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Orthosilicates with glaserite-type crystal structures: $Na_2BaZr[SiO_4]_2$ and $Na_2BaHf[SiO_4]_2$

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

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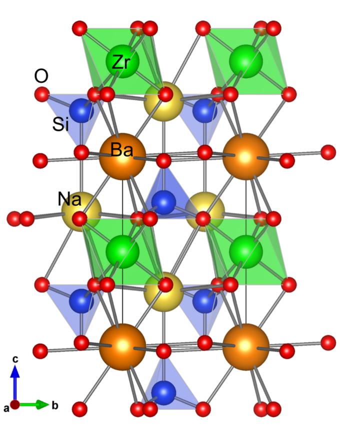
Single crystal particles of $Na_2BaZr[SiO_4]_2$ [systematic name: disodium barium zirconium bis(orthosilicate)] and $Na_2BaHf[SiO_4]_2$ [disodium barium hafnium bis(orthosilicate)] were extracted from grain-grown polycrystals obtained by heating compacts of binary oxide mixtures at 1473 K. Single crystal 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 $XY_2[M(TO_4)_2]$ are fully occupied by atoms of different elements. The crystal structures of the title compounds were refined in space group $P\overline{3}$ under consideration of a two-component twin model. The SiO_4 tetrahedra are rotated approximately $\pm 10.2°$ from the mirror plane of space group $P\overline{3}m$ 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 $X_{(\square;1)}Y_{(\square;2)}[M(TO_4)_2]$ 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 = Si), such as $BaMg[SiO_4]$ and Ba(Ba,Sr,Ca)$_2$Mg[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 $P\overline{3}$ to $P\overline{3}m$ (Yamagishi *et al.*, 2023). The rotation angle φ of the TO_4 tetrahedron was defined relative to the mirror plane of $P\overline{3}m$, and $BaCa_2Mg[SiO_4]_2$ with φ = 12.5° was proposed as a potential ferroaxial transition material. For the compounds with M = Zr, Kostov-Kytin and co-workers analysed the crystal structures of $Na_{3-x}H_{1+x}Zr(SiO)_4\cdot yH_2O$ 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, $Na_2BaZr[SiO_4]_2$ and $Na_2BaHf[SiO_4]_2$.

2. Structural commentary

According to the classification by Nikolova & Kostov-Kytin (2013) using the general formula $X_{(\square;1)}Y_{(\square;2)}[M(TO_4)_2]$ for compounds with glaserite-type crystal structures, Na_2BaZr

Table 1
Selected bond lengths (Å) for $Na_2BaZr[SiO_4]_2$.

Na1—O1^{i}	2.9791 (15)	Ba1—O2	3.1198 (2)
Na1—O1^{ii}	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) $x, y, z+1$.

Table 2
Selected bond lengths (Å) for $Na_2BaHf[SiO_4]_2$.

Na1—O1^{i}	2.4423 (15)	Ba1—O2	3.1158 (2)
Na1—O1^{ii}	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) $x, y, z+1$.

$[SiO_4]_2$ and $Na_2BaHf[SiO_4]_2$ 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 $P\overline{3}$. 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 $\overline{3}$ for Ba1, 1, *b* and $\overline{3}$ 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* = Zr- or Hf-centred oxygen octahedra and SiO_4 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 (×6) and 2.0600 (15) Å (×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 $Na_2BaZr[SiO_4]_2$ agree with those of 1.6354 (16) and 1.575 (2) Å for $Na_2BaHf[SiO_4]_2$. The Ba—O distances for the 12-coordinate *X* site are slightly longer for $Na_2BaZr[SiO_4]_2$ [2.8764 (15)–3.1198 (2) Å] than for $Na_2BaHf[SiO_4]_2$ [2.8687 (16)–3.1158 (2) Å]. The distances between O1 and Na1 at the tenfold coordination sites are slightly longer for $Na_2BaM[SiO_4]_2$ *M* = Zr [2.4461 (15)–3.1545 (19) Å] than for *M* = Hf [2.4423 (15)–3.145 (2) Å], while the Na1—O2 distance of 2.250 (3) Å for *M* = Zr is slightly shorter than that of 2.258 (3) Å for *M* = 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 $Na_2BaM[SiO_4]_2$ *M* = Zr, and 1.01, 1.89, 4.05, and 4.09 valence units for *M* = Hf. The rotation angles φ of the $[SiO_4]$ tetrahedra are 10.18° for *M* = Zr and 10.15° for *M* = Hf (Fig. 3).

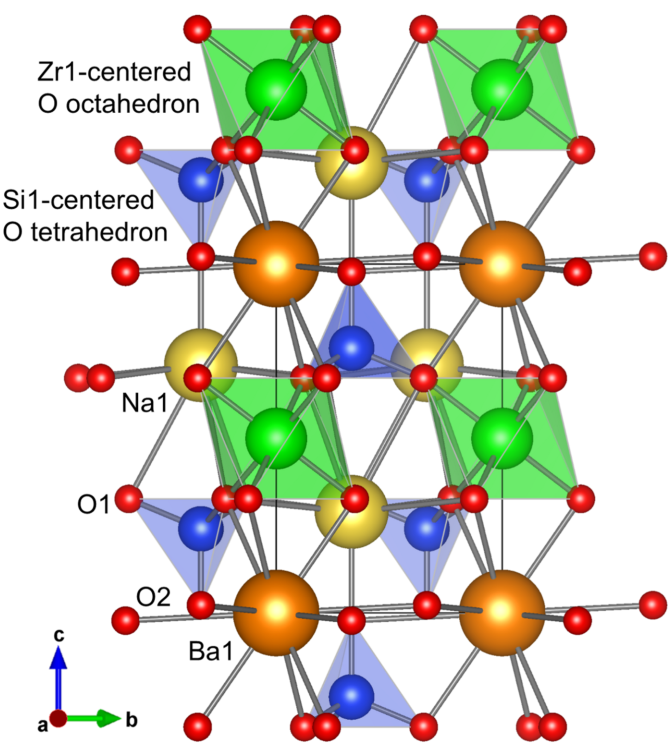


Figure 1
Crystal structure of $Na_2BaZr[SiO_4]_2$ in a projection along [100], drawn with Zr1-centered oxygen octahedra and Si1-centered oxygen tetrahedra.

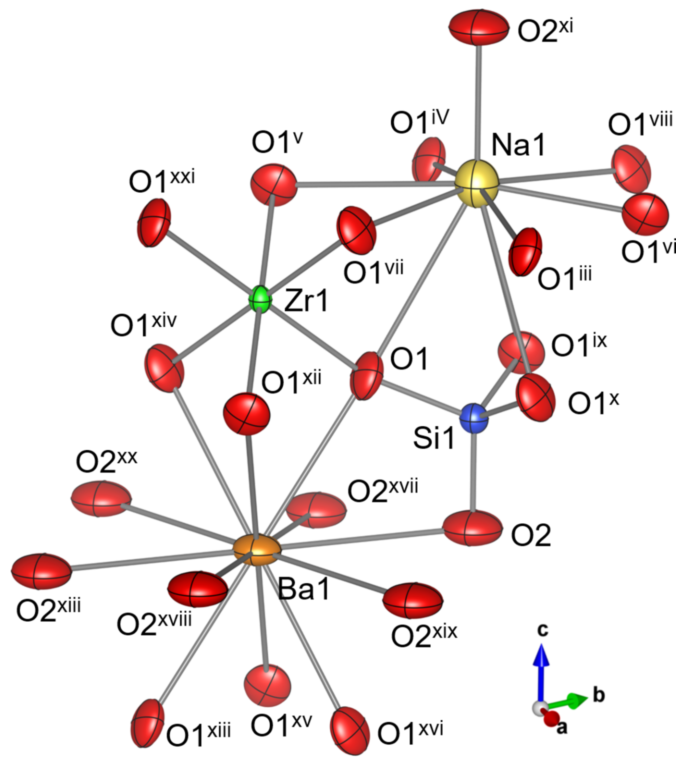


Figure 2
Atomic arrangements around Na1, Ba1, Zr1, and Si1 in the crystal structure of $Na_2BaZr[SiO_4]_2$. Displacement ellipsoids are depicted at the 90% probability level. [Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, -y+2, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $-x, -y+1, -z+1$; (v) $x-y, x, -z+1$; (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.

	$Na_2BaZr[SiO_4]_2$	$Na_2BaHf[SiO_4]_2$
Crystal data		
M_r	458.72	545.99
Crystal system, space group	Trigonal, $P\bar{3}$	Trigonal, $P\bar{3}$
Temperature (K)	293	293
a, *c* (Å)	5.3966 (2), 7.2153 (3)	5.3889 (2), 7.1996 (2)
V ($Å^3$)	181.98 (2)	181.07 (1)
Z	1	1
Radiation type	Mo $K\alpha$	Mo $K\alpha$
μ (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 (*CrysAlis PRO*; Rigaku OD, 2023)	Gaussian (*CrysAlis PRO*; Rigaku OD, 2023)
T_{min}, T_{max}	0.544, 0.817	0.641, 0.883
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9034, 587, 543	8609, 538, 532
R_{int}	0.043	0.045
$(\sin \theta/\lambda)_{max}$ ($Å^{-1}$)	0.832	0.806
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.016, 0.035, 1.11	0.010, 0.024, 1.11
No. of reflections	587	538
No. of parameters	24	24
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.52, −0.59	0.61, −0.60

Computer programs: *CrysAlis PRO* (Rigaku OD, 2023), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *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 $Na_2BaM[SiO_4]_2$ 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 + MO_2 + α-$Na_2Si_2O_5$ = $Na_2BaM[SiO_4]_2$ using *MAPLE* values calculated from the crystal structure data for BaO (–3.510 MJ mol^{-1}; Zollweg, 1955), ZrO_2 (–12.740 MJ mol^{-1}; Gualtieri *et al.*, 1996), HfO_2 (–12.740 MJ mol^{-1}; Pathak *et al.*, 2020) and α-$Na_2Si_2O_5$ (–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 of $Ca_2[SiO_4]$ ($P\bar{3}m$, *Z* = 2, *V* = 194.19 $Å^3$; Mumme *et al.*, 1996), $Ba_3Mg[SiO_4]_2$ ($P\bar{3}m$, *Z* = 1, *V* = 198.64 $Å^3$; Iwata *et al.*, 2009) and its superstructure ($P\bar{3}$, *Z* = 3, *V* = 594.71 $Å^3$; Park *et al.*, 2009), $BaCa_2Mg[SiO_4]_2$ ($P\bar{3}$, *Z* = 1, *V* = 173.31 $Å^3$; Park *et al.*, 2011), $Ba_xSr_{3-x}Mg[SiO_4]_2$ (*x* = 0.0 – 0.5, *C*2, *Z* = 4, *V* = 714.9 – 723.7 $Å^3$; *x* = 0.625 – 2.375, $P\bar{3}m$, *Z* = 1, *V* = 181.81 – 193.46 $Å^3$; *x* = 2.5 – 3.0, $P\bar{3}$, *Z* = 3, *V* = 583.2 – 594.72 $Å^3$; Yonezaki, 2015), $Ba(Sr_{1-x}Ca_x)_2Mg[SiO_4]_2$ (*x* = 0.0 – 0.5, $P\bar{3}m$, *Z* = 1, *V* = 182.76 – 178.70 $Å^3$; *x* = 0.5625 – 1.0, $P\bar{3}$, *Z* = 1, *V* = 177.97 – 174.00 $Å^3$; Yonesaki *et al.*, 2008; Yonesaki, 2013), $Ba_3Mn[SiO_4]$ ($P\bar{3}m$, *Z* = 1, *V* = 203.44 $Å^3$; Avdeev *et al.*, 2018), $Na_3HZr[SiO_4]_2$, $P\bar{1}$, *Z* = 2, *V* = 350.12 $Å^3$; $Na_3HZr[SiO_4]_2{\cdot}0.4H_2O$, $P\bar{1}$, *Z* = 2, *V* = 350.19 $Å^3$; $Na_3HZr[SiO_4]_2{\cdot}H_2O$, *C*2/*m*, Z = 4, *V* = 683.92 $Å^3$; Kostov-Kytin *et al.*, 2012).

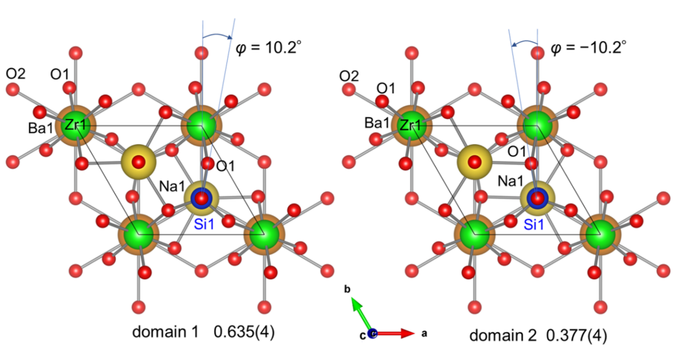


Figure 3
[001] projection of the twin domains in the crystal structure of $Na_2BaZr[SiO_4]_2$.

4. Synthesis and crystallization

The starting materials were powders of Na_2O (∼80%, Sigma-Aldrich), SiO_2 (99.9% Kojundo Chemical Lab. Co., Ltd.), BaO (99.99%, Sigma-Aldrich), ZrO_2 (99%, Sigma-Aldrich), and HfO_2 (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 $Na_2BaZr[SiO_4]_2$ 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 $Na_2BaHf[SiO_4]_2$ 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 $Na_2BaZr[SiO_4]_2$ and $Na_2BaHf[SiO_4]_2$ 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 $Na_2BaZr[SiO_4]_2$ and Na:Ba:Zr:Si = 2.3 (4):1.2 (1):1.3 (1): 2.0 (1) for $Na_2BaHf[SiO_4]_2$, 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 $P\overline{3}m$ was adopted and the $R1$ values were 0.032 and 0.018 for $Na_2BaM[SiO_4]_2$ for M = 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 = Zr) and 22.4 (M = Hf). Subsequently, when the refinement was performed in $P\overline{3}$ removing mirror symmetry operation from $P\overline{3}m$, the $R1$ values were 0.035 and 0.020, and the displacement ratios were still large at 27.6 and 18.2, for M = Zr and Hf, respectively. Further analysis in space group $P\overline{3}$ under consideration of twinning (twin matrix 010, 100, 00$\overline{1}$) resulted in $R1$ values of 0.016 and 0.010 for M = 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 = Zr and 0.623 (4):0.377 (4) for M = Hf.

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supporting information

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Hisanori Yamane, Shiro Funahashi, Naoto Hirosaki and Takashi Takeda

Computing details

Disodium barium zirconium bis(orthosilicate) (I)

Crystal data

$Na_2BaZr[SiO_4]_2$	D_x = 4.186 Mg m^{-3}
M_r = 458.72	Mo $K\alpha$ radiation, λ = 0.71073 Å
Trigonal, $P\overline{3}$	Cell parameters from 5734 reflections
a = 5.3966 (2) Å	θ = 2.8–47.6°
c = 7.2153 (3) Å	μ = 7.27 mm^{-1}
V = 181.98 (2) Å^3	T = 293 K
Z = 1	Plate, colourless
F(000) = 210	0.04 × 0.03 × 0.01 mm

Data collection

ROD, Synergy Custom system, HyPix-Arc 150 diffractometer	T_{min} = 0.544, T_{max} = 0.817
Radiation source: Rotating-anode X-ray tube, Rigaku (Mo) X-ray Source	9034 measured reflections
Mirror monochromator	587 independent reflections
Detector resolution: 10.0000 pixels mm^{-1}	543 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.043
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2023)	θ_{max} = 36.2°, θ_{min} = 2.8°
	h = −8→7
	k = −8→8
	l = −12→12

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	Primary atom site location: dual
$R[F^2 > 2\sigma(F^2)]$ = 0.016	$w = 1/[\sigma^2(F_o^2) + (0.0092P)^2 + 0.1709P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.035	$(\Delta/\sigma)_{max}$ < 0.001
S = 1.11	$\Delta\rho_{max}$ = 0.52 e Å^{-3}
587 reflections	$\Delta\rho_{min}$ = −0.59 e Å^{-3}
24 parameters	

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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 (Å, º)

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^{xiii}	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^{xii}—Ba1—O2^{xviii}	52.70 (5)
O1^{xii}—Ba1—O2^{xvii}	127.30 (5)
O1^{xiii}—Ba1—O2	127.30 (5)
O1—Ba1—O2	52.70 (5)
O1^{xiii}—Ba1—O2^{xvii}	108.70 (5)
O1^{xiii}—Ba1—O2^{xviii}	71.30 (5)
O1—Ba1—O2^{xvii}	71.30 (5)
O1^{xiv}—Ba1—O2	108.70 (5)
O1^{xvi}—Ba1—O2^{xvii}	99.18 (4)
O1—Ba1—O2^{xviii}	108.70 (5)
O1^{xv}—Ba1—O2^{xvii}	52.70 (5)
O1^{xiii}—Ba1—O2^{xiii}	52.70 (5)
O1^{xvi}—Ba1—O2^{xviii}	80.82 (4)
O1^{xv}—Ba1—O2^{xx}	71.30 (5)
O2^{xvii}—Ba1—O2^{xix}	119.741 (7)
O2^{xvii}—Ba1—O2^{xx}	60.259 (7)
O2^{xviii}—Ba1—O2^{xiii}	60.259 (7)
O2^{xvii}—Ba1—O2^{xiii}	119.741 (7)
O2—Ba1—O2^{xx}	119.740 (7)
O2^{xiii}—Ba1—O2^{xx}	60.260 (7)
O2^{xiii}—Ba1—O2^{xix}	119.740 (7)
O2^{xviii}—Ba1—O2^{xix}	60.259 (7)
O2—Ba1—O2^{xiii}	180.0
O2^{xviii}—Ba1—O2^{xx}	119.741 (7)
O2^{xvii}—Ba1—O2	60.259 (7)
O2—Ba1—O2^{xix}	60.260 (7)
O2^{xviii}—Ba1—O2	119.741 (7)
O2^{xvii}—Ba1—O2^{xviii}	180.00 (8)
O2^{xix}—Ba1—O2^{xx}	180.00 (8)
Na1^{iv}—Zr1—Na1^{xx}	77.74 (2)
Na1—Zr1—Na1^{xx}	102.26 (2)
Na1^{xviii}—Zr1—Na1	102.26 (2)
Na1^{iv}—Zr1—Na1^{xxi}	102.26 (2)
Na1^{xxi}—Zr1—Na1^{xx}	77.74 (2)
O1^{x}—Si1—Ba1^{i}	134.92 (5)
O1^{ix}—Si1—O1	106.53 (6)
O1—Si1—O1^{x}	106.53 (6)
O1^{ix}—Si1—O1^{x}	106.53 (6)
O2—Si1—Na1	180.0
O2—Si1—Na1^{ii}	96.45 (3)
O2—Si1—Na1^{iv}	96.45 (3)
O2—Si1—Na1^{iii}	96.45 (3)
O2—Si1—Ba1	60.849 (10)
O2—Si1—Ba1^{xxii}	60.849 (10)
O2—Si1—Ba1^{i}	60.849 (10)
O2—Si1—O1	112.28 (6)
O2—Si1—O1^{ix}	112.28 (6)
O2—Si1—O1^{x}	112.28 (6)
Na1^{iv}—O1—Na1^{iii}	168.17 (9)
Na1^{iv}—O1—Ba1	89.26 (5)
Ba1—O1—Na1^{iii}	79.67 (4)
Zr1—O1—Na1^{iv}	100.01 (6)
Zr1—O1—Na1^{iii}	84.71 (5)
Zr1—O1—Ba1	92.27 (5)
Si1—O1—Na1^{iii}	79.82 (5)
Si1—O1—Na1^{iv}	98.38 (6)
Si1—O1—Ba1	100.86 (7)
Si1—O1—Zr1	157.49 (9)
Na1^{xxiii}—O2—Ba1^{xxii}	87.07 (4)
Na1^{xxiii}—O2—Ba1	87.07 (4)
Na1^{xxiii}—O2—Ba1^{i}	87.07 (4)
Ba1—O2—Ba1^{xxii}	119.741 (7)
Ba1^{i}—O2—Ba1	119.741 (7)
Ba1^{i}—O2—Ba1^{xxii}	119.741 (7)
Si1—O2—Na1^{xxiii}	180.0
Si1—O2—Ba1^{i}	92.93 (4)
Si1—O2—Ba1^{xxii}	92.93 (4)
Si1—O2—Ba1	92.93 (4)

Na1^{ii}—Si1—O1—Na1^{iv}	80.07 (11)
Na1—Si1—O1—Na1^{iv}	100.39 (6)
Na1^{iii}—Si1—O1—Na1^{iv}	−168.16 (9)
Na1—Si1—O1—Na1^{iii}	−91.46 (4)
Na1^{iv}—Si1—O1—Na1^{iii}	168.16 (9)
Na1^{ii}—Si1—O1—Na1^{iii}	−111.77 (9)
Na1—Si1—O1—Ba1	−168.75 (6)
Na1^{iv}—Si1—O1—Ba1	90.86 (7)
Na1^{iii}—Si1—O1—Ba1	−77.30 (5)
Na1^{ii}—Si1—O1—Ba1	170.93 (5)
Na1^{iii}—Si1—O1—Zr1	47.3 (2)
Na1—Si1—O1—Zr1	−44.1 (2)
Ba1^{i}—Si1—O1—Zr1	−156.5 (2)
Ba1—Si1—O1—Zr1	124.6 (3)
Ba1^{xxii}—Si1—O1—Zr1	65.4 (3)
Ba1—Si1—O2—Ba1^{xxii}	−120.0
Ba1^{i}—Si1—O2—Ba1	−120.000 (1)
Ba1^{xxii}—Si1—O2—Ba1	120.0
Ba1^{i}—Si1—O2—Ba1^{xxii}	120.000 (1)
Ba1^{xxii}—Si1—O2—Ba1^{i}	−120.0
Ba1—Si1—O2—Ba1^{i}	120.0
O1^{ix}—Si1—O1—Na1^{iii}	−148.17 (6)
O1^{x}—Si1—O1—Na1^{iii}	−34.74 (9)
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

$Na_2BaHf[SiO_4]_2$
M_r = 545.99
Trigonal, $P\overline{3}$
a = 5.3889 (2) Å
c = 7.1996 (2) Å
V = 181.07 (1) Å^3
Z = 1
$F(000)$ = 242
D_x = 5.007 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7145 reflections
θ = 2.8–51.0°
μ = 20.19 mm^{-1}
T = 293 K
Plate, colourless
0.03 × 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} = 0.641, T_{max} = 0.883
8609 measured reflections
538 independent reflections
532 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 35.0°, θ_{min} = 2.8°
h = −8→7
k = −8→8
l = −11→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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.61$ e Å^{-3}
$\Delta\rho_{min} = -0.60$ 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: 0.623 (4) 0.377 (4)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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 (Å, º)

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) $x, y, z-1$.