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$Na_3MgB_{37}Si_9$: an icosahedral B_{12} cluster framework containing $\{Si_8\}$ units

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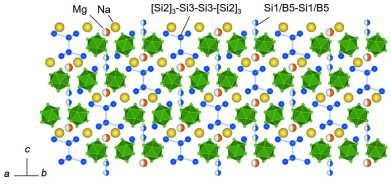
Single crystals of a novel sodium–magnesium boride silicide, $Na_3MgB_{37}Si_9$ [a = 10.1630 (3) Å, c = 16.5742 (6) Å, space group $R\bar{3}m$ (No. 166)], were synthesized by heating a mixture of Na, Si and crystalline B with B_2O_3 flux in Mg vapor at 1373 K. The Mg atoms in the title compound are located at an interstitial site of the $Dy_{2.1}B_{37}Si_9$-type structure with an occupancy of 0.5. The (001) layers of B_{12} icosahedra stack along the c-axis direction with shifting in the [–a/3, b/3, c/3] direction. A three-dimensional framework structure of the layers is formed *via* B—Si bonds and $\{Si_8\}$ units of $[Si]_3$—Si—Si—$[Si]_3$.

1. Chemical context

Boron-rich compounds composed of B_{12} icosahedral clusters are attracting attention as thermoelectric materials because of their low thermal conductivity resulting from their complicated crystal structures (Cahill *et al.*, 1977). In our previous study, a novel ternary borosilicide, $Na_8B_{74.5}Si_{17.5}$, was synthesized, and its crystal structure (Morito *et al.* 2010) and electronic structure measured using soft X-ray spectrometry (Terauchi *et al.* 2018), have been reported. This compound has a three-dimensional framework structure with layers composed of B_{12} icosahedral clusters and Si chains in the channels of the B_{12} clusters. During the investigation of this compound, a new crystalline phase was synthesized in which the stacking sequence of the B_{12} cluster layers differed from that of $Na_8B_{74.5}Si_{17.5}$. The composition analysis revealed that the new phase contained a small amount of Mg derived from an impurity in the starting material of amorphous B powder. Single crystals of this phase were prepared in the present study by heating a starting mixture of Na, crystalline B, a flux of B_2O_3 with Mg vapor, and the crystal structure was determined using single-crystal X-ray diffraction.



2. Structural commentary

The crystal structure of the new phase of composition $Na_3MgB_{37}Si_9$ is trigonal (space group $R\bar{3}m$, No. 166), and the hexagonal lattice constants are a = 10.1630 (3) Å and c = 16.5742 (6) Å. The structure is composed of B_{12} icosahedral clusters: the B—B distances of the 30 distinct bonds in the cluster are in the range of 1.791 (3)–1.843 (5) Å and the average distance is 1.811 Å (Table 1). The B_{12} icosahedral clusters are connected by a B2—B2 bond [1.761 (5) Å] on the

Table 1
Selected geometric parameters (Å, °).

Na1—B2^{i}	2.793 (2)	B2—B2^{viii}	1.761 (5)
Na1—B1	2.811 (2)	B3—B5^{i}	1.689 (7)
Na1—Si2^{i}	2.8621 (4)	B3—Si1^{i}	1.888 (4)
Na1—B4^{i}	2.9605 (16)	B4—Si2	2.082 (3)
Mg1—B2^{ii}	2.333 (3)	B5—B3^{iii}	1.689 (7)
B1—B3^{iii}	1.791 (3)	B5—Si1^{ix}	1.96 (2)
B1—B2^{iv}	1.798 (3)	B5—B5^{ix}	2.47 (4)
B1—B1^{v}	1.806 (4)	Si1—Si1^{ix}	1.460 (10)
B1—B2^{vi}	1.813 (3)	Si2—Si3^{x}	2.3951 (9)
B1—B4^{vii}	1.815 (3)	Si3—Si3^{xi}	2.304 (3)
B1—Si2^{i}	2.043 (2)		
Si3^{xi}—Si3—Si2^{x}	104.62 (4)	Si2^{x}—Si3—Si2^{xii}	113.86 (3)

Symmetry codes: (i) $-x+\frac{2}{3}, -y+\frac{1}{3}, -z+\frac{1}{3}$; (ii) $-y, x-y, z$; (iii) $x-y-\frac{1}{3}, x-\frac{2}{3}, -z+\frac{1}{3}$; (iv) $x-y+\frac{2}{3}, -y+\frac{1}{3}, -z+\frac{1}{3}$; (v) $-x+\frac{2}{3}, -x+y+\frac{1}{3}, -z+\frac{1}{3}$; (vi) $-x+y, -x, z$; (vii) $-x+y+\frac{1}{3}, -x+\frac{2}{3}, z-\frac{1}{3}$; (viii) $-x+y, y, z$; (ix) $-x, -y, -z$; (x) $-x+\frac{1}{3}, -y+\frac{2}{3}, -z+\frac{2}{3}$; (xi) $-x, -y, -z+1$; (xii) $y-\frac{2}{3}, -x+y-\frac{1}{3}, -z+\frac{2}{3}$.

(001) plane and form layers that stack along the *c* axis with a sequence of *ABCABC* by shifts of [–*a*/3, *b*/3, *c*/3] (Figs. 1 and 2).

Six B_{12} units in the layers surround $\{Si_8\}$ units of composition $[Si2]_3$—Si3—Si3—$[Si2]_3$. The bond lengths of 2.304 (3) Å for Si3—Si3 and 2.3951 (9) Å for Si2—Si3 are comparable with the bond length in crystalline silicon (2.35 Å). The bond angles of Si2—Si3—Si2 and Si2—Si3—Si3 are 113.86 (3)° and 104.61 (4)°, respectively, which are distorted from the regular tetrahedral bond angle of 109.47°. The Si2—B1 distance is 2.043 (2) Å, which is close to the Si—B distances (1.973–2.027 Å) found in *β*-silicon boride, SiB_3 (Salvador *et al.* 2003).

The framework structure of B_{12} icosahedra and $\{Si_8\}$ units of the title compound has also been reported in the structures of $Mg_3B_{36}Si_9C$ (Ludwig *et al.* 2013), $RE_{1-x}B_{12}Si_{3.3-\delta}$ (*RE* = Y, Gd–Lu) ($0 \le x \le 0.5$, $\delta \sim 0.3$) (Zhang *et al.* 2003) and $RE_{1-x}B_{36}Si_9C$ (*RE* = Y, Gd–Lu) (Ludwig *et al.* 2013) with the same space group of $R\bar{3}m$. The $\{Si_8\}$ units with Si2—B4 bonds [2.082 (3) Å] and Si1/B5—Si1/B5 pairs that bind to the B atoms at B3 connect the B_{12} layers of $Na_3MgB_{37}Si_9$ (Fig. 1). Because the Si1—Si1 distance of 1.460 (10) Å is short for an Si—Si bond and the B5—B5 distance 2.47 (4) Å is long for a B—B bond, it was concluded that disordered pairs of Si1—B5 and B5—Si1 [B—Si = 1.96 (2) Å] are statistically present with equal occupancies. Similar disordered Si/B—Si/B pairs have been reported in $Dy_{0.7}B_{12.33}Si_3$ (Si/B occupancy 0.5/0.5, Si—B length = 1.838 Å; Zhang *et al.* 2003). Instead of Si/B—Si/B pairs (Ludwig *et al.* 2013), $Mg_3B_{36}Si_9C$ contains Si/C—Si/C pairs (Si/C occupancy 0.507/0.493, Si—C length = 1.881 Å).

The Na1 site in the title compound is located around the $\{Si_8\}$ unit between the B_{12} cluster layers. The Na1—Si2 distance is 2.8620 (4) Å and the Na1—B1 and Na1—B2 distances are 2.811 (2) and 2.793 (2) Å, respectively. These distances are almost the same as the Na—Si distance of Na_4Si_4 [2.878 (3) Å; Morito *et al.*, 2015] and Na—B distance of NaB_{15} (2.798 Å; Naslain & Kasper, 1970). The Mg1 atom is situated above and below the $\{Si_8\}$ unit along the *c*-axis direction with an occupancy of 0.5. The Mg1—Si3 and Mg1—B2 distances are 2.403 (4) Å and 2.333 (3) Å, respectively, which are close to the Mg—Si (2.436 Å) and Mg—B distances (2.353 Å) in $MgB_{12}Si_2$ (Ludwig & Hillebrecht, 2006). The Na1—Mg1 distance in the title compound is 3.0389 (9) Å, which is close to the Na—Mg distance (3.120 Å) reported in $Na_4Mg_4Sn_3$ (Yamada *et al.* 2015). The site corresponding to the location of Mg1 in the title compound does not exist in $Mg_3B_{36}Si_9C$ (Ludwig *et al.* 2013), $RE_{1-x}B_{12}Si_{3.3-\delta}$ (*RE* = Y, Gd–Lu) ($0 \le x \le 0.5$, $\delta \sim 0.3$) (Zhang *et al.* 2003) and $RE_{1-x}B_{36}Si_9C$ (*RE* = Y, Gd–Lu) (Ludwig *et al.* 2013).

The number of electrons provided from Na and Mg to the framework of $B_{37}Si_9$ is five in $Na_3MgB_{37}Si_9$. In related compounds, the Mg atom in $Mg_3B_{36}Si_9C$ and the Dy atom in $Dy_{0.7}B_{12.33}Si_3$ ($Dy_{2.1}B_{37}Si_9$) provide six and 6.3 electrons, respectively, and approximately six electrons are supplied from *RE* in $RE_{1-x}B_{12}Si_{3.3-\delta}$ (*RE* = Y, Gd–Lu) ($0 \le x \le 0.5$, $\delta \sim 0.3$) and $RE_{1-x}B_{36}Si_9C$ (*RE* = Y, Gd–Lu). The lattice constants and unit-cell volume of $Mg_3B_{36}Si_9C$ are a = 10.0793 Å, c = 16.372 Å, and V = 1440.4 Å^3 (Ludwig *et al.*

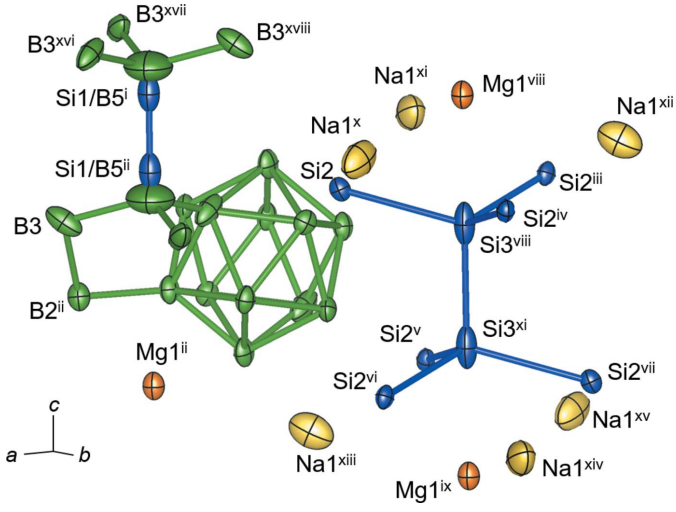


Figure 1
Interconnection of B_{12} clusters, Si1/B5—Si1/B5 bonds, $\{Si_8\}$ units and Na and Mg atoms in $Na_3MgB_{37}Si_9$. Displacement ellipsoids are drawn at the 90% probability level. Symmetry codes: (i) $x+\frac{2}{3}, y+\frac{1}{3}, z+\frac{1}{3}$; (ii) $-x+\frac{2}{3}, -y+\frac{1}{3}, -z+\frac{1}{3}$; (iii) $-x+y, 1-x, z$; (iv) $1-y, 1+x-y, z$; (v) $y-\frac{1}{3}, -x+y+\frac{1}{3}, -z+\frac{1}{3}$; (vi) $x-y+\frac{2}{3}, x+\frac{1}{3}, -z+\frac{1}{3}$; (vii) $-x+\frac{2}{3}, -y-\frac{2}{3}, -z+\frac{1}{3}$; (viii) $-x+\frac{1}{3}, -y+\frac{2}{3}, -z+\frac{2}{3}$; (ix) $x+\frac{1}{3}, y+\frac{2}{3}, z-\frac{1}{3}$; (*x*) $-y+\frac{2}{3}, x-y+\frac{1}{3}, z+\frac{1}{3}$; (xi) $x-\frac{1}{3}, y+\frac{1}{3}, z+\frac{1}{3}$; (xii) $-x+y+\frac{2}{3}, -x+\frac{4}{3}, z+\frac{1}{3}$; (xiii) $1-x+y, 1-x, z$; (xiv) $x, 1+y, z$; (xv) $-y, x-y, z$; (xvi) $x-y+\frac{1}{3}, x-\frac{1}{3}, -z+\frac{2}{3}$; (xvii) $y+\frac{1}{3}, -x+y+\frac{2}{3}, -z+\frac{2}{3}$; (xviii) $-x+\frac{4}{3}, -y+\frac{2}{3}, -z+\frac{2}{3}$.

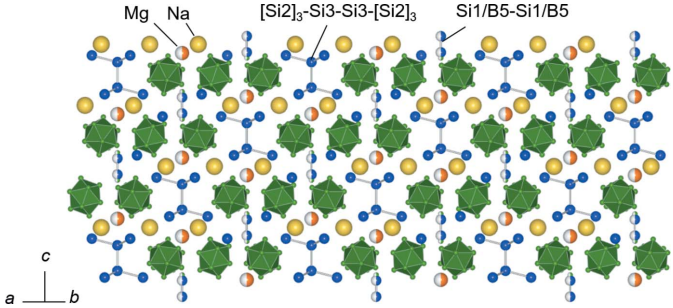


Figure 2
[110] projection of the crystal structure of $Na_3MgB_{37}Si_9$.

Table 2
Cell parameters (Å), cell volumes (Å^3) and selected bond lengths (Å) of $Na_3MgB_{37}Si_9$, $Dy_{2.1}B_{37}Si_9$[a] and $Mg_3B_{36}Si_9C$.

	$Na_3MgB_{37}Si_9$	$Dy_{2.1}B_{37}Si_9$	$Mg_3B_{36}Si_9C$
a	10.1630 (3)	10.078	10.079
c	16.5742 (6)	16.465	16.372
V	1482.54 (10)	1448.3	1440.4
B—B_{av} of B_{12} icosahedron	1.811	1.805	1.798
B2—B2	1.761 (5)	1.738	1.738
Si1—B3	1.887 (4)	1.877	1.851
Si1—B5/C	1.96 (2)	1.84	1.88
Si2—B1	2.043 (2)	2.032	2.035
Si2—B4	2.082 (3)	2.053	2.038
Si3—Si2	2.3951 (9)	2.366	2.362
Si3—Si3	2.304 (3)	2.343	2.341
Na1—B1	2.811 (2)	2.794	2.792
Na1—B2	2.793 (2)	2.751	2.729
Na1—B4	2.9604 (16)	2.934	2.934
Na1—Si2	2.8620 (4)	2.835	2.832
Mg1—B2	2.333 (3)		
Mg1—B4	2.568 (3)		
Mg1—Si3	2.403 (4)		

Notes: (*a*) Zhang *et al.* (2003); (*b*) Ludwig *et al.* (2013).

2013), those of $RE_{1-x}B_{12}Si_{3.3-\delta}$ (*RE* = Y, Gd–Lu) ($0 \le x \le 0.5$, $\delta \sim 0.3$) are *a* = 10.046–10.095 Å, *c* = 16.298–16.467 Å, and *V* = 1429–1454 Å^3 (Zhang *et al.* 2003) and those of $RE_{1-x}B_{36}Si_9C$ (*RE* = Y, Gd–Lu) are *a* = 10.000–10.096 Å, *c* = 16.225–16.454 Å, and *V* = 1405–1452 Å^3 (Ludwig *et al.* 2013). Thus, it may be seen that the lattice constants of $Na_3MgB_{37}Si_9$ are larger than those of related compounds and the unit-cell volume of $Na_3MgB_{37}Si_9$ is approximately 2% larger than the maximum unit-cell volume of 1454 Å^3 for the $RE_{1-x}B_{12}Si_{3.3-\delta}$ series with *RE* = Yb (Zhang *et al.* 2003). This increase in the lattice constants could be related to the occupancy of the Mg1 site, which is not found in other compounds.

Table 2 compares the interatomic distances for $Na_3MgB_{37}Si_9$, $Dy_{2.1}B_{37}Si_9$ and $Mg_3B_{36}Si_9C$. The average B—B distances of B_{12} icosahedra, B2—B2 distances between clusters, and Si2—B4 distances for $Na_3MgB_{37}Si_9$ are longer than those of other compounds. However, only the bond distance of Si3—Si3, in which Si3 only binds to Si, is specifically shorter. It is assumed that this bond became shorter because of an increase in the bond order from 1 because of a decrease in the number of electrons in the antibonding orbitals of the Si3—Si3 unit with a decrease in the electron count for the entire framework. Assuming that the main cause of the lattice expansion of $Na_3MgB_{37}Si_9$ is a decrease in the bonding force between B—B and B—Si atoms because of electron deficiency in the bonding orbitals of the $B_{37}Si_9$ framework, the lattice constant can be reduced by increasing the Mg occupancy, which can be attained by increasing the Mg vapor pressure during the synthesis.

3. Database survey

In space group $R\bar{3}m$, the framework structures of B_{12} icosahedral clusters containing {Si_8} units similar to $Na_3MgB_{37}Si_9$ have been reported for $Mg_3B_{36}Si_9C$ (Ludwig *et al.* 2013), $RE_{1-x}B_{12}Si_{3.3-\delta}$ (*RE* = Y, Gd–Lu) ($0 \le x \le 0.5$, $\delta \sim 0.3$) (Zhang *et al.* 2003) and $RE_{1-x}B_{36}Si_9C$ (*RE* = Y, Gd–Lu) (Ludwig *et al.* 2013).

Table 3
Experimental details.

Crystal data	
Chemical formula	$Na_3MgB_{37}Si_9$
M_r	746.06
Crystal system, space group	Trigonal, $R\bar{3}m$
Temperature (K)	298
a, *c* (Å)	10.1630 (3), 16.5742 (6)
V (Å^3)	1482.54 (10)
Z	3
Radiation type	Mo *Kα*
μ (mm^{-1})	0.72
Crystal size (mm)	0.20 × 0.16 × 0.02
Data collection	
Diffractometer	Burker, D8 QUEST
Absorption correction	Multi-scan (*SADABS*; Bruker, 2018)
T_{min}, T_{max}	0.911, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8352, 562, 540
R_{int}	0.032
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.703
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.035, 0.076, 1.31
No. of reflections	562
No. of parameters	57
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.58, −0.53

Computer programs: *APEX3* and *SAINT* (Bruker, 2018), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*), *VESTA* (Momma & Izumi, 2011) and *publCIF* (Westrip, 2010).

4. Synthesis and crystallization

Na metal pieces (purity 99.95%, Nippon Soda Co., Ltd.), crystalline B powder (99.9%, FUJIFILM Wako Pure Chemical Industries Co., Ltd.) and Si powder (99.999%, Kojundo Chemical Lab. Co., Ltd.) were weighed in a BN crucible (99.5%, Showa Denko K. K., outer diameter = 8.5 mm, inner diameter = 6.5 mm, depth = 18 mm), with a molar ratio of Na:B:Si = 5:4:3 (a total weight 280 mg) in a high-purity Ar-filled glove box (O_2 < 1 ppm, H_2O < 1 ppm). Then, 10 mg of B_2O_3 powder (90%, FUJIFILM Wako Pure Chemical Industries, Ltd.) were added to the crucible, which was stacked on another BN crucible containing 30 mg of Mg powder (99.9%, rare metallic), and these crucibles were encapsulated in a stainless steel container (SUS316, outer diameter = 12.7 mm, inner diameter = 10.75 mm, length 80 mm) with Ar gas. The container was heated at 1373 K for 24 h using an electric furnace. After cooling, the crucible was taken out from the reaction container, and any Na and NaSi remaining in the crucible were reacted and removed with 2-propanol and ethanol. Then, the sample was washed with pure water to remove water-soluble compounds such as sodium borate and alkoxide produced by the reaction of Na and alcohol to leave black plates of the title compound. An electron probe microanalyzer (EPMA; JEOL Ltd., JXA-8200) was used to analyze the composition of the obtained single crystal as Na

5.49 (8), Mg 2.37 (7), B 74.8 (7), Si 17.3 (4) atom %, which is nearly matched by $Na_3MgB_{37}Si_9$ (Na 6.0, Mg 2.0, B 74.0, Si 18.0 atom %). Other elements such as O were not found.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The occupancy of the Mg1 site in the analysis of the initial model was 0.506 (10), whereas the occupancy of the B5 and Si1 sites was 0.519 (15) and 0.481, respectively. These occupancies were fixed at 0.5, and the composition formula was determined to be $Na_3MgB_{37}Si_9$. The crystal structure was refined by considering (001) twinning, which reduced the *R*-value (all data) from 0.0651 to 0.0380.

Acknowledgements

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supporting information

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$Na_3MgB_{37}Si_9$: an icosahedral B_{12} cluster framework containing {Si_8} units

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Computing details

Data collection: Instrument Service (Bruker, 2018); cell refinement: *APEX3* (Bruker, 2018); data reduction: *SAINT* (Bruker, 2018); program(s) used to solve structure: *SHELXT2014/5* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015b); molecular graphics: *VESTA* (Momma & Izumi, 2011); software used to prepare material for publication: *publCIF* (Westrip, 2010).

3 sodium 1 magnesium 37 boron 9 silicon

Crystal data

$Na_3MgB_{37}Si_9$
M_r = 746.06
Trigonal, $R\bar{3}m$
a = 10.1630 (3) Å
c = 16.5742 (6) Å
V = 1482.54 (10) Å^3
Z = 3
$F(000)$ = 1068
D_x = 2.507 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6032 reflections
θ = 3.7–41.2°
μ = 0.72 mm^{-1}
T = 298 K
Plate, black
0.20 × 0.16 × 0.02 mm

Data collection

Burker, D8 QUEST diffractometer
Detector resolution: 10 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2018)
T_{min} = 0.911, T_{max} = 1.000
8352 measured reflections
562 independent reflections
540 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 30.0°, θ_{min} = 2.6°
h = −14→14
k = −14→14
l = −23→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.076
S = 1.31
562 reflections
57 parameters
0 restraints
$w = 1/[\sigma^2(F_o^2) + 11.3797P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −0.53 e Å^{-3}
Extinction correction: SHELXL2014/7 (Sheldrick 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0030 (6)

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 inversion twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Na1	0.5000	0.0000	0.0000	0.0179 (5)	
Mg1	0.0000	0.0000	0.2855 (2)	0.0074 (7)	0.5
B1	0.3002 (3)	0.0065 (2)	0.11511 (13)	0.0064 (4)	
B2	0.0027 (3)	0.1787 (3)	0.19610 (13)	0.0072 (4)	
B3	0.7591 (2)	0.2409 (2)	0.2315 (2)	0.0116 (7)	
B4	0.47839 (19)	0.52161 (19)	0.39743 (19)	0.0079 (6)	
B5	0.0000	0.0000	0.0744 (12)	0.026 (5)	0.5
Si1	0.0000	0.0000	0.0441 (3)	0.0103 (9)	0.5
Si2	0.46499 (5)	0.53501 (5)	0.27264 (5)	0.0056 (2)	
Si3	0.0000	0.0000	0.43049 (10)	0.0120 (3)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.0137 (7)	0.0265 (11)	0.0178 (8)	0.0132 (6)	0.0027 (4)	0.0054 (8)
Mg1	0.0060 (9)	0.0060 (9)	0.0102 (15)	0.0030 (5)	0.000	0.000
B1	0.0064 (9)	0.0041 (9)	0.0080 (8)	0.0020 (8)	−0.0004 (7)	0.0001 (8)
B2	0.0054 (9)	0.0053 (9)	0.0102 (9)	0.0022 (8)	−0.0005 (8)	−0.0009 (8)
B3	0.0087 (10)	0.0087 (10)	0.0116 (13)	0.0001 (12)	0.0035 (7)	−0.0035 (7)
B4	0.0050 (9)	0.0050 (9)	0.0116 (13)	0.0009 (11)	−0.0004 (6)	0.0004 (6)
B5	0.033 (8)	0.033 (8)	0.012 (9)	0.017 (4)	0.000	0.000
Si1	0.0061 (11)	0.0061 (11)	0.019 (3)	0.0031 (5)	0.000	0.000
Si2	0.0044 (3)	0.0044 (3)	0.0073 (4)	0.0015 (3)	0.00040 (14)	−0.00040 (14)
Si3	0.0055 (4)	0.0055 (4)	0.0249 (8)	0.0028 (2)	0.000	0.000

Geometric parameters (Å, º)

Na1—B2^{i}	2.793 (2)	B3—Si1^{i}	1.888 (4)
Na1—B2^{ii}	2.793 (2)	B3—B5^{xxx}	3.343 (19)
Na1—B2^{iii}	2.793 (2)	B3—Na1^{xxx}	4.123 (3)
Na1—B2^{iv}	2.793 (2)	B3—Na1^{xxxi}	4.123 (3)
Na1—B1^{v}	2.811 (2)	B3—Na1^{xxxii}	4.605 (3)
Na1—B1^{vi}	2.811 (2)	B4—B3^{xxviii}	1.799 (5)
Na1—B1^{vii}	2.811 (2)	B4—B1^{xxxiii}	1.815 (3)
Na1—B1	2.811 (2)	B4—B1^{xxxiv}	1.815 (3)
Na1—Si2^{viii}	2.8620 (4)	B4—B2^{xxxv}	1.824 (4)
Na1—Si2^{ix}	2.8620 (4)	B4—B2^{xv}	1.824 (4)
Na1—Si2^{i}	2.8621 (4)	B4—Si2	2.082 (3)

Na1—Si2^{ii}	2.8621 (4)	B4—Mg1^{xv}	2.568 (3)
Na1—B4^{viii}	2.9604 (16)	B4—Na1^{xxiv}	2.9605 (16)
Na1—B4^{ix}	2.9604 (16)	B4—Na1^{xxxiii}	2.9605 (16)
Na1—B4^{i}	2.9605 (16)	B4—B5^{xxx}	3.319 (3)
Na1—B4^{ii}	2.9605 (16)	B4—B5^{i}	4.031 (12)
Na1—Mg1^{i}	3.0389 (9)	B4—B5^{xv}	4.117 (16)
Na1—Mg1^{ii}	3.0389 (9)	B5—Si1	0.503 (18)
Mg1—B2^{x}	2.333 (3)	B5—B3^{xviii}	1.689 (7)
Mg1—B2^{xi}	2.333 (3)	B5—B3^{xxxvi}	1.689 (7)
Mg1—B2^{xii}	2.333 (3)	B5—B3^{i}	1.689 (7)
Mg1—B2^{xiii}	2.333 (3)	B5—Si1^{xxi}	1.96 (2)
Mg1—B2^{xiv}	2.333 (3)	B5—B5^{xxi}	2.47 (4)
Mg1—B2	2.333 (3)	B5—B2^{xiii}	2.705 (16)
Mg1—Si3	2.403 (4)	B5—B2^{xiv}	2.705 (16)
Mg1—B4^{xv}	2.568 (3)	B5—B2^{xi}	2.705 (16)
Mg1—B4^{xvi}	2.568 (3)	B5—B2^{xii}	2.705 (16)
Mg1—B4^{xvii}	2.568 (3)	B5—B2^{x}	2.705 (16)
Mg1—Si2^{xv}	2.933 (2)	Si1—Si1^{xxi}	1.460 (10)
Mg1—Si2^{xvii}	2.933 (2)	Si1—B3^{xviii}	1.887 (4)
B1—B3^{xviii}	1.791 (3)	Si1—B3^{xxxvi}	1.887 (4)
B1—B2^{iv}	1.798 (3)	Si1—B3^{i}	1.888 (4)
B1—B1^{xix}	1.806 (4)	Si1—B5^{xxi}	1.96 (2)
B1—B2^{xiv}	1.813 (3)	Si1—Na1^{xiv}	5.1337 (7)
B1—B4^{ix}	1.815 (3)	Si1—Na1^{xxii}	5.1337 (7)
B1—Si2^{i}	2.043 (2)	Si1—Na1^{xxxvii}	5.1337 (7)
B1—B5	3.093 (5)	Si1—Na1^{xxxviii}	5.1337 (7)
B1—Na1^{xx}	3.954 (2)	Si1—Na1^{x}	5.1337 (7)
B1—B5^{i}	4.268 (12)	Si2—B1^{i}	2.043 (2)
B1—B5^{xxi}	4.356 (15)	Si2—B1^{xxix}	2.043 (2)
B1—Na1^{xxii}	4.768 (2)	Si2—Si3^{xv}	2.3951 (9)
B2—B2^{xiii}	1.761 (5)	Si2—Na1^{xxxiii}	2.8621 (4)
B2—B1^{xxiii}	1.798 (3)	Si2—Na1^{xxiv}	2.8621 (4)
B2—B1^{x}	1.813 (3)	Si2—Mg1^{xv}	2.933 (2)
B2—B3^{i}	1.816 (4)	Si2—B5^{i}	3.5572 (16)
B2—B4^{xv}	1.824 (4)	Si2—B5^{xxx}	4.197 (11)
B2—B2^{xi}	1.843 (5)	Si2—Na1^{xxii}	4.5605 (8)
B2—B5	2.705 (16)	Si2—Na1^{xxxix}	5.3470 (8)
B2—Na1^{xxiv}	2.793 (2)	Si3—Si3^{xl}	2.304 (3)
B2—Na1^{xxv}	4.143 (2)	Si3—Si2^{xv}	2.3951 (9)
B2—B5^{xxvi}	4.537 (5)	Si3—Si2^{xvi}	2.3952 (9)
B2—Na1^{x}	4.617 (2)	Si3—Si2^{xvii}	2.3952 (9)
B3—B5^{i}	1.689 (7)	Si3—Na1^{xx}	3.3466 (8)
B3—B1^{xxvii}	1.791 (3)	Si3—Na1^{xxv}	3.3467 (8)
B3—B1^{iv}	1.791 (3)	Si3—Na1^{xxiv}	3.3467 (8)
B3—B4^{xxviii}	1.799 (5)	Si3—Na1^{xli}	4.8918 (14)
B3—B2^{i}	1.816 (4)	Si3—Na1^{xlii}	4.8918 (14)
B3—B2^{xxix}	1.816 (4)	Si3—Na1^{xliii}	4.8918 (14)

B2^{i}—Na1—B2^{ii}	180.00 (5)	B1^{iv}—B3—B2^{xxix}	60.33 (12)
B2^{i}—Na1—B2^{iii}	143.25 (9)	B4^{xxviii}—B3—B2^{xxix}	109.8 (2)
B2^{ii}—Na1—B2^{iii}	36.75 (9)	B2^{i}—B3—B2^{xxix}	60.99 (18)
B2^{i}—Na1—B2^{iv}	36.75 (9)	B5^{i}—B3—Si1^{i}	14.9 (6)
B2^{ii}—Na1—B2^{iv}	143.25 (9)	B1^{xxvii}—B3—Si1^{i}	123.43 (12)
B2^{iii}—Na1—B2^{iv}	180.00 (11)	B1^{iv}—B3—Si1^{i}	123.43 (12)
B2^{i}—Na1—B1^{v}	109.34 (7)	B4^{xxviii}—B3—Si1^{i}	129.2 (2)
B2^{ii}—Na1—B1^{v}	70.66 (7)	B2^{i}—B3—Si1^{i}	113.5 (2)
B2^{iii}—Na1—B1^{v}	37.43 (6)	B2^{xxix}—B3—Si1^{i}	113.5 (2)
B2^{iv}—Na1—B1^{v}	142.57 (6)	B5^{i}—B3—B5^{xxx}	45.3 (8)
B2^{i}—Na1—B1^{vi}	37.43 (6)	B1^{xxvii}—B3—B5^{xxx}	112.55 (16)
B2^{ii}—Na1—B1^{vi}	142.57 (6)	B1^{iv}—B3—B5^{xxx}	112.55 (16)
B2^{iii}—Na1—B1^{vi}	109.34 (7)	B4^{xxviii}—B3—B5^{xxx}	98.8 (3)
B2^{iv}—Na1—B1^{vi}	70.66 (7)	B2^{i}—B3—B5^{xxx}	136.96 (19)
B1^{v}—Na1—B1^{vi}	85.53 (9)	B2^{xxix}—B3—B5^{xxx}	136.96 (19)
B2^{i}—Na1—B1^{vii}	142.57 (6)	Si1^{i}—B3—B5^{xxx}	30.4 (3)
B2^{ii}—Na1—B1^{vii}	37.43 (6)	B5^{i}—B3—Na1^{xxx}	122.5 (5)
B2^{iii}—Na1—B1^{vii}	70.66 (7)	B1^{xxvii}—B3—Na1^{xxx}	99.85 (16)
B2^{iv}—Na1—B1^{vii}	109.34 (7)	B1^{iv}—B3—Na1^{xxx}	33.59 (11)
B1^{v}—Na1—B1^{vii}	94.47 (9)	B4^{xxviii}—B3—Na1^{xxx}	39.37 (5)
B1^{vi}—Na1—B1^{vii}	180.00 (6)	B2^{i}—B3—Na1^{xxx}	133.94 (17)
B2^{i}—Na1—B1	70.66 (7)	B2^{xxix}—B3—Na1^{xxx}	93.92 (11)
B2^{ii}—Na1—B1	109.34 (7)	Si1^{i}—B3—Na1^{xxx}	111.86 (14)
B2^{iii}—Na1—B1	142.57 (6)	B5^{xxx}—B3—Na1^{xxx}	88.28 (16)
B2^{iv}—Na1—B1	37.43 (6)	B5^{i}—B3—Na1^{xxxi}	122.5 (5)
B1^{v}—Na1—B1	180.0	B1^{xxvii}—B3—Na1^{xxxi}	33.59 (11)
B1^{vi}—Na1—B1	94.47 (9)	B1^{iv}—B3—Na1^{xxxi}	99.85 (16)
B1^{vii}—Na1—B1	85.53 (9)	B4^{xxviii}—B3—Na1^{xxxi}	39.37 (5)
B2^{i}—Na1—Si2^{viii}	78.17 (5)	B2^{i}—B3—Na1^{xxxi}	93.92 (11)
B2^{ii}—Na1—Si2^{viii}	101.83 (5)	B2^{xxix}—B3—Na1^{xxxi}	133.94 (17)
B2^{iii}—Na1—Si2^{viii}	76.28 (5)	Si1^{i}—B3—Na1^{xxxi}	111.86 (14)
B2^{iv}—Na1—Si2^{viii}	103.72 (5)	B5^{xxx}—B3—Na1^{xxxi}	88.28 (16)
B1^{v}—Na1—Si2^{viii}	73.21 (5)	Na1^{xxx}—B3—Na1^{xxxi}	76.09 (7)
B1^{vi}—Na1—Si2^{viii}	42.21 (5)	B5^{i}—B3—Na1	101.0 (6)
B1^{vii}—Na1—Si2^{viii}	137.79 (5)	B1^{xxvii}—B3—Na1	57.83 (11)
B1—Na1—Si2^{viii}	106.79 (5)	B1^{iv}—B3—Na1	111.50 (15)
B2^{i}—Na1—Si2^{ix}	101.83 (5)	B4^{xxviii}—B3—Na1	108.78 (14)
B2^{ii}—Na1—Si2^{ix}	78.17 (5)	B2^{i}—B3—Na1	3.02 (8)
B2^{iii}—Na1—Si2^{ix}	103.72 (5)	B2^{xxix}—B3—Na1	63.98 (11)
B2^{iv}—Na1—Si2^{ix}	76.28 (5)	Si1^{i}—B3—Na1	113.12 (15)
B1^{v}—Na1—Si2^{ix}	106.79 (5)	B5^{xxx}—B3—Na1	135.32 (13)
B1^{vi}—Na1—Si2^{ix}	137.79 (5)	Na1^{xxx}—B3—Na1	134.78 (8)
B1^{vii}—Na1—Si2^{ix}	42.21 (5)	Na1^{xxxi}—B3—Na1	91.40 (4)
B1—Na1—Si2^{ix}	73.21 (5)	B5^{i}—B3—Na1^{xxxii}	101.0 (6)
Si2^{viii}—Na1—Si2^{ix}	180.00 (3)	B1^{xxvii}—B3—Na1^{xxxii}	111.50 (15)
B2^{i}—Na1—Si2^{i}	103.71 (5)	B1^{iv}—B3—Na1^{xxxii}	57.83 (11)
B2^{ii}—Na1—Si2^{i}	76.29 (5)	B4^{xxviii}—B3—Na1^{xxxii}	108.78 (14)
B2^{iii}—Na1—Si2^{i}	101.83 (5)	B2^{i}—B3—Na1^{xxxii}	63.98 (11)

B2^{iv}—Na1—Si2^{i}	78.17 (5)	B2^{xxix}—B3—Na1^{xxxii}	3.02 (8)
B1^{v}—Na1—Si2^{i}	137.79 (5)	Si1^{i}—B3—Na1^{xxxii}	113.12 (15)
B1^{vi}—Na1—Si2^{i}	106.80 (5)	B5^{xxx}—B3—Na1^{xxxii}	135.32 (13)
B1^{vii}—Na1—Si2^{i}	73.20 (5)	Na1^{xxx}—B3—Na1^{xxxii}	91.40 (4)
B1—Na1—Si2^{i}	42.21 (5)	Na1^{xxxi}—B3—Na1^{xxxii}	134.78 (8)
Si2^{viii}—Na1—Si2^{i}	89.06 (3)	Na1—B3—Na1^{xxxii}	66.97 (5)
Si2^{ix}—Na1—Si2^{i}	90.94 (3)	B3^{xxviii}—B4—B1^{xxxiii}	59.41 (12)
B2^{i}—Na1—Si2^{ii}	76.29 (5)	B3^{xxviii}—B4—B1^{xxxiv}	59.41 (12)
B2^{ii}—Na1—Si2^{ii}	103.71 (5)	B1^{xxxiii}—B4—B1^{xxxiv}	107.0 (2)
B2^{iii}—Na1—Si2^{ii}	78.17 (5)	B3^{xxviii}—B4—B2^{xxxv}	106.60 (19)
B2^{iv}—Na1—Si2^{ii}	101.83 (5)	B1^{xxxiii}—B4—B2^{xxxv}	59.22 (12)
B1^{v}—Na1—Si2^{ii}	42.21 (5)	B1^{xxxiv}—B4—B2^{xxxv}	107.49 (19)
B1^{vi}—Na1—Si2^{ii}	73.20 (5)	B3^{xxviii}—B4—B2^{xv}	106.60 (19)
B1^{vii}—Na1—Si2^{ii}	106.80 (5)	B1^{xxxiii}—B4—B2^{xv}	107.49 (19)
B1—Na1—Si2^{ii}	137.79 (5)	B1^{xxxiv}—B4—B2^{xv}	59.22 (12)
Si2^{viii}—Na1—Si2^{ii}	90.94 (3)	B2^{xxxv}—B4—B2^{xv}	60.69 (17)
Si2^{ix}—Na1—Si2^{ii}	89.06 (3)	B3^{xxviii}—B4—Si2	116.8 (2)
Si2^{i}—Na1—Si2^{ii}	180.00 (3)	B1^{xxxiii}—B4—Si2	120.31 (12)
B2^{i}—Na1—B4^{viii}	109.24 (8)	B1^{xxxiv}—B4—Si2	120.31 (12)
B2^{ii}—Na1—B4^{viii}	70.76 (8)	B2^{xxxv}—B4—Si2	126.71 (16)
B2^{iii}—Na1—B4^{viii}	36.82 (8)	B2^{xv}—B4—Si2	126.71 (16)
B2^{iv}—Na1—B4^{viii}	143.18 (8)	B3^{xxviii}—B4—Mg1^{xv}	165.7 (2)
B1^{v}—Na1—B4^{viii}	36.55 (7)	B1^{xxxiii}—B4—Mg1^{xv}	114.65 (14)
B1^{vi}—Na1—B4^{viii}	72.94 (8)	B1^{xxxiv}—B4—Mg1^{xv}	114.65 (14)
B1^{vii}—Na1—B4^{viii}	107.06 (8)	B2^{xxxv}—B4—Mg1^{xv}	61.46 (13)
B1—Na1—B4^{viii}	143.45 (7)	B2^{xv}—B4—Mg1^{xv}	61.46 (13)
Si2^{viii}—Na1—B4^{viii}	41.86 (6)	Si2—B4—Mg1^{xv}	77.46 (13)
Si2^{ix}—Na1—B4^{viii}	138.14 (6)	B3^{xxviii}—B4—Na1^{xxiv}	117.95 (7)
Si2^{i}—Na1—B4^{viii}	107.63 (6)	B1^{xxxiii}—B4—Na1^{xxiv}	173.12 (16)
Si2^{ii}—Na1—B4^{viii}	72.37 (6)	B1^{xxxiv}—B4—Na1^{xxiv}	67.24 (8)
B2^{i}—Na1—B4^{ix}	70.76 (8)	B2^{xxxv}—B4—Na1^{xxiv}	118.03 (15)
B2^{ii}—Na1—B4^{ix}	109.24 (8)	B2^{xv}—B4—Na1^{xxiv}	66.59 (8)
B2^{iii}—Na1—B4^{ix}	143.18 (8)	Si2—B4—Na1^{xxiv}	66.54 (6)
B2^{iv}—Na1—B4^{ix}	36.82 (8)	Mg1^{xv}—B4—Na1^{xxiv}	66.25 (7)
B1^{v}—Na1—B4^{ix}	143.45 (7)	B3^{xxviii}—B4—Na1^{xxxiii}	117.95 (7)
B1^{vi}—Na1—B4^{ix}	107.06 (8)	B1^{xxxiii}—B4—Na1^{xxxiii}	67.24 (8)
B1^{vii}—Na1—B4^{ix}	72.94 (8)	B1^{xxxiv}—B4—Na1^{xxxiii}	173.12 (16)
B1—Na1—B4^{ix}	36.55 (7)	B2^{xxxv}—B4—Na1^{xxxiii}	66.59 (8)
Si2^{viii}—Na1—B4^{ix}	138.14 (6)	B2^{xv}—B4—Na1^{xxxiii}	118.03 (15)
Si2^{ix}—Na1—B4^{ix}	41.86 (6)	Si2—B4—Na1^{xxxiii}	66.54 (6)
Si2^{i}—Na1—B4^{ix}	72.37 (6)	Mg1^{xv}—B4—Na1^{xxxiii}	66.25 (7)
Si2^{ii}—Na1—B4^{ix}	107.63 (6)	Na1^{xxiv}—B4—Na1^{xxxiii}	118.24 (11)
B4^{viii}—Na1—B4^{ix}	180.00 (18)	B3^{xxviii}—B4—B5^{xxx}	17.4 (4)
B2^{i}—Na1—B4^{i}	143.17 (8)	B1^{xxxiii}—B4—B5^{xxx}	66.8 (2)
B2^{ii}—Na1—B4^{i}	36.83 (8)	B1^{xxxiv}—B4—B5^{xxx}	66.8 (2)
B2^{iii}—Na1—B4^{i}	70.76 (8)	B2^{xxxv}—B4—B5^{xxx}	121.1 (3)
B2^{iv}—Na1—B4^{i}	109.24 (8)	B2^{xv}—B4—B5^{xxx}	121.1 (3)
B1^{v}—Na1—B4^{i}	107.06 (8)	Si2—B4—B5^{xxx}	99.4 (4)

B1^{vi}—Na1—B4^{i}	143.45 (7)	Mg1^{xv}—B4—B5^{xxx}	176.9 (4)
B1^{vii}—Na1—B4^{i}	36.55 (7)	Na1^{xxiv}—B4—B5^{xxx}	112.64 (15)
B1—Na1—B4^{i}	72.94 (8)	Na1^{xxxiii}—B4—B5^{xxx}	112.64 (15)
Si2^{viii}—Na1—B4^{i}	107.63 (6)	B3^{xxviii}—B4—B5^{i}	55.0 (3)
Si2^{ix}—Na1—B4^{i}	72.37 (6)	B1^{xxxiii}—B4—B5^{i}	87.8 (2)
Si2^{i}—Na1—B4^{i}	41.85 (6)	B1^{xxxiv}—B4—B5^{i}	87.8 (2)
Si2^{ii}—Na1—B4^{i}	138.15 (6)	B2^{xxxv}—B4—B5^{i}	146.20 (15)
B4^{viii}—Na1—B4^{i}	96.65 (12)	B2^{xv}—B4—B5^{i}	146.20 (15)
B4^{ix}—Na1—B4^{i}	83.35 (12)	Si2—B4—B5^{i}	61.8 (3)
B2^{i}—Na1—B4^{ii}	36.83 (8)	Mg1^{xv}—B4—B5^{i}	139.3 (3)
B2^{ii}—Na1—B4^{ii}	143.17 (8)	Na1^{xxiv}—B4—B5^{i}	95.59 (14)
B2^{iii}—Na1—B4^{ii}	109.24 (8)	Na1^{xxxiii}—B4—B5^{i}	95.59 (14)
B2^{iv}—Na1—B4^{ii}	70.76 (8)	B5^{xxx}—B4—B5^{i}	37.6 (6)
B1^{v}—Na1—B4^{ii}	72.94 (8)	B3^{xxviii}—B4—B5^{xv}	108.0 (2)
B1^{vi}—Na1—B4^{ii}	36.55 (7)	B1^{xxxiii}—B4—B5^{xv}	82.20 (16)
B1^{vii}—Na1—B4^{ii}	143.45 (7)	B1^{xxxiv}—B4—B5^{xv}	82.20 (16)
B1—Na1—B4^{ii}	107.06 (8)	B2^{xxxv}—B4—B5^{xv}	30.37 (9)
Si2^{viii}—Na1—B4^{ii}	72.37 (6)	B2^{xv}—B4—B5^{xv}	30.37 (9)
Si2^{ix}—Na1—B4^{ii}	107.63 (6)	Si2—B4—B5^{xv}	135.2 (2)
Si2^{i}—Na1—B4^{ii}	138.15 (6)	Mg1^{xv}—B4—B5^{xv}	57.7 (2)
Si2^{ii}—Na1—B4^{ii}	41.85 (6)	Na1^{xxiv}—B4—B5^{xv}	93.09 (12)
B4^{viii}—Na1—B4^{ii}	83.35 (12)	Na1^{xxxiii}—B4—B5^{xv}	93.09 (12)
B4^{ix}—Na1—B4^{ii}	96.65 (12)	B5^{xxx}—B4—B5^{xv}	125.4 (2)
B4^{i}—Na1—B4^{ii}	180.00 (13)	B5^{i}—B4—B5^{xv}	163.0 (4)
B2^{i}—Na1—Mg1^{i}	46.93 (7)	Si1—B5—B3^{xviii}	105.6 (7)
B2^{ii}—Na1—Mg1^{i}	133.07 (7)	Si1—B5—B3^{xxxvi}	105.6 (7)
B2^{iii}—Na1—Mg1^{i}	133.07 (7)	B3^{xviii}—B5—B3^{xxxvi}	113.0 (6)
B2^{iv}—Na1—Mg1^{i}	46.93 (7)	Si1—B5—B3^{i}	105.6 (7)
B1^{v}—Na1—Mg1^{i}	101.34 (6)	B3^{xviii}—B5—B3^{i}	113.0 (6)
B1^{vi}—Na1—Mg1^{i}	78.66 (6)	B3^{xxxvi}—B5—B3^{i}	113.0 (6)
B1^{vii}—Na1—Mg1^{i}	101.34 (6)	Si1—B5—Si1^{xxi}	0.0
B1—Na1—Mg1^{i}	78.65 (6)	B3^{xviii}—B5—Si1^{xxi}	105.6 (7)
Si2^{viii}—Na1—Mg1^{i}	120.47 (4)	B3^{xxxvi}—B5—Si1^{xxi}	105.6 (7)
Si2^{ix}—Na1—Mg1^{i}	59.53 (4)	B3^{i}—B5—Si1^{xxi}	105.6 (7)
Si2^{i}—Na1—Mg1^{i}	120.47 (4)	Si1—B5—B5^{xxi}	0.000 (1)
Si2^{ii}—Na1—Mg1^{i}	59.53 (4)	B3^{xviii}—B5—B5^{xxi}	105.6 (7)
B4^{viii}—Na1—Mg1^{i}	129.34 (6)	B3^{xxxvi}—B5—B5^{xxi}	105.6 (7)
B4^{ix}—Na1—Mg1^{i}	50.66 (6)	B3^{i}—B5—B5^{xxi}	105.6 (7)
B4^{i}—Na1—Mg1^{i}	129.34 (6)	Si1^{xxi}—B5—B5^{xxi}	0.0
B4^{ii}—Na1—Mg1^{i}	50.66 (6)	Si1—B5—B2	138.2 (3)
B2^{i}—Na1—Mg1^{ii}	133.07 (7)	B3^{xviii}—B5—B2	77.9 (5)
B2^{ii}—Na1—Mg1^{ii}	46.93 (7)	B3^{xxxvi}—B5—B2	111.0 (9)
B2^{iii}—Na1—Mg1^{ii}	46.93 (7)	B3^{i}—B5—B2	41.2 (4)
B2^{iv}—Na1—Mg1^{ii}	133.07 (7)	Si1^{xxi}—B5—B2	138.2 (3)
B1^{v}—Na1—Mg1^{ii}	78.66 (6)	B5^{xxi}—B5—B2	138.2 (3)
B1^{vi}—Na1—Mg1^{ii}	101.34 (6)	Si1—B5—B2^{xiii}	138.2 (3)
B1^{vii}—Na1—Mg1^{ii}	78.66 (6)	B3^{xviii}—B5—B2^{xiii}	41.2 (4)
B1—Na1—Mg1^{ii}	101.35 (6)	B3^{xxxvi}—B5—B2^{xiii}	111.1 (9)

Si2^{viii}—Na1—Mg1^{ii}	59.53 (4)	B3^{i}—B5—B2^{xiii}	77.9 (5)
Si2^{ix}—Na1—Mg1^{ii}	120.47 (4)	Si1^{xxi}—B5—B2^{xiii}	138.2 (3)
Si2^{i}—Na1—Mg1^{ii}	59.53 (4)	B5^{xxi}—B5—B2^{xiii}	138.2 (3)
Si2^{ii}—Na1—Mg1^{ii}	120.47 (4)	B2—B5—B2^{xiii}	38.0 (2)
B4^{viii}—Na1—Mg1^{ii}	50.66 (6)	Si1—B5—B2^{xiv}	138.2 (3)
B4^{ix}—Na1—Mg1^{ii}	129.34 (6)	B3^{xviii}—B5—B2^{xiv}	41.2 (4)
B4^{i}—Na1—Mg1^{ii}	50.66 (6)	B3^{xxxvi}—B5—B2^{xiv}	77.9 (5)
B4^{ii}—Na1—Mg1^{ii}	129.34 (6)	B3^{i}—B5—B2^{xiv}	111.1 (9)
Mg1^{i}—Na1—Mg1^{ii}	180.00 (13)	Si1^{xxi}—B5—B2^{xiv}	138.2 (3)
B2^{x}—Mg1—B2^{xi}	44.34 (12)	B5^{xxi}—B5—B2^{xiv}	138.2 (3)
B2^{x}—Mg1—B2^{xii}	46.53 (12)	B2—B5—B2^{xiv}	70.5 (5)
B2^{xi}—Mg1—B2^{xii}	83.96 (13)	B2^{xiii}—B5—B2^{xiv}	39.8 (3)
B2^{x}—Mg1—B2^{xiii}	101.12 (17)	Si1—B5—B2^{xi}	138.2 (3)
B2^{xi}—Mg1—B2^{xiii}	83.96 (13)	B3^{xviii}—B5—B2^{xi}	111.0 (9)
B2^{xii}—Mg1—B2^{xiii}	83.96 (13)	B3^{xxxvi}—B5—B2^{xi}	77.9 (5)
B2^{x}—Mg1—B2^{xiv}	83.96 (13)	B3^{i}—B5—B2^{xi}	41.2 (4)
B2^{xi}—Mg1—B2^{xiv}	101.12 (17)	Si1^{xxi}—B5—B2^{xi}	138.2 (3)
B2^{xii}—Mg1—B2^{xiv}	44.34 (12)	B5^{xxi}—B5—B2^{xi}	138.2 (3)
B2^{xiii}—Mg1—B2^{xiv}	46.53 (12)	B2—B5—B2^{xi}	39.8 (3)
B2^{x}—Mg1—B2	83.96 (13)	B2^{xiii}—B5—B2^{xi}	70.5 (5)
B2^{xi}—Mg1—B2	46.52 (12)	B2^{xiv}—B5—B2^{xi}	83.5 (6)
B2^{xii}—Mg1—B2	101.12 (17)	Si1—B5—B2^{xii}	138.2 (3)
B2^{xiii}—Mg1—B2	44.34 (12)	B3^{xviii}—B5—B2^{xii}	77.9 (5)
B2^{xiv}—Mg1—B2	83.96 (13)	B3^{xxxvi}—B5—B2^{xii}	41.2 (4)
B2^{x}—Mg1—Si3	129.43 (9)	B3^{i}—B5—B2^{xii}	111.1 (9)
B2^{xi}—Mg1—Si3	129.43 (9)	Si1^{xxi}—B5—B2^{xii}	138.2 (3)
B2^{xii}—Mg1—Si3	129.43 (9)	B5^{xxi}—B5—B2^{xii}	138.2 (3)
B2^{xiii}—Mg1—Si3	129.43 (9)	B2—B5—B2^{xii}	83.5 (6)
B2^{xiv}—Mg1—Si3	129.43 (9)	B2^{xiii}—B5—B2^{xii}	70.5 (5)
B2—Mg1—Si3	129.43 (9)	B2^{xiv}—B5—B2^{xii}	38.0 (2)
B2^{x}—Mg1—B4^{xv}	85.59 (9)	B2^{xi}—B5—B2^{xii}	70.5 (5)
B2^{xi}—Mg1—B4^{xv}	43.37 (9)	Si1—B5—B2^{x}	138.2 (3)
B2^{xii}—Mg1—B4^{xv}	127.11 (15)	B3^{xviii}—B5—B2^{x}	111.1 (9)
B2^{xiii}—Mg1—B4^{xv}	85.59 (9)	B3^{xxxvi}—B5—B2^{x}	41.2 (4)
B2^{xiv}—Mg1—B4^{xv}	127.11 (15)	B3^{i}—B5—B2^{x}	77.9 (5)
B2—Mg1—B4^{xv}	43.37 (9)	Si1^{xxi}—B5—B2^{x}	138.2 (3)
Si3—Mg1—B4^{xv}	96.04 (11)	B5^{xxi}—B5—B2^{x}	138.2 (3)
B2^{x}—Mg1—B4^{xvi}	43.37 (9)	B2—B5—B2^{x}	70.5 (5)
B2^{xi}—Mg1—B4^{xvi}	85.59 (9)	B2^{xiii}—B5—B2^{x}	83.5 (6)
B2^{xii}—Mg1—B4^{xvi}	43.37 (9)	B2^{xiv}—B5—B2^{x}	70.5 (5)
B2^{xiii}—Mg1—B4^{xvi}	127.11 (15)	B2^{xi}—B5—B2^{x}	38.0 (2)
B2^{xiv}—Mg1—B4^{xvi}	85.59 (9)	B2^{xii}—B5—B2^{x}	39.8 (3)
B2—Mg1—B4^{xvi}	127.11 (15)	B5—Si1—Si1^{xxi}	180.0
Si3—Mg1—B4^{xvi}	96.04 (11)	B5—Si1—B3^{xviii}	59.53 (17)
B4^{xv}—Mg1—B4^{xvi}	118.91 (4)	Si1^{xxi}—Si1—B3^{xviii}	120.47 (17)
B2^{x}—Mg1—B4^{xvii}	127.11 (15)	B5—Si1—B3^{xxxvi}	59.53 (17)
B2^{xi}—Mg1—B4^{xvii}	127.11 (15)	Si1^{xxi}—Si1—B3^{xxxvi}	120.47 (17)
B2^{xii}—Mg1—B4^{xvii}	85.59 (9)	B3^{xviii}—Si1—B3^{xxxvi}	96.6 (2)

B2^{xiii}—Mg1—B4^{xvii}	43.37 (9)	B5—Si1—B3^{i}	59.53 (17)
B2^{xiv}—Mg1—B4^{xvii}	43.37 (9)	Si1^{xxi}—Si1—B3^{i}	120.47 (17)
B2—Mg1—B4^{xvii}	85.59 (9)	B3^{xviii}—Si1—B3^{i}	96.6 (2)
Si3—Mg1—B4^{xvii}	96.04 (11)	B3^{xxxvi}—Si1—B3^{i}	96.6 (2)
B4^{xv}—Mg1—B4^{xvii}	118.91 (4)	B5—Si1—B5^{xxi}	180.0
B4^{xvi}—Mg1—B4^{xvii}	118.91 (4)	Si1^{xxi}—Si1—B5^{xxi}	0.0
B2^{x}—Mg1—Si2^{xv}	112.42 (6)	B3^{xviii}—Si1—B5^{xxi}	120.47 (17)
B2^{xi}—Mg1—Si2^{xv}	82.24 (6)	B3^{xxxvi}—Si1—B5^{xxi}	120.47 (17)
B2^{xii}—Mg1—Si2^{xv}	157.19 (6)	B3^{i}—Si1—B5^{xxi}	120.47 (17)
B2^{xiii}—Mg1—Si2^{xv}	112.42 (6)	B5—Si1—Na1^{xiv}	98.18 (5)
B2^{xiv}—Mg1—Si2^{xv}	157.19 (6)	Si1^{xxi}—Si1—Na1^{xiv}	81.82 (5)
B2—Mg1—Si2^{xv}	82.24 (6)	B3^{xviii}—Si1—Na1^{xiv}	144.19 (12)
Si3—Mg1—Si2^{xv}	52.19 (6)	B3^{xxxvi}—Si1—Na1^{xiv}	48.18 (10)
B4^{xv}—Mg1—Si2^{xv}	43.85 (8)	B3^{i}—Si1—Na1^{xiv}	94.136 (18)
B4^{xvi}—Mg1—Si2^{xv}	117.22 (8)	B5^{xxi}—Si1—Na1^{xiv}	81.82 (5)
B4^{xvii}—Mg1—Si2^{xv}	117.22 (8)	B5—Si1—Na1^{xxii}	98.18 (5)
B2^{x}—Mg1—Si2^{xvii}	157.19 (6)	Si1^{xxi}—Si1—Na1^{xxii}	81.82 (5)
B2^{xi}—Mg1—Si2^{xvii}	157.19 (6)	B3^{xviii}—Si1—Na1^{xxii}	48.18 (10)
B2^{xii}—Mg1—Si2^{xvii}	112.42 (6)	B3^{xxxvi}—Si1—Na1^{xxii}	144.19 (12)
B2^{xiii}—Mg1—Si2^{xvii}	82.24 (6)	B3^{i}—Si1—Na1^{xxii}	94.136 (18)
B2^{xiv}—Mg1—Si2^{xvii}	82.24 (6)	B5^{xxi}—Si1—Na1^{xxii}	81.82 (5)
B2—Mg1—Si2^{xvii}	112.42 (6)	Na1^{xiv}—Si1—Na1^{xxii}	163.65 (11)
Si3—Mg1—Si2^{xvii}	52.19 (6)	B5—Si1—Na1^{xxxvii}	98.18 (5)
B4^{xv}—Mg1—Si2^{xvii}	117.22 (8)	Si1^{xxi}—Si1—Na1^{xxxvii}	81.82 (5)
B4^{xvi}—Mg1—Si2^{xvii}	117.21 (8)	B3^{xviii}—Si1—Na1^{xxxvii}	144.19 (12)
B4^{xvii}—Mg1—Si2^{xvii}	43.85 (8)	B3^{xxxvi}—Si1—Na1^{xxxvii}	94.135 (18)
Si2^{xv}—Mg1—Si2^{xvii}	86.35 (8)	B3^{i}—Si1—Na1^{xxxvii}	48.18 (10)
B3^{xviii}—B1—B2^{iv}	108.06 (16)	B5^{xxi}—Si1—Na1^{xxxvii}	81.82 (5)
B3^{xviii}—B1—B1^{xix}	107.43 (15)	Na1^{xiv}—Si1—Na1^{xxxvii}	59.328 (9)
B2^{iv}—B1—B1^{xix}	60.40 (13)	Na1^{xxii}—Si1—Na1^{xxxvii}	118.01 (3)
B3^{xviii}—B1—B2^{xiv}	60.52 (15)	B5—Si1—Na1^{xxxviii}	98.18 (5)
B2^{iv}—B1—B2^{xiv}	108.83 (15)	Si1^{xxi}—Si1—Na1^{xxxviii}	81.82 (5)
B1^{xix}—B1—B2^{xiv}	59.60 (13)	B3^{xviii}—Si1—Na1^{xxxviii}	94.137 (18)
B3^{xviii}—B1—B4^{ix}	59.85 (16)	B3^{xxxvi}—Si1—Na1^{xxxviii}	48.19 (10)
B2^{iv}—B1—B4^{ix}	60.63 (15)	B3^{i}—Si1—Na1^{xxxviii}	144.19 (12)
B1^{xix}—B1—B4^{ix}	108.74 (15)	B5^{xxi}—Si1—Na1^{xxxviii}	81.82 (5)
B2^{xiv}—B1—B4^{ix}	109.26 (16)	Na1^{xiv}—Si1—Na1^{xxxviii}	59.328 (9)
B3^{xviii}—B1—Si2^{i}	110.42 (15)	Na1^{xxii}—Si1—Na1^{xxxviii}	118.01 (3)
B2^{iv}—B1—Si2^{i}	136.22 (14)	Na1^{xxxvii}—Si1—Na1^{xxxviii}	118.01 (3)
B1^{xix}—B1—Si2^{i}	123.70 (8)	B5—Si1—Na1	98.18 (5)
B2^{xiv}—B1—Si2^{i}	107.77 (13)	Si1^{xxi}—Si1—Na1	81.82 (5)
B4^{ix}—B1—Si2^{i}	125.94 (15)	B3^{xviii}—Si1—Na1	48.19 (10)
B3^{xviii}—B1—Na1	125.76 (15)	B3^{xxxvi}—Si1—Na1	94.137 (18)
B2^{iv}—B1—Na1	70.74 (10)	B3^{i}—Si1—Na1	144.19 (12)
B1^{xix}—B1—Na1	116.13 (15)	B5^{xxi}—Si1—Na1	81.82 (5)
B2^{xiv}—B1—Na1	173.69 (13)	Na1^{xiv}—Si1—Na1	118.01 (3)
B4^{ix}—B1—Na1	76.20 (11)	Na1^{xxii}—Si1—Na1	59.328 (9)
Si2^{i}—B1—Na1	70.23 (6)	Na1^{xxxvii}—Si1—Na1	163.65 (11)

B3^{xviii}—B1—B5	26.44 (12)	Na1^{xxxviii}—Si1—Na1	59.329 (9)
B2^{iv}—B1—B5	134.42 (13)	B5—Si1—Na1^{x}	98.18 (5)
B1^{xix}—B1—B5	118.8 (4)	Si1^{xxi}—Si1—Na1^{x}	81.82 (5)
B2^{xiv}—B1—B5	60.4 (4)	B3^{xviii}—Si1—Na1^{x}	94.135 (18)
B4^{ix}—B1—B5	80.5 (2)	B3^{xxxvi}—Si1—Na1^{x}	144.19 (12)
Si2^{i}—B1—B5	85.06 (18)	B3^{i}—Si1—Na1^{x}	48.18 (10)
Na1—B1—B5	124.6 (4)	B5^{xxi}—Si1—Na1^{x}	81.82 (5)
B3^{xviii}—B1—Na1^{xx}	99.62 (14)	Na1^{xiv}—Si1—Na1^{x}	118.01 (3)
B2^{iv}—B1—Na1^{xx}	99.93 (10)	Na1^{xxii}—Si1—Na1^{x}	59.328 (9)
B1^{xix}—B1—Na1^{xx}	39.67 (11)	Na1^{xxxvii}—Si1—Na1^{x}	59.328 (9)
B2^{xiv}—B1—Na1^{xx}	39.15 (8)	Na1^{xxxviii}—Si1—Na1^{x}	163.65 (11)
B4^{ix}—B1—Na1^{xx}	139.11 (13)	Na1—Si1—Na1^{x}	118.01 (3)
Si2^{i}—B1—Na1^{xx}	93.52 (7)	B1^{i}—Si2—B1^{xxix}	99.44 (13)
Na1—B1—Na1^{xx}	134.55 (7)	B1^{i}—Si2—B4	112.65 (8)
B5—B1—Na1^{xx}	94.3 (3)	B1^{xxix}—Si2—B4	112.65 (8)
B3^{xviii}—B1—B5^{i}	102.63 (12)	B1^{i}—Si2—Si3^{xv}	110.23 (7)
B2^{iv}—B1—B5^{i}	23.0 (2)	B1^{xxix}—Si2—Si3^{xv}	110.23 (7)
B1^{xix}—B1—B5^{i}	39.4 (2)	B4—Si2—Si3^{xv}	111.12 (10)
B2^{xiv}—B1—B5^{i}	86.6 (2)	B1^{i}—Si2—Na1^{xxxiii}	166.61 (7)
B4^{ix}—B1—B5^{i}	72.9 (2)	B1^{xxix}—Si2—Na1^{xxxiii}	67.56 (6)
Si2^{i}—B1—B5^{i}	146.89 (9)	B4—Si2—Na1^{xxxiii}	71.60 (4)
Na1—B1—B5^{i}	92.17 (19)	Si3^{xv}—Si2—Na1^{xxxiii}	78.52 (2)
B5—B1—B5^{i}	127.32 (17)	B1^{i}—Si2—Na1^{xxiv}	67.56 (6)
Na1^{xx}—B1—B5^{i}	78.9 (2)	B1^{xxix}—Si2—Na1^{xxiv}	166.61 (7)
B3^{xviii}—B1—B5^{xxi}	45.13 (19)	B4—Si2—Na1^{xxiv}	71.60 (4)
B2^{iv}—B1—B5^{xxi}	127.76 (14)	Si3^{xv}—Si2—Na1^{xxiv}	78.52 (2)
B1^{xix}—B1—B5^{xxi}	151.4 (2)	Na1^{xxxiii}—Si2—Na1^{xxiv}	125.18 (3)
B2^{xiv}—B1—B5^{xxi}	93.9 (2)	B1^{i}—Si2—Mg1^{xv}	130.08 (7)
B4^{ix}—B1—B5^{xxi}	67.63 (14)	B1^{xxix}—Si2—Mg1^{xv}	130.08 (6)
Si2^{i}—B1—B5^{xxi}	71.88 (9)	B4—Si2—Mg1^{xv}	58.69 (11)
Na1—B1—B5^{xxi}	91.1 (2)	Si3^{xv}—Si2—Mg1^{xv}	52.42 (7)
B5—B1—B5^{xxi}	33.5 (6)	Na1^{xxxiii}—Si2—Mg1^{xv}	63.235 (15)
Na1^{xx}—B1—B5^{xxi}	124.81 (18)	Na1^{xxiv}—Si2—Mg1^{xv}	63.235 (15)
B5^{i}—B1—B5^{xxi}	138.30 (13)	B1^{i}—Si2—B5^{i}	60.03 (17)
B3^{xviii}—B1—Na1^{xxii}	58.43 (12)	B1^{xxix}—Si2—B5^{i}	60.03 (17)
B2^{iv}—B1—Na1^{xxii}	59.13 (9)	B4—Si2—B5^{i}	87.2 (3)
B1^{xix}—B1—Na1^{xxii}	105.05 (8)	Si3^{xv}—Si2—B5^{i}	161.7 (3)
B2^{xiv}—B1—Na1^{xxii}	105.67 (11)	Na1^{xxxiii}—Si2—B5^{i}	108.61 (12)
B4^{ix}—B1—Na1^{xxii}	4.27 (10)	Na1^{xxiv}—Si2—B5^{i}	108.61 (12)
Si2^{i}—B1—Na1^{xxii}	130.03 (8)	Mg1^{xv}—Si2—B5^{i}	145.8 (3)
Na1—B1—Na1^{xxii}	79.66 (5)	B1^{i}—Si2—B5^{xxx}	80.55 (17)
B5—B1—Na1^{xxii}	80.33 (15)	B1^{xxix}—Si2—B5^{xxx}	80.55 (17)
Na1^{xx}—B1—Na1^{xxii}	134.85 (5)	B4—Si2—B5^{xxx}	51.3 (3)
B5^{i}—B1—Na1^{xxii}	70.00 (18)	Si3^{xv}—Si2—B5^{xxx}	162.4 (2)
B5^{xxi}—B1—Na1^{xxii}	69.77 (5)	Na1^{xxxiii}—Si2—B5^{xxx}	93.66 (11)
B2^{xiii}—B2—B1^{xxiii}	131.14 (10)	Na1^{xxiv}—Si2—B5^{xxx}	93.66 (11)
B2^{xiii}—B2—B1^{x}	111.97 (10)	Mg1^{xv}—Si2—B5^{xxx}	110.0 (2)
B1^{xxiii}—B2—B1^{x}	60.00 (14)	B5^{i}—Si2—B5^{xxx}	35.9 (6)

B2^{xiii}—B2—B3^{i}	106.92 (13)	B1^{i}—Si2—Na1^{xxii}	59.92 (6)
B1^{xxiii}—B2—B3^{i}	106.68 (18)	B1^{xxix}—Si2—Na1^{xxii}	59.92 (6)
B1^{x}—B2—B3^{i}	59.15 (14)	B4—Si2—Na1^{xxii}	165.73 (10)
B2^{xiii}—B2—B4^{xv}	136.84 (12)	Si3^{xv}—Si2—Na1^{xxii}	83.15 (4)
B1^{xxiii}—B2—B4^{xv}	60.14 (13)	Na1^{xxxiii}—Si2—Na1^{xxii}	112.858 (15)
B1^{x}—B2—B4^{xv}	108.04 (17)	Na1^{xxiv}—Si2—Na1^{xxii}	112.858 (15)
B3^{i}—B2—B4^{xv}	106.97 (16)	Mg1^{xv}—Si2—Na1^{xxii}	135.57 (6)
B2^{xiii}—B2—B2^{xi}	120.000 (1)	B5^{i}—Si2—Na1^{xxii}	78.6 (3)
B1^{xxiii}—B2—B2^{xi}	107.39 (10)	B5^{xxx}—Si2—Na1^{xxii}	114.5 (2)
B1^{x}—B2—B2^{xi}	107.25 (10)	B1^{i}—Si2—Na1^{xxxix}	123.16 (7)
B3^{i}—B2—B2^{xi}	59.51 (9)	B1^{xxix}—Si2—Na1^{xxxix}	123.16 (7)
B4^{xv}—B2—B2^{xi}	59.65 (9)	B4—Si2—Na1^{xxxix}	85.66 (9)
B2^{xiii}—B2—Mg1	67.83 (6)	Si3^{xv}—Si2—Na1^{xxxix}	25.46 (4)
B1^{xxiii}—B2—Mg1	127.40 (14)	Na1^{xxxiii}—Si2—Na1^{xxxix}	69.017 (15)
B1^{x}—B2—Mg1	171.03 (15)	Na1^{xxiv}—Si2—Na1^{xxxix}	69.017 (15)
B3^{i}—B2—Mg1	112.01 (15)	Mg1^{xv}—Si2—Na1^{xxxix}	26.96 (6)
B4^{xv}—B2—Mg1	75.16 (13)	B5^{i}—Si2—Na1^{xxxix}	172.8 (3)
B2^{xi}—B2—Mg1	66.74 (6)	B5^{xxx}—Si2—Na1^{xxxix}	136.9 (2)
B2^{xiii}—B2—B5	71.01 (12)	Na1^{xxii}—Si2—Na1^{xxxix}	108.610 (15)
B1^{xxiii}—B2—B5	142.0 (3)	Si3^{xl}—Si3—Si2^{xv}	104.62 (4)
B1^{x}—B2—B5	83.9 (3)	Si3^{xl}—Si3—Si2^{xvi}	104.61 (4)
B3^{i}—B2—B5	37.8 (2)	Si2^{xv}—Si3—Si2^{xvi}	113.86 (3)
B4^{xv}—B2—B5	129.70 (16)	Si3^{xl}—Si3—Si2^{xvii}	104.61 (4)
B2^{xi}—B2—B5	70.08 (13)	Si2^{xv}—Si3—Si2^{xvii}	113.86 (3)
Mg1—B2—B5	87.7 (3)	Si2^{xvi}—Si3—Si2^{xvii}	113.86 (3)
B2^{xiii}—B2—Na1^{xxiv}	71.62 (5)	Si3^{xl}—Si3—Mg1	180.0
B1^{xxiii}—B2—Na1^{xxiv}	71.82 (10)	Si2^{xv}—Si3—Mg1	75.38 (4)
B1^{x}—B2—Na1^{xxiv}	116.66 (12)	Si2^{xvi}—Si3—Mg1	75.39 (4)
B3^{i}—B2—Na1^{xxiv}	175.02 (13)	Si2^{xvii}—Si3—Mg1	75.39 (4)
B4^{xv}—B2—Na1^{xxiv}	76.58 (10)	Si3^{xl}—Si3—Na1^{xx}	118.76 (3)
B2^{xi}—B2—Na1^{xxiv}	125.43 (5)	Si2^{xv}—Si3—Na1^{xx}	136.62 (7)
Mg1—B2—Na1^{xxiv}	72.08 (8)	Si2^{xvi}—Si3—Na1^{xx}	56.938 (18)
B5—B2—Na1^{xxiv}	142.00 (18)	Si2^{xvii}—Si3—Na1^{xx}	56.938 (18)
B2^{xiii}—B2—Na1^{xxv}	113.62 (3)	Mg1—Si3—Na1^{xx}	61.24 (3)
B1^{xxiii}—B2—Na1^{xxv}	98.99 (11)	Si3^{xl}—Si3—Na1^{xxv}	118.76 (3)
B1^{x}—B2—Na1^{xxv}	131.77 (12)	Si2^{xv}—Si3—Na1^{xxv}	56.938 (18)
B3^{i}—B2—Na1^{xxv}	92.82 (10)	Si2^{xvi}—Si3—Na1^{xxv}	56.940 (18)
B4^{xv}—B2—Na1^{xxv}	39.10 (9)	Si2^{xvii}—Si3—Na1^{xxv}	136.62 (7)
B2^{xi}—B2—Na1^{xxv}	33.32 (3)	Mg1—Si3—Na1^{xxv}	61.24 (3)
Mg1—B2—Na1^{xxv}	46.23 (4)	Na1^{xx}—Si3—Na1^{xxv}	98.79 (3)
B5—B2—Na1^{xxv}	96.5 (2)	Si3^{xl}—Si3—Na1^{xxiv}	118.76 (3)
Na1^{xxiv}—B2—Na1^{xxv}	92.11 (5)	Si2^{xv}—Si3—Na1^{xxiv}	56.938 (18)
B2^{xiii}—B2—B5^{xxvi}	157.80 (15)	Si2^{xvi}—Si3—Na1^{xxiv}	136.62 (7)
B1^{xxiii}—B2—B5^{xxvi}	29.13 (9)	Si2^{xvii}—Si3—Na1^{xxiv}	56.940 (18)
B1^{x}—B2—B5^{xxvi}	69.9 (2)	Mg1—Si3—Na1^{xxiv}	61.24 (3)
B3^{i}—B2—B5^{xxvi}	93.1 (3)	Na1^{xx}—Si3—Na1^{xxiv}	98.79 (3)
B4^{xv}—B2—B5^{xxvi}	38.8 (2)	Na1^{xxv}—Si3—Na1^{xxiv}	98.78 (3)
B2^{xi}—B2—B5^{xxvi}	78.28 (3)	Si3^{xl}—Si3—Na1^{xli}	36.851 (12)

Mg1—B2—B5^{xxvi}	113.9 (2)	Si2^{xv}—Si3—Na1^{xli}	67.76 (3)
B5—B2—B5^{xxvi}	130.32 (9)	Si2^{xvi}—Si3—Na1^{xli}	119.48 (4)
Na1^{xxiv}—B2—B5^{xxvi}	87.6 (2)	Si2^{xvii}—Si3—Na1^{xli}	119.48 (4)
Na1^{xxv}—B2—B5^{xxvi}	73.92 (14)	Mg1—Si3—Na1^{xli}	143.149 (12)
B2^{xiii}—B2—Na1^{x}	111.07 (3)	Na1^{xx}—Si3—Na1^{xli}	155.61 (4)
B1^{xxiii}—B2—Na1^{x}	57.51 (9)	Na1^{xxv}—Si3—Na1^{xli}	97.015 (14)
B1^{x}—B2—Na1^{x}	3.84 (8)	Na1^{xxiv}—Si3—Na1^{xli}	97.015 (14)
B3^{i}—B2—Na1^{x}	62.97 (11)	Si3^{xl}—Si3—Na1^{xlii}	36.852 (12)
B4^{xv}—B2—Na1^{x}	107.75 (13)	Si2^{xv}—Si3—Na1^{xlii}	119.48 (4)
B2^{xi}—B2—Na1^{x}	110.53 (3)	Si2^{xvi}—Si3—Na1^{xlii}	119.48 (4)
Mg1—B2—Na1^{x}	174.62 (10)	Si2^{xvii}—Si3—Na1^{xlii}	67.76 (3)
B5—B2—Na1^{x}	87.0 (3)	Mg1—Si3—Na1^{xlii}	143.148 (12)
Na1^{xxiv}—B2—Na1^{x}	112.83 (6)	Na1^{xx}—Si3—Na1^{xlii}	97.015 (14)
Na1^{xxv}—B2—Na1^{x}	133.76 (6)	Na1^{xxv}—Si3—Na1^{xlii}	155.61 (4)
B5^{xxvi}—B2—Na1^{x}	69.2 (2)	Na1^{xxiv}—Si3—Na1^{xlii}	97.016 (14)
B5^{i}—B3—B1^{xxvii}	125.38 (12)	Na1^{xli}—Si3—Na1^{xlii}	62.58 (2)
B5^{i}—B3—B1^{iv}	125.38 (12)	Si3^{xl}—Si3—Na1^{xliii}	36.852 (12)
B1^{xxvii}—B3—B1^{iv}	109.1 (2)	Si2^{xv}—Si3—Na1^{xliii}	119.48 (4)
B5^{i}—B3—B4^{xxviii}	144.1 (7)	Si2^{xvi}—Si3—Na1^{xliii}	67.76 (3)
B1^{xxvii}—B3—B4^{xxviii}	60.74 (14)	Si2^{xvii}—Si3—Na1^{xliii}	119.48 (4)
B1^{iv}—B3—B4^{xxviii}	60.74 (14)	Mg1—Si3—Na1^{xliii}	143.148 (12)
B5^{i}—B3—B2^{i}	101.0 (6)	Na1^{xx}—Si3—Na1^{xliii}	97.015 (14)
B1^{xxvii}—B3—B2^{i}	60.33 (12)	Na1^{xxv}—Si3—Na1^{xliii}	97.016 (14)
B1^{iv}—B3—B2^{i}	109.4 (2)	Na1^{xxiv}—Si3—Na1^{xliii}	155.61 (4)
B4^{xxviii}—B3—B2^{i}	109.8 (2)	Na1^{xli}—Si3—Na1^{xliii}	62.58 (2)
B5^{i}—B3—B2^{xxix}	101.0 (6)	Na1^{xlii}—Si3—Na1^{xliii}	62.58 (2)
B1^{xxvii}—B3—B2^{xxix}	109.4 (2)		

Symmetry codes: (i) −*x*+2/3, −*y*+1/3, −*z*+1/3; (ii) *x*+1/3, *y*−1/3, *z*−1/3; (iii) −*x*+*y*+1/3, *y*−1/3, *z*−1/3; (iv) *x*−*y*+2/3, −*y*+1/3, −*z*+1/3; (v) −*x*+1, −*y*, −*z*; (vi) −*x*+*y*+1, *y*, *z*; (vii) *x*−*y*, −*y*, −*z*; (viii) *x*−*y*+2/3, *x*−2/3, −*z*+1/3; (ix) −*x*+*y*+1/3, −*x*+2/3, *z*−1/3; (x) −*y*, *x*−*y*, *z*; (xi) −*y*, −*x*, *z*; (xii) *x*, *x*−*y*, *z*; (xiii) −*x*+*y*, *y*, *z*; (xiv) −*x*+*y*, −*x*, *z*; (xv) −*x*+1/3, −*y*+2/3, −*z*+2/3; (xvi) *y*−2/3, −*x*+*y*−1/3, −*z*+2/3; (xvii) *x*−*y*+1/3, *x*−1/3, −*z*+2/3; (xviii) *x*−*y*−1/3, *x*−2/3, −*z*+1/3; (xix) −*x*+2/3, −*x*+*y*+1/3, −*z*+1/3; (xx) −*x*+*y*+2/3, −*x*+1/3, *z*+1/3; (xxi) −*x*, −*y*, −*z*; (xxii) −*x*+*y*+1, −*x*+1, *z*; (xxiii) *x*−*y*−1/3, −*y*+1/3, −*z*+1/3; (xxiv) *x*−1/3, *y*+1/3, *z*+1/3; (xxv) −*y*−1/3, *x*−*y*−2/3, *z*+1/3; (xxvi) −*x*−1/3, −*y*+1/3, −*z*+1/3; (xxvii) *y*+2/3, −*x*+*y*+1/3, −*z*+1/3; (xxviii) −*x*+4/3, −*y*+2/3, −*z*+2/3; (xxix) *y*+2/3, *x*+1/3, −*z*+1/3; (xxx) *x*+2/3, *y*+1/3, *z*+1/3; (xxxi) −*y*+2/3, *x*−*y*−2/3, *z*+1/3; (xxxii) −*y*+1, *x*−*y*, *z*; (xxxiii) −*y*+2/3, *x*−*y*+1/3, *z*+1/3; (xxxiv) −*x*+*y*+2/3, *y*+1/3, *z*+1/3; (xxxv) *y*+1/3, *x*+2/3, −*z*+2/3; (xxxvi) *y*−1/3, −*x*+*y*+1/3, −*z*+1/3; (xxxvii) *x*−1, *y*, *z*; (xxxviii) −*y*, *x*−*y*−1, *z*; (xxxix) −*x*+*y*+2/3, −*x*+4/3, *z*+1/3; (xl) −*x*, −*y*, −*z*+1; (xli) −*x*+*y*+1/3, −*x*+2/3, *z*+2/3; (xlii) −*y*+1/3, *x*−*y*−1/3, *z*+2/3; (xliii) *x*−2/3, *y*−1/3, *z*+2/3.