.00784 (18)	0.000	0.000
Ba1	0.01899 (9)	0.01899 (9)	0.00767 (9)	0.00950 (4)	0.000	0.000
Zr1	0.00436 (8)	0.00436 (8)	0.00620 (12)	0.00218 (4)	0.000	0.000
Si1	0.00661 (17)	0.00661 (17)	0.0073 (3)	0.00331 (9)	0.000	0.000
O1	0.0154 (7)	0.0082 (5)	0.0175 (6)	0.0043 (5)	0.0010 (5)	0.0046 (4)
O2	0.0287 (8)	0.0287 (8)	0.0093 (8)	0.0144 (4)	0.000	0.000

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

Na1—Zr1 ⁱ	3.4657 (6)	Ba1—O1 ^{xvi}	2.8763 (15)
Na1—Si1 ⁱⁱ	3.1356 (2)	Ba1—O1	2.8763 (15)
Na1—Si1 ⁱⁱⁱ	3.1356 (2)	Ba1—O2 ^{xvii}	3.1198 (2)
Na1—Si1	3.3875 (15)	Ba1—O2	3.1198 (2)
Na1—Si1 ^{iv}	3.1356 (2)	Ba1—O2 ^{xviii}	3.1198 (2)
Na1—O1 ^v	2.9791 (15)	Ba1—O2 ^{xix}	3.1198 (2)
Na1—O1 ^{vi}	2.4461 (15)	Ba1—O2 ^{xxi}	3.1198 (2)
Na1—O1 ^{iv}	2.4461 (14)	Ba1—O2 ^{xx}	3.1198 (2)
Na1—O1 ^{vii}	2.4461 (14)	Zr1—O1 ^{xxi}	2.0666 (13)
Na1—O1 ^{viii}	2.9791 (15)	Zr1—O1 ^{vii}	2.0666 (14)
Na1—O1 ⁱⁱⁱ	2.9791 (15)	Zr1—O1	2.0667 (13)
Na1—O1	3.1545 (19)	Zr1—O1 ^v	2.0667 (13)
Na1—O1 ^{ix}	3.1545 (19)	Zr1—O1 ^{xiv}	2.0666 (14)
Na1—O1 ^x	3.1545 (19)	Zr1—O1 ^{xii}	2.0667 (13)
Na1—O2 ^{xi}	2.250 (3)	Si1—O1 ^x	1.6373 (13)
Ba1—O1 ^{xii}	2.8764 (15)	Si1—O1 ^{ix}	1.6373 (13)
Ba1—O1 ^{xiii}	2.8763 (15)	Si1—O1	1.6373 (13)
Ba1—O1 ^{xiv}	2.8763 (15)	Si1—O2	1.578 (2)
Ba1—O1 ^{xv}	2.8764 (15)		
Si1 ⁱⁱⁱ —Na1—Zr1 ⁱ	160.48 (5)	Na1—Zr1—Na1 ⁱⁱⁱ	77.74 (2)
Si1 ^{iv} —Na1—Zr1 ⁱ	66.579 (9)	Na1—Zr1—Na1 ^{xxi}	180.0
Si1 ⁱⁱ —Na1—Zr1 ⁱ	66.579 (9)	Na1 ⁱⁱⁱ —Zr1—Na1 ^{xx}	180.0
Si1—Na1—Zr1 ⁱ	64.03 (2)	Na1 ^{iv} —Zr1—Na1 ⁱⁱⁱ	102.26 (2)
Si1 ⁱⁱⁱ —Na1—Si1	96.45 (3)	Na1 ^{xviii} —Zr1—Na1 ^{iv}	180.0
Si1 ^{iv} —Na1—Si1 ⁱⁱⁱ	118.756 (11)	Na1 ^{xxi} —Zr1—Na1 ⁱⁱⁱ	102.26 (2)

Si1 ^{iv} —Na1—Si1	96.45 (3)	Na1 ^{xviii} —Zr1—Na1 ^{xxi}	77.74 (2)
Si1 ⁱⁱ —Na1—Si1 ^{iv}	118.757 (11)	Na1 ^{iv} —Zr1—Na1	77.74 (2)
Si1 ⁱⁱ —Na1—Si1 ⁱⁱⁱ	118.756 (11)	Na1 ^{xviii} —Zr1—Na1 ^{xx}	102.26 (2)
Si1 ⁱⁱ —Na1—Si1	96.45 (3)	Na1 ^{xviii} —Zr1—Na1 ⁱⁱⁱ	77.74 (2)
O1 ⁱⁱⁱ —Na1—Zr1 ⁱ	138.23 (4)	O1—Zr1—Na1 ^{xviii}	135.97 (4)
O1 ^{vii} —Na1—Zr1 ⁱ	137.54 (5)	O1 ^{vii} —Zr1—Na1 ^{xviii}	58.86 (4)
O1 ^{iv} —Na1—Zr1 ⁱ	35.96 (3)	O1 ^{xxi} —Zr1—Na1 ^{xx}	58.86 (4)
O1 ^{viii} —Na1—Zr1 ⁱ	36.43 (3)	O1 ^{vii} —Zr1—Na1 ⁱⁱⁱ	63.77 (5)
O1 ^v —Na1—Zr1 ⁱ	86.58 (3)	O1 ^{xii} —Zr1—Na1 ^{xx}	135.97 (4)
O1 ^{vi} —Na1—Zr1 ⁱ	85.84 (4)	O1 ^{xxi} —Zr1—Na1	116.23 (5)
O1 ^{iv} —Na1—Si1	83.70 (5)	O1 ^v —Zr1—Na1 ^{xx}	44.03 (4)
O1 ^{vi} —Na1—Si1	83.70 (5)	O1 ^v —Zr1—Na1 ^{xviii}	116.23 (5)
O1 ^{vii} —Na1—Si1 ⁱⁱⁱ	31.10 (3)	O1 ^v —Zr1—Na1 ⁱⁱⁱ	135.97 (4)
O1 ^{vii} —Na1—Si1	83.70 (5)	O1 ^{xii} —Zr1—Na1 ⁱⁱⁱ	44.03 (4)
O1 ⁱⁱⁱ —Na1—Si1	84.83 (4)	O1 ^{xiv} —Zr1—Na1 ^{xviii}	121.14 (4)
O1 ^v —Na1—Si1	84.83 (4)	O1 ^{xii} —Zr1—Na1 ^{xviii}	63.77 (5)
O1 ^v —Na1—Si1 ⁱⁱⁱ	91.85 (3)	O1 ^{xiv} —Zr1—Na1 ^{iv}	58.86 (4)
O1 ⁱⁱⁱ —Na1—Si1 ^{iv}	148.85 (3)	O1—Zr1—Na1 ^{iv}	44.03 (4)
O1 ^v —Na1—Si1 ⁱⁱ	148.85 (3)	O1 ^{xxi} —Zr1—Na1 ^{xviii}	44.03 (4)
O1 ^{viii} —Na1—Si1	84.83 (4)	O1 ^{xii} —Zr1—Na1	121.14 (4)
O1 ⁱⁱⁱ —Na1—Si1 ⁱⁱ	91.85 (3)	O1 ^v —Zr1—Na1 ^{iv}	63.77 (5)
O1 ^{vii} —Na1—Si1 ⁱⁱ	148.63 (3)	O1—Zr1—Na1 ⁱⁱⁱ	58.86 (4)
O1 ^{iv} —Na1—Si1 ^{iv}	31.10 (3)	O1—Zr1—Na1 ^{xxi}	116.23 (5)
O1 ^{viii} —Na1—Si1 ⁱⁱⁱ	148.85 (3)	O1 ^{xxi} —Zr1—Na1 ^{iv}	135.97 (4)
O1 ^{vi} —Na1—Si1 ^{iv}	148.63 (3)	O1 ^v —Zr1—Na1 ^{xxi}	121.14 (4)
O1 ^{viii} —Na1—Si1 ⁱⁱ	30.93 (3)	O1 ^{xii} —Zr1—Na1 ^{iv}	116.23 (5)
O1 ^{vii} —Na1—Si1 ^{iv}	92.26 (3)	O1 ^{xii} —Zr1—Na1 ^{xxi}	58.86 (4)
O1 ^{iv} —Na1—Si1 ⁱⁱ	92.26 (3)	O1 ^{vii} —Zr1—Na1 ^{xx}	116.23 (5)
O1 ^{viii} —Na1—Si1 ^{iv}	91.85 (3)	O1 ^{vii} —Zr1—Na1 ^{iv}	121.14 (4)
O1 ⁱⁱⁱ —Na1—Si1 ⁱⁱⁱ	30.93 (3)	O1—Zr1—Na1 ^{xx}	121.14 (4)
O1 ^v —Na1—Si1 ^{iv}	30.93 (3)	O1 ^{xxi} —Zr1—Na1 ^{xxi}	63.77 (5)
O1 ^{iv} —Na1—Si1 ⁱⁱⁱ	148.63 (3)	O1 ^{xiv} —Zr1—Na1 ^{xx}	63.77 (5)
O1 ^{vi} —Na1—Si1 ⁱⁱ	31.10 (3)	O1 ^{vii} —Zr1—Na1	44.03 (4)
O1 ^{vi} —Na1—Si1 ⁱⁱⁱ	92.26 (3)	O1 ^{xxi} —Zr1—Na1 ⁱⁱⁱ	121.14 (4)
O1 ^{vii} —Na1—O1 ⁱⁱⁱ	56.84 (6)	O1 ^{xiv} —Zr1—Na1	135.97 (4)
O1 ^{vi} —Na1—O1 ^{viii}	56.84 (6)	O1 ^{vii} —Zr1—Na1 ^{xxi}	135.97 (4)
O1 ^{iv} —Na1—O1 ^{vii}	118.811 (19)	O1 ^v —Zr1—Na1	58.86 (4)
O1 ^{iv} —Na1—O1 ^{viii}	62.52 (6)	O1 ^{xiv} —Zr1—Na1 ⁱⁱⁱ	116.23 (5)
O1 ^{vi} —Na1—O1 ⁱⁱⁱ	62.52 (6)	O1 ^{xiv} —Zr1—Na1 ^{xxi}	44.03 (4)
O1 ^{vi} —Na1—O1 ^v	168.18 (9)	O1—Zr1—Na1	63.77 (5)
O1 ^v —Na1—O1 ⁱⁱⁱ	119.197 (12)	O1 ^{xxi} —Zr1—O1 ^{xii}	92.75 (6)
O1 ^{vii} —Na1—O1 ^v	62.52 (6)	O1 ^{xiv} —Zr1—O1	87.25 (6)
O1 ^{iv} —Na1—O1 ^v	56.84 (6)	O1 ^{xxi} —Zr1—O1 ^{xiv}	92.75 (6)
O1 ^{vii} —Na1—O1 ^{viii}	168.18 (9)	O1 ^{xxi} —Zr1—O1	180.0
O1 ^{iv} —Na1—O1 ^{vi}	118.810 (18)	O1 ^{xxi} —Zr1—O1 ^{vii}	87.25 (6)
O1 ^{viii} —Na1—O1 ⁱⁱⁱ	119.197 (13)	O1 ^{xiv} —Zr1—O1 ^v	92.75 (6)
O1 ^{viii} —Na1—O1 ^v	119.196 (13)	O1—Zr1—O1 ^{xii}	87.25 (6)
O1 ^{vi} —Na1—O1 ^{vii}	118.812 (19)	O1 ^{vii} —Zr1—O1 ^{xii}	92.75 (6)

O1 ^{iv} —Na1—O1 ⁱⁱⁱ	168.18 (9)	O1 ^{vii} —Zr1—O1 ^v	87.25 (6)
O2 ^{xi} —Na1—Zr1 ⁱ	115.97 (2)	O1 ^{xxi} —Zr1—O1 ^v	87.25 (6)
O2 ^{xi} —Na1—Si1	180.0	O1—Zr1—O1 ^v	92.75 (6)
O2 ^{xi} —Na1—Si1 ^{iv}	83.55 (3)	O1 ^{xiv} —Zr1—O1 ^{xii}	87.25 (6)
O2 ^{xi} —Na1—Si1 ⁱⁱⁱ	83.55 (3)	O1 ^{vii} —Zr1—O1	92.75 (6)
O2 ^{xi} —Na1—Si1 ⁱⁱ	83.55 (3)	O1 ^{vii} —Zr1—O1 ^{xiv}	180.0
O2 ^{xi} —Na1—O1 ^v	95.17 (4)	O1 ^v —Zr1—O1 ^{xii}	180.0
O2 ^{xi} —Na1—O1 ^{iv}	96.30 (5)	Na1 ⁱⁱⁱ —Si1—Na1	83.55 (3)
O2 ^{xi} —Na1—O1 ^{vi}	96.30 (5)	Na1 ⁱⁱ —Si1—Na1 ⁱⁱⁱ	118.756 (11)
O2 ^{xi} —Na1—O1 ^{vii}	96.30 (5)	Na1 ⁱⁱ —Si1—Na1	83.55 (3)
O2 ^{xi} —Na1—O1 ^{viii}	95.17 (4)	Na1 ^{iv} —Si1—Na1	83.55 (3)
O2 ^{xi} —Na1—O1 ⁱⁱⁱ	95.17 (4)	Na1 ^{iv} —Si1—Na1 ⁱⁱⁱ	118.756 (11)
O1—Ba1—O1 ^{xiv}	59.43 (4)	Na1 ⁱⁱ —Si1—Na1 ^{iv}	118.757 (11)
O1 ^{xiii} —Ba1—O1 ^{xv}	59.43 (4)	Na1 ⁱⁱ —Si1—Ba1 ⁱ	67.716 (15)
O1—Ba1—O1 ^{xvi}	120.57 (4)	Na1 ^{iv} —Si1—Ba1	67.715 (15)
O1—Ba1—O1 ^{xii}	59.43 (4)	Na1 ⁱⁱ —Si1—Ba1	157.30 (3)
O1 ^{xiii} —Ba1—O1 ^{xiv}	120.57 (4)	Na1 ^{iv} —Si1—Ba1 ^{xxii}	157.30 (3)
O1 ^{xiv} —Ba1—O1 ^{xii}	59.43 (4)	Na1 ^{iv} —Si1—Ba1 ⁱ	67.716 (15)
O1 ^{xvi} —Ba1—O1 ^{xiv}	180.00 (10)	Na1—Si1—Ba1	119.151 (10)
O1 ^{xvi} —Ba1—O1 ^{xii}	120.57 (4)	Na1 ⁱⁱⁱ —Si1—Ba1 ^{xxii}	67.715 (15)
O1 ^{xiii} —Ba1—O1	180.0	Na1 ⁱⁱⁱ —Si1—Ba1 ⁱ	157.30 (3)
O1 ^{xiii} —Ba1—O1 ^{xii}	120.57 (4)	Na1 ⁱⁱⁱ —Si1—Ba1	67.715 (15)
O1 ^{xiii} —Ba1—O1 ^{xvi}	59.43 (4)	Na1—Si1—Ba1 ^{xxii}	119.151 (10)
O1—Ba1—O1 ^{xv}	120.57 (4)	Na1 ⁱⁱ —Si1—Ba1 ^{xxii}	67.715 (15)
O1 ^{xv} —Ba1—O1 ^{xii}	180.00 (10)	Na1—Si1—Ba1 ⁱ	119.151 (10)
O1 ^{xiv} —Ba1—O1 ^{xv}	120.57 (4)	Ba1—Si1—Ba1 ^{xxii}	98.284 (12)
O1 ^{xvi} —Ba1—O1 ^{xv}	59.43 (4)	Ba1 ⁱ —Si1—Ba1	98.284 (12)
O1 ^{xiv} —Ba1—O2 ^{xix}	127.30 (5)	Ba1 ⁱ —Si1—Ba1 ^{xxii}	98.284 (12)
O1 ^{xiv} —Ba1—O2 ^{xvii}	80.82 (4)	O1 ^x —Si1—Na1 ⁱⁱⁱ	50.51 (5)
O1 ^{xvi} —Ba1—O2 ^{xix}	52.70 (5)	O1—Si1—Na1 ⁱⁱⁱ	69.25 (5)
O1 ^{xii} —Ba1—O2	99.18 (4)	O1 ^{ix} —Si1—Na1 ⁱⁱⁱ	149.59 (7)
O1 ^{xv} —Ba1—O2 ^{xiii}	99.18 (4)	O1 ^{ix} —Si1—Na1 ^{iv}	69.25 (5)
O1—Ba1—O2 ^{xix}	80.82 (4)	O1 ^{ix} —Si1—Na1 ⁱⁱ	50.51 (5)
O1 ^{xiii} —Ba1—O2 ^{xx}	80.82 (4)	O1—Si1—Na1	67.72 (6)
O1 ^{xii} —Ba1—O2 ^{xix}	71.30 (5)	O1 ^x —Si1—Na1	67.72 (6)
O1 ^{xvi} —Ba1—O2 ^{xiii}	108.70 (5)	O1 ^x —Si1—Na1 ⁱⁱ	69.25 (5)
O1 ^{xiv} —Ba1—O2 ^{xiii}	71.30 (5)	O1—Si1—Na1 ⁱⁱ	149.59 (7)
O1 ^{xiii} —Ba1—O2 ^{xix}	99.18 (4)	O1—Si1—Na1 ^{iv}	50.51 (5)
O1—Ba1—O2 ^{xx}	99.18 (4)	O1 ^x —Si1—Na1 ^{iv}	149.59 (7)
O1 ^{xv} —Ba1—O2 ^{xix}	108.70 (5)	O1 ^{ix} —Si1—Na1	67.72 (6)
O1 ^{xvi} —Ba1—O2	71.30 (5)	O1—Si1—Ba1 ^{xxii}	134.92 (5)
O1 ^{xvi} —Ba1—O2 ^{xx}	127.30 (5)	O1—Si1—Ba1 ⁱ	117.30 (5)
O1 ^{xiv} —Ba1—O2 ^{xx}	52.70 (5)	O1—Si1—Ba1	52.35 (6)
O1 ^{xv} —Ba1—O2	80.82 (4)	O1 ^{ix} —Si1—Ba1 ⁱ	52.36 (6)
O1—Ba1—O2 ^{xiii}	127.30 (5)	O1 ^x —Si1—Ba1	117.30 (5)
O1 ^{xiv} —Ba1—O2 ^{xviii}	99.18 (4)	O1 ^{ix} —Si1—Ba1 ^{xxii}	117.30 (5)
O1 ^{xii} —Ba1—O2 ^{xx}	108.70 (5)	O1 ^{ix} —Si1—Ba1	134.92 (5)
O1 ^{xv} —Ba1—O2 ^{xviii}	127.30 (5)	O1 ^x —Si1—Ba1 ^{xxii}	52.35 (6)

O1 ^{xii} —Ba1—O2 ^{xiii}	80.82 (4)	O1 ^x —Si1—Ba1 ⁱ	134.92 (5)
O1 ^{xii} —Ba1—O2 ^{xviii}	52.70 (5)	O1 ^{ix} —Si1—O1	106.53 (6)
O1 ^{xii} —Ba1—O2 ^{xvii}	127.30 (5)	O1—Si1—O1 ^x	106.53 (6)
O1 ^{xiii} —Ba1—O2	127.30 (5)	O1 ^{ix} —Si1—O1 ^x	106.53 (6)
O1—Ba1—O2	52.70 (5)	O2—Si1—Na1	180.0
O1 ^{xiii} —Ba1—O2 ^{xvii}	108.70 (5)	O2—Si1—Na1 ⁱⁱ	96.45 (3)
O1 ^{xiii} —Ba1—O2 ^{xviii}	71.30 (5)	O2—Si1—Na1 ^{iv}	96.45 (3)
O1—Ba1—O2 ^{xvii}	71.30 (5)	O2—Si1—Na1 ⁱⁱⁱ	96.45 (3)
O1 ^{xiv} —Ba1—O2	108.70 (5)	O2—Si1—Ba1	60.849 (10)
O1 ^{xvi} —Ba1—O2 ^{xvii}	99.18 (4)	O2—Si1—Ba1 ^{xxii}	60.849 (10)
O1—Ba1—O2 ^{xviii}	108.70 (5)	O2—Si1—Ba1 ⁱ	60.849 (10)
O1 ^{xv} —Ba1—O2 ^{xvii}	52.70 (5)	O2—Si1—O1	112.28 (6)
O1 ^{xiii} —Ba1—O2 ^{xiii}	52.70 (5)	O2—Si1—O1 ^{ix}	112.28 (6)
O1 ^{xvi} —Ba1—O2 ^{xviii}	80.82 (4)	O2—Si1—O1 ^x	112.28 (6)
O1 ^{xv} —Ba1—O2 ^{xx}	71.30 (5)	Na1 ^{iv} —O1—Na1 ⁱⁱⁱ	168.17 (9)
O2 ^{xvii} —Ba1—O2 ^{xix}	119.741 (7)	Na1 ^{iv} —O1—Ba1	89.26 (5)
O2 ^{xvii} —Ba1—O2 ^{xx}	60.259 (7)	Ba1—O1—Na1 ⁱⁱⁱ	79.67 (4)
O2 ^{xviii} —Ba1—O2 ^{xiii}	60.259 (7)	Zr1—O1—Na1 ^{iv}	100.01 (6)
O2 ^{xvii} —Ba1—O2 ^{xiii}	119.741 (7)	Zr1—O1—Na1 ⁱⁱⁱ	84.71 (5)
O2—Ba1—O2 ^{xx}	119.740 (7)	Zr1—O1—Ba1	92.27 (5)
O2 ^{xiii} —Ba1—O2 ^{xx}	60.260 (7)	Si1—O1—Na1 ⁱⁱⁱ	79.82 (5)
O2 ^{xiii} —Ba1—O2 ^{xix}	119.740 (7)	Si1—O1—Na1 ^{iv}	98.38 (6)
O2 ^{xviii} —Ba1—O2 ^{xix}	60.259 (7)	Si1—O1—Ba1	100.86 (7)
O2—Ba1—O2 ^{xiii}	180.0	Si1—O1—Zr1	157.49 (9)
O2 ^{xviii} —Ba1—O2 ^{xx}	119.741 (7)	Na1 ^{xxiii} —O2—Ba1 ^{xxii}	87.07 (4)
O2 ^{xvii} —Ba1—O2	60.259 (7)	Na1 ^{xxiii} —O2—Ba1	87.07 (4)
O2—Ba1—O2 ^{xix}	60.260 (7)	Na1 ^{xxiii} —O2—Ba1 ⁱ	87.07 (4)
O2 ^{xviii} —Ba1—O2	119.741 (7)	Ba1—O2—Ba1 ^{xxii}	119.741 (7)
O2 ^{xvii} —Ba1—O2 ^{xviii}	180.00 (8)	Ba1 ⁱ —O2—Ba1	119.741 (7)
O2 ^{xix} —Ba1—O2 ^{xx}	180.00 (8)	Ba1 ⁱ —O2—Ba1 ^{xxii}	119.741 (7)
Na1 ^{iv} —Zr1—Na1 ^{xx}	77.74 (2)	Si1—O2—Na1 ^{xxiii}	180.0
Na1—Zr1—Na1 ^{xx}	102.26 (2)	Si1—O2—Ba1 ⁱ	92.93 (4)
Na1 ^{xviii} —Zr1—Na1	102.26 (2)	Si1—O2—Ba1 ^{xxii}	92.93 (4)
Na1 ^{iv} —Zr1—Na1 ^{xxi}	102.26 (2)	Si1—O2—Ba1	92.93 (4)
Na1 ^{xxi} —Zr1—Na1 ^{xx}	77.74 (2)		
Na1 ⁱⁱ —Si1—O1—Na1 ^{iv}	80.07 (11)	Ba1 ⁱ —Si1—O1—Zr1	-156.5 (2)
Na1—Si1—O1—Na1 ^{iv}	100.39 (6)	Ba1—Si1—O1—Zr1	124.6 (3)
Na1 ⁱⁱⁱ —Si1—O1—Na1 ^{iv}	-168.16 (9)	Ba1 ^{xxii} —Si1—O1—Zr1	65.4 (3)
Na1—Si1—O1—Na1 ⁱⁱⁱ	-91.46 (4)	Ba1—Si1—O2—Ba1 ^{xxii}	-120.0
Na1 ^{iv} —Si1—O1—Na1 ⁱⁱⁱ	168.16 (9)	Ba1 ⁱ —Si1—O2—Ba1	-120.000 (1)
Na1 ⁱⁱ —Si1—O1—Na1 ⁱⁱⁱ	-111.77 (9)	Ba1 ^{xxii} —Si1—O2—Ba1	120.0
Na1—Si1—O1—Ba1	-168.75 (6)	Ba1 ⁱ —Si1—O2—Ba1 ^{xxii}	120.000 (1)
Na1 ^{iv} —Si1—O1—Ba1	90.86 (7)	Ba1 ^{xxii} —Si1—O2—Ba1 ⁱ	-120.0
Na1 ⁱⁱⁱ —Si1—O1—Ba1	-77.30 (5)	Ba1—Si1—O2—Ba1 ⁱ	120.0
Na1 ⁱⁱ —Si1—O1—Ba1	170.93 (5)	O1 ^{ix} —Si1—O1—Na1 ⁱⁱⁱ	-148.17 (6)
Na1 ⁱⁱⁱ —Si1—O1—Zr1	47.3 (2)	O1 ^x —Si1—O1—Na1 ⁱⁱⁱ	-34.74 (9)
Na1—Si1—O1—Zr1	-44.1 (2)	O1 ^{ix} —Si1—O1—Na1 ^{iv}	43.67 (12)

Na1 ⁱⁱ —Si1—O1—Zr1	−64.5 (3)	O1 ^x —Si1—O1—Na1 ^{iv}	157.10 (5)
Na1 ^{iv} —Si1—O1—Zr1	−144.5 (3)	O1 ^{ix} —Si1—O1—Ba1	134.53 (8)
Na1 ^{iv} —Si1—O2—Ba1	−60.0	O1 ^x —Si1—O1—Ba1	−112.04 (9)
Na1 ⁱⁱⁱ —Si1—O2—Ba1 ⁱ	180.0	O1 ^{ix} —Si1—O1—Zr1	−100.85 (18)
Na1 ⁱⁱ —Si1—O2—Ba1	180.0	O1 ^x —Si1—O1—Zr1	12.6 (3)
Na1 ⁱⁱ —Si1—O2—Ba1 ^{xxii}	60.0	O1 ^{ix} —Si1—O2—Ba1 ^{xxii}	109.82 (5)
Na1 ^{iv} —Si1—O2—Ba1 ^{xxii}	180.000 (1)	O1 ^x —Si1—O2—Ba1	109.81 (5)
Na1 ⁱⁱⁱ —Si1—O2—Ba1 ^{xxii}	−60.0	O1—Si1—O2—Ba1	−10.18 (5)
Na1 ^{iv} —Si1—O2—Ba1 ⁱ	60.0	O1 ^{ix} —Si1—O2—Ba1 ⁱ	−10.18 (5)
Na1 ⁱⁱⁱ —Si1—O2—Ba1	60.0	O1 ^x —Si1—O2—Ba1 ^{xxii}	−10.19 (5)
Na1 ⁱⁱ —Si1—O2—Ba1 ⁱ	−60.000 (1)	O1 ^x —Si1—O2—Ba1 ⁱ	−130.19 (5)
Ba1—Si1—O1—Na1 ^{iv}	−90.86 (7)	O1—Si1—O2—Ba1 ⁱ	109.82 (5)
Ba1 ^{xxii} —Si1—O1—Na1 ⁱⁱⁱ	18.11 (8)	O1 ^{ix} —Si1—O2—Ba1	−130.18 (5)
Ba1 ⁱ —Si1—O1—Na1 ^{iv}	−12.01 (8)	O1—Si1—O2—Ba1 ^{xxii}	−130.18 (5)
Ba1—Si1—O1—Na1 ⁱⁱⁱ	77.30 (5)	O2—Si1—O1—Na1 ^{iv}	−79.61 (6)
Ba1 ⁱ —Si1—O1—Na1 ⁱⁱⁱ	156.15 (4)	O2—Si1—O1—Na1 ⁱⁱⁱ	88.54 (4)
Ba1 ^{xxii} —Si1—O1—Na1 ^{iv}	−150.05 (5)	O2—Si1—O1—Ba1	11.25 (6)
Ba1 ⁱ —Si1—O1—Ba1	78.85 (6)	O2—Si1—O1—Zr1	135.9 (2)
Ba1 ^{xxii} —Si1—O1—Ba1	−59.19 (9)		

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

Disodium barium hafnium bis(orthosilicate) (II)

Crystal data

Na₂BaHf[SiO₄]₂

$M_r = 545.99$

Trigonal, $P\bar{3}$

$a = 5.3889$ (2) Å

$c = 7.1996$ (2) Å

$V = 181.07$ (1) Å³

$Z = 1$

$F(000) = 242$

$D_x = 5.007$ Mg m⁻³

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

Cell parameters from 7145 reflections

$\theta = 2.8$ – 51.0°

$\mu = 20.19$ mm⁻¹

$T = 293$ K

Plate, colourless

$0.03 \times 0.03 \times 0.01$ mm

Data collection

ROD, Synergy Custom system, HyPix-Arc 150 diffractometer

Radiation source: Rotating-anode X-ray tube, Rigaku (Mo) X-ray Source

Mirror monochromator

Detector resolution: 10.0000 pixels mm⁻¹

ω scans

Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2023)

$T_{\min} = 0.641, T_{\max} = 0.883$

8609 measured reflections

538 independent reflections

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

$R_{\text{int}} = 0.045$

$\theta_{\max} = 35.0^\circ, \theta_{\min} = 2.8^\circ$

$h = -8 \rightarrow 7$

$k = -8 \rightarrow 8$

$l = -11 \rightarrow 11$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.010$

$wR(F^2) = 0.024$

$S = 1.11$

538 reflections

24 parameters

0 restraints

Primary atom site location: dual

$$w = 1/[\sigma^2(F_o^2) + (0.0035P)^2 + 0.1631P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.61 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.60 \text{ e } \text{\AA}^{-3}$$

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. Refined as a 2-component twin. 1. Twinned data refinement Scales: 0.623 (4) 0.377 (4)

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Na1	0.333333	0.666667	0.7096 (2)	0.0148 (2)
Ba1	0.000000	0.000000	0.000000	0.01327 (5)
Hf1	0.000000	0.000000	0.500000	0.00516 (4)
Si1	0.333333	0.666667	0.24191 (11)	0.00532 (12)
O1	0.1238 (3)	0.3468 (3)	0.3269 (2)	0.0118 (4)
O2	0.333333	0.666667	0.0232 (3)	0.0187 (5)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0142 (4)	0.0142 (4)	0.0159 (6)	0.00710 (18)	0.000	0.000
Ba1	0.01685 (8)	0.01685 (8)	0.00611 (10)	0.00842 (4)	0.000	0.000
Hf1	0.00461 (5)	0.00461 (5)	0.00626 (7)	0.00231 (2)	0.000	0.000
Si1	0.00477 (18)	0.00477 (18)	0.0064 (3)	0.00239 (9)	0.000	0.000
O1	0.0111 (9)	0.0074 (6)	0.0146 (7)	0.0030 (5)	0.0012 (5)	0.0043 (5)
O2	0.0245 (7)	0.0245 (7)	0.0073 (9)	0.0122 (4)	0.000	0.000

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

Na1—Hf1 ⁱ	3.4579 (6)	Ba1—O1 ^{xv}	2.8687 (16)
Na1—Si1	3.3670 (16)	Ba1—O1 ^{xvi}	2.8687 (16)
Na1—Si1 ⁱⁱ	3.1308 (2)	Ba1—O2 ^{xvii}	3.1157 (2)
Na1—Si1 ⁱⁱⁱ	3.1308 (2)	Ba1—O2 ^{xviii}	3.1158 (2)
Na1—Si1 ^{iv}	3.1308 (2)	Ba1—O2 ^{xiv}	3.1158 (2)
Na1—O1 ^v	2.4423 (15)	Ba1—O2 ^{xix}	3.1157 (2)
Na1—O1 ^{iv}	2.4423 (15)	Ba1—O2	3.1158 (2)
Na1—O1 ^{vi}	2.4423 (15)	Ba1—O2 ^{xx}	3.1158 (2)
Na1—O1 ^{vii}	2.9738 (15)	Hf1—O1 ^v	2.0600 (15)
Na1—O1 ^{viii}	2.9738 (15)	Hf1—O1 ^{xxi}	2.0600 (15)
Na1—O1 ⁱⁱⁱ	2.9738 (15)	Hf1—O1 ^{xiii}	2.0600 (15)
Na1—O1	3.145 (2)	Hf1—O1	2.0600 (15)
Na1—O1 ^{ix}	3.145 (2)	Hf1—O1 ^{vii}	2.0600 (15)
Na1—O1 ^x	3.145 (2)	Hf1—O1 ^{xvi}	2.0600 (15)
Na1—O2 ^{xi}	2.258 (3)	Si1—O1 ^x	1.6354 (16)
Ba1—O1 ^{xii}	2.8687 (16)	Si1—O1	1.6354 (16)

Ba1—O1 ^{xiii}	2.8687 (16)	Si1—O1 ^{ix}	1.6354 (16)
Ba1—O1 ^{xiv}	2.8687 (16)	Si1—O2	1.575 (2)
Ba1—O1	2.8687 (16)		
Si1 ⁱⁱⁱ —Na1—Hf1 ⁱ	160.53 (5)	Na1 ^{xix} —Hf1—Na1 ^{iv}	180.0
Si1 ⁱⁱ —Na1—Hf1 ⁱ	66.522 (10)	Na1 ^{xix} —Hf1—Na1 ^{xxi}	77.62 (3)
Si1 ^{iv} —Na1—Hf1 ⁱ	66.522 (10)	Na1 ^{xix} —Hf1—Na1 ⁱⁱⁱ	77.62 (3)
Si1—Na1—Hf1 ⁱ	64.13 (2)	Na1—Hf1—Na1 ^{xxi}	180.0
Si1 ⁱⁱ —Na1—Si1 ⁱⁱⁱ	118.773 (12)	Na1—Hf1—Na1 ⁱⁱⁱ	77.62 (3)
Si1 ⁱⁱ —Na1—Si1 ^{iv}	118.773 (12)	Na1 ^{iv} —Hf1—Na1 ^{xx}	77.62 (3)
Si1 ^{iv} —Na1—Si1 ⁱⁱⁱ	118.773 (12)	Na1 ^{xxi} —Hf1—Na1 ⁱⁱⁱ	102.38 (3)
Si1 ⁱⁱ —Na1—Si1	96.40 (3)	Na1 ^{xxi} —Hf1—Na1 ^{xx}	77.62 (3)
Si1 ^{iv} —Na1—Si1	96.40 (3)	Na1 ^{xix} —Hf1—Na1	102.38 (3)
Si1 ⁱⁱⁱ —Na1—Si1	96.40 (3)	Na1 ^{iv} —Hf1—Na1	77.62 (3)
O1 ⁱⁱⁱ —Na1—Hf1 ⁱ	138.33 (5)	O1 ^{vii} —Hf1—Na1 ^{xix}	116.29 (5)
O1 ^{viii} —Na1—Hf1 ⁱ	36.38 (3)	O1 ^{xvi} —Hf1—Na1 ^{xx}	63.71 (5)
O1 ^{vii} —Na1—Hf1 ⁱ	86.70 (3)	O1 ^v —Hf1—Na1	44.07 (4)
O1 ^{iv} —Na1—Hf1 ⁱ	35.92 (4)	O1 ^{xiii} —Hf1—Na1 ^{xix}	63.71 (5)
O1 ^v —Na1—Hf1 ⁱ	137.65 (5)	O1 ^{xxi} —Hf1—Na1 ^{xx}	58.91 (4)
O1 ^{vi} —Na1—Hf1 ⁱ	85.99 (4)	O1 ^{xxi} —Hf1—Na1 ^{xix}	44.07 (4)
O1 ^{iv} —Na1—Si1 ⁱⁱ	92.15 (4)	O1 ^{vii} —Hf1—Na1 ^{iv}	63.71 (5)
O1 ⁱⁱⁱ —Na1—Si1 ⁱⁱⁱ	30.94 (3)	O1 ^{xxi} —Hf1—Na1	116.29 (5)
O1 ^{iv} —Na1—Si1 ⁱⁱⁱ	148.71 (4)	O1 ^{vii} —Hf1—Na1 ^{xx}	44.07 (4)
O1 ^{vi} —Na1—Si1 ⁱⁱ	31.12 (4)	O1 ^v —Hf1—Na1 ^{iv}	121.09 (4)
O1 ^{viii} —Na1—Si1	84.93 (4)	O1 ^{xxi} —Hf1—Na1 ^{iv}	135.93 (4)
O1 ^v —Na1—Si1 ⁱⁱ	148.71 (4)	O1 ^{xvi} —Hf1—Na1 ⁱⁱⁱ	116.29 (5)
O1 ^{viii} —Na1—Si1 ⁱⁱⁱ	148.92 (3)	O1 ^{vii} —Hf1—Na1 ⁱⁱⁱ	135.93 (4)
O1 ^{viii} —Na1—Si1 ⁱⁱ	30.94 (3)	O1—Hf1—Na1 ⁱⁱⁱ	58.91 (4)
O1 ^{vi} —Na1—Si1	83.83 (5)	O1 ^v —Hf1—Na1 ^{xx}	116.29 (5)
O1 ^{vii} —Na1—Si1 ⁱⁱ	148.92 (3)	O1 ^{xvi} —Hf1—Na1 ^{xxi}	44.07 (4)
O1 ⁱⁱⁱ —Na1—Si1	84.93 (4)	O1—Hf1—Na1 ^{xx}	121.09 (4)
O1 ⁱⁱⁱ —Na1—Si1 ⁱⁱ	91.76 (3)	O1—Hf1—Na1 ^{xxi}	116.29 (5)
O1 ^v —Na1—Si1 ⁱⁱⁱ	31.12 (4)	O1 ^{xiii} —Hf1—Na1 ^{xx}	135.93 (4)
O1 ^{iv} —Na1—Si1 ^{iv}	31.12 (4)	O1 ^{vii} —Hf1—Na1 ^{xxi}	121.09 (4)
O1 ^{vii} —Na1—Si1 ⁱⁱⁱ	91.76 (3)	O1 ^{xxi} —Hf1—Na1 ⁱⁱⁱ	121.09 (4)
O1 ^{vi} —Na1—Si1 ^{iv}	148.71 (4)	O1 ^{xiii} —Hf1—Na1 ^{xxi}	58.91 (4)
O1 ^{iv} —Na1—Si1	83.83 (5)	O1—Hf1—Na1 ^{xix}	135.93 (4)
O1 ^v —Na1—Si1 ^{iv}	92.15 (4)	O1 ^{xxi} —Hf1—Na1 ^{xxi}	63.71 (5)
O1 ^v —Na1—Si1	83.83 (5)	O1 ^v —Hf1—Na1 ⁱⁱⁱ	63.71 (5)
O1 ^{viii} —Na1—Si1 ^{iv}	91.76 (3)	O1 ^{xvi} —Hf1—Na1 ^{iv}	58.91 (4)
O1 ^{vii} —Na1—Si1	84.93 (4)	O1—Hf1—Na1 ^{iv}	44.07 (4)
O1 ^{vii} —Na1—Si1 ^{iv}	30.94 (3)	O1 ^v —Hf1—Na1 ^{xxi}	135.93 (4)
O1 ⁱⁱⁱ —Na1—Si1 ^{iv}	148.92 (3)	O1 ^{xiii} —Hf1—Na1 ⁱⁱⁱ	44.07 (4)
O1 ^{vi} —Na1—Si1 ⁱⁱⁱ	92.15 (4)	O1 ^{xvi} —Hf1—Na1	135.93 (4)
O1 ^v —Na1—O1 ⁱⁱⁱ	57.02 (7)	O1 ^v —Hf1—Na1 ^{xix}	58.91 (4)
O1 ^{iv} —Na1—O1 ^{viii}	62.36 (7)	O1—Hf1—Na1	63.71 (5)
O1 ^{vi} —Na1—O1 ^{vii}	168.44 (9)	O1 ^{xvi} —Hf1—Na1 ^{xix}	121.09 (4)
O1 ^v —Na1—O1 ^{vii}	62.36 (7)	O1 ^{vii} —Hf1—Na1	58.91 (4)

O1 ^v —Na1—O1 ^{viii}	168.44 (9)	O1 ^{xiii} —Hf1—Na1	121.09 (4)
O1 ^{viii} —Na1—O1 ⁱⁱⁱ	119.229 (13)	O1 ^{xiii} —Hf1—Na1 ^{iv}	116.29 (5)
O1 ^{vi} —Na1—O1 ^v	118.859 (19)	O1 ^v —Hf1—O1 ^{xxi}	87.19 (7)
O1 ^{vii} —Na1—O1 ⁱⁱⁱ	119.229 (13)	O1 ^v —Hf1—O1 ^{vii}	87.19 (7)
O1 ^{vi} —Na1—O1 ^{viii}	57.02 (7)	O1—Hf1—O1 ^{xiii}	87.19 (7)
O1 ^{iv} —Na1—O1 ⁱⁱⁱ	168.44 (9)	O1 ^{xvi} —Hf1—O1 ^{xxi}	92.81 (7)
O1 ^{iv} —Na1—O1 ^{vii}	57.02 (7)	O1 ^v —Hf1—O1 ^{xiii}	92.81 (7)
O1 ^{vi} —Na1—O1 ⁱⁱⁱ	62.36 (7)	O1—Hf1—O1 ^{xxi}	180.0
O1 ^{iv} —Na1—O1 ^{vi}	118.859 (19)	O1 ^{xvi} —Hf1—O1	87.19 (7)
O1 ^{iv} —Na1—O1 ^v	118.859 (19)	O1 ^{vii} —Hf1—O1 ^{xxi}	87.19 (7)
O1 ^{viii} —Na1—O1 ^{vii}	119.229 (13)	O1—Hf1—O1 ^{vii}	92.81 (7)
O2 ^{xi} —Na1—Hf1 ⁱ	115.87 (2)	O1 ^{xiii} —Hf1—O1 ^{xxi}	92.81 (7)
O2 ^{xi} —Na1—Si1 ⁱⁱⁱ	83.60 (3)	O1 ^{xvi} —Hf1—O1 ^{xiii}	87.19 (7)
O2 ^{xi} —Na1—Si1	180.0	O1 ^v —Hf1—O1 ^{xvi}	180.0
O2 ^{xi} —Na1—Si1 ^{iv}	83.60 (3)	O1 ^{vii} —Hf1—O1 ^{xiii}	180.0
O2 ^{xi} —Na1—Si1 ⁱⁱ	83.60 (3)	O1 ^v —Hf1—O1	92.81 (7)
O2 ^{xi} —Na1—O1 ^{vii}	95.07 (4)	O1 ^{xvi} —Hf1—O1 ^{vii}	92.81 (7)
O2 ^{xi} —Na1—O1 ^v	96.17 (5)	Na1 ⁱⁱ —Si1—Na1 ^{iv}	118.773 (12)
O2 ^{xi} —Na1—O1 ^{viii}	95.07 (4)	Na1 ⁱⁱⁱ —Si1—Na1	83.60 (3)
O2 ^{xi} —Na1—O1 ^{vi}	96.17 (5)	Na1 ^{iv} —Si1—Na1	83.60 (3)
O2 ^{xi} —Na1—O1 ^{iv}	96.17 (5)	Na1 ^{iv} —Si1—Na1 ⁱⁱⁱ	118.772 (12)
O2 ^{xi} —Na1—O1 ⁱⁱⁱ	95.07 (4)	Na1 ⁱⁱ —Si1—Na1	83.60 (3)
O1 ^{xiii} —Ba1—O1	59.36 (5)	Na1 ⁱⁱ —Si1—Na1 ⁱⁱⁱ	118.772 (12)
O1 ^{xiv} —Ba1—O1	180.0	Na1 ⁱⁱ —Si1—Ba1 ⁱ	67.724 (16)
O1 ^{xv} —Ba1—O1 ^{xvi}	120.64 (5)	Na1 ^{iv} —Si1—Ba1 ^{xxii}	157.16 (4)
O1 ^{xii} —Ba1—O1 ^{xvi}	180.00 (8)	Na1—Si1—Ba1	119.240 (11)
O1 ^{xiv} —Ba1—O1 ^{xvi}	120.64 (5)	Na1 ⁱⁱⁱ —Si1—Ba1 ⁱ	157.16 (4)
O1 ^{xiv} —Ba1—O1 ^{xii}	59.36 (5)	Na1—Si1—Ba1 ^{xxii}	119.240 (11)
O1 ^{xiii} —Ba1—O1 ^{xvi}	59.36 (5)	Na1—Si1—Ba1 ⁱ	119.240 (11)
O1 ^{xv} —Ba1—O1 ^{xii}	59.36 (5)	Na1 ⁱⁱ —Si1—Ba1 ^{xxii}	67.723 (16)
O1 ^{xiii} —Ba1—O1 ^{xii}	120.64 (5)	Na1 ⁱⁱ —Si1—Ba1	157.16 (4)
O1 ^{xv} —Ba1—O1	120.64 (5)	Na1 ⁱⁱⁱ —Si1—Ba1 ^{xxii}	67.723 (16)
O1 ^{xiv} —Ba1—O1 ^{xv}	59.36 (5)	Na1 ^{iv} —Si1—Ba1	67.723 (16)
O1 ^{xii} —Ba1—O1	120.64 (5)	Na1 ⁱⁱⁱ —Si1—Ba1	67.723 (16)
O1 ^{xiv} —Ba1—O1 ^{xiii}	120.64 (5)	Na1 ^{iv} —Si1—Ba1 ⁱ	67.724 (16)
O1 ^{xv} —Ba1—O1 ^{xiii}	180.00 (10)	Ba1—Si1—Ba1 ^{xxii}	98.169 (14)
O1 ^{xvi} —Ba1—O1	59.36 (5)	Ba1 ⁱ —Si1—Ba1	98.169 (14)
O1 ^{xii} —Ba1—O2 ^{xviii}	52.61 (5)	Ba1 ⁱ —Si1—Ba1 ^{xxii}	98.169 (14)
O1—Ba1—O2	52.61 (5)	O1 ^{ix} —Si1—Na1 ⁱⁱ	50.52 (5)
O1 ^{xv} —Ba1—O2 ^{xviii}	108.55 (5)	O1 ^x —Si1—Na1	68.03 (6)
O1—Ba1—O2 ^{xviii}	80.96 (5)	O1—Si1—Na1 ⁱⁱ	149.93 (7)
O1 ^{xii} —Ba1—O2 ^{xiv}	108.55 (5)	O1 ^x —Si1—Na1 ^{iv}	149.94 (7)
O1 ^{xv} —Ba1—O2 ^{xx}	71.45 (5)	O1 ^{ix} —Si1—Na1 ^{iv}	69.22 (5)
O1 ^{xiii} —Ba1—O2	99.04 (5)	O1 ^{ix} —Si1—Na1 ⁱⁱⁱ	149.94 (7)
O1 ^{xii} —Ba1—O2 ^{xx}	127.39 (5)	O1—Si1—Na1	68.03 (6)
O1 ^{xv} —Ba1—O2 ^{xiv}	99.04 (5)	O1—Si1—Na1 ⁱⁱⁱ	69.22 (5)
O1—Ba1—O2 ^{xx}	99.04 (5)	O1 ^x —Si1—Na1 ⁱⁱ	69.22 (5)
O1—Ba1—O2 ^{xiv}	127.39 (5)	O1 ^x —Si1—Na1 ⁱⁱⁱ	50.51 (5)

O1—Ba1—O2 ^{xvii}	71.45 (5)	O1—Si1—Na1 ^{iv}	50.51 (5)
O1 ^{xv} —Ba1—O2	80.96 (5)	O1 ^{ix} —Si1—Na1	68.03 (6)
O1 ^{xiv} —Ba1—O2 ^{xix}	71.45 (5)	O1—Si1—Ba1 ^{xxii}	134.78 (5)
O1 ^{xii} —Ba1—O2	71.45 (5)	O1 ^{ix} —Si1—Ba1 ⁱ	52.13 (6)
O1 ^{xv} —Ba1—O2 ^{xix}	127.39 (5)	O1 ^{ix} —Si1—Ba1 ^{xxii}	117.23 (5)
O1 ^{xiv} —Ba1—O2 ^{xiv}	52.61 (5)	O1 ^x —Si1—Ba1 ^{xxii}	52.13 (6)
O1 ^{xiii} —Ba1—O2 ^{xix}	52.61 (5)	O1—Si1—Ba1 ⁱ	117.23 (5)
O1 ^{xiii} —Ba1—O2 ^{xiv}	80.96 (5)	O1 ^x —Si1—Ba1	117.23 (5)
O1 ^{xii} —Ba1—O2 ^{xix}	80.96 (5)	O1—Si1—Ba1	52.13 (6)
O1 ^{xvi} —Ba1—O2 ^{xiv}	71.45 (5)	O1 ^x —Si1—Ba1 ⁱ	134.78 (5)
O1 ^{xvi} —Ba1—O2 ^{xix}	99.04 (5)	O1 ^{ix} —Si1—Ba1	134.78 (6)
O1 ^{xiv} —Ba1—O2 ^{xviii}	99.04 (5)	O1 ^{ix} —Si1—O1	106.86 (7)
O1—Ba1—O2 ^{xix}	108.55 (5)	O1—Si1—O1 ^x	106.86 (7)
O1 ^{xiii} —Ba1—O2 ^{xviii}	71.45 (5)	O1 ^{ix} —Si1—O1 ^x	106.86 (7)
O1 ^{xiv} —Ba1—O2	127.39 (5)	O2—Si1—Na1	180.0
O1 ^{xvi} —Ba1—O2 ^{xviii}	127.39 (5)	O2—Si1—Na1 ⁱⁱⁱ	96.40 (3)
O1 ^{xiv} —Ba1—O2 ^{xvii}	108.55 (5)	O2—Si1—Na1 ^{iv}	96.40 (3)
O1 ^{xiv} —Ba1—O2 ^{xx}	80.96 (5)	O2—Si1—Na1 ⁱⁱ	96.40 (3)
O1 ^{xv} —Ba1—O2 ^{xvii}	52.61 (5)	O2—Si1—Ba1	60.760 (11)
O1 ^{xiii} —Ba1—O2 ^{xx}	108.55 (5)	O2—Si1—Ba1 ^{xxii}	60.760 (11)
O1 ^{xiii} —Ba1—O2 ^{xvii}	127.39 (5)	O2—Si1—Ba1 ⁱ	60.760 (11)
O1 ^{xvi} —Ba1—O2 ^{xx}	52.61 (5)	O2—Si1—O1	111.97 (6)
O1 ^{xii} —Ba1—O2 ^{xvii}	99.04 (5)	O2—Si1—O1 ^x	111.97 (6)
O1 ^{xvi} —Ba1—O2 ^{xvii}	80.96 (5)	O2—Si1—O1 ^{ix}	111.97 (6)
O1 ^{xvi} —Ba1—O2	108.55 (5)	Na1 ^{iv} —O1—Na1 ⁱⁱⁱ	168.44 (9)
O2 ^{xvii} —Ba1—O2 ^{xviii}	119.716 (8)	Na1 ^{iv} —O1—Ba1	89.42 (6)
O2 ^{xvii} —Ba1—O2 ^{xiv}	119.716 (8)	Ba1—O1—Na1 ⁱⁱⁱ	79.80 (5)
O2 ^{xiv} —Ba1—O2 ^{xx}	60.285 (8)	Hf1—O1—Na1 ⁱⁱⁱ	84.71 (5)
O2 ^{xix} —Ba1—O2 ^{xviii}	60.284 (8)	Hf1—O1—Na1 ^{iv}	100.01 (6)
O2 ^{xix} —Ba1—O2 ^{xx}	119.716 (8)	Hf1—O1—Ba1	92.35 (6)
O2—Ba1—O2 ^{xviii}	60.285 (8)	Si1—O1—Na1 ^{iv}	98.37 (7)
O2 ^{xvii} —Ba1—O2 ^{xix}	180.0	Si1—O1—Na1 ⁱⁱⁱ	79.84 (6)
O2 ^{xiv} —Ba1—O2 ^{xviii}	119.715 (8)	Si1—O1—Ba1	101.12 (7)
O2 ^{xvii} —Ba1—O2 ^{xx}	60.284 (8)	Si1—O1—Hf1	157.27 (10)
O2—Ba1—O2 ^{xiv}	180.0	Na1 ^{xxiii} —O2—Ba1 ^{xxii}	86.93 (4)
O2—Ba1—O2 ^{xx}	119.715 (8)	Na1 ^{xxiii} —O2—Ba1 ⁱ	86.93 (4)
O2 ^{xvii} —Ba1—O2	60.285 (8)	Na1 ^{xxiii} —O2—Ba1	86.93 (4)
O2 ^{xix} —Ba1—O2 ^{xiv}	60.284 (8)	Ba1 ⁱ —O2—Ba1 ^{xxii}	119.715 (8)
O2 ^{xix} —Ba1—O2	119.715 (8)	Ba1—O2—Ba1 ^{xxii}	119.715 (8)
O2 ^{xviii} —Ba1—O2 ^{xx}	180.0	Ba1 ⁱ —O2—Ba1	119.715 (8)
Na1 ^{iv} —Hf1—Na1 ⁱⁱⁱ	102.38 (3)	Si1—O2—Na1 ^{xxiii}	180.0
Na1 ^{iv} —Hf1—Na1 ^{xxi}	102.38 (3)	Si1—O2—Ba1	93.07 (4)
Na1—Hf1—Na1 ^{xx}	102.38 (3)	Si1—O2—Ba1 ⁱ	93.07 (4)
Na1 ^{xx} —Hf1—Na1 ⁱⁱⁱ	180.0	Si1—O2—Ba1 ^{xxii}	93.07 (4)
Na1 ^{xix} —Hf1—Na1 ^{xx}	102.38 (3)		
Na1 ⁱⁱ —Si1—O1—Na1 ^{iv}	79.72 (11)	Ba1 ⁱ —Si1—O1—Hf1	−156.1 (2)
Na1—Si1—O1—Na1 ⁱⁱⁱ	−91.40 (4)	Ba1—Si1—O1—Hf1	125.3 (3)

Na1 ^{iv} —Si1—O1—Na1 ⁱⁱⁱ	168.43 (9)	Ba1 ^{xxii} —Si1—O1—Hf1	66.5 (3)
Na1 ⁱⁱⁱ —Si1—O1—Na1 ^{iv}	-168.43 (9)	Ba1 ^{xxii} —Si1—O2—Ba1 ⁱ	-120.0
Na1 ⁱⁱ —Si1—O1—Na1 ⁱⁱⁱ	-111.84 (10)	Ba1 ^{xxii} —Si1—O2—Ba1	120.0
Na1—Si1—O1—Na1 ^{iv}	100.17 (6)	Ba1 ⁱ —Si1—O2—Ba1	-120.000 (1)
Na1 ⁱⁱ —Si1—O1—Ba1	170.78 (6)	Ba1—Si1—O2—Ba1 ⁱ	120.0
Na1—Si1—O1—Ba1	-168.78 (6)	Ba1—Si1—O2—Ba1 ^{xxii}	-120.0
Na1 ⁱⁱⁱ —Si1—O1—Ba1	-77.38 (5)	Ba1 ⁱ —Si1—O2—Ba1 ^{xxii}	120.0
Na1 ^{iv} —Si1—O1—Ba1	91.06 (7)	O1 ^{ix} —Si1—O1—Na1 ⁱⁱⁱ	-148.46 (7)
Na1 ^{iv} —Si1—O1—Hf1	-143.7 (3)	O1 ^{ix} —Si1—O1—Na1 ^{iv}	43.11 (12)
Na1 ⁱⁱⁱ —Si1—O1—Hf1	47.9 (2)	O1 ^x —Si1—O1—Na1 ^{iv}	157.23 (5)
Na1 ⁱⁱ —Si1—O1—Hf1	-63.9 (3)	O1 ^x —Si1—O1—Na1 ⁱⁱⁱ	-34.34 (9)
Na1—Si1—O1—Hf1	-43.5 (2)	O1 ^{ix} —Si1—O1—Ba1	134.17 (9)
Na1 ⁱⁱ —Si1—O2—Ba1 ⁱ	-60.000 (1)	O1 ^x —Si1—O1—Ba1	-111.72 (10)
Na1 ^{iv} —Si1—O2—Ba1	-60.0	O1 ^{ix} —Si1—O1—Hf1	-100.56 (19)
Na1 ⁱⁱ —Si1—O2—Ba1 ^{xxii}	60.0	O1 ^x —Si1—O1—Hf1	13.6 (3)
Na1 ⁱⁱⁱ —Si1—O2—Ba1 ^{xxii}	-60.0	O1 ^{ix} —Si1—O2—Ba1 ⁱ	-10.14 (6)
Na1 ⁱⁱⁱ —Si1—O2—Ba1	60.0	O1 ^x —Si1—O2—Ba1 ⁱ	-130.14 (6)
Na1 ⁱⁱⁱ —Si1—O2—Ba1 ⁱ	180.0	O1 ^{ix} —Si1—O2—Ba1	-130.14 (6)
Na1 ^{iv} —Si1—O2—Ba1 ^{xxii}	180.000 (1)	O1—Si1—O2—Ba1	-10.14 (6)
Na1 ⁱⁱ —Si1—O2—Ba1	180.0	O1 ^x —Si1—O2—Ba1	109.86 (6)
Na1 ^{iv} —Si1—O2—Ba1 ⁱ	60.0	O1—Si1—O2—Ba1 ^{xxii}	-130.14 (6)
Ba1—Si1—O1—Na1 ^{iv}	-91.06 (7)	O1 ^x —Si1—O2—Ba1 ^{xxii}	-10.14 (6)
Ba1—Si1—O1—Na1 ⁱⁱⁱ	77.38 (5)	O1 ^{ix} —Si1—O2—Ba1 ^{xxii}	109.86 (6)
Ba1 ⁱ —Si1—O1—Na1 ⁱⁱⁱ	155.97 (4)	O1—Si1—O2—Ba1 ⁱ	109.86 (6)
Ba1 ^{xxii} —Si1—O1—Na1 ^{iv}	-149.85 (6)	O2—Si1—O1—Na1 ^{iv}	-79.83 (6)
Ba1 ⁱ —Si1—O1—Na1 ^{iv}	-12.46 (9)	O2—Si1—O1—Na1 ⁱⁱⁱ	88.60 (4)
Ba1 ^{xxii} —Si1—O1—Na1 ⁱⁱⁱ	18.58 (9)	O2—Si1—O1—Ba1	11.22 (6)
Ba1 ⁱ —Si1—O1—Ba1	78.60 (6)	O2—Si1—O1—Hf1	136.5 (2)
Ba1 ^{xxii} —Si1—O1—Ba1	-58.80 (9)		

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