Na$_3$MgB$_{37}$Si$_9$: an icosahedral B$_{12}$ cluster framework containing \{Si$_8$\} units

Haruhiko Morito,$^a$* Takuji Ikeda,$^b$ Yukari Katsura$^c$ and Hisanori Yamane$^d$

$^a$Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan, $^b$Research Institute for Chemical Process Technology, National Institute of Advanced Industrial Science and Technology, 4-2-1, Nigatake, Miyagino-ku, Sendai 983-8551, Japan, $^c$National Institute for Materials Science, 1-2-1 Sengen, Tsukuba, Ibaraki, 305-0047, Japan, and $^d$Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan. *Correspondence e-mail: haruhiko.morito.b5@tohoku.ac.jp

Single crystals of a novel sodium–magnesium boride silicide, Na$_3$MgB$_{37}$Si$_9$ [$a = 10.1630$ (3) Å, $c = 16.5742$ (6) Å, space group $R3m$ (No. 166)], were synthesized by heating a mixture of Na, Si and crystalline B with B$_2$O$_3$ 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$_4$]$_3$—Si—Si—[Si$_4$].

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$_8$B$_{74.5}$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$_8$B$_{74.5}$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$_2$O$_3$, 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$_3$MgB$_{37}$Si$_9$ is trigonal (space group $R3m$, 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 B$_2$–B$_2$ bond [1.761 (5) Å] on the...
Table 1
Selected geometric parameters (Å, °).

| Bond                | Length/Angle |
|---------------------|--------------|
| Na1—B2’             | 2.793 (2)    |
| Na1—B1              | 2.811 (2)    |
| Na1—Si2             | 2.8621 (4)   |
| Na1—B4’             | 2.9065 (16)  |
| Mg1—B2ii            | 2.333 (3)    |
| B1—B3iii            | 1.791 (3)    |
| B1—B2’              | 1.798 (3)    |
| Si2—Si3             | 2.3951 (9)   |
| Mg1—Si1             | 2.062 (3)    |
| Si2—Si3             | 2.082 (3)    |
| B1—Si1              | 2.027 (2)    |
| Si2—Si3             | 2.043 (2)    |

Si3x—Si3—Si2x        104.62 (4) Si2x—Si3—Si2xii 113.86 (3)

Symmetry codes: (i) x, y, z; (ii) x, −y, z; (iii) −x, −y, z; (iv) x, −y, z; (v) x, −y, z; (vi) x, y, z; (vii) x, y, z; (viii) x, −y, −z; (x) x, y, z; (xi) y −z, −x + z; (xii) x, −y, z; (xiii) −x, −y, z; (xiv) x, y, z; (xv) −x, −y, z; (xvi) −x, y, z; (xvii) x, y, z; (xviii) x, −y, z; (xix) −x, −y, z; (xx) −x, −y, z; (xxi) x, y, z; (xxii) x, −y, −z; (xxiii) x, y, z; (xxiv) x, −y, z; (xxv) x, y, z; (xxvi) x, −y, z; (xxvii) x, y, z; (xxviii) x, −y, z; (xxix) −x, −y, z; (xxx) −x, −y, z.

(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 B12 units in the layers surround [Si6] units of composition [Si21]−Si3−Si3−[Si20]. 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 104.62 (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, SiB3 (Salvador et al. 2003).

The framework structure of B12 icosahedra and [Si6] units of the title compound has also been reported in the structures of Mg3B90Si6C (Ludwig et al. 2013), RE1−xB12Si3.3−x (RE = Y, Gd–Lu) (0 ≤ x ≤ 0.5, δ ~ 0.3) (Zhang et al. 2003) and RE1−xB12SiC (RE = Y, Gd–Lu) (Ludwig et al. 2013) with the same space group of R3m. The [Si6] 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 B12 layers of Na3MgB2Si3 (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 Dy2B37Si9 (Zhang et al. 2003). Instead of Si/B−Si/B pairs (Ludwig et al. 2013), Mg6B90Si6C contains SiC−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 [Si6] unit between the B12 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 Na3Si4 [2.878 (3) Å; Morito et al. 2015] and Na−B distance of NaB13 (2.798 Å; Naslain & Kasper, 1970). The Mg1 atom is situated above and below the [Si6] 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 MgB12Si2 (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 Na4Mg4Sn3 (Yamada et al. 2015). The site corresponding to the location of Mg1 in the title compound does not exist in Mg3B90Si6C (Ludwig et al. 2013), RE1−xB12Si3.3−x (RE = Y, Gd–Lu) (0 ≤ x ≤ 0.5, δ ~ 0.3) (Zhang et al. 2003) and RE1−xB12SiC (RE = Y, Gd–Lu) (Ludwig et al. 2013).

The number of electrons provided from Na and Mg to the framework of B7Si3 is five in Na3MgB7Si3. In related compounds, the Mg atom in Mg6B90Si6C and the Dy atom in Dy2B37Si9 (Dy2.1B37Si9) provide six and 6.3 electrons, respectively, and approximately six electrons are supplied from RE in RE1−xB12Si3.3−x (RE = Y, Gd–Lu) (0 ≤ x ≤ 0.5, δ ~ 0.3) and RE1−xB12SiC (RE = Y, Gd–Lu). The lattice constants and unit-cell volume of Mg3B90Si6C are a = 10.0793 Å, c = 16.372 Å, and V = 1400.4 Å³ (Ludwig et al. 2013).
2013), those of $RE_{1-x}B_{12}Si_{35-x,y}$ ($RE = Y, Gd–Lu$) ($0 \leq x \leq 0.5, \delta \sim 0.3$) 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 $RE_{1-x}B_{36}Si_{9}C$ ($RE = Y, Gd–Lu$) 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 $RE_{1-x}B_{12}Si_{35-x,y}$ 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 $Na_3MgB_{37}Si_9$, $Dy_2B_2Si_6$, and $MgB_2Si_5C$.

### Table 2

|        | $Na_3MgB_{37}Si_9$ | $Dy_2B_2Si_6$ | $MgB_2Si_5C$ |
|--------|-------------------|---------------|--------------|
| $a$    | 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         | 1.794        |
| $Si_3 – Si_3$ | 2.304 (3)       | 2.343         | 2.341        |
| $Si_2 – Si_2$ | 2.3951 (9)      | 2.366         | 2.362        |
| $Si_1 – B_{5/C}$ | 1.96 (2)       | 1.84          | 1.88         |
| $Si_2 – B_4$ | 2.082 (3)       | 2.032         | 2.035        |
| $Si_3 – B_4$ | 2.079 (2)       | 2.032         | 2.035        |
| $Na_1 – B_4$ | 2.8620 (4)      | 2.835         | 2.832        |

### Notes:

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

3. Database survey

In space group $R3m$, the framework structures of $B_{12}$ icosahedral clusters containing $Si_8$ units similar to $Na_3MgB_{37}Si_9$ have been reported for $MgB_{36}Si_9C$ (Ludwig et al. 2013), $RE_{1-x}B_{12}Si_{35-x,y}$ ($RE = Y, Gd–Lu$) ($0 \leq x \leq 0.5, \delta \sim 0.3$) (Zhang et al. 2013) and $RE_{1-x}B_{36}Si_9C$ ($RE = Y, Gd–Lu$) (Ludwig et al. 2013).

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, 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 = 8.5 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$_3$MgB$_{37}$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$_3$MgB$_{37}$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

We thank T. Kamaya for his help with the EPMA analysis.

Funding information

Funding for this research was provided by: the Japan Science and Technology Agency (JST) CREST (grant No. JPMJCR19J1).

References

Bruker (2018). APEX3, SAINT and SADABS. Bruker AXS inc., Madison, Wisconsin, USA.

Cahill, D. G., Fischer, H. E., Watson, S. K., Pohl, R. O. & Slack, G. A. (1989). Phys. Rev. B, 40, 3254–3260.

Ludwig, T. & Hillebrecht, H. (2006). J. Solid State Chem. 179, 1623–1629.

Ludwig, T., Pediaditakis, A., Sagawe, V. & Hillebrecht, H. (2013). J. Solid State Chem. 204, 113–122.

Momma, K. & Izumi, F. (2011). J. Appl. Cryst. 44, 1272–1276.

Morito, H., Eck, B., Dronskowski, R. & Yamane, H. (2010). Dalton Trans. 39, 10197–10202.

Morito, H., Momma, K. & Yamane, H. (2015). J. Alloys Compd. 623, 473–479.

Naslain, R. & Kasper, J. S. (1970). J. Solid State Chem. 1, 150–151.

Salvador, J. R., Bic, D., Mahanti, S. D. & Kanatzidis, M. G. (2003). Angew. Chem. Int. Ed. 42, 1929–1932.

Sheldrick, G. M. (2015a). Acta Cryst. A71, 3–8.

Sheldrick, G. M. (2015b). Acta Cryst. C71, 3–8.

Terauchi, M., Morito, H., Yamane, H., Koshiya, S. & Kimoto, K. (2018). Microscopy, 67, i72–i77.

Westrip, S. P. (2010). J. Appl. Cryst. 43, 920–925.

Yamada, T., Ishiyama, R. & Yamane, H. (2015). Jpn. J. Appl. Phys. 54, 07J, C04.

Zhang, F. X., Xu, F. F., Mori, T., Liu, Q. L. & Tanaka, T. (2003). J. Solid State Chem. 170, 75–81.
Na$_3$MgB$_{37}$Si$_9$: an icosahedral B$_{12}$ cluster framework containing \{Si$_8$\} units

Haruhiko Morito, Takuji Ikeda, Yukari Katsura and Hisanori Yamane

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$_3$MgB$_{37}$Si$_9$

$M_r = 746.06$

Trigonal, $R\overline{3}m$

$a = 10.1630 (3)$ Å

c = 16.5742 (6) Å

$V = 1482.54 (10)$ Å$^3$

$Z = 3$

$F(000) = 1068$

$D_v = 2.507$ Mg m$^{-3}$

Mo Kα radiation, $\lambda = 0.71073$ Å

Cell parameters from 6032 reflections

$\theta = 3.7$–$41.2^\circ$

$\mu = 0.72$ mm$^{-1}$

$T = 298$ K

Plate, black

0.20 × 0.16 × 0.02 mm

Data collection

Bruker, D8 QUEST
diffractometer

Detector resolution: 10 pixels mm$^{-1}$

$\omega$ scans

Absorption correction: multi-scan

(SADABS; Bruker, 2018)

$T_{\text{min}} = 0.911$, $T_{\text{max}} = 1.000$

8352 measured reflections

562 independent reflections

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

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

$\Delta\rho_{\text{max}} = 0.58$ e Å$^{-3}$

$\Delta\rho_{\text{min}} = -0.53$ e Å$^{-3}$

Extinction correction: SHELXL2014/7

(Sheldrick 2015),

$Fc^2 = kFc[1+0.001xFc^2\lambda^2/\sin(2\theta)]^{-1/4}$

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     | U₁₁   | U₂₂   | U₃₃   | U₁₂   | U₁₃   | U₂₃   | Occ. (<1) |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----------|
| Na1 | 0.500 | 0.000 | 0.000 | 0.0179(5) | | | | | | |
| Mg1 | 0.000 | 0.000 | 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)

|     | U₁₁   | U₂₂   | U₃₃   | U₁₂   | U₁₃   | U₂₃   |
|-----|-------|-------|-------|-------|-------|-------|
| 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, °)

Na1—B2i 2.793(2) B3—Si1iv 1.888(4)
Na1—B2ii 2.793(2) B3—B5xxx 3.343(19)
Na1—B2iii 2.793(2) B3—Na1vxxx 4.123(3)
Na1—B2iv 2.793(2) B3—Na1vxxxii 4.123(3)
Na1—B1v 2.811(2) B3—Na1vxxxii 4.605(3)
Na1—B1vi 2.811(2) B4—B3viii 1.799(5)
Na1—B1vii 2.811(2) B4—B1viii 1.815(3)
Na1—B1 2.811(2) B4—B1iv 1.815(3)
Na1—Si2viii 2.8620(4) B4—B2xv 1.824(4)
Na1—Si2ix 2.8620(4) B4—B2iv 1.824(4)
Na1—Si2i 2.8621(4) B4—Si2 2.082(3)
Na1—Si2ii 2.8621 (4) B4—Mg1iv 2.568 (3)
Na1—B4viii 2.9604 (16) B4—Na1xviii 2.9605 (16)
Na1—B4ix 2.9604 (16) B4—Na1xxiii 2.9605 (16)
Na1—B4i 2.9605 (16) B4—B5xxx 3.319 (3)
Na1—B4iv 2.9605 (16) B4—B5i 4.031 (12)
Na1—Mg1 3.0389 (9) B4—B5xv 4.117 (16)
Na1—Mg1ii 3.0389 (9) B5—Si1 0.503 (18)
Mg1—B2x 2.333 (3) B5—B3viii 1.689 (7)
Mg1—B2xi 2.333 (3) B5—B3xxiii 1.96 (2)
Mg1—B2xii 2.333 (3) B5—B5xxiv 2.47 (4)
Mg1—B2xiii 2.333 (3) B5—B2xxv 2.705 (16)
Mg1—Si3 2.403 (4) B5—B2xxvi 2.705 (16)
Mg1—B4xv 2.568 (3) B5—B2xxvii 2.705 (16)
Mg1—B4xvi 2.568 (3) B5—B2xxviii 2.705 (16)
Mg1—B4xvii 2.568 (3) B5—B2xxix 2.705 (16)
Mg1—Si2xx 2.933 (2) Si1—Si1xxi 1.460 (10)
Mg1—Si2xxi 2.933 (2) Si1—B3viii 1.887 (4)
B1—B3viii 1.791 (3) Si1—B3xxiv 1.887 (4)
B1—B2xiv 1.806 (4) Si1—B5xxvi 1.96 (2)
B1—B2xiv 1.813 (3) Si1—Na1xxv 5.1337 (7)
B1—B4xx 1.815 (3) Si1—Na1xxvii 5.1337 (7)
B1—Si2i 2.043 (2) Si1—Si1xxviii 5.1337 (7)
B1—B5 3.093 (5) Si1—Si1xxviii 5.1337 (7)
B1—Na1xx 3.954 (2) Si1—Na1xxviii 5.1337 (7)
B1—B5i 4.268 (12) Si1—Na1xxviii 5.1337 (7)
B1—B5iv 4.356 (15) Si2—B1i 2.043 (2)
B1—Na1xxii 4.768 (2) Si2—B1xxvii 2.043 (2)
B2—B2xiii 1.761 (5) Si2—B3ii 2.3951 (9)
B2—B2xiii 1.798 (3) Si2—Si3xxiv 2.8621 (4)
B2—B1xvii 1.798 (3) Si2—Na1xxix 2.8621 (4)
B2—B1xxxiii 1.813 (3) Si2—Si1xxiv 2.8621 (4)
B2—B1xv 1.813 (3) Si2—Na1xxv 5.1337 (7)
B2—B3i 1.816 (4) Si2—Mg1xxv 5.1337 (7)
B2—B4ix 1.824 (4) Si2—B5iv 3.5572 (16)
B2—B4iv 1.843 (5) Si2—B5v 4.197 (11)
B2—B5 2.705 (16) Si2—Na1xxvi 4.5605 (8)
B2—Na1xxiv 2.793 (2) Si2—Na1xxvii 5.3470 (8)
B2—Na1xxv 4.143 (2) Si3—Si3iv 2.304 (3)
B2—B5vii 4.537 (5) Si3—Si2xxvii 2.3951 (9)
B2—Na1x 4.617 (2) Si3—Si2xxvi 2.3952 (9)
B3—B5i 1.689 (7) Si3—Si1ii 2.3952 (9)
B3—B1xxiii 1.791 (3) Si3—Na1xxv 3.3466 (8)
B3—B1xxxiii 1.791 (3) Si3—Na1xxiv 3.3467 (8)
B3—B4xxiv 1.799 (5) Si3—Na1xiii 3.3467 (8)
B3—B2i 1.816 (4) Si3—Na1xii 5.1337 (7)
B3—B2xxxix 1.816 (4) Si3—Na1viii 4.8918 (14)
| Bond  | Angle (°) (E78) | Bond  | Angle (°) (E78) |
|-------|----------------|-------|----------------|
| B2—Na1—B2i | 180.00 (5) | B1iv—B3—B2xxix | 60.33 (12) |
| B2—Na1—B2ii | 143.25 (9) | B4xxiii—B3—B2xxix | 109.8 (2) |
| B2—Na1—B2iii | 36.75 (9) | B2i—B3—B2xxix | 60.99 (18) |
| B2—Na1—B2iv | 36.75 (9) | B5i—B3—Si1i | 14.9 (6) |
| B2—Na1—B2v | 143.25 (9) | B1xxviii—B3—Si1i | 123.43 (12) |
| B2—Na1—B2vi | 180.00 (11) | B1iv—B3—Si1i | 123.43 (12) |
| B2—Na1—B1v | 109.34 (7) | B4xxiii—B3—Si1i | 129.2 (2) |
| B2—Na1—B1vi | 70.66 (7) | B2i—B3—Si1i | 113.5 (2) |
| B2—Na1—B1vii | 37.43 (6) | B2xxix—B3—Si1i | 113.5 (2) |
| B2—Na1—B1viii | 142.57 (6) | B5i—B3—B5xxx | 45.3 (8) |
| B2—Na1—B1ix | 37.43 (6) | B1xxviii—B3—B5xxx | 112.55 (16) |
| B2—Na1—B1x | 142.57 (6) | B1iv—B3—B5xxx | 112.55 (16) |
| B2—Na1—B1xi | 109.34 (7) | B4xxiii—B3—B5xxx | 98.8 (3) |
| B2—Na1—B1xii | 70.66 (7) | B2i—B3—B5xxx | 136.96 (19) |
| B2—Na1—B1xiii | 85.53 (9) | B2xxix—B3—B5xxx | 136.96 (19) |
| B2—Na1—B1xiv | 142.57 (6) | Si1i—B3—B5xxx | 30.4 (3) |
| B2—Na1—B1xv | 37.43 (6) | B5i—B3—Na1xxx | 122.5 (5) |
| B2—Na1—B1xvi | 70.66 (7) | B1xxviii—B3—Na1xxx | 99.85 (16) |
| B2—Na1—B1xvii | 109.34 (7) | B1iv—B3—Na1xxx | 33.59 (11) |
| B2—Na1—B1xviii | 94.47 (9) | B4xxiii—B3—Na1xxx | 39.37 (5) |
| B2—Na1—B1xix | 180.00 (6) | B2i—B3—Na1xxx | 133.94 (17) |
| B2—Na1—B1xx | 70.66 (7) | B2xxix—B3—Na1xxx | 93.92 (11) |
| B2—Na1—B1xxi | 109.34 (7) | Si1i—B3—Na1xxx | 111.86 (14) |
| B2—Na1—B1xxii | 142.57 (6) | B5xxx—B3—Na1xxx | 88.28 (16) |
| B2—Na1—B1xxiii | 37.43 (6) | B5i—B3—Na1xxx | 122.5 (5) |
| B2—Na1—B1xxiv | 180.00 (6) | B1xxviii—B3—Na1xxx | 33.59 (11) |
| B2—Na1—B1xxv | 94.47 (9) | B1iv—B3—Na1xxx | 99.85 (16) |
| B2—Na1—B1xxvi | 85.53 (9) | B4xxiii—B3—Na1xxx | 39.37 (5) |
| B2—Na1—B1xxvii | 78.17 (5) | B2i—B3—Na1xxx | 93.92 (11) |
| B2—Na1—Si2iii | 101.83 (5) | B2xxix—B3—Na1xxx | 133.94 (17) |
| B2—Na1—Si2iv | 76.28 (5) | Si1i—B3—Na1xxx | 111.86 (14) |
| B2—Na1—Si2v | 103.72 (5) | B5xxx—B3—Na1xxx | 88.28 (16) |
| B2—Na1—Si2vi | 73.21 (5) | Na1xxx—B3—Na1xxx | 76.09 (7) |
| B2—Na1—Si2vii | 42.21 (5) | B5i—B3—Na1 | 101.0 (6) |
| B2—Na1—Si2viii | 137.79 (5) | B1xxviii—B3—Na1 | 57.83 (11) |
| B1—Na1—Si2vi | 106.79 (5) | B1iv—B3—Na1 | 111.50 (15) |
| B2—Na1—Si2ix | 101.83 (5) | B4xxiii—B3—Na1 | 108.78 (14) |
| B2—Na1—Si2x | 78.17 (5) | B2i—B3—Na1 | 3.02 (8) |
| B2—Na1—Si2yi | 103.72 (5) | B2xxix—B3—Na1 | 63.98 (11) |
| B2—Na1—Si2zi | 76.28 (5) | Si1i—B3—Na1 | 113.12 (15) |
| B1—Na1—Si2xi | 106.79 (5) | B5xxx—B3—Na1 | 135.32 (13) |
| B1—Na1—Si2xii | 137.79 (5) | Na1xxx—B3—Na1 | 134.78 (8) |
| B1—Na1—Si2xiii | 42.21 (5) | Na1xxx—B3—Na1 | 91.40 (4) |
| B1—Na1—Si2xiv | 73.21 (5) | B5i—B3—Na1xxi | 101.0 (6) |
| B1—Na1—Si2xv | 180.00 (3) | B1xxviii—B3—Na1xxi | 111.50 (15) |
| B2—Na1—Si2i | 103.71 (5) | B1iv—B3—Na1xxi | 57.83 (11) |
| B2—Na1—Si2ii | 76.29 (5) | B4xxiii—B3—Na1xxi | 108.78 (14) |
| B2—Na1—Si2iii | 101.83 (5) | B2i—B3—Na1xxxii | 63.98 (11) |
| Bond          | Distance (Å) | Standard Deviation (Å) |
|--------------|--------------|------------------------|
| B2ii—Na1—Si2i | 78.17 (5)    |                        |
| B1—Na1—Si2i  | 137.79 (5)   |                        |
| B1iv—Na1—Si2i| 106.80 (5)   |                        |
| B1—Na1—Si2i  | 73.20 (5)    |                        |
| Si2v—Na1—Si2i| 42.21 (5)    |                        |
| Si2v—Na1—Si2i| 89.06 (3)    |                        |
| Si2iv—Na1—Si2i| 90.94 (3)  |                        |
| B2i—Na1—Si2i | 76.29 (5)    |                        |
| B2iv—Na1—Si2ii| 103.71 (5) |                        |
| B2iv—Na1—Si2ii| 78.17 (5)  |                        |
| B2ii—Na1—Si2ii| 101.83 (5) |                        |
| B1—Na1—Si2ii | 42.21 (5)    |                        |
| B1iii—Na1—Si2ii| 73.20 (5) |                        |
| B1—Na1—Si2ii | 106.80 (5)   |                        |
| B1—Na1—Si2ii | 137.79 (5)   |                        |
| Si2v—Na1—Si2ii| 90.94 (3)  |                        |
| Si2iv—Na1—Si2ii| 89.06 (3) |                        |
| Si2v—Na1—Si2ii| 90.94 (3)  |                        |
| Si2iv—Na1—Si2ii| 90.94 (3) |                        |
| Si2i—Na1—Si2ii| 180.00 (3) |                        |
| B2i—Na1—B4viii| 109.24 (8) |                        |
| B2ii—Na1—B4viii| 70.76 (8) |                        |
| B2iii—Na1—B4viii| 36.82 (8) |                        |
| B2iv—Na1—B4viii| 143.18 (8) |                        |
| B1—Na1—B4viii| 36.55 (7)    |                        |
| B1iii—Na1—B4viii| 72.94 (8) |                        |
| B1—Na1—B4viii| 107.06 (8)   |                        |
| B1—Na1—B4viii| 143.45 (7)   |                        |
| Si2v—Na1—B4viii| 41.86 (6) |                        |
| Si2iv—Na1—B4viii| 138.14 (6) |                        |
| Si2i—Na1—B4viii| 107.63 (6) |                        |
| Si2iv—Na1—B4viii| 72.37 (6) |                        |
| Si2i—Na1—B4viii| 109.24 (8) |                        |
| B2i—Na1—B4viii| 143.18 (8) |                        |
| B2ii—Na1—B4viii| 36.82 (8) |                        |
| B1—Na1—B4viii| 143.45 (7)   |                        |
| B1—Na1—B4viii| 107.06 (8)   |                        |
| B1—Na1—B4viii| 137.79 (5)   |                        |
| B2iv—Na1—B4viii| 109.24 (8) |                        |
| B1—Na1—B4viii| 107.06 (8)   |                        |

**supporting information**

Acta Cryst. (2022). E78, 203-206

sup-5
B1vi—Na1—B4i 143.45 (7) Mg1v—B4—B5xx 176.9 (4)
B1v—Na1—B4i 36.55 (7) Na1xxv—B4—B5xx 112.64 (15)
B1—Na1—B4i 72.94 (8) Na1xxiii—B4—B5xx 112.64 (15)
Si2iii—Na1—B4i 107.63 (6) B3viii—B4—B5i 55.0 (3)
Si2iv—Na1—B4i 72.37 (6) B1xxix—B4—B5i 87.8 (2)
Si2v—Na1—B4i 41.85 (6) B1xxiv—B4—B5i 87.8 (2)
Si2vi—Na1—B4i 138.15 (6) B2xxv—B4—B5i 146.20 (15)
B4vii—Na1—B4i 96.65 (12) B2xxv—B4—B5i 146.20 (15)
B4iv—Na1—B4i 83.35 (12) Si2—B4—B5i 61.8 (3)
B2—Na1—B4iv 36.83 (8) Mg1v—B4—B5i 139.3 (3)
B2ii—Na1—B4iv 143.17 (8) Na1xxiv—B4—B5i 95.59 (14)
B2iii—Na1—B4iv 109.24 (8) Na1xxiii—B4—B5i 95.59 (14)
B2iv—Na1—B4iv 70.76 (8) B5xx—B4—B5i 37.6 (6)
B1v—Na1—B4iv 72.94 (8) B3viii—B4—B5iv 108.0 (2)
B1v—Na1—B4iv 36.55 (7) B1xxiv—B4—B5iv 82.20 (16)
B1—Na1—B4iv 143.45 (7) B1xxv—B4—B5iv 82.20 (16)
Si2v—Na1—B4iv 107.06 (8) B2xxv—B4—B5iv 30.37 (9)
Si2iv—Na1—B4iv 72.37 (6) B2xxv—B4—B5iv 30.37 (9)
Si2v—Na1—B4iv 120.47 (6) Si1—B5—B3 v 105.6 (7)
Si2v—Na1—B4iv 59.53 (4) B3xx—B5—B3v 105.6 (7)
Si2v—Na1—B4iv 120.47 (6) B3xx—B5—B3v 113.0 (6)
B4iv—Na1—B4iv 83.35 (12) B3xx—B5—B3v 113.0 (6)
B4iv—Na1—B4iv 96.65 (12) Si1—B5—Si1xiv 0.0
B4—Na1—B4iv 180.00 (13) B3xx—B5—B3v 113.0 (6)
B2—Na1—Mgiv 46.93 (7) B3xx—B5—B3v 105.6 (7)
B2ii—Na1—Mgiv 133.07 (7) Si1—B5—B3xiv 105.6 (7)
B2iii—Na1—Mgiv 133.07 (7) B3xx—B5—B3v 105.6 (7)
B2iv—Na1—Mgiv 46.93 (7) Si1—B5—B3xiv 113.0 (6)
B1v—Na1—Mgiv 101.34 (6) B3xx—B5—B3v 113.0 (6)
B1v—Na1—Mgiv 78.66 (6) Si1—B5—B3xiv 113.0 (6)
B1—Na1—Mgiv 101.34 (6) B5xiv—B5—B2 138.2 (3)
B1—Na1—Mgiv 78.66 (6) B5xiv—B5—B2 101.35 (6)
B2—Na1—Mgiv 129.34 (6) B5xiv—B5—B2 111.1 (9)
B2ii—Na1—Mgiv 50.66 (6) B5xiv—B5—B2 111.0 (9)
B2iii—Na1—Mgiv 129.34 (6) B3xx—B5—B2 111.0 (9)
B2iv—Na1—Mgiv 50.66 (6) B3xx—B5—B2 111.0 (9)
B2v—Na1—Mgiv 133.07 (7) B3xx—B5—B2 111.0 (9)
B2vi—Na1—Mgiv 46.93 (7) B3xx—B5—B2 111.0 (9)
B2vii—Na1—Mgiv 133.07 (7) B3xx—B5—B2 111.0 (9)
B1v—Na1—Mgiv 78.66 (6) B3xx—B5—B2 111.0 (9)
B1v—Na1—Mgiv 101.34 (6) B3xx—B5—B2 111.0 (9)
B1v—Na1—Mgiv 78.66 (6) B3xx—B5—B2 111.0 (9)
| Bond | 1st Atom | 2nd Atom | 3rd Atom | Bond Angle (°) | Thermal Parameter (Å²) |
|------|----------|----------|----------|---------------|------------------------|
| Si2viii—Na1—Mg1ii | 59.53 (4) | B3i—B5—B2viii | 77.9 (5) |
| Si2—Na1—Mg1ii | 120.47 (4) | Si1xvi—B5—B2viii | 138.2 (3) |
| Si2v—Na1—Mg1ii | 59.53 (4) | B5xxi—B5—B2viii | 138.2 (3) |
| B4vii—Na1—Mg1iv | 120.47 (4) | B2—B5—B2viii | 38.0 (2) |
| B4v—Na1—Mg1ii | 50.66 (6) | Si1—B5—B2xiv | 138.2 (3) |
| B4—Na1—Mg1ii | 129.34 (6) | B3viii—B5—B2xiv | 41.2 (4) |
| B4vii—Na1—Mg1iv | 50.66 (6) | B3xxvi—B5—B2xiv | 77.9 (5) |
| Mg1i—Na1—Mg1iv | 180.00 (13) | B3—B5—B2xiv | 111.1 (9) |
| B2v—Mg1—B2vii | 44.34 (12) | B3viii—B5—B2xi | 111.0 (9) |
| B2v—Mg1—B2vii | 46.53 (12) | B3xxvi—B5—B2xi | 77.9 (5) |
| B2v—Mg1—B2vii | 83.96 (13) | B3—B5—B2xi | 41.2 (4) |
| B2v—Mg1—B2vii | 101.12 (17) | Si1—B5—B2xi | 138.2 (3) |
| B2v—Mg1—B2vii | 83.96 (13) | B3xxvi—B5—B2xi | 41.2 (4) |
| B2v—Mg1—B2vii | 129.34 (6) | Si1—B5—B2xi | 138.2 (3) |
| B2v—Mg1—B2vii | 44.34 (12) | B3xxvi—B5—B2xi | 77.9 (5) |
| B2v—Mg1—B2vii | 46.53 (12) | B3—B5—B2xi | 41.2 (4) |
| B2v—Mg1—B2vii | 83.96 (13) | Si1—B5—B2xi | 138.2 (3) |
| B2v—Mg1—B2vii | 101.12 (17) | B3xxvi—B5—B2xi | 77.9 (5) |
| B2v—Mg1—B2vii | 44.34 (12) | B3xxvi—B5—B2xi | 77.9 (5) |
| B2v—Mg1—B2vii | 46.53 (12) | B3xxvi—B5—B2xi | 77.9 (5) |
| B2v—Mg1—B2vii | 83.96 (13) | B3—B5—B2xi | 41.2 (4) |
| B2v—Mg1—B2vii | 101.12 (17) | Si1—B5—B2xi | 138.2 (3) |
| B2v—Mg1—B2vii | 83.96 (13) | B3xxvi—B5—B2xi | 77.9 (5) |
| B2v—Mg1—B2vii | 129.34 (6) | Si1—B5—B2xi | 138.2 (3) |
| B2v—Mg1—B2vii | 44.34 (12) | B3xxvi—B5—B2xi | 77.9 (5) |
| B2v—Mg1—B2vii | 46.53 (12) | B3xxvi—B5—B2xi | 77.9 (5) |
| B2v—Mg1—B2vii | 83.96 (13) | B3—B5—B2xi | 41.2 (4) |
| B2v—Mg1—B2vii | 101.12 (17) | Si1—B5—B2xi | 138.2 (3) |
| B2v—Mg1—B2vii | 83.96 (13) | B3xxvi—B5—B2xi | 77.9 (5) |
| B2v—Mg1—B2vii | 129.34 (6) | Si1—B5—B2xi | 138.2 (3) |
| B2v—Mg1—B2vii | 44.34 (12) | B3xxvi—B5—B2xi | 77.9 (5) |
| B2v—Mg1—B2vii | 46.53 (12) | B3xxvi—B5—B2xi | 77.9 (5) |
| B2v—Mg1—B2vii | 83.96 (13) | B3—B5—B2xi | 41.2 (4) |
| B2v—Mg1—B2vii | 101.12 (17) | Si1—B5—B2xi | 138.2 (3) |
| B2v—Mg1—B2vii | 83.96 (13) | B3xxvi—B5—B2xi | 77.9 (5) |
| B2v—Mg1—B2vii | 129.34 (6) | Si1—B5—B2xi | 138.2 (3) |
| B2v—Mg1—B2vii | 44.34 (12) | B3xxvi—B5—B2xi | 77.9 (5) |
| B2v—Mg1—B2vii | 46.53 (12) | B3xxvi—B5—B2xi | 77.9 (5) |
| B2v—Mg1—B2vii | 83.96 (13) | B3—B5—B2xi | 41.2 (4) |
| B2v—Mg1—B2vii | 101.12 (17) | Si1—B5—B2xi | 138.2 (3) |
| Bond                  | Angle (°)  |
|-----------------------|------------|
| B3viii—B1—B5         | 26.44 (12) |
| B2vi—B1—B5           | 134.42 (13)|
| B1xx—B1—B5           | 118.8 (4)  |
| B2iv—B1—B5           | 60.4 (4)   |
| Si2—B1—B5            | 85.06 (18) |
| Na1—B1—B5            | 124.6 (4)  |
| B3viii—B1—Na1xx      | 99.62 (14) |
| B2vi—B1—Na1xx        | 99.93 (10) |
| B1xx—B1—Na1xx        | 39.67 (11) |
| B2iv—B1—Na1xx        | 39.15 (8)  |
| B4—B1—Na1xx          | 139.11 (13)|
| Si2—B1—Na1xx         | 93.52 (7)  |
| Na1—B1—Na1xx         | 134.55 (7) |
| B5—B1—Na1xx          | 94.3 (3)   |
| B3viii—B1—B5i        | 102.63 (12)|
| B2vi—B1—B5i          | 23.0 (2)   |
| B1xx—B1—B5i          | 39.4 (2)   |
| B2iv—B1—B5i          | 86.6 (2)   |
| B4—B1—B5i            | 72.9 (2)   |
| Si2—B1—B5i           | 146.89 (9) |
| Na1—B1—B5i           | 92.17 (19) |
| B5—B1—B5i            | 127.32 (17)|
| Na1xx—B1—B5i         | 78.9 (2)   |
| B3viii—B1—B5xi       | 45.13 (19) |
| B2vi—B1—B5xxi        | 127.76 (14)|
| B1xx—B1—B5xxi        | 151.4 (2)  |
| B2iv—B1—B5xxi        | 93.9 (2)   |
| B4—B1—B5xxi          | 67.63 (14) |
| Si2—B1—B5xxi         | 71.88 (9)  |
| Na1—B1—B5xxi         | 91.1 (2)   |
| B5—B1—B5xxi          | 33.5 (6)   |
| Na1xx—B1—B5xxi       | 124.81 (18)|
| B5—B1—B5xxi          | 138.30 (13)|
| B3viii—B1—Na1xxii    | 58.43 (12) |
| B2vi—B1—Na1xxii      | 59.13 (9)  |
| B1xx—B1—Na1xxii      | 105.05 (8) |
| B2iv—B1—Na1xxii      | 105.67 (11)|
| B4—B1—Na1xxii        | 4.27 (10)  |
| Si2—B1—Na1xxii       | 130.00 (8) |
| Na1—B1—Na1xxii       | 79.66 (5)  |
| B5—B1—Na1xxii        | 80.33 (15) |
| Na1xx—B1—Na1xxii     | 134.85 (5) |
| B5—B1—Na1xxii        | 70.00 (18) |
| B5xxi—B1—Na1xxii     | 69.77 (5)  |
| B2viii—B2—B1xxii     | 131.14 (10)|
| B2viii—B2—B1x        | 111.97 (10)|
| B1xxii—B2—B1x        | 60.00 (14) |

**Supporting Information**

*Acta Cryst.* (2022). E78, 203-206

sup-9
| Bond                  | Angle (°) (°) |
|-----------------------|--------------|
| B2xxiii—B2—B3i       | 106.92 (13)  |
| B1xxiv—B2—B3i       | 106.68 (18)  |
| B1—B2—B3           | 59.15 (14)   |
| B2xxiii—B2—B4iv     | 136.84 (12)  |
| B1xxiv—B2—B4iv     | 60.14 (13)   |
| B1—B2—B4          | 108.04 (17)  |
| B3—B2—B4          | 106.97 (16)  |
| B2xxii—B2—B3i       | 120.00 (1)   |
| B1xxiv—B2—B2i      | 107.39 (10)  |
| B1—B2—B2i        | 107.25 (10)  |
| B3—B2—B2i        | 59.51 (9)    |
| B4iv—B2—B2i       | 59.65 (9)    |
| B2xxii—B2—Mg1       | 67.83 (6)    |
| B1xxiv—B2—Mg1     | 127.40 (14)  |
| B1—B2—Mg1        | 171.03 (15)  |
| B3—B2—Mg1        | 112.01 (15)  |
| B4iv—B2—Mg1      | 75.16 (13)   |
| B2xxii—B2—Mg1      | 66.74 (6)    |
| B2xxii—B2—B5       | 71.01 (12)   |
| B1xxiv—B2—B5      | 142.0 (3)    |
| B1—B2—B5        | 83.9 (3)     |
| B3—B2—B5        | 37.8 (2)     |
| B4iv—B2—B5       | 129.70 (16)  |
| B2xxii—B2—B5      | 70.08 (13)   |
| Mg1—B2—B5        | 87.7 (3)     |
| B2xxii—B2—Na1xxiv  | 71.62 (5)    |
| B1xxiv—B2—Na1xxiv | 71.82 (10)   |
| B1—B2—Na1xxiv    | 116.66 (12)  |
| B3—B2—Na1xxiv    | 175.02 (13)  |
| B4iv—B2—Na1xxiv  | 76.58 (10)   |
| B2xxii—B2—Na1xxiv | 125.43 (5)   |
| Mg1—B2—Na1xxiv  | 72.08 (8)    |
| B5—B2—Na1xxiv    | 142.00 (18)  |
| B2xxii—B2—Na1xxv    | 113.62 (3)   |
| B1xxiv—B2—Na1xxv  | 98.99 (11)   |
| B1—B2—Na1xxv     | 131.77 (12)  |
| B3—B2—Na1xxv     | 92.82 (10)   |
| B4iv—B2—Na1xxv   | 39.10 (9)    |
| B2xxii—B2—Na1xxv  | 33.32 (3)    |
| Mg1—B2—Na1xxv    | 46.23 (4)    |
| B5—B2—Na1xxv    | 96.5 (2)     |
| Na1xxiv—B2—Na1xxv | 92.11 (5)    |
| Na1xx—B2—Na1xxv  | 157.80 (15)  |
| B1xxiv—B2—B5xxvi  | 29.13 (9)    |
| B1—B2—B5xxvi    | 69.9 (2)     |
| B3—B2—B5xxvi    | 93.1 (3)     |
| B4iv—B2—B5xxvi  | 38.8 (2)     |
| B2xxii—B2—B5xxvi | 78.28 (3)    |

sup-10

Acta Cryst. (2022). E78, 203-206
| Bond                        | Value 1   | Value 2   | Value 3   |
|-----------------------------|-----------|-----------|-----------|
| Mg1—B2—B5_{xxvi}           | 113.9 (2) | Si2_{xvi}—Si3—Na1_{xlii} | 67.76 (3) |
| B5—B2—B5_{xvi}             | 130.32 (9)| Si2_{xvi}—Si3—Na1_{xlii} | 119.48 (4)|
| Na1_{xxvi}—B2—B5_{xxvi}    | 87.6 (2)  | Si2_{xvi}—Si3—Na1_{xlii} | 119.48 (4)|
| Na1_{xxv}—B2—B5_{xxvi}     | 73.92 (14)| Mg1—Si3—Na1_{xlii} | 143.149 (12)|
| B2_{ii}—B2—Na1_{x}         | 111.07 (3)| Na1_{xvi}—Si3—Na1_{xlii} | 155.61 (4)|
| B1_{ii}—B2—Na1_{x}         | 57.51 (9) | Na1_{xvi}—Si3—Na1_{xlii} | 97.015 (14)|
| B1—B2—Na1_{x}              | 3.84 (8)  | Na1_{xiv}—Si3—Na1_{xlii} | 97.015 (14)|
| B3—B2—Na1_{x}              | 62.97 (11)| Si3_{xli}—Si3—Na1_{xlii} | 36.852 (12)|
| B4_{xvi}—B2—Na1_{x}        | 107.75 (13)| Si2_{xv}—Si3—Na1_{xlii} | 119.48 (4)|
| B2_{ii}—B2—Na1_{x}         | 110.53 (3)| Si2_{xv}—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_{xxv}—B2—Na1_{x}       | 118.32 (6)| Na1_{xvi}—Si3—Na1_{xlii} | 97.015 (14)|
| Na1_{xxv}—B2—Na1_{x}       | 133.76 (6)| Na1_{xvi}—Si3—Na1_{xlii} | 155.61 (4)|
| B5_{xvi}—B2—Na1_{x}        | 69.2 (2)  | Na1_{xvi}—Si3—Na1_{xlii} | 97.016 (14)|
| B5_{x}—B3—B1_{xvii}        | 125.38 (12)| Na1_{xx}—Si3—Na1_{xlii} | 62.58 (2)|
| B5—B3—B1_{xv}              | 125.38 (12)| Si3_{xli}—Si3—Na1_{xlii} | 36.852 (12)|
| B1_{xvii}—B3—B1_{xv}       | 109.1 (2) | Si2_{xvi}—Si3—Na1_{xlii} | 119.48 (4)|
| B5—B3—B4_{xvii}            | 144.1 (7) | Si2_{xvi}—Si3—Na1_{xlii} | 67.76 (3)|
| B1_{xvii}—B3—B4_{xvii}     | 60.74 (14)| Si2_{xv}—Si3—Na1_{xlii} | 119.48 (4)|
| B1_{x}—B3—B4_{xvii}        | 60.74 (14)| Mg1—Si3—Na1_{xlii} | 143.148 (12)|
| B5_{x}—B3—B2_{x}           | 101.0 (6) | Na1_{xvi}—Si3—Na1_{xlii} | 97.015 (14)|
| B1_{xvii}—B3—B2_{x}        | 60.33 (12)| Na1_{xvi}—Si3—Na1_{xlii} | 97.016 (14)|
| B1_{x}—B3—B2_{x}           | 109.4 (2) | Na1_{xvi}—Si3—Na1_{xlii} | 155.61 (4)|
| B4_{xvii}—B3—B2_{x}        | 109.8 (2) | Na1_{xvi}—Si3—Na1_{xlii} | 62.58 (2)|
| B5_{x}—B3—B2_{xxi}         | 101.0 (6) | Na1_{xvi}—Si3—Na1_{xlii} | 62.58 (2)|
| B1_{xvii}—B3—B2_{xxi}      | 109.4 (2) | Mg1—Si3—Na1_{xlii} | 143.148 (12)|

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, y, z; (xiii) −x+y, y, z; (xiv) −x+y, −z, z; (xv) x−y+1/3, −x+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, −x+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) y−1/3, −x+y+1/3, −z+1/3; (xxvii) y+2/3, −x+y+1/3, −z+1/3; (xxviii) y+4/3, −x+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; (xxxx) −y+2/3, x+1/3, −z+1/3; (xxxxi) −y+1, x−y, z; (xxxxii) −y+1, x−y, z; (xxxxiii) −y+2/3, x+1/3, z+1/3; (xxxxiv) −y+2/3, y+1/3, z+1/3; (xli) −x, −y, −z+1; (xlii) −x+y+1/3, −x+2/3, z+2/3; (xliii) −y+1/3, x−y−1/3, z+2/3; (xliii) x−2/3, y−1/3, z+2/3.