Crystal structures of the alkali aluminoboracites $A_4B_4Al_3O_{12}Cl$ (A = Li, Na)

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Single crystals of alkali aluminoboracites, $A_4B_4Al_3O_{12}Cl$ (A = Li, Na), were grown using the self-flux method, and their isotypic cubic crystal structures were determined by single-crystal X-ray diffraction. $Na_4B_4Al_3O_{12}Cl$ is the first reported sodium boracite, and its lattice parameter [13.5904 (1) Å] is the largest among the boracites consisting of a cation–oxygen framework reported so far. For both crystals, structure models refined in the cubic space group $F\bar{4}3c$, which assume that all cubic octant subcells in the unit cell are equivalent, converged with $R1$ factors of $\sim$0.03. However, the presence of weak hhl reflections with odd h and l values indicates that refinements in the space group $F23$, which presume a checkerboard-like ordering of two types of subcells with slightly different atomic positions, are more appropriate.

1. Chemical context

Boracite is originally known as a mineral with the formula $Mg_3B_7O_{13}Cl$. The name boracite also refers to borate compounds with the general formula $M_3B_7O_{13}X$, consisting of a negatively charged B–O framework, extraframework divalent cations M, such as Mg^{2+}, Cr^{2+}, Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+} and Cd^{2+}, and extraframework anions X, such as Cl^-, Br^-, I^- and S^{2-} (Schmid, 1965; Nelmes, 1974). The extraframework cations can also be an alkali ion, but only lithium variants $Li_{4-x}B_7O_{12+x/2}X$, $Li_4B_{7-3x}Al_{3x}O_{12}X$ and $Li_4B_{7-3x}Ga_{3x}O_{12}Cl$ (X = Cl, Br; x = 0–1) have been reported to date (Levasseur et al., 1971; Réau et al., 1976; Jeitschko et al., 1977; Calès et al., 1977; Sorokin, 2015; Tezuka et al., 2017; Kajihara et al., 2017; Katsumata et al., 2022). The latter two compounds (Kajihara et al., 2017; Katsumata et al., 2022) are the first examples of boracites containing framework cations other than B^{3+} ions. The lithium boracites are lithium-ion conducting, and their dc Li^+ ion conductivity can be increased to $\sim$10^{-5} S cm^{-1} at room temperature in glass-ceramics consisting mainly of $Li_4B_4M_3O_{12}Cl$ (M = Al, Ga; Kajihara et al., 2017). In addition, $Li_4B_4Al_3O_{12}Cl$ is stable in contact with Li metal and is water-resistant; solid-state cells consisting of an $Li_4B_4Al_3O_{12}Cl$-based glass-ceramic solid electrolyte, an $LiCoO_2$-based composite cathode containing an ionic liquid and an Li–Au alloy anode worked successfully (Saito et al., 2021). More recently, a thioboracite, $Li_6B_7S_{13}I$, a sulfide variant of lithium boracite with room-temperature Li^+ ion conductivity of $\sim$5 × 10^{-4} S cm^{-1} has been reported (Kaup et al., 2021). However, single crystals of $Li_4B_4Al_3O_{12}Cl$ have not yet been grown, and the preliminary crystal structure analysis of $Li_4B_4Al_3O_{12}Cl$ (Kajihara et al., 2017; Katsumata et al., 2022) was incomplete. In addition, boracites containing alkali ions other than Li^+ have not been reported. Furthermore, a rhombohedral distortion of the unit cell of single-crystalline

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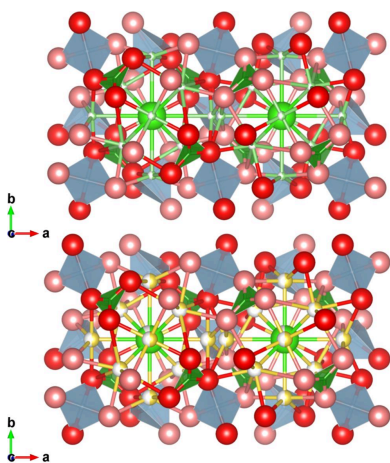
Table 1
Summary of the observed *hhl* reflections in $Li_4B_4Al_3O_{12}Cl$ and $Na_4B_4Al_3O_{12}Cl$.

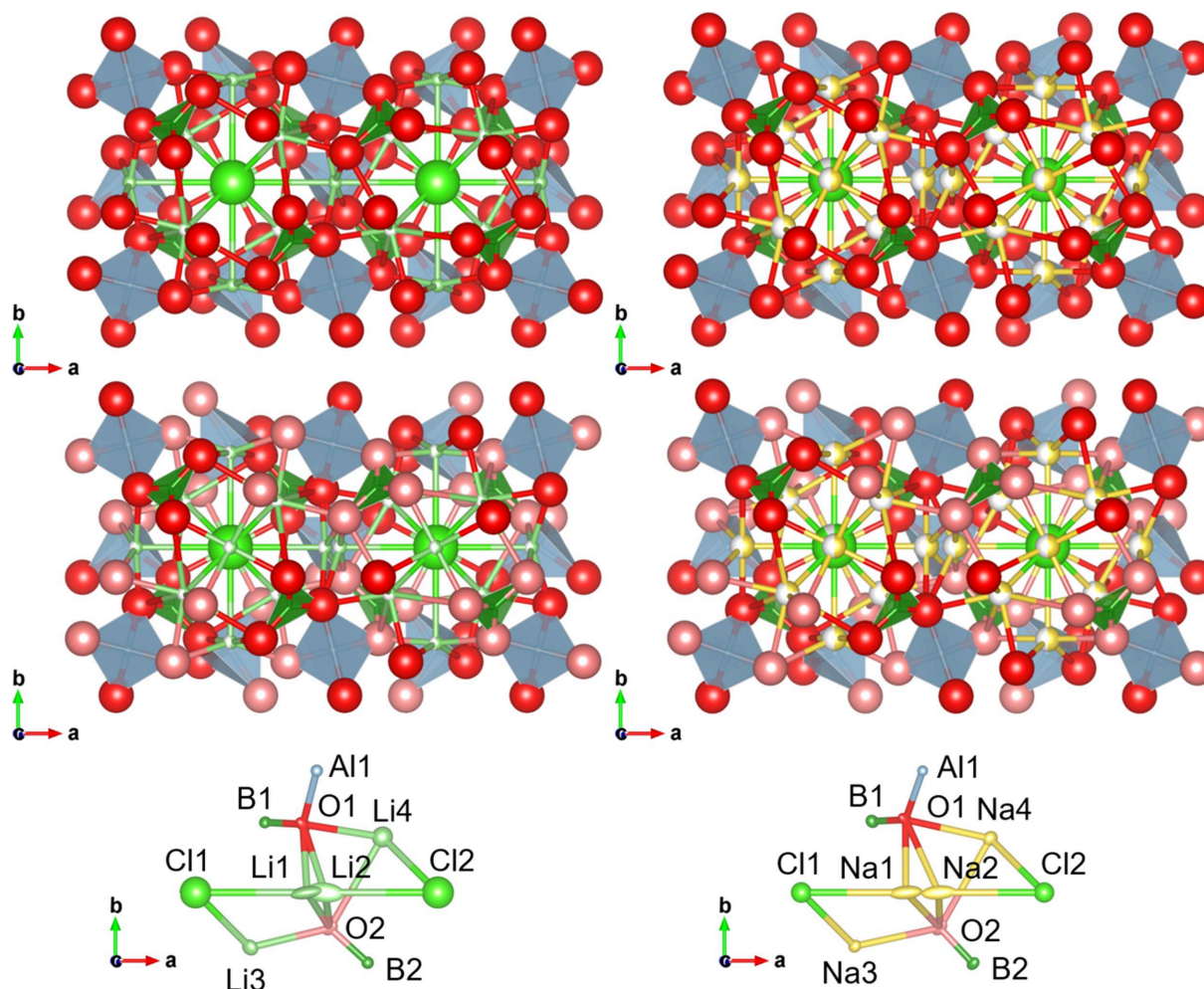|	$Li_4B_4Al_3O_{12}Cl$		$Na_4B_4Al_3O_{12}Cl$	
	$<I/\sigma(I)>$	Number of reflections	$<I/\sigma(I)>$	Number of reflections
No conditions	14.35	325	12.14	340
h even	30.24	153	24.96	165
h odd	0.21	172	0.04	175
l even	30.24	153	24.96	165
l odd	0.21	172	0.04	175
h + *l* even	14.35	325	12.14	340
h + *l* odd	0.00	0	0.00	0

$Li_4B_7O_{12}Cl$ was experimentally observed at room temperature (Jeitschko *et al.*, 1977) and was recently theoretically confirmed (Li & Holzwarth, 2022), raising the question whether similar unit-cell distortions occur in other alkali boracites.

In the present study, we report the growth of single crystals of $A_4B_4Al_3O_{12}Cl$ (*A* = Li, Na) using the self-flux method and

their structural characterization by single-crystal X-ray diffraction (XRD).

2. Structural commentary

The crystallites of $Li_4B_4Al_3O_{12}Cl$ exhibit complete extinction under cross-polarized light, supporting cubic symmetry. Hence, the unit cell of $Li_4B_4Al_3O_{12}Cl$ is not distorted. At first,

Figure 1
Schematic illustrations of two neighbouring cubic octant subcells in the unit cell of $Li_4B_4Al_3O_{12}Cl$ in the space groups $F\bar{4}3c$ (top left) and $F23$ (middle left), those of $Na_4B_4Al_3O_{12}Cl$ in the space groups $F\bar{4}3c$ (top right) and $F23$ (middle right), and asymmetric units with displacement ellipsoids at the 50% probability level of $Li_4B_4Al_3O_{12}Cl$ (bottom left) and $Na_4B_4Al_3O_{12}Cl$ (bottom right) in the space group $F23$. Red, large green, small green and yellow spheres denote O, Cl, Li and Na atoms, respectively. Green triangles and gray tetrahedra denote BO_3 and AlO_4 units, respectively. The forefront Al atoms located at *z* = 0.5 are not shown for clarity. In the middle and bottom figures, red and pale-red spheres denote O1 and O2 atoms, respectively.

Table 2
Selected bond lengths and angles (Å, °) in $A_4B_4Al_3O_{12}Cl$ crystal structures.

	Space group $F\bar{4}3c$			Space group $F23$	
	A = Li	A = Na		A = Li	A = Na
$A1{-}O1$	2.0828 (17)	2.2588 (16)	$A1{-}O1$	2.053 (3)	2.2585 (18)
$A1{-}O1^{i}$	2.0828 (17)	2.446 (2)	$A1{-}O2^{ii}$	2.143 (16)	2.452 (3)
			$A2{-}O2^{iii}$	2.056 (4)	2.2602 (18)
			$A2{-}O1^{iv}$	2.132 (16)	2.442 (3)
$A1{-}Cl1$	3.2460 (1)	2.936 (4)	$A1{-}Cl1$	2.98 (6)	2.925 (6)
			$A2{-}Cl2$	3.03 (6)	2.948 (6)
$A2{-}O1^{v}$	2.22 (3)	2.484 (5)	$A3{-}O2^{vi}$	2.23 (3)	2.488 (6)
$A2{-}O1^{vii}$	2.828 (8)	2.913 (2)	$A3{-}O1^{vii}$	2.824 (8)	2.912 (2)
			$A4{-}O1^{viii}$	2.23 (3)	2.480 (6)
			$A4{-}O2^{ix}$	2.826 (8)	2.914 (2)
$A2{-}Cl1$	2.57 (5)	2.605 (9)	$A3{-}Cl1$	2.55 (6)	2.599 (10)
			$A4{-}Cl2$	2.55 (5)	2.612 (10)
$B1{-}O1$	1.3700 (16)	1.3693 (15)	$B1{-}O1$	1.3693 (17)	1.3684 (16)
			$B2{-}O2^{x}$	1.3702 (17)	1.3684 (16)
$Al1{-}O1^{xi}$	1.7533 (17)	1.7506 (16)	$Al1{-}O1^{xi}$	1.754 (2)	1.7495 (18)
			$Al1{-}O2^{xii}$	1.754 (2)	1.7522 (18)
$B1{-}O1{-}Al1^{xiii}$	118.97 (12)	128.59 (12)	$B1{-}O1{-}Al1^{xiii}$	119.05 (13)	128.62 (14)
			$B2^{xiv}{-}O2{-}Al1^{vii}$	118.94 (13)	128.66 (14)

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

the crystal structure was refined in the noncentrosymmetric cubic space group $F\bar{4}3c$ following the model from the Rietveld refinement of powder X-ray diffraction data (Kajihara *et al.*, 2017; Katsumata *et al.*, 2022). The occupancy (g) of Cl1 converged to the upper bound [$g(Cl1) = 1$] and was fixed at this value. The reliability factor $R1$ converged to 0.031, and the refinement results agreed well with those derived from the powder samples (Kajihara *et al.*, 2017; Katsumata *et al.*, 2022). The unit cell of $Li_4B_4Al_3O_{12}Cl$ can be divided into eight equivalent cubic subcells, each containing one Cl1 at the cube centre. The Cl1 site is surrounded by six sites with multiplicity 24 (Wyckoff letter c) and four sites with multiplicity 32 (Wyckoff letter e) containing four Li atoms in total, and the resulting $ClLi_4$ moiety is embedded in a negatively charged framework consisting of alternating corner-shared bridges of planar BO_3 triangles and AlO_4 tetrahedra. The occupancy of Li1 is close to 1, whereas that of Li2 is $\sim\frac{1}{4}$. The lattice parameter of $Li_4B_4Al_3O_{12}Cl$ [$a = 12.9839$ (1) Å] is similar to that of the polycrystalline sample obtained by solid-state synthesis [$a = 12.9687$ (1) Å; Katsumata *et al.*, 2022] but larger than that crystallized from glass-ceramics [$a = 12.9149$ (5) Å; Kajihara *et al.*, 2017], probably because of an incomplete uptake of Al in crystals obtained from glass-ceramics.

Similar to $Li_4B_4Al_3O_{12}Cl$, the crystallites of $Na_4B_4Al_3O_{12}Cl$ exhibit complete cross-polarized extinction. Refinement in the space group $F\bar{4}3c$ resulted in a reliability factor $R1$ of 0.022, and the results indicate that $Na_4B_4Al_3O_{12}Cl$ is isostructural with $Li_4B_4Al_3O_{12}Cl$, except that Na1 is located at the 48 g site and displaced from the 24 c site at the midpoint between neighbouring Cl1 atoms. The lattice parameter of $Na_4B_4Al_3O_{12}Cl$ [$a = 13.5904$ (1) Å] is the largest among known cubic boracites, apart from the sulfide variant $Li_6B_7S_{13}I$ [$a = 15.245$ (2) Å; Kaup *et al.*, 2021]. The occupancy of Cl1 is less than 1 ($\sim$0.92), possibly because of its higher growth temperature compared to that of $Li_4B_4Al_3O_{12}Cl$. The equivalent

isotropic displacement parameters (U_{eq}) of extraframework species [Cl1, 0.0350 (9) Å^2; Na1, 0.0422 (14) Å^2; Na2, 0.017 (2) Å^2] of $Na_4B_4Al_3O_{12}Cl$ are notably smaller than those of $Li_4B_4Al_3O_{12}Cl$ [Cl1, 0.0787 (15) Å^2; Li1, 0.066 (6) Å^2; Li2, 0.028 (11) Å^2], despite that the species in the framework (B1, Al1 and O1) are similar or even larger in $Na_4B_4Al_3O_{12}Cl$. These observations suggest that replacing Li with Na increases the packing density at the extraframework sites and suppresses the thermal motion of the atoms located therein.

The convergence of the structure refinements of $Li_4B_4Al_3O_{12}Cl$ and $Na_4B_4Al_3O_{12}Cl$ in the space group $F\bar{4}3c$ was satisfactory ($R1 \simeq 0.03$). However, these crystals both exhibit weak hhl reflections with odd h and l, which violate the extinction conditions in space group $F\bar{4}3c$, as listed in Table 1. The noncentrosymmetric cubic space groups compatible with the observed reflection condition (hhl: $h + l = 2n$) are $F23$, $F432$ and $F\bar{4}3m$. Among them, only the structure analyses in the space group $F23$ were successful. The conversion of the space group from $F\bar{4}3c$ to $F23$ is accompanied by the splitting of atoms except for Al1. This conversion also splits Li1 at the 24 c site of $F\bar{4}3c$ into Li1 and Li2 at the 24 g site of $F23$. The occupancies of $A1$ and $A2$ (A = Li, Na) converged to the upper bound [$g(A1) = g(A2) = 0.5$] both in $Li_4B_4Al_3O_{12}Cl$ and $Na_4B_4Al_3O_{12}Cl$, and were fixed at this value. The slightly larger $R1$ factors in $F23$ compared to $F\bar{4}3c$ are due to an increased number of measured reflections partially with low intensities.

Fig. 1 summarizes the schematic illustrations of two adjacent cubic octant subcells of the unit cells of $Li_4B_4Al_3O_{12}Cl$ and $Na_4B_4Al_3O_{12}Cl$, along with their asymmetric units derived from the analyses in the space group $F23$. In the space group $F\bar{4}3c$, the eight subcells in a unit cell are equivalent. In contrast, in the space group $F23$, they are classified into two types of subcells stacked alternately in three dimensions. Nevertheless, the atomic displacements associated with the

Table 3
Experimental details.

	Li$_4$B$_4$Al$_3$O$_{12}$Cl in $F\bar{4}3c$	Li$_4$B$_4$Al$_3$O$_{12}$Cl in $F23$	Na$_{3.92}$B$_4$Al$_3$O$_{12}$Cl$_{0.92}$ in $F\bar{4}3c$	Na$_{3.92}$B$_4$Al$_3$O$_{12}$Cl$_{0.92}$ in $F23$
Crystal data				
Chemical formula	Li$_4$B$_4$Al$_3$O$_{12}$Cl	Li$_4$B$_4$Al$_3$O$_{12}$Cl	Na$_{3.92}$B$_4$Al$_3$O$_{12}$Cl$_{0.92}$	Na$_{3.92}$B$_4$Al$_3$O$_{12}$Cl$_{0.92}$
M_r	379.39	379.39	438.91	438.91
Crystal system, space group	Cubic, $F\bar{4}3c$	Cubic, $F23$	Cubic, $F\bar{4}3c$	Cubic, $F23$
Temperature (K)	297	297	294	294
a (Å)	12.9839 (1)	12.9839 (1)	13.5904 (1)	13.5904 (1)
V (Å^3)	2188.85 (5)	2188.85 (5)	2510.13 (6)	2510.13 (6)
Z	8	8	8	8
Radiation type	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	6.12	6.12	6.78	6.78
Crystal size (mm)	0.11 × 0.10 × 0.06	0.11 × 0.10 × 0.06	0.08 × 0.06 × 0.04	0.08 × 0.06 × 0.04
Data collection				
Diffractometer	Bruker D8 goniometer	Bruker D8 goniometer	Bruker D8 goniometer	Bruker D8 goniometer
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.62, 0.75	0.62, 0.75	0.66, 0.75	0.66, 0.75
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	3843, 193, 191	4728, 389, 317	4504, 218, 216	5514, 437, 355
R_{int}	0.023	0.024	0.027	0.028
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.621	0.621	0.624	0.624
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.031, 0.075, 1.16	0.032, 0.081, 1.17	0.022, 0.055, 1.20	0.024, 0.066, 1.12
No. of reflections	193	389	218	437
No. of parameters	23	50	27	52
No. of restraints	1	1	1	1
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.63	0.20, −0.91	0.15, −0.45	0.17, −0.58
Absolute structure	Flack x determined using 80 quotients [$(I^+) - (I^-)$]/[$(I^+) + (I^-)$] (Parsons *et al.*, 2013)	Flack x determined using 132 quotients [$(I^+) - (I^-)$]/[$(I^+) + (I^-)$] (Parsons *et al.*, 2013).	Flack x determined using 89 quotients [$(I^+) - (I^-)$]/[$(I^+) + (I^-)$] (Parsons *et al.*, 2013)	Flack x determined using 142 quotients [$(I^+) - (I^-)$]/[$(I^+) + (I^-)$] (Parsons *et al.*, 2013).
Absolute structure parameter	−0.03 (3)	−0.03 (2)	0.01 (3)	0.01 (2)

Computer programs: *BIS* (Bruker, 2021), *SAINT* (Bruker, 2019), *SHELXTL* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *ShelXle* (Hübschle *et al.*, 2011), *VESTA* (Momma & Izumi, 2011) and *publCIF* (Westrip, 2010).

conversion of the space group from $F\bar{4}3c$ to $F23$ are small, and the structures solved in these two space groups are very similar, apart from the splitting of Li1 in space group $F\bar{4}3c$ into Li1 and Li2 in space group $F23$. Such subcell ordering is also observed in the lithium-rich boracite Li$_5$B$_7$O$_{12.5}$Cl (space group $F23$) (Vlasse *et al.*, 1981; Tezuka *et al.*, 2017; Li & Holzwarth, 2022); in Li$_5$B$_7$O$_{12.5}$Cl, the chemical compositions of adjacent subcells differ notably as a result of the incorporation of excess Li and O and the resulting partial conversion of BO$_3$ triangles to BO$_4$ tetrahedra, as well as the ordering of Li. In contrast, in the title compounds Li$_4$B$_4$Al$_3$O$_{12}$Cl and Na$_4$B$_4$Al$_3$O$_{12}$Cl, such a distinct structural ordering associated with a compositional change is not observed, as the conversion of BO$_3$ triangles to BO$_4$ tetrahedra is unlikely even under alkali-rich conditions.

Table 2 lists selected atomic distances and angles. The B—O and Al—O distances are similar between Li$_4$B$_4$Al$_3$O$_{12}$Cl and Na$_4$B$_4$Al$_3$O$_{12}$Cl. In contrast, the B—O—Al angles in Na$_4$B$_4$Al$_3$O$_{12}$Cl are larger than those in Li$_4$B$_4$Al$_3$O$_{12}$Cl by ∼10°. This widening in the B—O—Al angles is responsible for the expansion of the unit cell in Na$_4$B$_4$Al$_3$O$_{12}$Cl. The increase in A—O (A = Li, Na) distances from Li$_4$B$_4$Al$_3$O$_{12}$Cl and Na$_4$B$_4$Al$_3$O$_{12}$Cl amounts to ∼0.2–0.3 Å, and is consistent with the difference in the ionic radii between Li and Na with the same coordination numbers (1.13–0.73 Å = 0.40 Å for fourfold

corrdination and 1.16–0.90 Å = 0.26 Å for sixfold coordination; Shannon, 1976). In contrast, the increase in A—Cl distances is notably smaller (∼0.05 Å) or even negative, indicating an increase in the packing density of extraframework A and Cl. This observation is consistent with the smaller atomic displacement parameters of extraframework A and Cl in Na$_4$B$_4$Al$_3$O$_{12}$Cl compared to Li$_4$B$_4$Al$_3$O$_{12}$Cl (see above).

3. Synthesis and crystallization

Li$_2$CO$_3$ (Fujifilm Wako Chemicals, 99%), Na$_2$CO$_3$ (Fujifilm Wako Chemicals, 99%), B$_2$O$_3$ (Kojundo Chemical Laboratory, 99.9%), γ-Al$_2$O$_3$ (Kojundo Chemical Laboratory, 99.99%), LiCl (Kanto Chemical, 99.9%) and NaCl (Kojundo Chemical Laboratory, 99.9%) were mixed in an A_2CO$_3$:B$_2$O$_3$:γ-Al$_2$O$_3$: ACl (A = Li, Na) molar ratio of 3:4:3:14, with a B$_2$O$_3$ content of 10 mmol. LiCl (melting point: 878 K) and NaCl (melting point: 1074 K), acting as self-fluxes, were added in excess. The mixture of sample 1 (A = Li) or 2 (A = Na) was placed in a platinum crucible covered by an alumina crucible, heated to 1073 K for 3 h (sample 1) or 1123 K for 4 h (sample 2), maintained for 5 h, cooled at a rate of 3 K h^{-1} for 50 h, and then cooled to room temperature in the furnace by turning off the power.

The resulting mixtures were washed with water to leach out water-soluble components. The residues were characterized by powder X-ray diffraction (SmartLab diffractometer, Rigaku) using Cu $K\alpha$ radiation. The main impurity phases in the residues of samples 1 and 2 were Li_2BAlO_4 (space group $P2_1/c$) and $LiAl_5O_8$ (space group $P4_132$), and $Na_2Al_2B_4O_7$ (space group $P\overline{3}1c$), respectively. Single-crystal particles with cubic symmetry were selected using an optical microscope (BH2, Olympus), showing complete light extinction under crossed polarizers.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The crystal structures of $Li_4B_4Al_3O_{12}Cl$ and $Na_4B_4Al_3O_{12}Cl$ were solved both in the space groups $F\overline{4}3c$ and $F23$ using the same hkl file. In the refinements in the space group $F23$, all reflections were used. In the refinements in the space group $F\overline{4}3c$, reflections that violate the extinction conditions (885 in $Li_4B_4Al_3O_{12}Cl$ and 1010 in $Na_4B_4Al_3O_{12}Cl$) were rejected by *SHELXL* (Sheldrick, 2015b), but few rejected reflections had intensities with $I/\sigma(I) > 3$ (3 in $Li_4B_4Al_3O_{12}Cl$ and 4 in $Na_4B_4Al_3O_{12}Cl$). To maintain charge neutrality, the occupancies, g, of A (A = Li, Na) and Cl were refined under the restraint that the total number of A in the unit cell was larger by 24 than that of Cl [*e.g.* $24g(\mathrm{Li}1) + 32g(\mathrm{Li}2) - 8g(\mathrm{Cl}1) = 24$ for $Li_4B_4Al_3O_{12}Cl$ solved in $F\overline{4}3c$], while permitting possible Cl deficiency. The summary of reflections was derived by the program *Space-Group* in *WinGX* (Farrugia, 2012).

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supporting information

Crystal structures of the alkali aluminoboracites $A_4B_4Al_3O_{12}Cl$ (A = Li, Na)

Sho Yoshino, Hidechika Arima, Masanao Ishijima and Koichi Kajihara

Computing details

Lithium aluminoboracite (kjh0818yoshinoL14_0m_a)

Crystal data

$Li_4B_4Al_3O_{12}Cl$	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$M_r = 379.39$	Cell parameters from 2808 reflections
Cubic, $F\bar{4}3c$	$\theta = 6.8–73.2°$
$a = 12.9839$ (1) Å	$\mu = 6.12$ mm^{-1}
$V = 2188.85$ (5) Å^3	$T = 297$ K
$Z = 8$	Plate, colorless
$F(000) = 1472$	$0.11 \times 0.10 \times 0.06$ mm
$D_x = 2.303$ Mg m^{-3}	

Data collection

Bruker D8 goniometer diffractometer	3843 measured reflections
Radiation source: sealed tube	193 independent reflections
Detector resolution: 7.3910 pixels mm^{-1}	191 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.023$
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)	$\theta_{max} = 73.2°$, $\theta_{min} = 6.8°$
	$h = -15 \rightarrow 12$
	$k = -15 \rightarrow 16$
$T_{min} = 0.62$, $T_{max} = 0.75$	$l = -16 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0536P)^2 + 3.2978P]$ where $P = (F_o^2 + 2F_c^2)/3$
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.031$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.075$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
$S = 1.16$	$\Delta\rho_{min} = -0.63$ e Å^{-3}
193 reflections	Absolute structure: Flack x determined using 80 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
23 parameters	
1 restraint	Absolute structure parameter: −0.03 (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.

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

	x	*y*	*z*	$U_{iso}*/U_{eq}$	Occ. (<1)
Li1	0.000000	0.250000	0.250000	0.066 (6)	0.991 (13)
Li2	0.364 (2)	0.364 (2)	0.364 (2)	0.028 (11)	0.256 (10)
B1	0.1057 (3)	0.1057 (3)	0.1057 (3)	0.0114 (10)	
Al1	0.250000	0.000000	0.000000	0.0118 (6)	
O1	0.02786 (13)	0.11000 (13)	0.17680 (15)	0.0166 (6)	
Cl1	0.250000	0.250000	0.250000	0.0787 (15)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Li1	0.156 (18)	0.021 (4)	0.021 (4)	0.000	0.000	0.000
Li2	0.028 (11)	0.028 (11)	0.028 (11)	0.000 (9)	0.000 (9)	0.000 (9)
B1	0.0114 (10)	0.0114 (10)	0.0114 (10)	−0.0014 (14)	−0.0014 (14)	−0.0014 (14)
Al1	0.0115 (8)	0.0120 (6)	0.0120 (6)	0.000	0.000	0.000
O1	0.0185 (11)	0.0154 (10)	0.0158 (9)	0.0048 (7)	0.0067 (10)	0.0044 (9)
Cl1	0.0787 (15)	0.0787 (15)	0.0787 (15)	0.000	0.000	0.000

Geometric parameters (Å, º)

Li1—O1	2.0828 (17)	Li2—O1[xiii]	2.22 (3)
Li1—O1[i]	2.0828 (17)	Li2—Cl1	2.57 (5)
Li1—O1[ii]	2.0828 (17)	Li2—O1[ix]	2.828 (8)
Li1—O1[iii]	2.0828 (17)	Li2—O1[xiv]	2.828 (8)
Li1—Li2[iv]	2.740 (13)	Li2—O1[vi]	2.828 (8)
Li1—Li2[v]	2.740 (13)	Li2—Al1[xv]	2.90 (2)
Li1—Li2[vi]	2.740 (13)	Li2—Al1[xvi]	2.90 (2)
Li1—Li2[vii]	2.740 (13)	B1—O1[x]	1.3700 (16)
Li1—Cl1	3.2460 (1)	B1—O1[xvii]	1.3700 (16)
Li1—Al1[viii]	3.2460 (1)	B1—O1	1.3700 (16)
Li1—Al1[ix]	3.2460 (1)	Al1—O1[xviii]	1.7533 (17)
Li1—Al1[x]	3.2460 (1)	Al1—O1[xix]	1.7533 (17)
Li2—O1[xi]	2.22 (3)	Al1—O1[xvii]	1.7533 (17)
Li2—O1[xii]	2.22 (3)	Al1—O1[xx]	1.7533 (17)
O1—Li1—O1[i]	160.00 (10)	O1[ix]—Li2—O1[vi]	118.0 (5)
O1—Li1—O1[ii]	91.729 (17)	O1[xiv]—Li2—O1[vi]	118.0 (5)
O1[i]—Li1—O1[ii]	91.729 (17)	O1[xi]—Li2—Al1[xv]	69.0 (7)
O1—Li1—O1[iii]	91.729 (17)	O1[xii]—Li2—Al1[xv]	37.1 (3)
O1[i]—Li1—O1[iii]	91.729 (17)	O1[xiii]—Li2—Al1[xv]	123 (2)
O1[ii]—Li1—O1[iii]	160.00 (10)	Cl1—Li2—Al1[xv]	114.0 (9)
O1—Li1—Li2[iv]	52.6 (10)	Li1[xiv]—Li2—Al1[xv]	171 (2)
O1[i]—Li1—Li2[iv]	146.2 (9)	Li1[ix]—Li2—Al1[xv]	70.20 (14)
O1[ii]—Li1—Li2[iv]	70.29 (8)	Li1[vi]—Li2—Al1[xv]	70.20 (14)
O1[iii]—Li1—Li2[iv]	96.5 (4)	O1[ix]—Li2—Al1[xv]	106.4 (4)
O1—Li1—Li2[v]	96.5 (4)	O1[xiv]—Li2—Al1[xv]	134.8 (7)

O1^{i}—Li1—Li2^{v}	70.29 (8)	O1^{vi}—Li2—Al1^{xv}	35.62 (12)
O1^{ii}—Li1—Li2^{v}	52.6 (10)	O1^{xi}—Li2—Al1^{xvi}	123 (2)
O1^{iii}—Li1—Li2^{v}	146.2 (9)	O1^{xii}—Li2—Al1^{xvi}	69.0 (7)
Li2^{iv}—Li1—Li2^{v}	114.4 (12)	O1^{xiii}—Li2—Al1^{xvi}	37.1 (3)
O1—Li1—Li2^{vi}	70.29 (8)	Cl1—Li2—Al1^{xvi}	114.0 (9)
O1^{i}—Li1—Li2^{vi}	96.5 (4)	Li1^{xiv}—Li2—Al1^{xvi}	70.20 (14)
O1^{ii}—Li1—Li2^{vi}	146.2 (9)	Li1^{ix}—Li2—Al1^{xvi}	70.20 (14)
O1^{iii}—Li1—Li2^{vi}	52.6 (10)	Li1^{vi}—Li2—Al1^{xvi}	171 (2)
Li2^{iv}—Li1—Li2^{vi}	114.4 (12)	O1^{ix}—Li2—Al1^{xvi}	35.62 (12)
Li2^{v}—Li1—Li2^{vi}	100 (2)	O1^{xiv}—Li2—Al1^{xvi}	106.4 (4)
O1—Li1—Li2^{vii}	146.2 (9)	O1^{vi}—Li2—Al1^{xvi}	134.8 (7)
O1^{i}—Li1—Li2^{vii}	52.6 (10)	Al1^{xv}—Li2—Al1^{xvi}	104.6 (11)
O1^{ii}—Li1—Li2^{vii}	96.5 (4)	O1^{x}—B1—O1^{xvii}	119.981 (12)
O1^{iii}—Li1—Li2^{vii}	70.29 (8)	O1^{x}—B1—O1	119.980 (12)
Li2^{iv}—Li1—Li2^{vii}	100 (2)	O1^{xvii}—B1—O1	119.982 (12)
Li2^{v}—Li1—Li2^{vii}	114.4 (12)	O1^{xviii}—Al1—O1^{xix}	107.09 (6)
Li2^{vi}—Li1—Li2^{vii}	114.4 (12)	O1^{xviii}—Al1—O1^{xvii}	114.35 (13)
O1—Li1—Cl1	80.00 (5)	O1^{xix}—Al1—O1^{xvii}	107.09 (6)
O1^{i}—Li1—Cl1	80.00 (5)	O1^{xviii}—Al1—O1^{xx}	107.09 (6)
O1^{ii}—Li1—Cl1	100.00 (5)	O1^{xix}—Al1—O1^{xx}	114.35 (13)
O1^{iii}—Li1—Cl1	100.00 (5)	O1^{xvii}—Al1—O1^{xx}	107.09 (6)
Li2^{iv}—Li1—Cl1	130.0 (11)	O1^{xviii}—Al1—Li2^{i}	153.8 (2)
Li2^{v}—Li1—Cl1	50.0 (11)	O1^{xix}—Al1—Li2^{i}	49.7 (3)
Li2^{vi}—Li1—Cl1	50.0 (11)	O1^{xvii}—Al1—Li2^{i}	69.9 (9)
Li2^{vii}—Li1—Cl1	130.0 (11)	O1^{xx}—Al1—Li2^{i}	95.3 (7)
O1—Li1—Al1^{viii}	150.78 (5)	O1^{xviii}—Al1—Li2^{xxi}	69.9 (9)
O1^{i}—Li1—Al1^{viii}	29.22 (5)	O1^{xix}—Al1—Li2^{xxi}	95.3 (7)
O1^{ii}—Li1—Al1^{viii}	62.85 (5)	O1^{xvii}—Al1—Li2^{xxi}	153.8 (2)
O1^{iii}—Li1—Al1^{viii}	117.15 (5)	O1^{xx}—Al1—Li2^{xxi}	49.7 (3)
Li2^{iv}—Li1—Al1^{viii}	122.8 (6)	Li2^{i}—Al1—Li2^{xxi}	118.5 (19)
Li2^{v}—Li1—Al1^{viii}	57.2 (6)	O1^{xviii}—Al1—Li2^{xxii}	95.3 (7)
Li2^{vi}—Li1—Al1^{viii}	122.8 (6)	O1^{xix}—Al1—Li2^{xxii}	153.8 (2)
Li2^{vii}—Li1—Al1^{viii}	57.2 (6)	O1^{xvii}—Al1—Li2^{xxii}	49.7 (3)
Cl1—Li1—Al1^{viii}	90.0	O1^{xx}—Al1—Li2^{xxii}	69.9 (9)
O1—Li1—Al1^{ix}	117.15 (5)	Li2^{i}—Al1—Li2^{xxii}	105.2 (9)
O1^{i}—Li1—Al1^{ix}	62.85 (5)	Li2^{xxi}—Al1—Li2^{xxii}	105.2 (9)
O1^{ii}—Li1—Al1^{ix}	150.78 (5)	O1^{xviii}—Al1—Li2^{xxiii}	49.7 (3)
O1^{iii}—Li1—Al1^{ix}	29.22 (5)	O1^{xix}—Al1—Li2^{xxiii}	69.9 (9)
Li2^{iv}—Li1—Al1^{ix}	122.8 (6)	O1^{xvii}—Al1—Li2^{xxiii}	95.3 (7)
Li2^{v}—Li1—Al1^{ix}	122.8 (6)	O1^{xx}—Al1—Li2^{xxiii}	153.8 (2)
Li2^{vi}—Li1—Al1^{ix}	57.2 (6)	Li2^{i}—Al1—Li2^{xxiii}	105.2 (9)
Li2^{vii}—Li1—Al1^{ix}	57.2 (6)	Li2^{xxi}—Al1—Li2^{xxiii}	105.2 (9)
Cl1—Li1—Al1^{ix}	90.0	Li2^{xxii}—Al1—Li2^{xxiii}	118.5 (19)
Al1^{viii}—Li1—Al1^{ix}	90.0	O1^{xviii}—Al1—Li1^{xxiv}	78.09 (5)
O1—Li1—Al1^{x}	29.22 (5)	O1^{xix}—Al1—Li1^{xxiv}	144.55 (6)
O1^{i}—Li1—Al1^{x}	150.78 (5)	O1^{xvii}—Al1—Li1^{xxiv}	101.91 (5)
O1^{ii}—Li1—Al1^{x}	117.15 (5)	O1^{xx}—Al1—Li1^{xxiv}	35.45 (6)
O1^{iii}—Li1—Al1^{x}	62.85 (5)	Li2^{i}—Al1—Li1^{xxiv}	127.4 (4)

Li2^{iv}—Li1—Al1^{x}	57.2 (6)	Li2^{xxi}—Al1—Li1^{xxiv}	52.6 (4)
Li2^{v}—Li1—Al1^{x}	122.8 (6)	Li2^{xxii}—Al1—Li1^{xxiv}	52.6 (4)
Li2^{vi}—Li1—Al1^{x}	57.2 (6)	Li2^{xxiii}—Al1—Li1^{xxiv}	127.4 (4)
Li2^{vii}—Li1—Al1^{x}	122.8 (6)	O1^{xviii}—Al1—Li1^{x}	101.91 (5)
Cl1—Li1—Al1^{x}	90.0	O1^{xix}—Al1—Li1^{x}	35.45 (6)
Al1^{viii}—Li1—Al1^{x}	180.0	O1^{xvii}—Al1—Li1^{x}	78.09 (5)
Al1^{ix}—Li1—Al1^{x}	90.0	O1^{xx}—Al1—Li1^{x}	144.55 (6)
O1^{xi}—Li2—O1^{xii}	97.0 (15)	Li2^{i}—Al1—Li1^{x}	52.6 (4)
O1^{xi}—Li2—O1^{xiii}	97.0 (15)	Li2^{xxi}—Al1—Li1^{x}	127.4 (4)
O1^{xii}—Li2—O1^{xiii}	97.0 (15)	Li2^{xxii}—Al1—Li1^{x}	127.4 (4)
O1^{xi}—Li2—Cl1	120.1 (12)	Li2^{xxiii}—Al1—Li1^{x}	52.6 (4)
O1^{xii}—Li2—Cl1	120.1 (12)	Li1^{xxiv}—Al1—Li1^{x}	180.0
O1^{xiii}—Li2—Cl1	120.1 (12)	O1^{xviii}—Al1—Li1^{xvii}	144.55 (6)
O1^{xi}—Li2—Li1^{xiv}	107.0 (3)	O1^{xix}—Al1—Li1^{xvii}	101.91 (5)
O1^{xii}—Li2—Li1^{xiv}	139.1 (8)	O1^{xvii}—Al1—Li1^{xvii}	35.45 (6)
O1^{xiii}—Li2—Li1^{xiv}	48.29 (9)	O1^{xx}—Al1—Li1^{xvii}	78.09 (5)
Cl1—Li2—Li1^{xiv}	75.3 (11)	Li2^{i}—Al1—Li1^{xvii}	52.6 (4)
O1^{xi}—Li2—Li1^{ix}	139.1 (8)	Li2^{xxi}—Al1—Li1^{xvii}	127.4 (4)
O1^{xii}—Li2—Li1^{ix}	48.29 (9)	Li2^{xxii}—Al1—Li1^{xvii}	52.6 (4)
O1^{xiii}—Li2—Li1^{ix}	107.0 (3)	Li2^{xxiii}—Al1—Li1^{xvii}	127.4 (4)
Cl1—Li2—Li1^{ix}	75.3 (11)	Li1^{xxiv}—Al1—Li1^{xvii}	90.0
Li1^{xiv}—Li2—Li1^{ix}	113.8 (9)	Li1^{x}—Al1—Li1^{xvii}	90.0
O1^{xi}—Li2—Li1^{vi}	48.29 (9)	O1^{xviii}—Al1—Li1^{xviii}	35.45 (6)
O1^{xii}—Li2—Li1^{vi}	107.0 (3)	O1^{xix}—Al1—Li1^{xviii}	78.09 (5)
O1^{xiii}—Li2—Li1^{vi}	139.1 (8)	O1^{xvii}—Al1—Li1^{xviii}	144.55 (6)
Cl1—Li2—Li1^{vi}	75.3 (11)	O1^{xx}—Al1—Li1^{xviii}	101.91 (5)
Li1^{xiv}—Li2—Li1^{vi}	113.8 (9)	Li2^{i}—Al1—Li1^{xviii}	127.4 (4)
Li1^{ix}—Li2—Li1^{vi}	113.8 (9)	Li2^{xxi}—Al1—Li1^{xviii}	52.6 (4)
O1^{xi}—Li2—O1^{ix}	158 (2)	Li2^{xxii}—Al1—Li1^{xviii}	127.4 (4)
O1^{xii}—Li2—O1^{ix}	71.54 (19)	Li2^{xxiii}—Al1—Li1^{xviii}	52.6 (4)
O1^{xiii}—Li2—O1^{ix}	66.73 (16)	Li1^{xxiv}—Al1—Li1^{xviii}	90.0
Cl1—Li2—O1^{ix}	81.8 (11)	Li1^{x}—Al1—Li1^{xviii}	90.0
Li1^{xiv}—Li2—O1^{ix}	74.1 (3)	Li1^{xvii}—Al1—Li1^{xviii}	180.0
Li1^{ix}—Li2—O1^{ix}	43.90 (17)	B1—O1—Al1^{x}	118.97 (12)
Li1^{vi}—Li2—O1^{ix}	152.3 (17)	B1—O1—Li1	118.1 (2)
O1^{xi}—Li2—O1^{xiv}	66.73 (16)	Al1^{x}—O1—Li1	115.33 (9)
O1^{xii}—Li2—O1^{xiv}	158 (2)	B1—O1—Li2^{iv}	123.5 (10)
O1^{xiii}—Li2—O1^{xiv}	71.54 (19)	Al1^{x}—O1—Li2^{iv}	93.18 (8)
Cl1—Li2—O1^{xiv}	81.8 (11)	Li1—O1—Li2^{iv}	79.2 (11)
Li1^{xiv}—Li2—O1^{xiv}	43.90 (17)	Li2—Cl1—Li2^{i}	109.471 (6)
Li1^{ix}—Li2—O1^{xiv}	152.3 (17)	Li2—Cl1—Li2^{vi}	109.471 (1)
Li1^{vi}—Li2—O1^{xiv}	74.1 (3)	Li2^{i}—Cl1—Li2^{vi}	109.5
O1^{ix}—Li2—O1^{xiv}	118.0 (5)	Li2—Cl1—Li2^{v}	109.471 (3)
O1^{xi}—Li2—O1^{vi}	71.54 (19)	Li2^{i}—Cl1—Li2^{v}	109.471 (1)
O1^{xii}—Li2—O1^{vi}	66.73 (16)	Li2^{vi}—Cl1—Li2^{v}	109.471 (1)
O1^{xiii}—Li2—O1^{vi}	158 (2)	Li2—Cl1—Li1	125.264 (1)
Cl1—Li2—O1^{vi}	81.8 (11)	Li2^{i}—Cl1—Li1	125.264 (1)
Li1^{xiv}—Li2—O1^{vi}	152.3 (17)	Li2^{vi}—Cl1—Li1	54.736 (1)

| Li1^{ix}—Li2—O1^{vi} | 74.1 (3) | Li2^{v}—Cl1—Li1 | 54.736 (1) |
| Li1^{vi}—Li2—O1^{vi} | 43.90 (17) | | |

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

Lithium aluminoboracite (kjh0818yoshinoL14_0m_a_1)

Crystal data

$Li_4B_4Al_3O_{12}Cl$	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$M_r = 379.39$	Cell parameters from 2808 reflections
Cubic, $F23$	$\theta = 6.8$–$73.2°$
$a = 12.9839$ (1) Å	$\mu = 6.12$ mm^{-1}
$V = 2188.85$ (5) Å^3	$T = 297$ K
$Z = 8$	Plate, colorless
$F(000) = 1472$	$0.11 \times 0.10 \times 0.06$ mm
$D_x = 2.303$ Mg m^{-3}	

Data collection

Bruker D8 goniometer diffractometer	4728 measured reflections
Radiation source: sealed tube	389 independent reflections
Detector resolution: 7.3910 pixels mm^{-1}	317 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.024$
Absorption correction: multi-scan (SADABS; Krause et al., 2015)	$\theta_{max} = 73.2°$, $\theta_{min} = 5.9°$
$T_{min} = 0.62$, $T_{max} = 0.75$	$h = -15 \rightarrow 12$
	$k = -15 \rightarrow 16$
	$l = -16 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0537P)^2 + 1.5774P]$ where $P = (F_o^2 + 2F_c^2)/3$
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.032$	$(\Delta/\sigma)_{max} = 0.003$
$wR(F^2) = 0.081$	$\Delta\rho_{max} = 0.20$ e Å^{-3}
$S = 1.17$	$\Delta\rho_{min} = -0.91$ e Å^{-3}
389 reflections	Absolute structure: Flack x determined using 132 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons et al., 2013).
50 parameters	
1 restraint	Absolute structure parameter: -0.03 (2)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	y	z	$U_{iso}*/U_{eq}$	Occ. (<1)
Li1	0.020 (4)	0.250000	0.250000	0.047 (13)	0.5
Li2	0.517 (5)	0.750000	0.750000	0.050 (15)	0.5
Li3	0.363 (3)	0.363 (3)	0.363 (3)	0.020 (12)	0.205 (14)
Li4	0.864 (2)	0.864 (2)	0.864 (2)	0.035 (12)	0.295 (14)

B1	0.1060 (3)	0.1060 (3)	0.1060 (3)	0.0112 (10)
B2	0.6057 (3)	0.6057 (3)	0.6057 (3)	0.0119 (10)
Al1	0.24997 (11)	0.000000	0.000000	0.0118 (5)
O1	0.02797 (13)	0.11005 (14)	0.17683 (14)	0.0170 (5)
O2	0.02784 (13)	0.17681 (14)	0.61004 (14)	0.0171 (5)
Cl1	0.250000	0.250000	0.250000	0.0774 (16)
Cl2	0.750000	0.750000	0.750000	0.0786 (16)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Li1	0.08 (3)	0.015 (11)	0.040 (17)	0.000	0.000	−0.012 (14)
Li2	0.11 (5)	0.031 (14)	0.010 (11)	0.000	0.000	−0.008 (13)
Li3	0.020 (12)	0.020 (12)	0.020 (12)	−0.004 (10)	−0.004 (10)	−0.004 (10)
Li4	0.035 (12)	0.035 (12)	0.035 (12)	0.000 (10)	0.000 (10)	0.000 (10)
B1	0.0112 (10)	0.0112 (10)	0.0112 (10)	−0.0005 (15)	−0.0005 (15)	−0.0005 (15)
B2	0.0119 (10)	0.0119 (10)	0.0119 (10)	−0.0001 (15)	−0.0001 (15)	−0.0001 (15)
Al1	0.0115 (6)	0.0119 (6)	0.0120 (6)	0.000	0.000	0.0003 (4)
O1	0.0185 (10)	0.0161 (9)	0.0164 (10)	0.0050 (6)	0.0069 (9)	0.0048 (9)
O2	0.0196 (11)	0.0164 (10)	0.0154 (9)	0.0071 (9)	0.0050 (6)	0.0048 (9)
Cl1	0.0774 (16)	0.0774 (16)	0.0774 (16)	0.000	0.000	0.000
Cl2	0.0786 (16)	0.0786 (16)	0.0786 (16)	0.000	0.000	0.000

Geometric parameters (Å, º)

Li1—Li2[i]	0.48 (10)	Li3—O2[xxiii]	2.23 (3)
Li1—O1[ii]	2.053 (3)	Li3—O2[xxiv]	2.23 (3)
Li1—O1	2.053 (3)	Li3—Cl1	2.55 (6)
Li1—O2[iii]	2.143 (16)	Li3—O1[xxv]	2.824 (8)
Li1—O2[iv]	2.143 (16)	Li3—O1[xxvi]	2.824 (8)
Li1—Li3[v]	2.57 (4)	Li3—O1[vi]	2.824 (8)
Li1—Li3[vi]	2.57 (4)	Li4—O1[xxvii]	2.23 (3)
Li1—Li4[vii]	2.91 (4)	Li4—O1[xxviii]	2.23 (3)
Li1—Li4[viii]	2.91 (4)	Li4—O1[xxix]	2.23 (3)
Li1—Cl1	2.98 (6)	Li4—Cl2	2.55 (5)
Li1—Al1[ix]	3.256 (5)	Li4—O2[xxx]	2.826 (8)
Li1—Al1[x]	3.256 (5)	Li4—O2[xxxi]	2.826 (8)
Li2—O2[xi]	2.056 (4)	Li4—O2[xxxii]	2.826 (8)
Li2—O2[xii]	2.056 (4)	Li4—Al1[xxxiii]	2.91 (2)
Li2—O1[xiii]	2.132 (16)	Li4—Al1[xxxiv]	2.91 (2)
Li2—O1[xiv]	2.132 (16)	B1—O1	1.3693 (17)
Li2—Li4[xv]	2.60 (4)	B1—O1[ix]	1.3693 (17)
Li2—Li4[xvi]	2.60 (4)	B1—O1[x]	1.3693 (17)
Li2—Li3[xvii]	2.88 (4)	B2—O2[xxxv]	1.3702 (17)
Li2—Li3[xviii]	2.88 (4)	B2—O2[xii]	1.3702 (17)
Li2—Cl2	3.03 (6)	B2—O2[xxxvi]	1.3702 (17)
Li2—Al1[xix]	3.253 (4)	Al1—O1[xxxvii]	1.754 (2)
Li2—Al1[xx]	3.253 (4)	Al1—O2[xxxviii]	1.754 (2)

Li2—Al1^{xxi}	3.253 (4)	Al1—O1^{x}	1.754 (2)
Li3—O2^{xxii}	2.23 (3)	Al1—O2^{xxxix}	1.754 (2)
Li2^{i}—Li1—O1^{ii}	92.8 (16)	Li2^{xvi}—Li4—Li2^{xliii}	110.8 (14)
Li2^{i}—Li1—O1	92.8 (16)	Li2^{xlii}—Li4—Li2^{xliii}	110.9 (14)
O1^{ii}—Li1—O1	174 (3)	O1^{xxvii}—Li4—O2^{xxx}	157 (2)
Li2^{i}—Li1—O2^{iii}	73.1 (14)	O1^{xxviii}—Li4—O2^{xxx}	71.5 (2)
O1^{ii}—Li1—O2^{iii}	90.8 (4)	O1^{xxix}—Li4—O2^{xxx}	66.70 (16)
O1—Li1—O2^{iii}	90.8 (4)	Cl2—Li4—O2^{xxx}	82.1 (11)
Li2^{i}—Li1—O2^{iv}	73.1 (14)	Li2^{xvi}—Li4—O2^{xxx}	44.3 (2)
O1^{ii}—Li1—O2^{iv}	90.8 (4)	Li2^{xlii}—Li4—O2^{xxx}	74.0 (4)
O1—Li1—O2^{iv}	90.8 (4)	Li2^{xliii}—Li4—O2^{xxx}	150 (2)
O2^{iii}—Li1—O2^{iv}	146 (3)	O1^{xxvii}—Li4—O2^{xxxi}	66.70 (16)
Li2^{i}—Li1—Li3^{v}	126.0 (15)	O1^{xxviii}—Li4—O2^{xxxi}	157 (2)
O1^{ii}—Li1—Li3^{v}	74.3 (8)	O1^{xxix}—Li4—O2^{xxxi}	71.5 (2)
O1—Li1—Li3^{v}	102.3 (12)	Cl2—Li4—O2^{xxxi}	82.1 (11)
O2^{iii}—Li1—Li3^{v}	55.4 (12)	Li2^{xvi}—Li4—O2^{xxxi}	150 (2)
O2^{iv}—Li1—Li3^{v}	155 (2)	Li2^{xlii}—Li4—O2^{xxxi}	44.3 (2)
Li2^{i}—Li1—Li3^{vi}	126.0 (15)	Li2^{xliii}—Li4—O2^{xxxi}	74.0 (4)
O1^{ii}—Li1—Li3^{vi}	102.3 (12)	O2^{xxx}—Li4—O2^{xxxi}	118.2 (5)
O1—Li1—Li3^{vi}	74.3 (8)	O1^{xxvii}—Li4—O2^{xxxii}	71.5 (2)
O2^{iii}—Li1—Li3^{vi}	155 (2)	O1^{xxviii}—Li4—O2^{xxxii}	66.70 (16)
O2^{iv}—Li1—Li3^{vi}	55.4 (12)	O1^{xxix}—Li4—O2^{xxxii}	157 (2)
Li3^{v}—Li1—Li3^{vi}	108 (3)	Cl2—Li4—O2^{xxxii}	82.1 (11)
Li2^{i}—Li1—Li4^{vii}	45.7 (13)	Li2^{xvi}—Li4—O2^{xxxii}	74.0 (4)
O1^{ii}—Li1—Li4^{vii}	136 (2)	Li2^{xlii}—Li4—O2^{xxxii}	150 (2)
O1—Li1—Li4^{vii}	49.6 (13)	Li2^{xliii}—Li4—O2^{xxxii}	44.3 (2)
O2^{iii}—Li1—Li4^{vii}	65.9 (10)	O2^{xxx}—Li4—O2^{xxxii}	118.2 (5)
O2^{iv}—Li1—Li4^{vii}	90.1 (14)	O2^{xxxi}—Li4—O2^{xxxii}	118.2 (5)
Li3^{v}—Li1—Li4^{vii}	114.3 (10)	O1^{xxvii}—Li4—Al1^{xxxiii}	68.7 (7)
Li3^{vi}—Li1—Li4^{vii}	114.3 (10)	O1^{xxviii}—Li4—Al1^{xxxiii}	37.0 (3)
Li2^{i}—Li1—Li4^{viii}	45.7 (13)	O1^{xxix}—Li4—Al1^{xxxiii}	122 (2)
O1^{ii}—Li1—Li4^{viii}	49.6 (13)	Cl2—Li4—Al1^{xxxiii}	114.3 (9)
O1—Li1—Li4^{viii}	136 (2)	Li2^{xvi}—Li4—Al1^{xxxiii}	72.2 (6)
O2^{iii}—Li1—Li4^{viii}	90.1 (14)	Li2^{xlii}—Li4—Al1^{xxxiii}	174 (2)
O2^{iv}—Li1—Li4^{viii}	65.9 (10)	Li2^{xliii}—Li4—Al1^{xxxiii}	72.2 (6)
Li3^{v}—Li1—Li4^{viii}	114.3 (10)	O2^{xxx}—Li4—Al1^{xxxiii}	106.3 (4)
Li3^{vi}—Li1—Li4^{viii}	114.3 (10)	O2^{xxxi}—Li4—Al1^{xxxiii}	134.6 (7)
Li4^{vii}—Li1—Li4^{viii}	91 (3)	O2^{xxxii}—Li4—Al1^{xxxiii}	35.59 (12)
Li2^{i}—Li1—Cl1	180.0	O1^{xxvii}—Li4—Al1^{xxxiv}	37.0 (3)
O1^{ii}—Li1—Cl1	87.2 (16)	O1^{xxviii}—Li4—Al1^{xxxiv}	122 (2)
O1—Li1—Cl1	87.2 (16)	O1^{xxix}—Li4—Al1^{xxxiv}	68.7 (7)
O2^{iii}—Li1—Cl1	106.9 (14)	Cl2—Li4—Al1^{xxxiv}	114.3 (9)
O2^{iv}—Li1—Cl1	106.9 (14)	Li2^{xvi}—Li4—Al1^{xxxiv}	174 (2)
Li3^{v}—Li1—Cl1	54.0 (15)	Li2^{xlii}—Li4—Al1^{xxxiv}	72.2 (6)
Li3^{vi}—Li1—Cl1	54.0 (15)	Li2^{xliii}—Li4—Al1^{xxxiv}	72.2 (6)
Li4^{vii}—Li1—Cl1	134.3 (13)	O2^{xxx}—Li4—Al1^{xxxiv}	134.6 (7)
Li4^{viii}—Li1—Cl1	134.3 (13)	O2^{xxxi}—Li4—Al1^{xxxiv}	35.59 (12)

Li2^{i}—Li1—Al1^{ix}	85.4 (10)	O2^{xxxii}—Li4—Al1^{xxxiv}	106.3 (4)
O1^{ii}—Li1—Al1^{ix}	152.41 (19)	Al1^{xxxiii}—Li4—Al1^{xxxiv}	104.3 (11)
O1—Li1—Al1^{ix}	28.56 (17)	O1—B1—O1^{ix}	119.972 (15)
O2^{iii}—Li1—Al1^{ix}	114.7 (7)	O1—B1—O1^{x}	119.972 (15)
O2^{iv}—Li1—Al1^{ix}	62.3 (2)	O1^{ix}—B1—O1^{x}	119.972 (15)
Li3^{v}—Li1—Al1^{ix}	128.1 (12)	O2^{xxxv}—B2—O2^{xii}	119.982 (12)
Li3^{vi}—Li1—Al1^{ix}	58.5 (7)	O2^{xxxv}—B2—O2^{xxxvi}	119.982 (13)
Li4^{vii}—Li1—Al1^{ix}	55.9 (7)	O2^{xii}—B2—O2^{xxxvi}	119.982 (12)
Li4^{viii}—Li1—Al1^{ix}	116.6 (14)	O1^{xxxvii}—Al1—O2^{xxxviii}	107.12 (9)
Cl1—Li1—Al1^{ix}	94.6 (10)	O1^{xxxvii}—Al1—O1^{x}	114.42 (15)
Li2^{i}—Li1—Al1^{x}	85.4 (10)	O2^{xxxviii}—Al1—O1^{x}	107.03 (8)
O1^{ii}—Li1—Al1^{x}	117.73 (11)	O1^{xxxvii}—Al1—O2^{xxxix}	107.03 (8)
O1—Li1—Al1^{x}	62.78 (10)	O2^{xxxviii}—Al1—O2^{xxxix}	114.35 (15)
O2^{iii}—Li1—Al1^{x}	29.72 (10)	O1^{x}—Al1—O2^{xxxix}	107.12 (9)
O2^{iv}—Li1—Al1^{x}	145.3 (15)	O1^{xxxvii}—Al1—Li4^{xliv}	95.5 (7)
Li3^{v}—Li1—Al1^{x}	58.5 (7)	O2^{xxxviii}—Al1—Li4^{xliv}	153.8 (2)
Li3^{vi}—Li1—Al1^{x}	128.1 (12)	O1^{x}—Al1—Li4^{xliv}	49.8 (3)
Li4^{vii}—Li1—Al1^{x}	55.9 (7)	O2^{xxxix}—Al1—Li4^{xliv}	69.7 (8)
Li4^{viii}—Li1—Al1^{x}	116.6 (14)	O1^{xxxvii}—Al1—Li4^{xlv}	49.8 (3)
Cl1—Li1—Al1^{x}	94.6 (10)	O2^{xxxviii}—Al1—Li4^{xlv}	69.7 (8)
Al1^{ix}—Li1—Al1^{x}	89.62 (17)	O1^{x}—Al1—Li4^{xlv}	95.5 (7)
O2^{xi}—Li2—O2^{xii}	172 (3)	O2^{xxxix}—Al1—Li4^{xlv}	153.8 (2)
O2^{xi}—Li2—O1^{xiii}	91.1 (4)	Li4^{xliv}—Al1—Li4^{xlv}	119.1 (19)
O2^{xii}—Li2—O1^{xiii}	91.1 (4)	O1^{xxxvii}—Al1—Li3^{ii}	153.8 (2)
O2^{xi}—Li2—O1^{xiv}	91.1 (4)	O2^{xxxviii}—Al1—Li3^{ii}	49.8 (3)
O2^{xii}—Li2—O1^{xiv}	91.1 (4)	O1^{x}—Al1—Li3^{ii}	69.5 (9)
O1^{xiii}—Li2—O1^{xiv}	148 (3)	O2^{xxxix}—Al1—Li3^{ii}	95.6 (7)
O2^{xi}—Li2—Li4^{xv}	101.4 (13)	Li4^{xliv}—Al1—Li3^{ii}	104.9 (7)
O2^{xii}—Li2—Li4^{xv}	73.7 (9)	Li4^{xlv}—Al1—Li3^{ii}	104.9 (7)
O1^{xiii}—Li2—Li4^{xv}	154 (2)	O1^{xxxvii}—Al1—Li3^{xli}	69.5 (9)
O1^{xiv}—Li2—Li4^{xv}	55.1 (12)	O2^{xxxviii}—Al1—Li3^{xli}	95.6 (7)
O2^{xi}—Li2—Li4^{xvi}	73.7 (9)	O1^{x}—Al1—Li3^{xli}	153.8 (2)
O2^{xii}—Li2—Li4^{xvi}	101.4 (13)	O2^{xxxix}—Al1—Li3^{xli}	49.8 (3)
O1^{xiii}—Li2—Li4^{xvi}	55.1 (12)	Li4^{xliv}—Al1—Li3^{xli}	104.9 (7)
O1^{xiv}—Li2—Li4^{xvi}	154 (2)	Li4^{xlv}—Al1—Li3^{xli}	104.9 (7)
Li4^{xv}—Li2—Li4^{xvi}	107 (3)	Li3^{ii}—Al1—Li3^{xli}	119 (2)
O2^{xi}—Li2—Li3^{xvii}	137 (2)	O1^{xxxvii}—Al1—Li2^{xlvi}	37.0 (5)
O2^{xii}—Li2—Li3^{xvii}	50.2 (14)	O2^{xxxviii}—Al1—Li2^{xlvi}	74.9 (9)
O1^{xiii}—Li2—Li3^{xvii}	66.6 (10)	O1^{x}—Al1—Li2^{xlvi}	143.0 (5)
O1^{xiv}—Li2—Li3^{xvii}	91.1 (15)	O2^{xxxix}—Al1—Li2^{xlvi}	105.1 (9)
Li4^{xv}—Li2—Li3^{xvii}	114.4 (10)	Li4^{xliv}—Al1—Li2^{xlvi}	130.5 (9)
Li4^{xvi}—Li2—Li3^{xvii}	114.4 (10)	Li4^{xlv}—Al1—Li2^{xlvi}	49.5 (9)
O2^{xi}—Li2—Li3^{xviii}	50.2 (13)	Li3^{ii}—Al1—Li2^{xlvi}	124.6 (9)
O2^{xii}—Li2—Li3^{xviii}	137 (2)	Li3^{xli}—Al1—Li2^{xlvi}	55.4 (9)
O1^{xiii}—Li2—Li3^{xviii}	91.1 (15)	O1^{xxxvii}—Al1—Li2^{xlvii}	98.7 (9)
O1^{xiv}—Li2—Li3^{xviii}	66.6 (10)	O2^{xxxviii}—Al1—Li2^{xlvii}	34.2 (3)
Li4^{xv}—Li2—Li3^{xviii}	114.4 (10)	O1^{x}—Al1—Li2^{xlvii}	81.3 (9)
Li4^{xvi}—Li2—Li3^{xviii}	114.4 (10)	O2^{xxxix}—Al1—Li2^{xlvii}	145.8 (3)

Angle	Value	Angle	Value
Li3ˣᵛⁱⁱ—Li2—Li3ˣᵛⁱⁱⁱ	92 (3)	Li4ˣˡⁱᵛ—Al1—Li2ˣˡᵛⁱⁱ	130.5 (9)
O2ˣⁱ—Li2—Cl2	86.0 (17)	Li4ˣˡᵛ—Al1—Li2ˣˡᵛⁱⁱ	49.5 (9)
O2ˣⁱⁱ—Li2—Cl2	86.0 (17)	Li3ⁱⁱ—Al1—Li2ˣˡᵛⁱⁱ	55.4 (9)
O1ˣⁱⁱⁱ—Li2—Cl2	105.9 (15)	Li3ˣˡⁱ—Al1—Li2ˣˡᵛⁱⁱ	124.6 (9)
O1ˣⁱᵛ—Li2—Cl2	105.9 (15)	Li2ˣˡᵛⁱ—Al1—Li2ˣˡᵛⁱⁱ	82 (2)
Li4ˣᵛ—Li2—Cl2	53.3 (15)	O1ˣˣˣᵛⁱⁱ—Al1—Li2ˣˡᵛⁱⁱⁱ	81.3 (9)
Li4ˣᵛⁱ—Li2—Cl2	53.3 (15)	O2ˣˣˣᵛⁱⁱⁱ—Al1—Li2ˣˡᵛⁱⁱⁱ	145.8 (3)
Li3ˣᵛⁱⁱ—Li2—Cl2	133.8 (13)	O1ˣ—Al1—Li2ˣˡᵛⁱⁱⁱ	98.7 (9)
Li3ˣᵛⁱⁱⁱ—Li2—Cl2	133.8 (13)	O2ˣˣˣⁱˣ—Al1—Li2ˣˡᵛⁱⁱⁱ	34.2 (3)
O2ˣⁱ—Li2—Al1ˣⁱˣ	117.76 (6)	Li4ˣˡⁱᵛ—Al1—Li2ˣˡᵛⁱⁱⁱ	49.5 (9)
O2ˣⁱⁱ—Li2—Al1ˣⁱˣ	62.84 (9)	Li4ˣˡᵛ—Al1—Li2ˣˡᵛⁱⁱⁱ	130.5 (9)
O1ˣⁱⁱⁱ—Li2—Al1ˣⁱˣ	29.66 (11)	Li3ⁱⁱ—Al1—Li2ˣˡᵛⁱⁱⁱ	124.6 (9)
O1ˣⁱᵛ—Li2—Al1ˣⁱˣ	146.3 (15)	Li3ˣˡⁱ—Al1—Li2ˣˡᵛⁱⁱⁱ	55.4 (9)
Li4ˣᵛ—Li2—Al1ˣⁱˣ	127.3 (13)	Li2ˣˡᵛⁱ—Al1—Li2ˣˡᵛⁱⁱⁱ	98 (2)
Li4ˣᵛⁱ—Li2—Al1ˣⁱˣ	58.3 (7)	Li2ˣˡᵛⁱⁱ—Al1—Li2ˣˡᵛⁱⁱⁱ	179.99 (5)
Li3ˣᵛⁱⁱ—Li2—Al1ˣⁱˣ	56.2 (7)	O1ˣˣˣᵛⁱⁱ—Al1—Li2ˣˡⁱˣ	143.0 (5)
Li3ˣᵛⁱⁱⁱ—Li2—Al1ˣⁱˣ	117.5 (15)	O2ˣˣˣᵛⁱⁱⁱ—Al1—Li2ˣˡⁱˣ	105.1 (9)
Cl2—Li2—Al1ˣⁱˣ	93.9 (10)	O1ˣ—Al1—Li2ˣˡⁱˣ	37.0 (5)
O2ˣⁱ—Li2—Al1ˣˣ	152.45 (6)	O2ˣˣˣⁱˣ—Al1—Li2ˣˡⁱˣ	74.9 (9)
O2ˣⁱⁱ—Li2—Al1ˣˣ	28.68 (17)	Li4ˣˡⁱᵛ—Al1—Li2ˣˡⁱˣ	49.5 (9)
O1ˣⁱⁱⁱ—Li2—Al1ˣˣ	115.2 (7)	Li4ˣˡᵛ—Al1—Li2ˣˡⁱˣ	130.5 (9)
O1ˣⁱᵛ—Li2—Al1ˣˣ	62.41 (19)	Li3ⁱⁱ—Al1—Li2ˣˡⁱˣ	55.4 (9)
Li4ˣᵛ—Li2—Al1ˣˣ	58.3 (7)	Li3ˣˡⁱ—Al1—Li2ˣˡⁱˣ	124.6 (9)
Li4ˣᵛⁱ—Li2—Al1ˣˣ	127.3 (13)	Li2ˣˡᵛⁱ—Al1—Li2ˣˡⁱˣ	180.0 (17)
Li3ˣᵛⁱⁱ—Li2—Al1ˣˣ	56.2 (7)	Li2ˣˡᵛⁱⁱ—Al1—Li2ˣˡⁱˣ	98 (2)
Li3ˣᵛⁱⁱⁱ—Li2—Al1ˣˣ	117.5 (15)	Li2ˣˡᵛⁱⁱⁱ—Al1—Li2ˣˡⁱˣ	82 (2)
Cl2—Li2—Al1ˣˣ	93.9 (10)	B1—O1—Al1ⁱˣ	119.05 (13)
Al1ˣⁱˣ—Li2—Al1ˣˣ	89.75 (15)	B1—O1—Li1	112.4 (12)
O2ˣⁱ—Li2—Al1ˣˣⁱ	28.68 (17)	Al1ⁱˣ—O1—Li1	117.4 (4)
O2ˣⁱⁱ—Li2—Al1ˣˣⁱ	152.45 (6)	B1—O1—Li2ⁱ	122.3 (12)
O1ˣⁱⁱⁱ—Li2—Al1ˣˣⁱ	62.41 (19)	Al1ⁱˣ—O1—Li2ⁱ	113.4 (6)
O1ˣⁱᵛ—Li2—Al1ˣˣⁱ	115.2 (7)	Li1—O1—Li2ⁱ	13 (3)
Li4ˣᵛ—Li2—Al1ˣˣⁱ	127.3 (13)	B1—O1—Li4ᵛⁱⁱ	123.9 (9)
Li4ˣᵛⁱ—Li2—Al1ˣˣⁱ	58.3 (7)	Al1ⁱˣ—O1—Li4ᵛⁱⁱ	93.12 (8)
Li3ˣᵛⁱⁱ—Li2—Al1ˣˣⁱ	117.5 (15)	Li1—O1—Li4ᵛⁱⁱ	85.7 (19)
Li3ˣᵛⁱⁱⁱ—Li2—Al1ˣˣⁱ	56.2 (7)	Li2ⁱ—O1—Li4ᵛⁱⁱ	73.2 (19)
Cl2—Li2—Al1ˣˣⁱ	93.9 (10)	B1—O1—Li3ᵛⁱ	102.2 (9)
Al1ˣⁱˣ—Li2—Al1ˣˣⁱ	89.73 (15)	Al1ⁱˣ—O1—Li3ᵛⁱ	74.9 (10)
Al1ˣˣ—Li2—Al1ˣˣⁱ	172 (2)	Li1—O1—Li3ᵛⁱ	61.3 (10)
O2ˣˣⁱⁱ—Li3—O2ˣˣⁱⁱⁱ	96.4 (16)	Li2ⁱ—O1—Li3ᵛⁱ	69.5 (10)
O2ˣˣⁱⁱ—Li3—O2ˣˣⁱᵛ	96.4 (16)	Li4ᵛⁱⁱ—O1—Li3ᵛⁱ	131.5 (12)
O2ˣˣⁱⁱⁱ—Li3—O2ˣˣⁱᵛ	96.4 (16)	B1—O1—Li3	75.8 (3)
O2ˣˣⁱⁱ—Li3—Cl1	120.6 (12)	Al1ⁱˣ—O1—Li3	112.35 (10)
O2ˣˣⁱⁱⁱ—Li3—Cl1	120.6 (12)	Li1—O1—Li3	50.3 (16)
O2ˣˣⁱᵛ—Li3—Cl1	120.6 (12)	Li2ⁱ—O1—Li3	63.2 (15)
O2ˣˣⁱⁱ—Li3—Li1ᵛⁱ	108.9 (5)	Li4ᵛⁱⁱ—O1—Li3	135.3 (9)
O2ˣˣⁱⁱⁱ—Li3—Li1ᵛⁱ	140.8 (8)	Li3ᵛⁱ—O1—Li3	38.8 (10)
O2ˣˣⁱᵛ—Li3—Li1ᵛⁱ	52.5 (10)	B2ˡ—O2—Al1ˣˣᵛⁱ	118.94 (13)

Cl1—Li3—Li1^vi	71.3 (15)	B2^l—O2—Li2^l	113.5 (13)
O2^xxii—Li3—Li1^xxvi	52.4 (10)	Al1^xxvi—O2—Li2^l	117.1 (5)
O2^xxiii—Li3—Li1^xxvi	108.9 (5)	B2^l—O2—Li1^li	123.2 (11)
O2^xxiv—Li3—Li1^xxvi	140.8 (8)	Al1^xxvi—O2—Li1^li	113.0 (5)
Cl1—Li3—Li1^xxvi	71.3 (15)	Li2^l—O2—Li1^li	13 (3)
Li1^vi—Li3—Li1^xxvi	110.2 (15)	B2^l—O2—Li3^lii	123.8 (10)
O2^xxii—Li3—Li1^xxv	140.8 (8)	Al1^xxvi—O2—Li3^lii	93.19 (8)
O2^xxiii—Li3—Li1^xxv	52.4 (10)	Li2^l—O2—Li3^lii	85 (2)
O2^xxiv—Li3—Li1^xxv	108.9 (5)	Li1^li—O2—Li3^lii	72.1 (18)
Cl1—Li3—Li1^xxv	71.3 (15)	B2^l—O2—Li4^liii	102.4 (9)
Li1^vi—Li3—Li1^xxv	110.2 (15)	Al1^xxvi—O2—Li4^liii	74.7 (10)
Li1^xxvi—Li3—Li1^xxv	110.2 (15)	Li2^l—O2—Li4^liii	62.0 (11)
O2^xxii—Li3—O1^xxv	157 (2)	Li1^li—O2—Li4^liii	70.2 (10)
O2^xxiii—Li3—O1^xxv	71.5 (2)	Li3^lii—O2—Li4^liii	131.4 (12)
O2^xxiv—Li3—O1^xxv	66.68 (17)	B2^l—O2—Li4	82.6 (3)
Cl1—Li3—O1^xxv	82.2 (11)	Al1^xxvi—O2—Li4	90.33 (9)
Li1^vi—Li3—O1^xxv	74.0 (4)	Li2^l—O2—Li4	64.2 (14)
Li1^xxvi—Li3—O1^xxv	149 (2)	Li1^li—O2—Li4	75.6 (13)
Li1^xxv—Li3—O1^xxv	44.4 (3)	Li3^lii—O2—Li4	146.2 (12)
O2^xxii—Li3—O1^xxvi	71.5 (2)	Li4^liii—O2—Li4	21.0 (10)
O2^xxiii—Li3—O1^xxvi	66.68 (17)	Li3—Cl1—Li3^ii	109.468 (7)
O2^xxiv—Li3—O1^xxvi	157 (2)	Li3—Cl1—Li3^v	109.473 (3)
Cl1—Li3—O1^xxvi	82.2 (11)	Li3^ii—Cl1—Li3^v	109.473 (1)
Li1^vi—Li3—O1^xxvi	149 (2)	Li3—Cl1—Li3^vi	109.473 (1)
Li1^xxvi—Li3—O1^xxvi	44.4 (3)	Li3^ii—Cl1—Li3^vi	109.5
Li1^xxv—Li3—O1^xxvi	73.9 (4)	Li3^v—Cl1—Li3^vi	109.468 (2)
O1^xxv—Li3—O1^xxvi	118.2 (5)	Li3—Cl1—Li1	125.266 (1)
O2^xxii—Li3—O1^vi	66.68 (17)	Li3^ii—Cl1—Li1	125.266 (4)
O2^xxiii—Li3—O1^vi	157 (2)	Li3^v—Cl1—Li1	54.734 (1)
O2^xxiv—Li3—O1^vi	71.5 (2)	Li3^vi—Cl1—Li1	54.734 (2)
Cl1—Li3—O1^vi	82.2 (11)	Li3—Cl1—Li1^xxvi	54.736 (2)
Li1^vi—Li3—O1^vi	44.4 (3)	Li3^ii—Cl1—Li1^xxvi	125.264 (3)
Li1^xxvi—Li3—O1^vi	73.9 (4)	Li3^v—Cl1—Li1^xxvi	54.736 (2)
Li1^xxv—Li3—O1^vi	149 (2)	Li3^vi—Cl1—Li1^xxvi	125.264 (2)
O1^xxv—Li3—O1^vi	118.2 (5)	Li1—Cl1—Li1^xxvi	90.000 (3)
O1^xxvi—Li3—O1^vi	118.2 (5)	Li3—Cl1—Li1^ix	125.264 (5)
O2^xxii—Li3—Li2^xl	45.2 (8)	Li3^ii—Cl1—Li1^ix	54.736 (1)
O2^xxiii—Li3—Li2^xl	105.2 (6)	Li3^v—Cl1—Li1^ix	54.736 (2)
O2^xxiv—Li3—Li2^xl	137.0 (11)	Li3^vi—Cl1—Li1^ix	125.264 (4)
Cl1—Li3—Li2^xl	79.1 (13)	Li1—Cl1—Li1^ix	90.000 (3)
Li1^vi—Li3—Li2^xl	113.8 (9)	Li1^xxvi—Cl1—Li1^ix	90.0
Li1^xxvi—Li3—Li2^xl	7.8 (17)	Li3—Cl1—Li1^xxv	54.736 (2)
Li1^xxv—Li3—Li2^xl	113.8 (9)	Li3^ii—Cl1—Li1^xxv	125.264 (1)
O1^xxv—Li3—Li2^xl	155.6 (18)	Li3^v—Cl1—Li1^xxv	125.264 (2)
O1^xxvi—Li3—Li2^xl	43.86 (15)	Li3^vi—Cl1—Li1^xxv	54.736 (2)
O1^vi—Li3—Li2^xl	74.5 (3)	Li1—Cl1—Li1^xxv	90.000 (3)
O2^xxii—Li3—Li2^xli	105.2 (6)	Li1^xxvi—Cl1—Li1^xxv	90.0
O2^xxiii—Li3—Li2^xli	137.0 (11)	Li1^ix—Cl1—Li1^xxv	180.0

O2^{xxiv}—Li3—Li2^{xli}	45.2 (8)	Li3—Cl1—Li1^{x}	125.264 (1)
Cl1—Li3—Li2^{xli}	79.1 (13)	Li3^{ii}—Cl1—Li1^{x}	54.736 (1)
Li1^{vi}—Li3—Li2^{xli}	7.8 (17)	Li3^{v}—Cl1—Li1^{x}	125.264 (4)
Li1^{xxvi}—Li3—Li2^{xli}	113.8 (9)	Li3^{vi}—Cl1—Li1^{x}	54.736 (1)
Li1^{xxv}—Li3—Li2^{xli}	113.8 (9)	Li1—Cl1—Li1^{x}	90.000 (4)
O1^{xxv}—Li3—Li2^{xli}	74.5 (3)	Li1^{xxvi}—Cl1—Li1^{x}	180.0
O1^{xxvi}—Li3—Li2^{xli}	155.6 (18)	Li1^{ix}—Cl1—Li1^{x}	90.000 (2)
O1^{vi}—Li3—Li2^{xli}	43.86 (15)	Li1^{xxv}—Cl1—Li1^{x}	90.0
Li2^{xl}—Li3—Li2^{xli}	116.5 (8)	Li3—Cl1—Li1^{vi}	54.734 (2)
O1^{xxvii}—Li4—O1^{xxviii}	96.6 (15)	Li3^{ii}—Cl1—Li1^{vi}	54.734 (3)
O1^{xxvii}—Li4—O1^{xxix}	96.6 (15)	Li3^{v}—Cl1—Li1^{vi}	125.266 (2)
O1^{xxviii}—Li4—O1^{xxix}	96.6 (15)	Li3^{vi}—Cl1—Li1^{vi}	125.266 (1)
O1^{xxvii}—Li4—Cl2	120.5 (12)	Li1—Cl1—Li1^{vi}	180.0
O1^{xxviii}—Li4—Cl2	120.5 (12)	Li1^{xxvi}—Cl1—Li1^{vi}	90.000 (5)
O1^{xxix}—Li4—Cl2	120.5 (12)	Li1^{ix}—Cl1—Li1^{vi}	90.0
O1^{xxvii}—Li4—Li2^{xvi}	140.6 (8)	Li1^{xxv}—Cl1—Li1^{vi}	90.000 (4)
O1^{xxviii}—Li4—Li2^{xvi}	51.7 (10)	Li1^{x}—Cl1—Li1^{vi}	90.000 (1)
O1^{xxix}—Li4—Li2^{xvi}	108.6 (5)	Li4—Cl2—Li4^{liv}	109.474 (11)
Cl2—Li4—Li2^{xvi}	71.9 (15)	Li4—Cl2—Li4^{xvi}	109.470 (2)
O1^{xxvii}—Li4—Li2^{xlii}	108.6 (5)	Li4^{liv}—Cl2—Li4^{xvi}	109.470 (3)
O1^{xxviii}—Li4—Li2^{xlii}	140.6 (8)	Li4—Cl2—Li4^{xv}	109.470 (6)
O1^{xxix}—Li4—Li2^{xlii}	51.7 (10)	Li4^{liv}—Cl2—Li4^{xv}	109.5
Cl2—Li4—Li2^{xlii}	71.9 (15)	Li4^{xvi}—Cl2—Li4^{xv}	109.474 (7)
Li2^{xvi}—Li4—Li2^{xlii}	110.8 (14)	Li4—Cl2—Li2	125.263 (4)
O1^{xxvii}—Li4—Li2^{xliii}	51.7 (10)	Li4^{liv}—Cl2—Li2	125.263 (12)
O1^{xxviii}—Li4—Li2^{xliii}	108.6 (5)	Li4^{xvi}—Cl2—Li2	54.737 (7)
O1^{xxix}—Li4—Li2^{xliii}	140.6 (8)	Li4^{xv}—Cl2—Li2	54.737 (6)
Cl2—Li4—Li2^{xliii}	71.9 (15)		

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

Sodium aluminoboracite (kjh230804yoshinoN4_0m_a)

Crystal data

Na$_{3.92}$B$_4$Al$_3$O$_{12}$Cl$_{0.92}$	Cu *Kα* radiation, λ = 1.54178 Å
M_r = 438.91	Cell parameters from 3423 reflections
Cubic, *F*4̄3*c*	θ = 4.6–74.3°
a = 13.5904 (1) Å	μ = 6.78 mm^{-1}
V = 2510.13 (6) Å^3	*T* = 294 K
Z = 8	Plate, colorless
F(000) = 1728	0.08 × 0.06 × 0.04 mm
D_x = 2.323 Mg m^{-3}	

Data collection

Bruker D8 goniometer diffractometer	4504 measured reflections
Radiation source: sealed tube	218 independent reflections
Detector resolution: 7.3910 pixels mm^{-1}	216 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.027$
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)	$\theta_{max} = 74.3°$, $\theta_{min} = 6.5°$
	$h = -16 \rightarrow 16$
$T_{min} = 0.66$, $T_{max} = 0.75$	$k = -16 \rightarrow 16$
	$l = -16 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0311P)^2 + 4.0293P]$ where $P = (F_o^2 + 2F_c^2)/3$
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.022$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.055$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
$S = 1.20$	$\Delta\rho_{min} = -0.45$ e Å^{-3}
218 reflections	Absolute structure: Flack x determined using 89 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
27 parameters	
1 restraint	
	Absolute structure parameter: 0.01 (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.

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

	x	y	z	$U_{iso}*/U_{eq}$	Occ. (<1)
Na1	0.0340 (3)	0.250000	0.250000	0.0422 (14)	0.499 (4)
Na2	0.3606 (4)	0.3606 (4)	0.3606 (4)	0.017 (2)	0.231 (6)
B1	0.1039 (2)	0.1039 (2)	0.1039 (2)	0.0143 (9)	
Al1	0.250000	0.000000	0.000000	0.0095 (4)	
O1	0.03513 (13)	0.10047 (12)	0.17745 (12)	0.0176 (5)	
Cl1	0.250000	0.250000	0.250000	0.0350 (9)	0.920 (10)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.096 (4)	0.0127 (18)	0.0182 (19)	0.000	0.000	−0.0066 (17)
Na2	0.017 (2)	0.017 (2)	0.017 (2)	−0.0006 (18)	−0.0006 (18)	−0.0006 (18)
B1	0.0143 (9)	0.0143 (9)	0.0143 (9)	0.0015 (12)	0.0015 (12)	0.0015 (12)
Al1	0.0096 (6)	0.0095 (5)	0.0095 (5)	0.000	0.000	0.000
O1	0.0189 (9)	0.0149 (8)	0.0188 (8)	0.0060 (6)	0.0102 (8)	0.0061 (7)
Cl1	0.0350 (9)	0.0350 (9)	0.0350 (9)	0.000	0.000	0.000

Geometric parameters (Å, º)

Na1—Na1^i	0.923 (8)	Na2—O1^x	2.484 (5)
Na1—O1^{ii}	2.2588 (16)	Na2—Cl1	2.605 (9)

Na1—O1	2.2588 (16)	Na2—O1xi	2.913 (2)
Na1—O1iii	2.446 (2)	Na2—O1v	2.913 (2)
Na1—O1i	2.446 (2)	Na2—O1xii	2.913 (2)
Na1—Na2iv	2.564 (4)	Na2—Al1xiii	3.072 (4)
Na1—Na2v	2.564 (4)	Na2—Al1xiv	3.072 (4)
Na1—Cl1	2.936 (4)	B1—O1xv	1.3692 (15)
Na1—B1ii	2.965 (3)	B1—O1xvi	1.3692 (15)
Na1—B1	2.965 (3)	B1—O1	1.3693 (15)
Na1—Na2vi	3.174 (3)	Al1—O1xvii	1.7506 (16)
Na1—Na2vii	3.174 (3)	Al1—O1xviii	1.7506 (16)
Na2—O1viii	2.484 (5)	Al1—O1xvi	1.7506 (16)
Na2—O1ix	2.484 (5)	Al1—O1xix	1.7506 (16)

Na1i—Na1—O1ii	90.40 (11)	O1—B1—Na1	46.75 (14)
Na1i—Na1—O1	90.40 (11)	O1xv—B1—Na1xv	46.75 (14)
O1ii—Na1—O1	179.2 (2)	O1xvi—B1—Na1xv	87.53 (15)
Na1i—Na1—O1iii	67.42 (9)	O1—B1—Na1xv	135.5 (3)
O1ii—Na1—O1iii	90.15 (4)	Na1—B1—Na1xv	88.88 (15)
O1—Na1—O1iii	90.15 (4)	O1xv—B1—Na1xvi	135.5 (3)
Na1i—Na1—O1i	67.42 (9)	O1xvi—B1—Na1xvi	46.75 (14)
O1ii—Na1—O1i	90.15 (4)	O1—B1—Na1xvi	87.53 (15)
O1—Na1—O1i	90.15 (4)	Na1—B1—Na1xvi	88.88 (15)
O1iii—Na1—O1i	134.84 (18)	Na1xv—B1—Na1xvi	88.88 (15)
Na1i—Na1—Na2iv	124.0 (2)	O1xvii—Al1—O1xviii	108.49 (6)
O1ii—Na1—Na2iv	74.01 (7)	O1xvii—Al1—O1xvi	111.44 (11)
O1—Na1—Na2iv	105.53 (9)	O1xviii—Al1—O1xvi	108.49 (6)
O1iii—Na1—Na2iv	59.39 (18)	O1xvii—Al1—O1xix	108.49 (6)
O1i—Na1—Na2iv	159.73 (13)	O1xviii—Al1—O1xix	111.44 (11)
Na1i—Na1—Na2v	124.0 (2)	O1xvi—Al1—O1xix	108.49 (6)
O1ii—Na1—Na2v	105.53 (9)	O1xvii—Al1—Na2ii	157.64 (7)
O1—Na1—Na2v	74.01 (7)	O1xviii—Al1—Na2ii	53.95 (9)
O1iii—Na1—Na2v	159.73 (13)	O1xvi—Al1—Na2ii	68.08 (15)
O1i—Na1—Na2v	59.39 (18)	O1xix—Al1—Na2ii	92.12 (11)
Na2iv—Na1—Na2v	112.1 (4)	O1xvii—Al1—Na2xx	68.08 (15)
Na1i—Na1—Cl1	180.0	O1xviii—Al1—Na2xx	92.12 (11)
O1ii—Na1—Cl1	89.60 (11)	O1xvi—Al1—Na2xx	157.64 (7)
O1—Na1—Cl1	89.60 (11)	O1xix—Al1—Na2xx	53.95 (9)
O1iii—Na1—Cl1	112.58 (9)	Na2ii—Al1—Na2xx	121.4 (3)
O1i—Na1—Cl1	112.58 (9)	O1xvii—Al1—Na2xxi	92.12 (11)
Na2iv—Na1—Cl1	56.0 (2)	O1xviii—Al1—Na2xxi	157.64 (7)
Na2v—Na1—Cl1	56.0 (2)	O1xvi—Al1—Na2xxi	53.95 (9)
Na1i—Na1—B1ii	108.69 (11)	O1xix—Al1—Na2xxi	68.08 (15)
O1ii—Na1—B1ii	26.20 (7)	Na2ii—Al1—Na2xxi	103.87 (13)
O1—Na1—B1ii	153.23 (14)	Na2xx—Al1—Na2xxi	103.87 (13)
O1iii—Na1—B1ii	114.17 (5)	O1xvii—Al1—Na2xxii	53.95 (9)
O1i—Na1—B1ii	80.59 (6)	O1xviii—Al1—Na2xxii	68.08 (15)
Na2iv—Na1—B1ii	79.69 (9)	O1xvi—Al1—Na2xxii	92.12 (11)
Na2v—Na1—B1ii	79.69 (9)	O1xix—Al1—Na2xxii	157.64 (7)

Cl1—Na1—B1ⁱⁱ	71.31 (11)	Na2ⁱⁱ—Al1—Na2ˣˣⁱⁱ	103.87 (13)
Na1ⁱ—Na1—B1	108.68 (11)	Na2ˣˣ—Al1—Na2ˣˣⁱⁱ	103.87 (13)
O1ⁱⁱ—Na1—B1	153.23 (14)	Na2ˣˣⁱ—Al1—Na2ˣˣⁱⁱ	121.4 (3)
O1—Na1—B1	26.20 (7)	O1ˣᵛⁱⁱ—Al1—Na1ˣˣⁱⁱⁱ	67.96 (7)
O1ⁱⁱⁱ—Na1—B1	80.59 (6)	O1ˣᵛⁱⁱⁱ—Al1—Na1ˣˣⁱⁱⁱ	137.41 (6)
O1ⁱ—Na1—B1	114.17 (5)	O1ˣᵛⁱ—Al1—Na1ˣˣⁱⁱⁱ	112.04 (7)
Na2ⁱᵛ—Na1—B1	79.69 (9)	O1ˣⁱˣ—Al1—Na1ˣˣⁱⁱⁱ	42.59 (6)
Na2ᵛ—Na1—B1	79.69 (9)	Na2ⁱⁱ—Al1—Na1ˣˣⁱⁱⁱ	133.95 (9)
Cl1—Na1—B1	71.32 (11)	Na2ˣˣ—Al1—Na1ˣˣⁱⁱⁱ	46.05 (9)
B1ⁱⁱ—Na1—B1	142.6 (2)	Na2ˣˣⁱ—Al1—Na1ˣˣⁱⁱⁱ	58.13 (7)
Na1ⁱ—Na1—Na2ᵛⁱ	42.07 (17)	Na2ˣˣⁱⁱ—Al1—Na1ˣˣⁱⁱⁱ	121.87 (7)
O1ⁱⁱ—Na1—Na2ᵛⁱ	129.7 (2)	O1ˣᵛⁱⁱ—Al1—Na1ˣᵛⁱⁱ	35.94 (5)
O1—Na1—Na2ᵛⁱ	51.10 (16)	O1ˣᵛⁱⁱⁱ—Al1—Na1ˣᵛⁱⁱ	80.49 (8)
O1ⁱⁱⁱ—Na1—Na2ᵛⁱ	60.81 (7)	O1ˣᵛⁱ—Al1—Na1ˣᵛⁱⁱ	144.06 (5)
O1ⁱ—Na1—Na2ᵛⁱ	85.28 (12)	O1ˣⁱˣ—Al1—Na1ˣᵛⁱⁱ	99.51 (8)
Na2ⁱᵛ—Na1—Na2ᵛⁱ	114.50 (19)	Na2ⁱⁱ—Al1—Na1ˣᵛⁱⁱ	133.95 (9)
Na2ᵛ—Na1—Na2ᵛⁱ	114.50 (19)	Na2ˣˣ—Al1—Na1ˣᵛⁱⁱ	46.05 (9)
Cl1—Na1—Na2ᵛⁱ	137.93 (17)	Na2ˣˣⁱ—Al1—Na1ˣᵛⁱⁱ	121.87 (7)
B1ⁱⁱ—Na1—Na2ᵛⁱ	150.8 (2)	Na2ˣˣⁱⁱ—Al1—Na1ˣᵛⁱⁱ	58.13 (7)
B1—Na1—Na2ᵛⁱ	66.6 (2)	Na1ˣˣⁱⁱⁱ—Al1—Na1ˣᵛⁱⁱ	74.52 (12)
Na1ⁱ—Na1—Na2ᵛⁱⁱ	42.07 (17)	O1ˣᵛⁱⁱ—Al1—Na1ˣᵛⁱ	144.06 (5)
O1ⁱⁱ—Na1—Na2ᵛⁱⁱ	51.10 (16)	O1ˣᵛⁱⁱⁱ—Al1—Na1ˣᵛⁱ	99.51 (8)
O1—Na1—Na2ᵛⁱⁱ	129.7 (2)	O1ˣᵛⁱ—Al1—Na1ˣᵛⁱ	35.94 (5)
O1ⁱⁱⁱ—Na1—Na2ᵛⁱⁱ	85.28 (12)	O1ˣⁱˣ—Al1—Na1ˣᵛⁱ	80.49 (8)
O1ⁱ—Na1—Na2ᵛⁱⁱ	60.81 (7)	Na2ⁱⁱ—Al1—Na1ˣᵛⁱ	46.05 (9)
Na2ⁱᵛ—Na1—Na2ᵛⁱⁱ	114.50 (19)	Na2ˣˣ—Al1—Na1ˣᵛⁱ	133.95 (9)
Na2ᵛ—Na1—Na2ᵛⁱⁱ	114.50 (19)	Na2ˣˣⁱ—Al1—Na1ˣᵛⁱ	58.13 (7)
Cl1—Na1—Na2ᵛⁱⁱ	137.93 (17)	Na2ˣˣⁱⁱ—Al1—Na1ˣᵛⁱ	121.87 (7)
B1ⁱⁱ—Na1—Na2ᵛⁱⁱ	66.6 (2)	Na1ˣˣⁱⁱⁱ—Al1—Na1ˣᵛⁱ	105.48 (12)
B1—Na1—Na2ᵛⁱⁱ	150.8 (2)	Na1ˣᵛⁱⁱ—Al1—Na1ˣᵛⁱ	180.00 (12)
Na2ᵛⁱ—Na1—Na2ᵛⁱⁱ	84.1 (3)	O1ˣᵛⁱⁱ—Al1—Na1ˣᵛ	112.04 (7)
O1ᵛⁱⁱⁱ—Na2—O1ⁱˣ	92.3 (2)	O1ˣᵛⁱⁱⁱ—Al1—Na1ˣᵛ	42.59 (6)
O1ᵛⁱⁱⁱ—Na2—O1ˣ	92.3 (2)	O1ˣᵛⁱ—Al1—Na1ˣᵛ	67.96 (7)
O1ⁱˣ—Na2—O1ˣ	92.3 (2)	O1ˣⁱˣ—Al1—Na1ˣᵛ	137.41 (6)
O1ᵛⁱⁱⁱ—Na2—Na1ˣⁱ	108.59 (7)	Na2ⁱⁱ—Al1—Na1ˣᵛ	46.05 (9)
O1ⁱˣ—Na2—Na1ˣⁱ	143.23 (13)	Na2ˣˣ—Al1—Na1ˣᵛ	133.95 (9)
O1ˣ—Na2—Na1ˣⁱ	57.95 (8)	Na2ˣˣⁱ—Al1—Na1ˣᵛ	121.87 (7)
O1ᵛⁱⁱⁱ—Na2—Na1ˣⁱⁱ	57.95 (8)	Na2ˣˣⁱⁱ—Al1—Na1ˣᵛ	58.13 (7)
O1ⁱˣ—Na2—Na1ˣⁱⁱ	108.59 (7)	Na1ˣˣⁱⁱⁱ—Al1—Na1ˣᵛ	180.0
O1ˣ—Na2—Na1ˣⁱⁱ	143.23 (13)	Na1ˣᵛⁱⁱ—Al1—Na1ˣᵛ	105.48 (12)
Na1ˣⁱ—Na2—Na1ˣⁱⁱ	108.1 (2)	Na1ˣᵛⁱ—Al1—Na1ˣᵛ	74.52 (12)
O1ᵛⁱⁱⁱ—Na2—Na1ᵛ	143.23 (13)	B1—O1—Al1ˣᵛ	128.59 (12)
O1ⁱˣ—Na2—Na1ᵛ	57.95 (8)	B1—O1—Na1	107.1 (2)
O1ˣ—Na2—Na1ᵛ	108.59 (7)	Al1ˣᵛ—O1—Na1	117.00 (8)
Na1ˣⁱ—Na2—Na1ᵛ	108.1 (2)	B1—O1—Na1ⁱ	121.89 (16)
Na1ˣⁱⁱ—Na2—Na1ᵛ	108.1 (2)	Al1ˣᵛ—O1—Na1ⁱ	108.44 (8)
O1ᵛⁱⁱⁱ—Na2—Cl1	123.62 (17)	Na1—O1—Na1ⁱ	22.18 (18)
O1ⁱˣ—Na2—Cl1	123.62 (17)	B1—O1—Na2ᵛⁱ	119.5 (2)

O1^{x}—Na2—Cl1	123.62 (17)	Al1^{xv}—O1—Na2^{vi}	91.32 (7)
Na1^{xi}—Na2—Cl1	69.2 (2)	Na1—O1—Na2^{vi}	83.85 (18)
Na1^{xii}—Na2—Cl1	69.2 (2)	Na1^{i}—O1—Na2^{vi}	62.66 (18)
Na1^{v}—Na2—Cl1	69.2 (2)	B1—O1—Na2^{v}	106.6 (3)
O1^{viii}—Na2—O1^{xi}	62.95 (7)	Al1^{xv}—O1—Na2^{v}	78.04 (18)
O1^{ix}—Na2—O1^{xi}	151.5 (3)	Na1—O1—Na2^{v}	57.80 (10)
O1^{x}—Na2—O1^{xi}	75.84 (7)	Na1^{i}—O1—Na2^{v}	72.03 (7)
Na1^{xi}—Na2—O1^{xi}	48.20 (5)	Na2^{vi}—O1—Na2^{v}	127.14 (10)
Na1^{xii}—Na2—O1^{xi}	71.49 (6)	Na2^{ii}—Cl1—Na2^{iv}	109.5
Na1^{v}—Na2—O1^{xi}	150.4 (3)	Na2^{ii}—Cl1—Na2^{v}	109.5
Cl1—Na2—O1^{xi}	83.80 (18)	Na2^{iv}—Cl1—Na2^{v}	109.5
O1^{viii}—Na2—O1^{v}	151.5 (3)	Na2^{ii}—Cl1—Na2	109.471 (1)
O1^{ix}—Na2—O1^{v}	75.84 (7)	Na2^{iv}—Cl1—Na2	109.471 (1)
O1^{x}—Na2—O1^{v}	62.95 (7)	Na2^{v}—Cl1—Na2	109.5
Na1^{xi}—Na2—O1^{v}	71.49 (6)	Na2^{ii}—Cl1—Na1	125.3
Na1^{xii}—Na2—O1^{v}	150.4 (3)	Na2^{iv}—Cl1—Na1	54.7
Na1^{v}—Na2—O1^{v}	48.20 (5)	Na2^{v}—Cl1—Na1	54.7
Cl1—Na2—O1^{v}	83.80 (18)	Na2—Cl1—Na1	125.3
O1^{xi}—Na2—O1^{v}	118.85 (6)	Na2^{ii}—Cl1—Na1^{xi}	125.3
O1^{viii}—Na2—O1^{xii}	75.84 (7)	Na2^{iv}—Cl1—Na1^{xi}	54.7
O1^{ix}—Na2—O1^{xii}	62.95 (7)	Na2^{v}—Cl1—Na1^{xi}	125.3
O1^{x}—Na2—O1^{xii}	151.5 (3)	Na2—Cl1—Na1^{xi}	54.7
Na1^{xi}—Na2—O1^{xii}	150.4 (3)	Na1—Cl1—Na1^{xi}	90.0
Na1^{xii}—Na2—O1^{xii}	48.20 (5)	Na2^{ii}—Cl1—Na1^{xv}	54.7
Na1^{v}—Na2—O1^{xii}	71.49 (6)	Na2^{iv}—Cl1—Na1^{xv}	54.7
Cl1—Na2—O1^{xii}	83.80 (18)	Na2^{v}—Cl1—Na1^{xv}	125.3
O1^{xi}—Na2—O1^{xii}	118.85 (6)	Na2—Cl1—Na1^{xv}	125.3
O1^{v}—Na2—O1^{xii}	118.85 (6)	Na1—Cl1—Na1^{xv}	90.0
O1^{viii}—Na2—Al1^{xiii}	117.7 (3)	Na1^{xi}—Cl1—Na1^{xv}	90.0
O1^{ix}—Na2—Al1^{xiii}	69.15 (13)	Na2^{ii}—Cl1—Na1^{xii}	125.3
O1^{x}—Na2—Al1^{xiii}	34.73 (6)	Na2^{iv}—Cl1—Na1^{xii}	125.3
Na1^{xi}—Na2—Al1^{xiii}	74.34 (5)	Na2^{v}—Cl1—Na1^{xii}	54.7
Na1^{xii}—Na2—Al1^{xiii}	175.4 (3)	Na2—Cl1—Na1^{xii}	54.7
Na1^{v}—Na2—Al1^{xiii}	74.34 (5)	Na1—Cl1—Na1^{xii}	90.0
Cl1—Na2—Al1^{xiii}	115.42 (15)	Na1^{xi}—Cl1—Na1^{xii}	90.0
O1^{xi}—Na2—Al1^{xiii}	108.42 (8)	Na1^{xv}—Cl1—Na1^{xii}	180.0
O1^{v}—Na2—Al1^{xiii}	33.89 (4)	Na2^{ii}—Cl1—Na1^{v}	54.7
O1^{xii}—Na2—Al1^{xiii}	130.79 (12)	Na2^{iv}—Cl1—Na1^{v}	125.3
O1^{viii}—Na2—Al1^{xiv}	69.15 (13)	Na2^{v}—Cl1—Na1^{v}	125.3
O1^{ix}—Na2—Al1^{xiv}	34.73 (6)	Na2—Cl1—Na1^{v}	54.7
O1^{x}—Na2—Al1^{xiv}	117.7 (3)	Na1—Cl1—Na1^{v}	180.0
Na1^{xi}—Na2—Al1^{xiv}	175.4 (3)	Na1^{xi}—Cl1—Na1^{v}	90.0
Na1^{xii}—Na2—Al1^{xiv}	74.34 (5)	Na1^{xv}—Cl1—Na1^{v}	90.0
Na1^{v}—Na2—Al1^{xiv}	74.34 (5)	Na1^{xii}—Cl1—Na1^{v}	90.0
Cl1—Na2—Al1^{xiv}	115.42 (15)	Na2^{ii}—Cl1—Na1^{xvi}	54.7
O1^{xi}—Na2—Al1^{xiv}	130.79 (12)	Na2^{iv}—Cl1—Na1^{xvi}	125.3
O1^{v}—Na2—Al1^{xiv}	108.42 (8)	Na2^{v}—Cl1—Na1^{xvi}	54.7
O1^{xii}—Na2—Al1^{xiv}	33.89 (4)	Na2—Cl1—Na1^{xvi}	125.3

Al1[xiii]—Na2—Al1[xiv]	102.92 (18)	Na1—Cl1—Na1[xvi]	90.0
O1[xv]—B1—O1[xvi]	119.993 (7)	Na1[xi]—Cl1—Na1[xvi]	180.0
O1[xv]—B1—O1	119.993 (7)	Na1[xv]—Cl1—Na1[xvi]	90.0
O1[xvi]—B1—O1	119.993 (7)	Na1[xii]—Cl1—Na1[xvi]	90.0
O1[xv]—B1—Na1	87.53 (15)	Na1[v]—Cl1—Na1[xvi]	90.0
O1[xvi]—B1—Na1	135.5 (3)		

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

Sodium aluminoboracite (kjh230804yoshinoN4_0m_a_1)

Crystal data

$Na_{3.92}B_4Al_3O_{12}Cl_{0.92}$	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$M_r = 438.91$	Cell parameters from 3423 reflections
Cubic, $F23$	$\theta = 4.6$–$74.3°$
$a = 13.5904$ (1) Å	$\mu = 6.78$ mm^{-1}
$V = 2510.13$ (6) Å^3	$T = 294$ K
$Z = 8$	Plate, colorless
$F(000) = 1728$	$0.08 \times 0.06 \times 0.04$ mm
$D_x = 2.323$ Mg m^{-3}	

Data collection

Bruker D8 goniometer diffractometer	5514 measured reflections
Radiation source: sealed tube	437 independent reflections
Detector resolution: 7.3910 pixels mm^{-1}	355 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.028$
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)	$\theta_{max} = 74.3°$, $\theta_{min} = 5.6°$
	$h = -16 \rightarrow 16$
	$k = -16 \rightarrow 16$
$T_{min} = 0.66$, $T_{max} = 0.75$	$l = -16 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 2.0455P]$ where $P = (F_o^2 + 2F_c^2)/3$
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.024$	$(\Delta/\sigma)_{max} = 0.006$
$wR(F^2) = 0.066$	$\Delta\rho_{max} = 0.17$ e Å^{-3}
$S = 1.12$	$\Delta\rho_{min} = -0.58$ e Å^{-3}
437 reflections	Absolute structure: Flack x determined using 142 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013).
52 parameters	
1 restraint	Absolute structure parameter: 0.01 (2)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Na1	0.0348 (5)	0.250000	0.250000	0.0429 (12)	0.5

Na2	0.5331 (5)	0.750000	0.750000	0.0430 (12)	0.5
Na3	0.3604 (4)	0.3604 (4)	0.3604 (4)	0.015 (2)	0.226 (7)
Na4	0.8610 (4)	0.8610 (4)	0.8610 (4)	0.020 (2)	0.235 (7)
B1	0.1039 (3)	0.1039 (3)	0.1039 (3)	0.0149 (10)	
B2	0.6039 (3)	0.6039 (3)	0.6039 (3)	0.0138 (10)	
Al1	0.25008 (10)	0.000000	0.000000	0.0099 (3)	
O1	0.03517 (13)	0.10051 (12)	0.17740 (13)	0.0181 (5)	
O2	0.03517 (13)	0.17741 (13)	0.60039 (12)	0.0182 (5)	
Cl1	0.250000	0.250000	0.250000	0.0359 (9)	0.921 (9)
Cl2	0.750000	0.750000	0.750000	0.0350 (9)	0.921 (9)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Na1	0.092 (4)	0.0156 (18)	0.0210 (19)	0.000	0.000	−0.0062 (17)
Na2	0.100 (4)	0.0169 (18)	0.0118 (17)	0.000	0.000	−0.0067 (16)
Na3	0.015 (2)	0.015 (2)	0.015 (2)	−0.0008 (19)	−0.0008 (19)	−0.0008 (19)
Na4	0.020 (2)	0.020 (2)	0.020 (2)	−0.002 (2)	−0.002 (2)	−0.002 (2)
B1	0.0149 (10)	0.0149 (10)	0.0149 (10)	0.0013 (13)	0.0013 (13)	0.0013 (13)
B2	0.0138 (10)	0.0138 (10)	0.0138 (10)	0.0030 (13)	0.0030 (13)	0.0030 (13)
Al1	0.0100 (5)	0.0099 (5)	0.0099 (5)	0.000	0.000	−0.0001 (4)
O1	0.0192 (9)	0.0153 (8)	0.0198 (10)	0.0061 (7)	0.0107 (8)	0.0059 (8)
O2	0.0194 (9)	0.0196 (10)	0.0156 (8)	0.0105 (8)	0.0056 (7)	0.0070 (8)
Cl1	0.0359 (9)	0.0359 (9)	0.0359 (9)	0.000	0.000	0.000
Cl2	0.0350 (9)	0.0350 (9)	0.0350 (9)	0.000	0.000	0.000

Geometric parameters (Å, º)

Na1—Na2[i]	0.922 (6)	Na3—Cl1	2.599 (10)
Na1—O1[ii]	2.2585 (18)	Na3—O1[xxi]	2.912 (2)
Na1—O1	2.2585 (18)	Na3—O1[xxii]	2.912 (2)
Na1—O2[iii]	2.452 (3)	Na3—O1[vi]	2.912 (2)
Na1—O2[iv]	2.452 (3)	Na3—Al1[xvii]	3.074 (4)
Na1—Na3[v]	2.556 (5)	Na3—Al1[xxiii]	3.074 (4)
Na1—Na3[vi]	2.556 (5)	Na4—O1[xxiv]	2.480 (6)
Na1—Cl1	2.925 (6)	Na4—O1[xxv]	2.480 (6)
Na1—B1[ii]	2.961 (4)	Na4—O1[xxvi]	2.480 (6)
Na1—B1	2.961 (4)	Na4—Cl2	2.612 (10)
Na1—Na4[vii]	3.182 (5)	Na4—O2[xxvii]	2.914 (2)
Na1—Na4[viii]	3.182 (5)	Na4—O2[xxviii]	2.914 (2)
Na2—O2[ix]	2.2602 (18)	Na4—O2[xxix]	2.914 (2)
Na2—O2[x]	2.2602 (18)	Na4—Al1[xxx]	3.069 (4)
Na2—O1[xi]	2.442 (3)	Na4—Al1[xxxi]	3.069 (4)
Na2—O1[xii]	2.442 (3)	B1—O1[xxxii]	1.3684 (16)
Na2—Na4[xiii]	2.573 (5)	B1—O1[xxxiii]	1.3684 (16)
Na2—Na4[xiv]	2.573 (5)	B1—O1	1.3684 (16)
Na2—Cl2	2.948 (6)	B2—O2[xxxiv]	1.3685 (16)
Na2—B2[xv]	2.969 (4)	B2—O2[xxxv]	1.3684 (16)

Na2—B2	2.969 (4)	B2—O2[x]	1.3684 (16)
Na2—Na3[xvi]	3.164 (5)	Al1—O2[xxxvi]	1.7495 (18)
Na2—Na3[xvii]	3.164 (5)	Al1—O2[xxxvii]	1.7495 (18)
Na3—O2[xviii]	2.488 (6)	Al1—O1[xxxviii]	1.7522 (18)
Na3—O2[xix]	2.488 (6)	Al1—O1[xxxii]	1.7522 (18)
Na3—O2[xx]	2.488 (6)		
Na2[i]—Na1—O1[ii]	90.14 (17)	Cl2—Na4—O2[xxix]	83.7 (2)
Na2[i]—Na1—O1	90.14 (17)	O2[xxvii]—Na4—O2[xxix]	118.80 (8)
O1[ii]—Na1—O1	179.7 (3)	O2[xxviii]—Na4—O2[xxix]	118.80 (8)
Na2[i]—Na1—O2[iii]	67.19 (14)	O1[xxiv]—Na4—Al1[xxx]	118.0 (4)
O1[ii]—Na1—O2[iii]	90.07 (9)	O1[xxv]—Na4—Al1[xxx]	69.23 (15)
O1—Na1—O2[iii]	90.04 (9)	O1[xxvi]—Na4—Al1[xxx]	34.80 (7)
Na2[i]—Na1—O2[iv]	67.19 (14)	Na2[xxxix]—Na4—Al1[xxx]	74.23 (8)
O1[ii]—Na1—O2[iv]	90.04 (9)	Na2[xiv]—Na4—Al1[xxx]	74.23 (8)
O1—Na1—O2[iv]	90.07 (9)	Na2[xl]—Na4—Al1[xxx]	175.4 (4)
O2[iii]—Na1—O2[iv]	134.4 (3)	Cl2—Na4—Al1[xxx]	115.28 (18)
Na2[i]—Na1—Na3[v]	123.9 (3)	O2[xxvii]—Na4—Al1[xxx]	33.88 (5)
O1[ii]—Na1—Na3[v]	74.16 (9)	O2[xxviii]—Na4—Al1[xxx]	130.86 (15)
O1—Na1—Na3[v]	105.68 (13)	O2[xxix]—Na4—Al1[xxx]	108.51 (9)
O2[iii]—Na1—Na3[v]	59.5 (2)	O1[xxiv]—Na4—Al1[xxxi]	34.80 (7)
O2[iv]—Na1—Na3[v]	159.92 (19)	O1[xxv]—Na4—Al1[xxxi]	118.0 (4)
Na2[i]—Na1—Na3[vi]	123.9 (3)	O1[xxvi]—Na4—Al1[xxxi]	69.23 (15)
O1[ii]—Na1—Na3[vi]	105.68 (13)	Na2[xxxix]—Na4—Al1[xxxi]	175.4 (4)
O1—Na1—Na3[vi]	74.16 (9)	Na2[xiv]—Na4—Al1[xxxi]	74.23 (8)
O2[iii]—Na1—Na3[vi]	159.92 (19)	Na2[xl]—Na4—Al1[xxxi]	74.23 (8)
O2[iv]—Na1—Na3[vi]	59.5 (2)	Cl2—Na4—Al1[xxxi]	115.28 (18)
Na3[v]—Na1—Na3[vi]	112.2 (5)	O2[xxvii]—Na4—Al1[xxxi]	130.86 (15)
Na2[i]—Na1—Cl1	180.0	O2[xxviii]—Na4—Al1[xxxi]	108.51 (9)
O1[ii]—Na1—Cl1	89.86 (17)	O2[xxix]—Na4—Al1[xxxi]	33.88 (5)
O1—Na1—Cl1	89.86 (17)	Al1[xxx]—Na4—Al1[xxxi]	103.1 (2)
O2[iii]—Na1—Cl1	112.81 (14)	O1[xxxii]—B1—O1[xxxiii]	119.995 (7)
O2[iv]—Na1—Cl1	112.81 (14)	O1[xxxii]—B1—O1	119.995 (7)
Na3[v]—Na1—Cl1	56.1 (3)	O1[xxxiii]—B1—O1	119.992 (7)
Na3[vi]—Na1—Cl1	56.1 (3)	O1[xxxii]—B1—Na1[xxxii]	46.89 (18)
Na2[i]—Na1—B1[ii]	108.51 (15)	O1[xxxiii]—B1—Na1[xxxii]	135.4 (3)
O1[ii]—Na1—B1[ii]	26.25 (9)	O1—B1—Na1[xxxii]	87.58 (17)
O1—Na1—B1[ii]	153.5 (2)	O1[xxxii]—B1—Na1[xxxiii]	87.58 (17)
O2[iii]—Na1—B1[ii]	114.16 (5)	O1[xxxiii]—B1—Na1[xxxiii]	46.89 (18)
O2[iv]—Na1—B1[ii]	80.61 (6)	O1—B1—Na1[xxxiii]	135.4 (3)
Na3[v]—Na1—B1[ii]	79.81 (13)	Na1[xxxii]—B1—Na1[xxxiii]	88.6 (2)
Na3[vi]—Na1—B1[ii]	79.81 (13)	O1[xxxii]—B1—Na1	135.4 (3)
Cl1—Na1—B1[ii]	71.49 (15)	O1[xxxiii]—B1—Na1	87.58 (17)
Na2[i]—Na1—B1	108.51 (15)	O1—B1—Na1	46.89 (18)
O1[ii]—Na1—B1	153.5 (2)	Na1[xxxii]—B1—Na1	88.6 (2)
O1—Na1—B1	26.25 (9)	Na1[xxxiii]—B1—Na1	88.6 (2)
O2[iii]—Na1—B1	80.61 (6)	O2[xxxiv]—B2—O2[xxxv]	119.993 (8)
O2[iv]—Na1—B1	114.16 (5)	O2[xxxiv]—B2—O2[x]	119.994 (8)

Na3^{v}—Na1—B1	79.81 (13)	O2^{xxxv}—B2—O2^{x}	119.995 (8)
Na3^{vi}—Na1—B1	79.81 (13)	O2^{xxxiv}—B2—Na2	135.7 (3)
Cl1—Na1—B1	71.49 (15)	O2^{xxxv}—B2—Na2	87.51 (17)
B1^{ii}—Na1—B1	143.0 (3)	O2^{x}—B2—Na2	46.65 (18)
Na2^{i}—Na1—Na4^{vii}	42.1 (2)	O2^{xxxiv}—B2—Na2^{xxxiii}	46.65 (18)
O1^{ii}—Na1—Na4^{vii}	129.4 (3)	O2^{xxxv}—B2—Na2^{xxxiii}	135.7 (3)
O1—Na1—Na4^{vii}	50.85 (19)	O2^{x}—B2—Na2^{xxxiii}	87.51 (17)
O2^{iii}—Na1—Na4^{vii}	60.65 (11)	Na2—B2—Na2^{xxxiii}	89.2 (2)
O2^{iv}—Na1—Na4^{vii}	85.09 (18)	O2^{xxxiv}—B2—Na2^{xxxii}	87.51 (17)
Na3^{v}—Na1—Na4^{vii}	114.45 (17)	O2^{xxxv}—B2—Na2^{xxxii}	46.65 (18)
Na3^{vi}—Na1—Na4^{vii}	114.45 (17)	O2^{x}—B2—Na2^{xxxii}	135.7 (3)
Cl1—Na1—Na4^{vii}	137.9 (2)	Na2—B2—Na2^{xxxii}	89.2 (2)
B1^{ii}—Na1—Na4^{vii}	150.6 (3)	Na2^{xxxiii}—B2—Na2^{xxxii}	89.2 (2)
B1—Na1—Na4^{vii}	66.4 (2)	O2^{xxxvi}—Al1—O2^{xxxvii}	111.44 (14)
Na2^{i}—Na1—Na4^{viii}	42.1 (2)	O2^{xxxvi}—Al1—O1^{xxxviii}	108.50 (8)
O1^{ii}—Na1—Na4^{viii}	50.85 (19)	O2^{xxxvii}—Al1—O1^{xxxviii}	108.53 (8)
O1—Na1—Na4^{viii}	129.4 (3)	O2^{xxxvi}—Al1—O1^{xxxii}	108.53 (8)
O2^{iii}—Na1—Na4^{viii}	85.09 (18)	O2^{xxxvii}—Al1—O1^{xxxii}	108.50 (8)
O2^{iv}—Na1—Na4^{viii}	60.65 (11)	O1^{xxxviii}—Al1—O1^{xxxii}	111.37 (14)
Na3^{v}—Na1—Na4^{viii}	114.45 (17)	O2^{xxxvi}—Al1—Na4^{xli}	157.72 (8)
Na3^{vi}—Na1—Na4^{viii}	114.45 (17)	O2^{xxxvii}—Al1—Na4^{xli}	68.19 (18)
Cl1—Na1—Na4^{viii}	137.9 (2)	O1^{xxxviii}—Al1—Na4^{xli}	92.00 (14)
B1^{ii}—Na1—Na4^{viii}	66.4 (2)	O1^{xxxii}—Al1—Na4^{xli}	53.90 (9)
B1—Na1—Na4^{viii}	150.6 (3)	O2^{xxxvi}—Al1—Na4^{xlii}	68.19 (18)
Na4^{vii}—Na1—Na4^{viii}	84.1 (4)	O2^{xxxvii}—Al1—Na4^{xlii}	157.72 (8)
Na1^{xii}—Na2—O2^{ix}	90.71 (17)	O1^{xxxviii}—Al1—Na4^{xlii}	53.90 (9)
Na1^{xii}—Na2—O2^{x}	90.71 (17)	O1^{xxxii}—Al1—Na4^{xlii}	92.00 (14)
O2^{ix}—Na2—O2^{x}	178.6 (3)	Na4^{xli}—Al1—Na4^{xlii}	121.1 (4)
Na1^{xii}—Na2—O1^{xi}	67.66 (14)	O2^{xxxvi}—Al1—Na3^{ii}	54.03 (9)
O2^{ix}—Na2—O1^{xi}	90.25 (9)	O2^{xxxvii}—Al1—Na3^{ii}	92.18 (13)
O2^{x}—Na2—O1^{xi}	90.29 (9)	O1^{xxxviii}—Al1—Na3^{ii}	157.61 (8)
Na1^{xii}—Na2—O1^{xii}	67.66 (15)	O1^{xxxii}—Al1—Na3^{ii}	67.99 (17)
O2^{ix}—Na2—O1^{xii}	90.29 (9)	Na4^{xli}—Al1—Na3^{ii}	103.88 (11)
O2^{x}—Na2—O1^{xii}	90.25 (9)	Na4^{xlii}—Al1—Na3^{ii}	103.88 (11)
O1^{xi}—Na2—O1^{xii}	135.3 (3)	O2^{xxxvi}—Al1—Na3^{xliii}	92.18 (13)
Na1^{xii}—Na2—Na4^{xiii}	124.0 (3)	O2^{xxxvii}—Al1—Na3^{xliii}	54.03 (9)
O2^{ix}—Na2—Na4^{xiii}	105.33 (14)	O1^{xxxviii}—Al1—Na3^{xliii}	67.99 (17)
O2^{x}—Na2—Na4^{xiii}	73.84 (9)	O1^{xxxii}—Al1—Na3^{xliii}	157.61 (8)
O1^{xi}—Na2—Na4^{xiii}	159.6 (2)	Na4^{xli}—Al1—Na3^{xliii}	103.88 (11)
O1^{xii}—Na2—Na4^{xiii}	59.2 (2)	Na4^{xlii}—Al1—Na3^{xliii}	103.88 (11)
Na1^{xii}—Na2—Na4^{xiv}	124.0 (3)	Na3^{ii}—Al1—Na3^{xliii}	121.6 (4)
O2^{ix}—Na2—Na4^{xiv}	73.84 (9)	O2^{xxxvi}—Al1—Na2^{xliv}	68.10 (10)
O2^{x}—Na2—Na4^{xiv}	105.33 (14)	O2^{xxxvii}—Al1—Na2^{xliv}	111.93 (11)
O1^{xi}—Na2—Na4^{xiv}	59.2 (2)	O1^{xxxviii}—Al1—Na2^{xliv}	42.50 (8)
O1^{xii}—Na2—Na4^{xiv}	159.6 (2)	O1^{xxxii}—Al1—Na2^{xliv}	137.46 (9)
Na4^{xiii}—Na2—Na4^{xiv}	111.9 (5)	Na4^{xli}—Al1—Na2^{xliv}	133.72 (12)
Na1^{xii}—Na2—Cl2	180.0	Na4^{xlii}—Al1—Na2^{xliv}	46.26 (12)
O2^{ix}—Na2—Cl2	89.29 (17)	Na3^{ii}—Al1—Na2^{xliv}	122.08 (10)

O2^{x}—Na2—Cl2	89.29 (17)	Na3^{xliii}—Al1—Na2^{xliv}	57.94 (10)
O1^{xi}—Na2—Cl2	112.34 (14)	O2^{xxxvi}—Al1—Na2^{xlv}	36.03 (6)
O1^{xii}—Na2—Cl2	112.34 (14)	O2^{xxxvii}—Al1—Na2^{xlv}	144.01 (8)
Na4^{xiii}—Na2—Cl2	56.0 (3)	O1^{xxxviii}—Al1—Na2^{xlv}	99.67 (11)
Na4^{xiv}—Na2—Cl2	56.0 (3)	O1^{xxxii}—Al1—Na2^{xlv}	80.31 (10)
Na1^{xii}—Na2—B2^{xv}	108.90 (15)	Na4^{xli}—Al1—Na2^{xlv}	133.72 (12)
O2^{ix}—Na2—B2^{xv}	26.12 (9)	Na4^{xlii}—Al1—Na2^{xlv}	46.26 (12)
O2^{x}—Na2—B2^{xv}	152.8 (2)	Na3^{ii}—Al1—Na2^{xlv}	57.94 (10)
O1^{xi}—Na2—B2^{xv}	114.17 (5)	Na3^{xliii}—Al1—Na2^{xlv}	122.08 (10)
O1^{xii}—Na2—B2^{xv}	80.61 (6)	Na2^{xliv}—Al1—Na2^{xlv}	74.9 (2)
Na4^{xiii}—Na2—B2^{xv}	79.56 (13)	O2^{xxxvi}—Al1—Na2^{xlvi}	144.01 (8)
Na4^{xiv}—Na2—B2^{xv}	79.56 (13)	O2^{xxxvii}—Al1—Na2^{xlvi}	36.03 (6)
Cl2—Na2—B2^{xv}	71.10 (15)	O1^{xxxviii}—Al1—Na2^{xlvi}	80.31 (10)
Na1^{xii}—Na2—B2	108.90 (15)	O1^{xxxii}—Al1—Na2^{xlvi}	99.67 (11)
O2^{ix}—Na2—B2	152.9 (2)	Na4^{xli}—Al1—Na2^{xlvi}	46.26 (12)
O2^{x}—Na2—B2	26.12 (9)	Na4^{xlii}—Al1—Na2^{xlvi}	133.72 (12)
O1^{xi}—Na2—B2	80.61 (6)	Na3^{ii}—Al1—Na2^{xlvi}	122.08 (10)
O1^{xii}—Na2—B2	114.17 (5)	Na3^{xliii}—Al1—Na2^{xlvi}	57.94 (10)
Na4^{xiii}—Na2—B2	79.56 (13)	Na2^{xliv}—Al1—Na2^{xlvi}	105.1 (2)
Na4^{xiv}—Na2—B2	79.56 (13)	Na2^{xlv}—Al1—Na2^{xlvi}	179.96 (4)
Cl2—Na2—B2	71.10 (15)	O2^{xxxvi}—Al1—Na2^{xlvii}	111.93 (11)
B2^{xv}—Na2—B2	142.2 (3)	O2^{xxxvii}—Al1—Na2^{xlvii}	68.10 (10)
Na1^{xii}—Na2—Na3^{xvi}	42.1 (2)	O1^{xxxviii}—Al1—Na2^{xlvii}	137.46 (9)
O2^{ix}—Na2—Na3^{xvi}	130.0 (3)	O1^{xxxii}—Al1—Na2^{xlvii}	42.50 (8)
O2^{x}—Na2—Na3^{xvi}	51.37 (19)	Na4^{xli}—Al1—Na2^{xlvii}	46.26 (12)
O1^{xi}—Na2—Na3^{xvi}	61.00 (11)	Na4^{xlii}—Al1—Na2^{xlvii}	133.72 (12)
O1^{xii}—Na2—Na3^{xvi}	85.47 (18)	Na3^{ii}—Al1—Na2^{xlvii}	57.94 (10)
Na4^{xiii}—Na2—Na3^{xvi}	114.53 (18)	Na3^{xliii}—Al1—Na2^{xlvii}	122.08 (10)
Na4^{xiv}—Na2—Na3^{xvi}	114.53 (18)	Na2^{xliv}—Al1—Na2^{xlvii}	179.96 (12)
Cl2—Na2—Na3^{xvi}	137.9 (2)	Na2^{xlv}—Al1—Na2^{xlvii}	105.1 (2)
B2^{xv}—Na2—Na3^{xvi}	151.0 (3)	Na2^{xlvi}—Al1—Na2^{xlvii}	74.9 (2)
B2—Na2—Na3^{xvi}	66.8 (2)	B1—O1—Al1^{xxxiii}	128.62 (14)
Na1^{xii}—Na2—Na3^{xvii}	42.1 (2)	B1—O1—Na1	106.9 (3)
O2^{ix}—Na2—Na3^{xvii}	51.37 (18)	Al1^{xxxiii}—O1—Na1	117.02 (10)
O2^{x}—Na2—Na3^{xvii}	130.0 (3)	B1—O1—Na2^{i}	121.75 (19)
O1^{xi}—Na2—Na3^{xvii}	85.47 (18)	Al1^{xxxiii}—O1—Na2^{i}	108.49 (10)
O1^{xii}—Na2—Na3^{xvii}	61.00 (11)	Na1—O1—Na2^{i}	22.20 (14)
Na4^{xiii}—Na2—Na3^{xvii}	114.53 (18)	B1—O1—Na4^{vii}	119.4 (2)
Na4^{xiv}—Na2—Na3^{xvii}	114.53 (18)	Al1^{xxxiii}—O1—Na4^{vii}	91.30 (7)
Cl2—Na2—Na3^{xvii}	137.9 (2)	Na1—O1—Na4^{vii}	84.2 (2)
B2^{xv}—Na2—Na3^{xvii}	66.8 (2)	Na2^{i}—O1—Na4^{vii}	63.0 (2)
B2—Na2—Na3^{xvii}	151.0 (3)	B1—O1—Na3^{vi}	106.5 (3)
Na3^{xvi}—Na2—Na3^{xvii}	84.2 (4)	Al1^{xxxiii}—O1—Na3^{vi}	78.1 (2)
O2^{xviii}—Na3—O2^{xix}	92.1 (3)	Na1—O1—Na3^{vi}	57.59 (12)
O2^{xviii}—Na3—O2^{xx}	92.1 (3)	Na2^{i}—O1—Na3^{vi}	71.84 (11)
O2^{xix}—Na3—O2^{xx}	92.1 (3)	Na4^{vii}—O1—Na3^{vi}	127.3 (2)
O2^{xviii}—Na3—Na1^{vi}	143.25 (16)	B2^{xlviii}—O2—Al1^{xxii}	128.66 (14)
O2^{xix}—Na3—Na1^{vi}	108.65 (10)	B2^{xlviii}—O2—Na2^{xlviii}	107.2 (3)

O2[xx]—Na3—Na1[vi]	58.15 (12)	Al1[xxii]—O2—Na2[xlviii]	116.89 (10)
O2[xviii]—Na3—Na1[xxi]	58.15 (12)	B2[xlviii]—O2—Na1[xlix]	121.99 (19)
O2[xix]—Na3—Na1[xxi]	143.26 (16)	Al1[xxii]—O2—Na1[xlix]	108.31 (10)
O2[xx]—Na3—Na1[xxi]	108.65 (10)	Na2[xlviii]—O2—Na1[xlix]	22.10 (14)
Na1[vi]—Na3—Na1[xxi]	108.1 (3)	B2[xlviii]—O2—Na3[l]	119.5 (2)
O2[xviii]—Na3—Na1[xxii]	108.65 (10)	Al1[xxii]—O2—Na3[l]	91.29 (7)
O2[xix]—Na3—Na1[xxii]	58.15 (12)	Na2[xlviii]—O2—Na3[l]	83.4 (2)
O2[xx]—Na3—Na1[xxii]	143.25 (16)	Na1[xlix]—O2—Na3[l]	62.3 (2)
Na1[vi]—Na3—Na1[xxii]	108.1 (3)	B2[xlviii]—O2—Na4[li]	106.8 (3)
Na1[xxi]—Na3—Na1[xxii]	108.1 (3)	Al1[xxii]—O2—Na4[li]	77.9 (2)
O2[xviii]—Na3—Cl1	123.8 (2)	Na2[xlviii]—O2—Na4[li]	58.00 (12)
O2[xix]—Na3—Cl1	123.8 (2)	Na1[xlix]—O2—Na4[li]	72.17 (10)
O2[xx]—Na3—Cl1	123.8 (2)	Na3[l]—O2—Na4[li]	126.9 (2)
Na1[vi]—Na3—Cl1	69.1 (3)	Na3—Cl1—Na3[ii]	109.472 (1)
Na1[xxi]—Na3—Cl1	69.1 (3)	Na3—Cl1—Na3[v]	109.5
Na1[xxii]—Na3—Cl1	69.1 (3)	Na3[ii]—Cl1—Na3[v]	109.5
O2[xviii]—Na3—O1[xxi]	75.84 (8)	Na3—Cl1—Na3[vi]	109.5
O2[xix]—Na3—O1[xxi]	151.3 (4)	Na3[ii]—Cl1—Na3[vi]	109.5
O2[xx]—Na3—O1[xxi]	62.94 (6)	Na3[v]—Cl1—Na3[vi]	109.5
Na1[vi]—Na3—O1[xxi]	71.52 (7)	Na3—Cl1—Na1[vi]	54.7
Na1[xxi]—Na3—O1[xxi]	48.25 (5)	Na3[ii]—Cl1—Na1[vi]	54.736 (1)
Na1[xxii]—Na3—O1[xxi]	150.4 (4)	Na3[v]—Cl1—Na1[vi]	125.3
Cl1—Na3—O1[xxi]	83.9 (2)	Na3[vi]—Cl1—Na1[vi]	125.3
O2[xviii]—Na3—O1[xxii]	62.94 (6)	Na3—Cl1—Na1[xxii]	54.7
O2[xix]—Na3—O1[xxii]	75.84 (8)	Na3[ii]—Cl1—Na1[xxii]	125.3
O2[xx]—Na3—O1[xxii]	151.3 (4)	Na3[v]—Cl1—Na1[xxii]	54.7
Na1[vi]—Na3—O1[xxii]	150.4 (4)	Na3[vi]—Cl1—Na1[xxii]	125.3
Na1[xxi]—Na3—O1[xxii]	71.53 (7)	Na1[vi]—Cl1—Na1[xxii]	90.0
Na1[xxii]—Na3—O1[xxii]	48.25 (5)	Na3—Cl1—Na1[xxxiii]	125.3
Cl1—Na3—O1[xxii]	83.9 (2)	Na3[ii]—Cl1—Na1[xxxiii]	54.7
O1[xxi]—Na3—O1[xxii]	118.89 (7)	Na3[v]—Cl1—Na1[xxxiii]	54.7
O2[xviii]—Na3—O1[vi]	151.3 (4)	Na3[vi]—Cl1—Na1[xxxiii]	125.3
O2[xix]—Na3—O1[vi]	62.94 (6)	Na1[vi]—Cl1—Na1[xxxiii]	90.0
O2[xx]—Na3—O1[vi]	75.84 (8)	Na1[xxii]—Cl1—Na1[xxxiii]	90.0
Na1[vi]—Na3—O1[vi]	48.25 (5)	Na3—Cl1—Na1[xxi]	54.7
Na1[xxi]—Na3—O1[vi]	150.4 (4)	Na3[ii]—Cl1—Na1[xxi]	125.3
Na1[xxii]—Na3—O1[vi]	71.52 (7)	Na3[v]—Cl1—Na1[xxi]	125.3
Cl1—Na3—O1[vi]	83.9 (2)	Na3[vi]—Cl1—Na1[xxi]	54.7
O1[xxi]—Na3—O1[vi]	118.88 (7)	Na1[vi]—Cl1—Na1[xxi]	90.0
O1[xxii]—Na3—O1[vi]	118.88 (7)	Na1[xxii]—Cl1—Na1[xxi]	90.0
O2[xviii]—Na3—Al1[xvii]	34.68 (7)	Na1[xxxiii]—Cl1—Na1[xxi]	180.0
O2[xix]—Na3—Al1[xvii]	69.06 (15)	Na3—Cl1—Na1[xxxii]	125.3
O2[xx]—Na3—Al1[xvii]	117.4 (4)	Na3[ii]—Cl1—Na1[xxxii]	54.7
Na1[vi]—Na3—Al1[xvii]	175.3 (4)	Na3[v]—Cl1—Na1[xxxii]	125.3
Na1[xxi]—Na3—Al1[xvii]	74.45 (8)	Na3[vi]—Cl1—Na1[xxxii]	54.7
Na1[xxii]—Na3—Al1[xvii]	74.45 (8)	Na1[vi]—Cl1—Na1[xxxii]	90.0
Cl1—Na3—Al1[xvii]	115.54 (18)	Na1[xxii]—Cl1—Na1[xxxii]	180.0
O1[xxi]—Na3—Al1[xvii]	108.38 (9)	Na1[xxxiii]—Cl1—Na1[xxxii]	90.0

O1^{xxii}—Na3—Al1^{xvii}	33.91 (5)	Na1^{xxi}—Cl1—Na1^{xxxii}	90.0
O1^{vi}—Na3—Al1^{xvii}	130.71 (15)	Na3—Cl1—Na1	125.3
O2^{xviii}—Na3—Al1^{xxiii}	117.4 (4)	Na3ⁱⁱ—Cl1—Na1	125.264 (1)
O2^{xix}—Na3—Al1^{xxiii}	34.68 (7)	Na3^v—Cl1—Na1	54.7
O2^{xx}—Na3—Al1^{xxiii}	69.06 (15)	Na3^{vi}—Cl1—Na1	54.7
Na1^{vi}—Na3—Al1^{xxiii}	74.45 (8)	Na1^{vi}—Cl1—Na1	180.0
Na1^{xxi}—Na3—Al1^{xxiii}	175.3 (4)	Na1^{xxii}—Cl1—Na1	90.0
Na1^{xxii}—Na3—Al1^{xxiii}	74.45 (8)	Na1^{xxxiii}—Cl1—Na1	90.0
Cl1—Na3—Al1^{xxiii}	115.54 (18)	Na1^{xxi}—Cl1—Na1	90.0
O1^{xxi}—Na3—Al1^{xxiii}	130.71 (14)	Na1^{xxii}—Cl1—Na1	90.0
O1^{xxii}—Na3—Al1^{xxiii}	108.38 (10)	Na4^{xiv}—Cl2—Na4^{xv}	109.472 (1)
O1^{vi}—Na3—Al1^{xxiii}	33.91 (5)	Na4^{xiv}—Cl2—Na4^{xiii}	109.470 (1)
Al1^{xvii}—Na3—Al1^{xxiii}	102.8 (2)	Na4^{xv}—Cl2—Na4^{xiii}	109.472 (1)
O1^{xxiv}—Na4—O1^{xxv}	92.5 (3)	Na4^{xiv}—Cl2—Na4	109.5
O1^{xxiv}—Na4—O1^{xxvi}	92.5 (3)	Na4^{xv}—Cl2—Na4	109.470 (2)
O1^{xxv}—Na4—O1^{xxvi}	92.5 (3)	Na4^{xiii}—Cl2—Na4	109.472 (1)
O1^{xxiv}—Na4—Na2^{xxxix}	143.20 (16)	Na4^{xiv}—Cl2—Na2^{xxxii}	54.7
O1^{xxv}—Na4—Na2^{xxxix}	57.75 (12)	Na4^{xv}—Cl2—Na2^{xxxii}	54.7
O1^{xxvi}—Na4—Na2^{xxxix}	108.55 (10)	Na4^{xiii}—Cl2—Na2^{xxxii}	125.264 (2)
O1^{xxiv}—Na4—Na2^{xiv}	108.55 (10)	Na4—Cl2—Na2^{xxxii}	125.3
O1^{xxv}—Na4—Na2^{xiv}	143.20 (16)	Na4^{xiv}—Cl2—Na2^{xxxix}	125.3
O1^{xxvi}—Na4—Na2^{xiv}	57.75 (12)	Na4^{xv}—Cl2—Na2^{xxxix}	125.264 (1)
Na2^{xxxix}—Na4—Na2^{xiv}	108.2 (3)	Na4^{xiii}—Cl2—Na2^{xxxix}	54.736 (1)
O1^{xxiv}—Na4—Na2^{xl}	57.75 (12)	Na4—Cl2—Na2^{xxxix}	54.7
O1^{xxv}—Na4—Na2^{xl}	108.55 (10)	Na2^{xxxii}—Cl2—Na2^{xxxix}	180.0
O1^{xxvi}—Na4—Na2^{xl}	143.20 (16)	Na4^{xiv}—Cl2—Na2^{xxxiii}	125.264 (1)
Na2^{xxxix}—Na4—Na2^{xl}	108.2 (3)	Na4^{xv}—Cl2—Na2^{xxxiii}	54.736 (1)
Na2^{xiv}—Na4—Na2^{xl}	108.2 (3)	Na4^{xiii}—Cl2—Na2^{xxxiii}	54.7
O1^{xxiv}—Na4—Cl2	123.5 (2)	Na4—Cl2—Na2^{xxxiii}	125.264 (1)
O1^{xxv}—Na4—Cl2	123.5 (2)	Na2^{xxxii}—Cl2—Na2^{xxxiii}	90.0
O1^{xxvi}—Na4—Cl2	123.5 (2)	Na2^{xxxix}—Cl2—Na2^{xxxiii}	90.0
Na2^{xxxix}—Na4—Cl2	69.3 (3)	Na4^{xiv}—Cl2—Na2^{xl}	54.736 (1)
Na2^{xiv}—Na4—Cl2	69.3 (3)	Na4^{xv}—Cl2—Na2^{xl}	125.3
Na2^{xl}—Na4—Cl2	69.3 (3)	Na4^{xiii}—Cl2—Na2^{xl}	125.264 (1)
O1^{xxiv}—Na4—O2^{xxvii}	151.8 (4)	Na4—Cl2—Na2^{xl}	54.736 (1)
O1^{xxv}—Na4—O2^{xxvii}	75.89 (8)	Na2^{xxxii}—Cl2—Na2^{xl}	90.0
O1^{xxvi}—Na4—O2^{xxvii}	62.98 (6)	Na2^{xxxix}—Cl2—Na2^{xl}	90.0
Na2^{xxxix}—Na4—O2^{xxvii}	48.16 (5)	Na2^{xxxiii}—Cl2—Na2^{xl}	180.0
Na2^{xiv}—Na4—O2^{xxvii}	71.42 (7)	Na4^{xiv}—Cl2—Na2	54.735 (1)
Na2^{xl}—Na4—O2^{xxvii}	150.3 (4)	Na4^{xv}—Cl2—Na2	125.265 (1)
Cl2—Na4—O2^{xxvii}	83.7 (2)	Na4^{xiii}—Cl2—Na2	54.735 (1)
O1^{xxiv}—Na4—O2^{xxviii}	75.89 (8)	Na4—Cl2—Na2	125.3
O1^{xxv}—Na4—O2^{xxviii}	62.98 (6)	Na2^{xxxii}—Cl2—Na2	90.000 (2)
O1^{xxvi}—Na4—O2^{xxviii}	151.8 (4)	Na2^{xxxix}—Cl2—Na2	90.0
Na2^{xxxix}—Na4—O2^{xxviii}	71.42 (7)	Na2^{xxxiii}—Cl2—Na2	90.000 (1)
Na2^{xiv}—Na4—O2^{xxviii}	150.3 (4)	Na2^{xl}—Cl2—Na2	90.0
Na2^{xl}—Na4—O2^{xxviii}	48.16 (5)	Na4^{xiv}—Cl2—Na2^{xiv}	125.3
Cl2—Na4—O2^{xxviii}	83.7 (2)	Na4^{xv}—Cl2—Na2^{xiv}	54.735 (1)

O2^{xxvii}—Na4—O2^{xxviii}	118.80 (8)	Na4^{xiii}—Cl2—Na2^{xiv}	125.265 (1)
O1^{xxiv}—Na4—O2^{xxix}	62.98 (6)	Na4—Cl2—Na2^{xiv}	54.735 (1)
O1^{xxv}—Na4—O2^{xxix}	151.8 (4)	Na2^{xxxii}—Cl2—Na2^{xiv}	90.0
O1^{xxvi}—Na4—O2^{xxix}	75.89 (8)	Na2^{xxxix}—Cl2—Na2^{xiv}	90.000 (2)
Na2^{xxxix}—Na4—O2^{xxix}	150.3 (4)	Na2^{xxxiii}—Cl2—Na2^{xiv}	90.0
Na2^{xiv}—Na4—O2^{xxix}	48.16 (5)	Na2^{xl}—Cl2—Na2^{xiv}	90.000 (1)
Na2^{xl}—Na4—O2^{xxix}	71.42 (7)	Na2—Cl2—Na2^{xiv}	180.0

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