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Crystal structure of $Li_3Ga(BO_3)_2$

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The crystal structure of trilithium gallium bis(orthoborate), $Li_3Ga(BO_3)_2$, is isotypic with $Li_3Al(BO_3)_2$ in a triclinic cell in space-group type $P\overline{1}$. The three Li and the unique Ga atom are coordinated by four O atoms each in tetrahedra, and the two B atoms are coordinated by three O atoms in orthoborate triangles. Chains with composition $[Ga_2(BO_3)_4]^{6-}$ extend along the *a* axis. The Li atoms interleave these chains in tetrahedral interstices. A comparison is made between the structure model of the title compound and that of a previously reported model for a compound with the same composition [Abdullaev & Mamedov (1972). *Zh. Strukt. Khim.* **13**, 943–946.]

1. Chemical context

We are examining the alkali metal/gallium/borate phase diagrams, investigations of which have revealed to date, among others, the homologous series $A_2Ga_2O(BO_3)_2$, in which A = Na, K, Rb, and Cs (Corbel & Leblanc, 2000; Smith, 1995; Smith *et al.*, 1997,2008, respectively) and the homologous series $A_3Ga(BO_3)_2$, in which A = Li, Na, K, Rb, and Cs. We report herein the crystal structure of the lithium analog (Fig. 1) of the latter series, which is the only one which melts congruently, which has a unique structure among the series, and which is isotypic with $Li_3Al(BO_3)_2$ (He *et al.*, 2002); the other analogs have yet to be crystallized in the form of single crystals, but are structurally distinct from the lithium analog and isotypic with each other based on their powder X-ray diffraction patterns.

A crystal structure for this compound was previously reported by Abdullaev & Mamedov (1972) in the same triclinic space-group type $P\overline{1}$, and with the same gallium-borate polyhedral pattern but with important differences with the structure reported herein, to wit: slightly different cell parameters and a different reduced cell, a significantly smaller cell volume (*i.e.*, 3% smaller), less regular bond-valence sums (BVS), greater deviations from expected interatomic distances, and irregular, five- and six-coordinate lithium-centered polyhedra. Table 1 compares interatomic distances from the structure reported by Addullaev & Mamedov (1972) and this report, with expected distances using Shannon's radii (Shannon, 1976); it also lists bond-valence sums for each structure. We have considered as bonds all Li—O distances under 3 Å from the 1972 report because doing so produces more reasonable BVS values, thus rendering some of the lithium atoms as being five- or six-coordinate in the previous structure report. It should be noted that the authors, however, reported all lithium atoms as tetrahedrally coordinated. The present structure model clearly differs from the 1972 structure

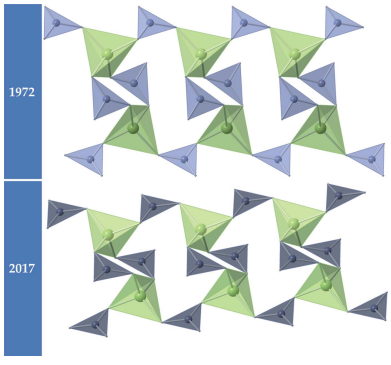

Table 1
Comparison of the two structures with composition $Li_3Ga(BO_3)_2$.

Structure model	Abdullaev & Mamedov (1972)	Current work	Shannon (1976)
Reduced cell (Å, °)	4.90 (2) 6.23 (3) 7.78 (5) 72.9 (5) 90.0 (5) 90.0 (5)	4.8731 (3) 6.2429 (4) 8.0130 (5) 73.346 (6) 89.701 (5) 89.698 (5)	
Range of interatomic distances (Å)			
Li—O	2.28±0.41	1.965±0.054	1.97
Ga—O	2.07±0.43	1.847±0.021	1.85
B—O	1.31±0.13	1.384±0.038	1.39
Bond-valence-sum values and coordination numbers (in brackets)			
Li (1, 2 & 3)	1.14 [4 + 1], 1.01 [4], 1.00 [6]	1.07 [4], 1.03 [4], 1.05 [4]	
Ga (1)	2.38 [4]	2.92 [4]	
B (1 & 2)	3.17 [3], 3.06 [3]	2.91 [3], 2.91 [3]	

model and hence indicates a second possible modification for this composition. Whether a polymorphic relation exists between the two phases remains unknown and needs additional proof by using complementary methods such as thermal analysis.

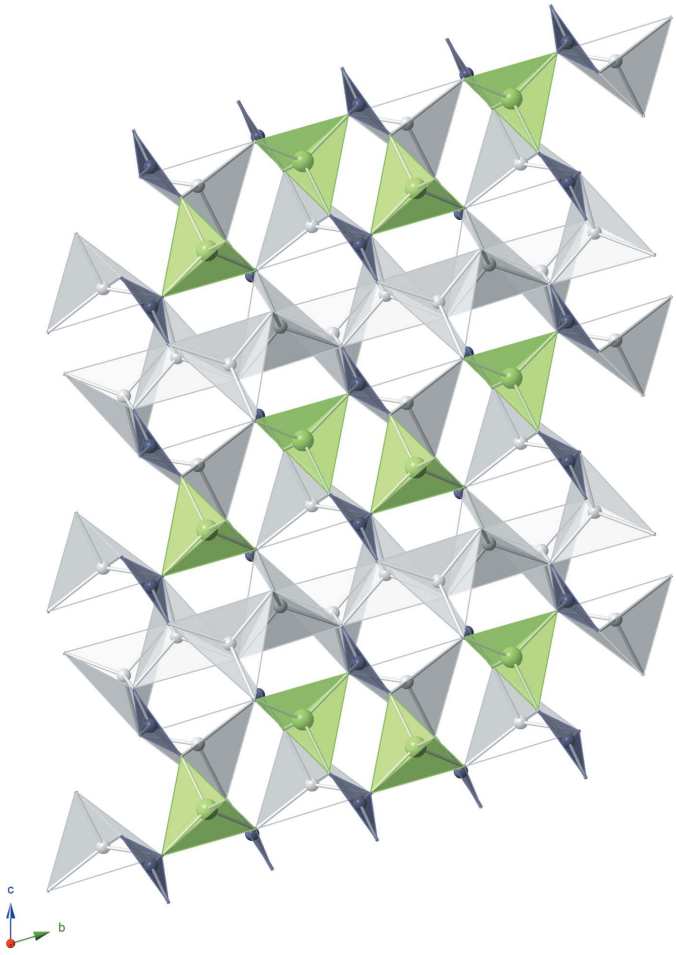

Figure 1
A projection of the crystal structure of $Li_3Ga(BO_3)_2$ along the *a* axis. Infinite $[Ga_2(BO_3)_4]^{6-}$ chains are linked together by sheets of Li atoms in tetrahedral voids. GaO_4 tetrahedra are light green, LiO_4 tetrahedra are light gray, and BO_3 triangles are blue–grey. Corner O atoms have been omitted for clarity.

2. Structural commentary

The crystal structure of the title compound consists of lithium- and gallium-centered tetrahedra and boron-centered triangles, all of which share oxygen vertices (Fig.1). Each GaO_4 tetrahedron is linked to four BO_3 triangles and six LiO_4 tetrahedra. The gallium-centered tetrahedra and boron-centered triangles adjoin through shared vertices to form infinite chains of composition $[Ga_2(BO_3)_4]^{6-}$, with the chains extending parallel to the *a* axis; lithium cations interleave the chains in tetrahedral interstices. Fig. 2 shows a comparison of the gallium-borate chains in both the previously reported structure (Abdullaev & Mamedov, 1972) and the structure presented here. The two exhibit the same connectivity but have sizeable

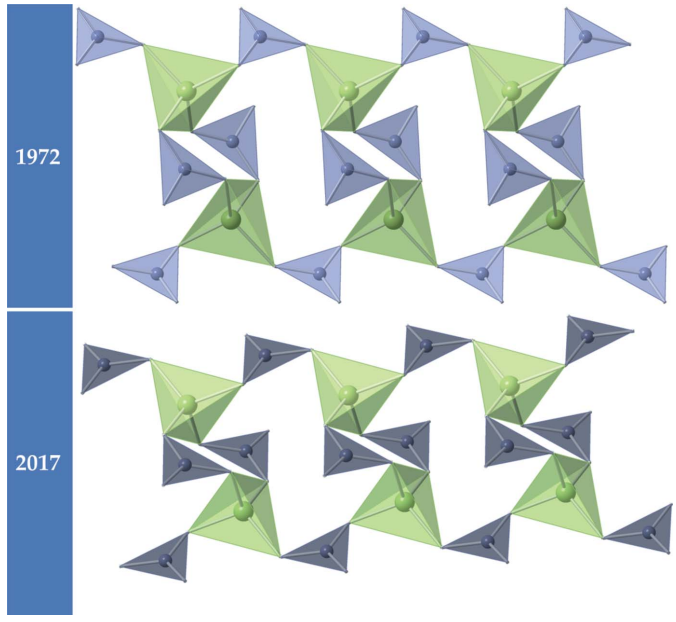

Figure 2
A comparison of the infinite $[Ga_2(BO_3)_4]^{6-}$ chains in the structures of $Li_3Ga(BO_3)_2$ with respect to the model by Abdullaev & Mamedov (1972) (top) and the structure model presented in this manuscript. The connectivity of these two chains are the same but there are important differences in the actual bonding. In our structure model, these chains run down the *c* axis. Here the GaO_4 tetrahedra are light green and the BO_3 triangles are blue–grey (which are shown in light blue–grey in the 1972 structure). Corner O atoms have been omitted for clarity.

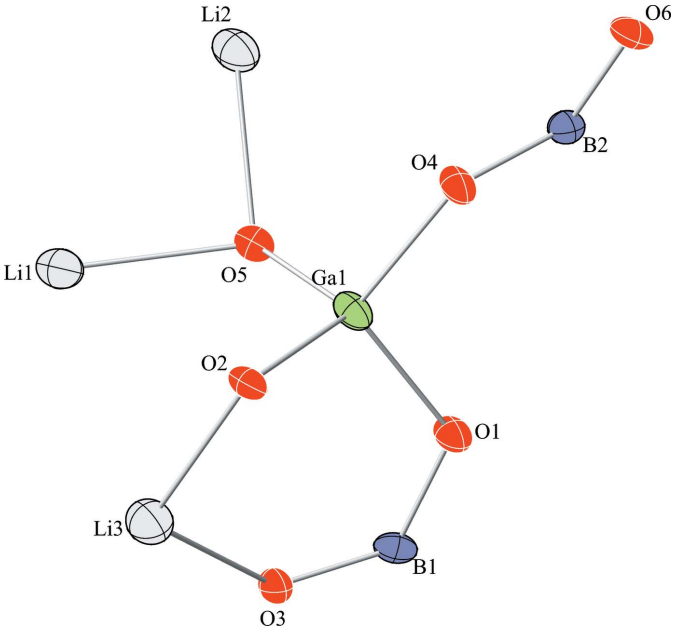

Figure 3
The asymmetric unit of the title structure with atom labelling. Displacement ellipsoids are drawn at the 75% probability level.

differences in bond lengths, bond angles and bond-valence-sum values (see Table 1). Averaged interatomic distances for the title structure are consistent with those determined from the ionic radii reported by Shannon (1976), *viz.* 1.97 (5), 1.85 (2), and 1.39 (4) Å for the experimentally determined Li—O, Ga—O, and B—O distances, respectively. We also calculated the bond-valence-um values for each element using the values provided by Brese & O'Keeffe (1991). The results (Table 1) are in good agreement with the expected values of 1, 3, 3 and 2 for Li, Ga, B and O atoms, respectively.

Lastly, Fig. 3 displays the anisotropic displacement parameters of the atoms within the asymmetric unit of the title structure.

3. Synthesis and crystallization

Powder samples were made by solid-state reactions starting with stoichiometric proportions of lithium nitrate, gallium(III) nitrate, and boric acid. We first ground the starting materials and fired them in an alumina crucible at 573 K for two h to decompose them to finely divided oxides, after which we progressively heated the samples to 973 K at 50 to 100 K and 24-hour increments, grinding the samples between each successive heat treatment. Samples were single-phase as revealed by powder X-ray diffraction.

Single crystals were grown from the melt. About 500 mg of sample were placed in a platinum dish, heated to 1033 K in a box oven, slow-cooled at 10 K h^{-1} to about 470 K, and then air-quenched. Several small, clear, colorless crystals were physically removed from the platinum crucible and mounted on a goniometer for a preliminary scan in order to find one of suitable quality.

Table 2
Experimental details.

Crystal data	
Chemical formula	$Li_3Ga(BO_3)_2$
M_r	208.16
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	4.8731 (3), 6.2429 (4), 8.0130 (5)
α, β, γ (°)	73.346 (6), 89.701 (5), 89.698 (5)
V (Å^3)	233.54 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	5.84
Crystal size (mm)	0.09 × 0.03 × 0.01
Data collection	
Diffractometer	Rigaku SCX mini diffractometer
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku Oxford Diffraction, 2015)
T_{min}, T_{max}	0.785, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2936, 1397, 1265
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.714
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.028, 0.067, 1.09
No. of reflections	1397
No. of parameters	109
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.04, −0.76

Computer programs: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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Computing details

Data collection: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015); cell refinement: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015); data reduction: *CrysAlis PRO* (Rigaku Oxford Diffraction, 2015); program(s) used to solve structure: SHELXT (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015*b*); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

Trilithium gallium bis(orthoborate)

Crystal data

$Li_3Ga(BO_3)_2$
M_r = 208.16
Triclinic, $P\overline{1}$
a = 4.8731 (3) Å
b = 6.2429 (4) Å
c = 8.0130 (5) Å
α = 73.346 (6)°
β = 89.701 (5)°
γ = 89.698 (5)°
V = 233.54 (3) Å^3
Z = 2
$F(000)$ = 196
D_x = 2.960 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 1687 reflections
θ = 2.7–32.5°
μ = 5.84 mm^{-1}
T = 293 K
Plate, clear light colourless
0.09 × 0.03 × 0.01 mm

Data collection

Rigaku SCX mini diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Rigaku Oxford Diffraction, 2015)
T_{min} = 0.785, T_{max} = 1.000
2936 measured reflections
1397 independent reflections
1265 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 30.5°, θ_{min} = 2.7°
h = −6→6
k = −8→8
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.067
S = 1.09
1397 reflections
109 parameters
0 restraints
Primary atom site location: dual
$w = 1/[\sigma^2(F_o^2) + (0.0282P)^2 + 0.1042P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.04 e Å^{-3}
$\Delta\rho_{min}$ = −0.76 e Å^{-3}

Special details

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

Refinement. Crystals of $Li_3Ga(BO_3)_2$ were mounted on MiTeGen Microloop with non-drying immersion oil. The crystal was then optically aligned on the Rigaku SCX-Mini diffractometer using a digital camera. Initial matrix images were collected to determine the unit cell, validity and proper exposure time. Three hemispheres (where φ= 0.0, 120.0 and 240.0) of data were collected with each consisting 180 images each with 1.00° widths and a 1.00° step. The structure of $Li_3Ga(BO_3)_2$ was refined using SHELXT (Sheldrick, 2015) Intrinsic Phasing and SHELXL (Sheldrick, 2015). Olex2 (Dolomanov *et al.*, 2009) was used as a graphical interface. Images of the above compound were made using CrystalMaker for Windows, version 9.2.8. The refinement proceeded without any incidents and without any need for modelling disorder or twinning or any constraints or restraints.
Refinement of the structure was based on F^2 against all reflections. The R-factor R is based on $F^2>2?(F^2)$, but is not relevant to the choice of reflections for refinement; whereas the weighted R-factor wR and goodness of fit S are based on F^2. The maximum electron denisty is 1.035 and is located 1.629 Å from Li(2), 1.960 Å from Li(1) and 2.169 Å from a different Li(1), which leads to nothing reasonable. All other maximum peaks are under 0.600.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ga1	0.65937 (6)	0.22951 (4)	0.60906 (4)	0.00968 (10)
B1	0.1691 (6)	0.0135 (5)	0.7454 (4)	0.0088 (5)
B2	0.6631 (6)	0.5014 (5)	0.2489 (4)	0.0094 (5)
O1	0.3037 (4)	0.1391 (3)	0.5958 (2)	0.0116 (4)
O2	−0.1202 (4)	−0.0028 (3)	0.7317 (2)	0.0101 (4)
O3	0.2978 (4)	−0.0830 (3)	0.8955 (2)	0.0109 (4)
O4	0.7953 (4)	0.3547 (3)	0.3900 (2)	0.0117 (4)
O5	0.3833 (4)	0.5529 (3)	0.2727 (2)	0.0100 (4)
O6	0.7921 (4)	0.5853 (3)	0.0967 (2)	0.0120 (4)
Li1	0.1828 (10)	−0.3717 (8)	1.0414 (6)	0.0154 (10)
Li2	1.1645 (10)	0.2738 (8)	0.3670 (6)	0.0143 (9)
Li3	0.6839 (10)	0.8785 (8)	−0.0399 (6)	0.0159 (10)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ga1	0.00877 (15)	0.01034 (15)	0.00789 (15)	−0.00023 (10)	0.00130 (10)	0.00064 (10)
B1	0.0103 (13)	0.0052 (11)	0.0106 (12)	0.0008 (9)	0.0021 (10)	−0.0018 (10)
B2	0.0091 (13)	0.0088 (12)	0.0095 (12)	−0.0013 (10)	0.0002 (10)	−0.0013 (10)
O1	0.0098 (9)	0.0134 (9)	0.0090 (8)	−0.0028 (7)	0.0011 (7)	0.0012 (7)
O2	0.0068 (8)	0.0105 (8)	0.0098 (8)	0.0013 (6)	0.0002 (7)	0.0020 (7)
O3	0.0107 (9)	0.0104 (8)	0.0094 (8)	−0.0007 (7)	−0.0018 (7)	0.0008 (7)
O4	0.0110 (9)	0.0138 (9)	0.0066 (8)	0.0017 (7)	0.0012 (7)	0.0030 (7)
O5	0.0088 (9)	0.0102 (8)	0.0104 (8)	0.0008 (7)	0.0013 (7)	−0.0017 (7)
O6	0.0136 (9)	0.0114 (9)	0.0088 (8)	−0.0001 (7)	0.0029 (7)	0.0005 (7)
Li1	0.019 (2)	0.013 (2)	0.013 (2)	−0.0038 (18)	0.0013 (18)	−0.0023 (18)
Li2	0.012 (2)	0.014 (2)	0.013 (2)	−0.0009 (17)	0.0008 (17)	0.0009 (17)
Li3	0.013 (2)	0.017 (2)	0.015 (2)	−0.0014 (18)	0.0000 (18)	−0.0016 (18)

Geometric parameters (Å, º)

Ga1—O1	1.8385 (18)	B1—O2	1.421 (3)
Ga1—O2^{i}	1.8440 (18)	B1—O3	1.339 (3)
Ga1—O4	1.8272 (18)	B2—O4	1.393 (3)
Ga1—O5^{ii}	1.8759 (18)	B2—O5	1.423 (3)
B1—O1	1.393 (3)	B2—O6	1.336 (3)
O1—Ga1—O2^{i}	111.84 (8)	Li1^{xii}—Li1—Li3^{vii}	149.2 (3)
O1—Ga1—O5^{ii}	102.08 (8)	Li1^{xii}—Li1—Li3^{ix}	72.2 (2)
O1—Ga1—Li1^{iii}	116.15 (10)	Li2^{ix}—Li1—Ga1^{iii}	63.94 (14)
O1—Ga1—Li2^{iv}	124.51 (10)	Li2^{ix}—Li1—Li3^{viii}	60.89 (16)
O1—Ga1—Li2^{v}	35.98 (10)	Li2^{ix}—Li1—Li3^{ii}	120.2 (2)
O1—Ga1—Li2^{vi}	86.55 (10)	Li3^{ii}—Li1—Ga1^{iii}	56.40 (12)
O1—Ga1—Li2	133.42 (11)	Li3^{vii}—Li1—Ga1^{iii}	74.07 (15)
O1—Ga1—Li3^{vii}	86.54 (11)	Li3^{viii}—Li1—Ga1^{iii}	117.59 (17)
O2^{i}—Ga1—O5^{ii}	111.37 (8)	Li3^{ix}—Li1—Ga1^{iii}	97.77 (17)
O2^{i}—Ga1—Li1^{iii}	76.62 (10)	Li3^{vii}—Li1—Li2^{ix}	117.0 (2)
O2^{i}—Ga1—Li2^{iv}	115.22 (10)	Li3^{ix}—Li1—Li2^{ix}	114.0 (2)
O2^{i}—Ga1—Li2^{v}	135.30 (11)	Li3^{ii}—Li1—Li3^{viii}	156.5 (2)
O2^{i}—Ga1—Li2^{vi}	37.59 (10)	Li3^{vii}—Li1—Li3^{viii}	107.55 (19)
O2^{i}—Ga1—Li2	77.78 (10)	Li3^{ix}—Li1—Li3^{viii}	129.60 (18)
O2^{i}—Ga1—Li3^{vii}	39.95 (11)	Li3^{vii}—Li1—Li3^{ii}	49.58 (19)
O4—Ga1—O1	109.76 (8)	Li3^{ix}—Li1—Li3^{ii}	73.05 (19)
O4—Ga1—O2^{i}	110.94 (8)	Li3^{ix}—Li1—Li3^{vii}	116.4 (2)
O4—Ga1—O5^{ii}	110.54 (8)	Ga1—Li2—Ga1^{vi}	105.15 (13)
O4—Ga1—Li1^{iii}	126.18 (10)	Ga1^{i}—Li2—Ga1^{iv}	70.59 (10)
O4—Ga1—Li2	34.37 (10)	Ga1—Li2—Ga1^{iv}	95.24 (13)
O4—Ga1—Li2^{vi}	96.01 (11)	Ga1^{i}—Li2—Ga1	104.73 (14)
O4—Ga1—Li2^{v}	74.92 (11)	Ga1^{i}—Li2—Ga1^{vi}	81.11 (11)
O4—Ga1—Li2^{iv}	78.99 (10)	Ga1^{vi}—Li2—Ga1^{iv}	148.57 (16)
O4—Ga1—Li3^{vii}	150.82 (11)	Ga1—Li2—Li3^{xiii}	135.80 (19)
O5^{ii}—Ga1—Li1^{iii}	34.75 (10)	Ga1^{i}—Li2—Li3^{xiii}	110.84 (17)
O5^{ii}—Ga1—Li2^{iv}	33.37 (10)	B1^{viii}—Li2—Ga1^{i}	136.51 (18)
O5^{ii}—Ga1—Li2^{v}	106.86 (11)	B1^{viii}—Li2—Ga1^{vi}	57.25 (11)
O5^{ii}—Ga1—Li2^{vi}	146.78 (10)	B1^{viii}—Li2—Ga1^{iv}	152.84 (18)
O5^{ii}—Ga1—Li2	116.90 (11)	B1^{viii}—Li2—Ga1	77.51 (13)
O5^{ii}—Ga1—Li3^{vii}	88.33 (11)	B1^{viii}—Li2—B2^{i}	135.2 (2)
Li1^{iii}—Ga1—Li2^{iv}	52.55 (11)	B1^{viii}—Li2—Li1^{xi}	97.11 (18)
Li2^{v}—Ga1—Li1^{iii}	137.36 (13)	B1^{viii}—Li2—Li3^{xiii}	58.70 (14)
Li2—Ga1—Li1^{iii}	110.42 (13)	B2^{i}—Li2—Ga1	146.69 (19)
Li2^{vi}—Ga1—Li1^{iii}	112.82 (12)	B2^{i}—Li2—Ga1^{vi}	100.55 (15)
Li2^{v}—Ga1—Li2	104.73 (14)	B2^{i}—Li2—Ga1^{i}	58.67 (11)
Li2—Ga1—Li2^{vi}	74.85 (13)	B2^{i}—Li2—Ga1^{iv}	53.11 (10)
Li2^{vi}—Ga1—Li2^{iv}	148.57 (16)	B2^{i}—Li2—Li1^{xi}	59.61 (14)
Li2^{v}—Ga1—Li2^{iv}	109.41 (10)	B2^{i}—Li2—Li3^{xiii}	76.46 (16)
Li2^{v}—Ga1—Li2^{vi}	98.89 (11)	O1^{i}—Li2—Ga1^{vi}	72.19 (15)
Li2—Ga1—Li2^{iv}	84.76 (13)	O1^{i}—Li2—Ga1	75.30 (16)

Li3^{vii}—Ga1—Li1^{iii}	59.79 (12)	O1^{i}—Li2—Ga1^{iv}	90.70 (18)
Li3^{vii}—Ga1—Li2^{vi}	59.91 (13)	O1^{i}—Li2—Ga1^{i}	34.43 (10)
Li3^{vii}—Ga1—Li2^{v}	121.95 (13)	O1^{i}—Li2—B1^{viii}	112.1 (2)
Li3^{vii}—Ga1—Li2	117.45 (13)	O1^{i}—Li2—B2^{i}	93.10 (19)
Li3^{vii}—Ga1—Li2^{iv}	112.26 (13)	O1^{i}—Li2—O2^{viii}	102.8 (2)
O1—B1—O2	115.8 (2)	O1^{i}—Li2—O5^{i}	105.5 (2)
O1—B1—Li2^{viii}	104.8 (2)	O1^{i}—Li2—Li1^{xi}	149.9 (3)
O1—B1—Li3^{ii}	113.6 (2)	O1^{i}—Li2—Li3^{xiii}	124.6 (2)
O2—B1—Li2^{viii}	47.04 (15)	O2^{viii}—Li2—Ga1^{vi}	32.82 (9)
O2—B1—Li3^{ii}	111.9 (2)	O2^{viii}—Li2—Ga1	102.44 (18)
O3—B1—O1	123.3 (2)	O2^{viii}—Li2—Ga1^{iv}	159.9 (2)
O3—B1—O2	120.9 (2)	O2^{viii}—Li2—Ga1^{i}	113.13 (19)
O3—B1—Li2^{viii}	113.91 (19)	O2^{viii}—Li2—B1^{viii}	30.07 (10)
O3—B1—Li3^{ii}	42.00 (16)	O2^{viii}—Li2—B2^{i}	110.6 (2)
Li3^{ii}—B1—Li2^{viii}	141.61 (18)	O2^{viii}—Li2—Li1^{xi}	99.0 (2)
O4—B2—O5	117.1 (2)	O2^{viii}—Li2—Li3^{xiii}	39.36 (13)
O4—B2—Li1^{viii}	106.0 (2)	O4—Li2—Ga1	33.11 (10)
O4—B2—Li2^{v}	88.65 (18)	O4—Li2—Ga1^{vi}	121.9 (2)
O4—B2—Li3	149.2 (2)	O4—Li2—Ga1^{i}	131.9 (2)
O5—B2—Li1^{viii}	119.8 (2)	O4—Li2—Ga1^{iv}	87.97 (18)
O5—B2—Li2^{v}	41.16 (15)	O4—Li2—B1^{viii}	71.58 (17)
O5—B2—Li3	88.65 (18)	O4—Li2—B2^{i}	136.5 (2)
O6—B2—O4	121.2 (2)	O4—Li2—O1^{i}	107.7 (2)
O6—B2—O5	121.6 (2)	O4—Li2—O2^{viii}	101.6 (2)
O6—B2—Li1^{viii}	40.79 (15)	O4—Li2—O5^{i}	108.5 (2)
O6—B2—Li2^{v}	137.1 (2)	O4—Li2—Li1^{xi}	87.7 (2)
O6—B2—Li3	37.74 (15)	O4—Li2—Li3^{xiii}	117.1 (2)
Li1^{viii}—B2—Li2^{v}	105.56 (17)	O5^{i}—Li2—Ga1^{iv}	31.06 (10)
Li1^{viii}—B2—Li3	70.99 (16)	O5^{i}—Li2—Ga1^{i}	74.16 (15)
Li3—B2—Li2^{v}	122.03 (17)	O5^{i}—Li2—Ga1^{vi}	127.9 (2)
Ga1—O1—Li2^{v}	109.59 (17)	O5^{i}—Li2—Ga1	125.0 (2)
B1—O1—Ga1	120.01 (17)	O5^{i}—Li2—B1^{viii}	140.4 (2)
B1—O1—Li2^{v}	129.9 (2)	O5^{i}—Li2—B2^{i}	27.93 (10)
Ga1^{v}—O2—Li2^{viii}	109.59 (15)	O5^{i}—Li2—O2^{viii}	129.2 (3)
Ga1^{v}—O2—Li3^{ix}	103.87 (16)	O5^{i}—Li2—Li1^{xi}	44.44 (15)
B1—O2—Ga1^{v}	123.74 (16)	O5^{i}—Li2—Li3^{xiii}	90.06 (19)
B1—O2—Li2^{viii}	102.9 (2)	Li1^{xi}—Li2—Ga1^{vi}	121.89 (19)
B1—O2—Li3^{ix}	114.5 (2)	Li1^{xi}—Li2—Ga1^{i}	116.94 (18)
Li3^{ix}—O2—Li2^{viii}	99.6 (2)	Li1^{xi}—Li2—Ga1	119.78 (18)
B1—O3—Li1	120.6 (2)	Li1^{xi}—Li2—Ga1^{iv}	63.51 (13)
B1—O3—Li3^{vii}	133.1 (2)	Li1^{xi}—Li2—Li3^{xiii}	64.81 (16)
B1—O3—Li3^{ii}	110.7 (2)	Li3^{xiii}—Li2—Ga1^{iv}	120.57 (17)
Li1—O3—Li3^{ii}	108.2 (2)	Li3^{xiii}—Li2—Ga1^{vi}	57.29 (12)
Li1—O3—Li3^{vii}	95.7 (2)	Ga1^{x}—Li3—Li1^{ii}	63.82 (13)
Li3^{vii}—O3—Li3^{ii}	81.0 (2)	Ga1^{x}—Li3—Li2^{xiii}	62.79 (13)
Ga1—O4—Li2	112.52 (17)	B1^{ii}—Li3—Ga1^{x}	121.35 (18)
B2—O4—Ga1	127.86 (17)	B1^{ii}—Li3—B2	69.64 (14)
B2—O4—Li2	119.6 (2)	B1^{ii}—Li3—Li1^{ii}	57.56 (14)

Ga1^{ii}—O5—Li1^{x}	113.47 (16)	B1^{ii}—Li3—Li1^{x}	106.5 (2)
Ga1^{ii}—O5—Li2^{v}	115.56 (17)	B1^{ii}—Li3—Li1^{xi}	80.20 (17)
B2—O5—Ga1^{ii}	113.05 (16)	B1^{ii}—Li3—Li2^{xiii}	150.9 (2)
B2—O5—Li1^{x}	110.1 (2)	B2—Li3—Ga1^{x}	168.9 (2)
B2—O5—Li2^{v}	110.9 (2)	B2—Li3—Li1^{x}	60.43 (15)
Li2^{v}—O5—Li1^{x}	92.0 (2)	B2—Li3—Li1^{ii}	127.1 (2)
B2—O6—Li1^{viii}	112.8 (2)	B2—Li3—Li1^{xi}	64.26 (15)
B2—O6—Li1^{xi}	130.9 (2)	B2—Li3—Li2^{xiii}	108.51 (19)
B2—O6—Li3	117.0 (2)	O2^{xi}—Li3—Ga1^{x}	36.18 (10)
Li1^{xi}—O6—Li1^{viii}	83.6 (2)	O2^{xi}—Li3—B1^{ii}	122.9 (2)
Li3—O6—Li1^{xi}	95.2 (2)	O2^{xi}—Li3—B2	141.0 (2)
Li3—O6—Li1^{viii}	112.6 (2)	O2^{xi}—Li3—Li1^{ii}	77.94 (18)
B2^{viii}—Li1—Ga1^{iii}	150.65 (19)	O2^{xi}—Li3—Li1^{x}	130.1 (2)
B2^{viii}—Li1—Li2^{ix}	115.6 (2)	O2^{xi}—Li3—Li1^{xi}	80.86 (19)
B2^{viii}—Li1—Li3^{ix}	107.8 (2)	O2^{xi}—Li3—Li2^{xiii}	41.01 (14)
B2^{viii}—Li1—Li3^{ii}	117.46 (19)	O2^{xi}—Li3—Li3^{xiv}	118.1 (3)
B2^{viii}—Li1—Li3^{vii}	81.65 (18)	O3^{ii}—Li3—Ga1^{x}	97.47 (18)
B2^{viii}—Li1—Li3^{viii}	54.76 (14)	O3^{x}—Li3—Ga1^{x}	73.34 (15)
O3—Li1—Ga1^{iii}	90.74 (18)	O3^{x}—Li3—B1^{ii}	116.5 (2)
O3—Li1—B2^{viii}	81.99 (18)	O3^{ii}—Li3—B1^{ii}	27.27 (10)
O3—Li1—O5^{vii}	110.1 (2)	O3^{x}—Li3—B2	101.3 (2)
O3—Li1—O6^{viii}	108.0 (2)	O3^{ii}—Li3—B2	92.9 (2)
O3—Li1—O6^{ix}	117.7 (3)	O3^{x}—Li3—O2^{xi}	103.3 (2)
O3—Li1—Li1^{xii}	125.5 (3)	O3^{ii}—Li3—O2^{xi}	112.5 (2)
O3—Li1—Li2^{ix}	153.3 (3)	O3^{x}—Li3—O3^{ii}	99.0 (2)
O3—Li1—Li3^{vii}	42.42 (15)	O3^{ii}—Li3—Li1^{x}	108.3 (2)
O3—Li1—Li3^{ii}	36.20 (14)	O3^{ii}—Li3—Li1^{xi}	103.2 (2)
O3—Li1—Li3^{viii}	133.3 (2)	O3^{x}—Li3—Li1^{x}	41.91 (14)
O3—Li1—Li3^{ix}	75.85 (19)	O3^{ii}—Li3—Li1^{ii}	35.65 (13)
O5^{vii}—Li1—Ga1^{iii}	31.78 (9)	O3^{x}—Li3—Li1^{ii}	99.1 (2)
O5^{vii}—Li1—B2^{viii}	126.2 (2)	O3^{x}—Li3—Li1^{xi}	153.9 (3)
O5^{vii}—Li1—Li1^{xii}	124.5 (3)	O3^{ii}—Li3—Li2^{xiii}	153.3 (2)
O5^{vii}—Li1—Li2^{ix}	43.60 (14)	O3^{x}—Li3—Li2^{xiii}	92.5 (2)
O5^{vii}—Li1—Li3^{viii}	86.42 (18)	O3^{ii}—Li3—Li3^{xiv}	49.37 (18)
O5^{vii}—Li1—Li3^{ix}	126.0 (2)	O3^{x}—Li3—Li3^{xiv}	49.60 (17)
O5^{vii}—Li1—Li3^{ii}	82.63 (18)	O6—Li3—Ga1^{x}	149.2 (2)
O5^{vii}—Li1—Li3^{vii}	76.30 (19)	O6—Li3—B1^{ii}	82.26 (18)
O6^{ix}—Li1—Ga1^{iii}	95.39 (18)	O6—Li3—B2	25.26 (10)
O6^{viii}—Li1—Ga1^{iii}	149.8 (2)	O6—Li3—O2^{xi}	115.8 (3)
O6^{viii}—Li1—B2^{viii}	26.37 (10)	O6—Li3—O3^{ii}	109.1 (2)
O6^{ix}—Li1—B2^{viii}	113.2 (2)	O6—Li3—O3^{x}	116.1 (3)
O6^{viii}—Li1—O5^{vii}	118.0 (2)	O6—Li3—Li1^{x}	74.64 (19)
O6^{ix}—Li1—O5^{vii}	106.5 (2)	O6—Li3—Li1^{xi}	42.94 (15)
O6^{ix}—Li1—O6^{viii}	96.4 (2)	O6—Li3—Li1^{ii}	135.9 (2)
O6^{viii}—Li1—Li1^{xii}	48.01 (17)	O6—Li3—Li2^{xiii}	86.9 (2)
O6^{ix}—Li1—Li1^{xii}	48.35 (17)	O6—Li3—Li3^{xiv}	126.2 (3)
O6^{viii}—Li1—Li2^{ix}	92.4 (2)	Li1^{x}—Li3—Ga1^{x}	112.15 (18)
O6^{ix}—Li1—Li2^{ix}	75.35 (18)	Li1^{xi}—Li3—Ga1^{x}	116.62 (19)

O6^{viii}—Li1—Li3^{vii}	103.7 (2)	Li1^{x}—Li3—Li1^{ii}	130.42 (19)
O6^{ix}—Li1—Li3^{ii}	106.1 (2)	Li1^{xi}—Li3—Li1^{x}	116.4 (2)
O6^{viii}—Li1—Li3^{ii}	143.8 (2)	Li1^{xi}—Li3—Li1^{ii}	106.95 (18)
O6^{ix}—Li1—Li3^{vii}	155.5 (3)	Li1^{x}—Li3—Li2^{xiii}	96.3 (2)
O6^{viii}—Li1—Li3^{ix}	109.5 (2)	Li1^{xi}—Li3—Li2^{xiii}	73.57 (18)
O6^{ix}—Li1—Li3^{ix}	41.90 (15)	Li2^{xiii}—Li3—Li1^{ii}	118.79 (19)
O6^{ix}—Li1—Li3^{viii}	96.9 (2)	Li3^{xiv}—Li3—Ga1^{x}	83.1 (2)
O6^{viii}—Li1—Li3^{viii}	33.21 (13)	Li3^{xiv}—Li3—B1^{ii}	70.0 (2)
Li1^{xii}—Li1—Ga1^{iii}	136.1 (3)	Li3^{xiv}—Li3—B2	100.9 (3)
Li1^{xii}—Li1—B2^{viii}	67.7 (2)	Li3^{xiv}—Li3—Li1^{xi}	150.0 (3)
Li1^{xii}—Li1—Li2^{ix}	81.0 (2)	Li3^{xiv}—Li3—Li1^{ii}	59.6 (2)
Li1^{xii}—Li1—Li3^{viii}	57.4 (2)	Li3^{xiv}—Li3—Li1^{x}	70.8 (2)
Li1^{xii}—Li1—Li3^{ii}	144.5 (3)	Li3^{xiv}—Li3—Li2^{xiii}	136.2 (3)
Ga1—O4—Li2—Ga1^{iv}	−102.80 (13)	O6—B2—O4—Li2	0.4 (4)
Ga1—O4—Li2—Ga1^{vi}	66.9 (3)	O6—B2—O5—Ga1^{ii}	−101.3 (3)
Ga1—O4—Li2—Ga1^{i}	−41.4 (3)	O6—B2—O5—Li1^{x}	26.8 (3)
Ga1—O4—Li2—B1^{viii}	95.37 (14)	O6—B2—O5—Li2^{v}	127.1 (3)
Ga1—O4—Li2—B2^{i}	−127.4 (3)	Li1^{iii}—Ga1—O1—B1	−37.0 (2)
Ga1—O4—Li2—O1^{i}	−12.7 (3)	Li1^{iii}—Ga1—O1—Li2^{v}	135.94 (19)
Ga1—O4—Li2—O2^{viii}	95.0 (2)	Li1^{iii}—Ga1—O4—B2	−105.3 (2)
Ga1—O4—Li2—O5^{i}	−126.46 (19)	Li1^{iii}—Ga1—O4—Li2	72.3 (2)
Ga1—O4—Li2—Li1^{xi}	−166.36 (14)	Li1^{viii}—B2—O4—Ga1	−140.43 (17)
Ga1—O4—Li2—Li3^{xiii}	133.58 (18)	Li1^{viii}—B2—O4—Li2	42.1 (3)
B2—O4—Li2—Ga1^{iv}	75.0 (2)	Li1^{viii}—B2—O5—Ga1^{ii}	−149.04 (15)
B2—O4—Li2—Ga1^{vi}	−115.2 (2)	Li1^{viii}—B2—O5—Li1^{x}	−21.0 (3)
B2—O4—Li2—Ga1^{i}	136.4 (2)	Li1^{viii}—B2—O5—Li2^{v}	79.3 (3)
B2—O4—Li2—Ga1	177.8 (3)	Li1^{viii}—B2—O6—Li1^{xi}	−101.9 (3)
B2—O4—Li2—B1^{viii}	−86.8 (2)	Li1^{viii}—B2—O6—Li3	133.1 (3)
B2—O4—Li2—B2^{i}	50.5 (4)	Li2^{vi}—Ga1—O1—B1	76.7 (2)
B2—O4—Li2—O1^{i}	165.1 (2)	Li2^{v}—Ga1—O1—B1	−173.0 (3)
B2—O4—Li2—O2^{viii}	−87.2 (3)	Li2^{iv}—Ga1—O1—B1	−98.1 (2)
B2—O4—Li2—O5^{i}	51.4 (3)	Li2—Ga1—O1—B1	142.1 (2)
B2—O4—Li2—Li1^{xi}	11.5 (3)	Li2—Ga1—O1—Li2^{v}	−44.96 (17)
B2—O4—Li2—Li3^{xiii}	−48.6 (3)	Li2^{vi}—Ga1—O1—Li2^{v}	−110.28 (16)
O1—Ga1—O4—B2	42.2 (2)	Li2^{iv}—Ga1—O1—Li2^{v}	74.9 (2)
O1—Ga1—O4—Li2	−140.21 (19)	Li2—Ga1—O4—B2	−177.6 (3)
O1—B1—O2—Ga1^{v}	−38.0 (3)	Li2^{iv}—Ga1—O4—B2	−80.7 (2)
O1—B1—O2—Li2^{viii}	86.5 (3)	Li2^{vi}—Ga1—O4—B2	130.6 (2)
O1—B1—O2—Li3^{ix}	−166.5 (2)	Li2^{v}—Ga1—O4—B2	33.0 (2)
O1—B1—O3—Li1	−143.3 (3)	Li2^{iv}—Ga1—O4—Li2	96.9 (2)
O1—B1—O3—Li3^{ii}	89.1 (3)	Li2^{vi}—Ga1—O4—Li2	−51.7 (2)
O1—B1—O3—Li3^{vii}	−8.1 (5)	Li2^{v}—Ga1—O4—Li2	−149.4 (3)
O2^{i}—Ga1—O1—B1	48.3 (2)	Li2^{viii}—B1—O1—Ga1	−145.49 (15)
O2^{i}—Ga1—O1—Li2^{v}	−138.71 (18)	Li2^{viii}—B1—O1—Li2^{v}	43.1 (4)
O2^{i}—Ga1—O4—B2	166.3 (2)	Li2^{viii}—B1—O2—Ga1^{v}	−124.5 (2)
O2^{i}—Ga1—O4—Li2	−16.1 (2)	Li2^{viii}—B1—O2—Li3^{ix}	107.0 (2)
O2—B1—O1—Ga1	165.44 (16)	Li2^{viii}—B1—O3—Li1	−14.5 (3)

O2—B1—O1—Li2^{v}	−5.9 (4)	Li2^{viii}—B1—O3—Li3^{vii}	120.7 (3)
O2—B1—O3—Li1	38.4 (4)	Li2^{viii}—B1—O3—Li3^{ii}	−142.1 (2)
O2—B1—O3—Li3^{ii}	−89.2 (3)	Li2^{v}—B2—O4—Ga1	−34.6 (2)
O2—B1—O3—Li3^{vii}	173.6 (3)	Li2^{v}—B2—O4—Li2	147.9 (3)
O3—B1—O1—Ga1	−13.0 (3)	Li2^{v}—B2—O5—Ga1^{ii}	131.7 (2)
O3—B1—O1—Li2^{v}	175.7 (3)	Li2^{v}—B2—O5—Li1^{x}	−100.3 (3)
O3—B1—O2—Ga1^{v}	140.4 (2)	Li2^{v}—B2—O6—Li1^{xi}	−151.7 (3)
O3—B1—O2—Li2^{viii}	−95.1 (3)	Li2^{v}—B2—O6—Li1^{viii}	−49.8 (4)
O3—B1—O2—Li3^{ix}	12.0 (3)	Li2^{v}—B2—O6—Li3	83.2 (4)
O4—Ga1—O1—B1	171.88 (18)	Li3^{vii}—Ga1—O1—B1	16.7 (2)
O4—Ga1—O1—Li2^{v}	−15.1 (2)	Li3^{vii}—Ga1—O1—Li2^{v}	−170.3 (2)
O4—B2—O5—Ga1^{ii}	80.4 (2)	Li3^{vii}—Ga1—O4—B2	162.9 (3)
O4—B2—O5—Li1^{x}	−151.6 (2)	Li3^{vii}—Ga1—O4—Li2	−19.4 (3)
O4—B2—O5—Li2^{v}	−51.3 (3)	Li3^{ii}—B1—O1—Ga1	33.9 (2)
O4—B2—O6—Li1^{viii}	78.0 (3)	Li3^{ii}—B1—O1—Li2^{v}	−137.4 (3)
O4—B2—O6—Li1^{xi}	−23.9 (4)	Li3^{ii}—B1—O2—Ga1^{v}	94.3 (2)
O4—B2—O6—Li3	−149.0 (3)	Li3^{ii}—B1—O2—Li2^{viii}	−141.2 (2)
O5^{ii}—Ga1—O1—B1	−70.85 (19)	Li3^{ii}—B1—O2—Li3^{ix}	−34.2 (3)
O5^{ii}—Ga1—O1—Li2^{v}	102.13 (18)	Li3^{ii}—B1—O3—Li1	127.6 (3)
O5^{ii}—Ga1—O4—B2	−69.7 (2)	Li3^{ii}—B1—O3—Li3^{vii}	−97.2 (3)
O5^{ii}—Ga1—O4—Li2	107.94 (19)	Li3—B2—O4—Ga1	139.9 (3)
O5—B2—O4—Ga1	−3.7 (3)	Li3—B2—O4—Li2	−37.5 (5)
O5—B2—O4—Li2	178.8 (2)	Li3—B2—O5—Ga1^{ii}	−81.93 (16)
O5—B2—O6—Li1^{viii}	−100.3 (3)	Li3—B2—O5—Li1^{x}	46.1 (2)
O5—B2—O6—Li1^{xi}	157.8 (3)	Li3—B2—O5—Li2^{v}	146.4 (2)
O5—B2—O6—Li3	32.7 (4)	Li3—B2—O6—Li1^{viii}	−133.1 (3)
O6—B2—O4—Ga1	177.91 (18)	Li3—B2—O6—Li1^{xi}	125.1 (4)

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, -y, -z+2$; (iv) $-x+2, -y+1, -z+1$; (v) $x-1, y, z$; (vi) $-x+2, -y, -z+1$; (vii) $x, y-1, z+1$; (viii) $-x+1, -y, -z+1$; (ix) $x-1, y-1, z+1$; (x) $x, y+1, z-1$; (xi) $x+1, y+1, z-1$; (xii) $-x, -y-1, -z+2$; (xiii) $-x+2, -y+1, -z$; (xiv) $-x+1, -y+2, -z$.