

Deep hydration of an $\text{Li}_{7-3x}\text{La}_3\text{Zr}_2\text{M}^{\text{III}}_x\text{O}_{12}$ solid-state electrolyte material: a case study on Al- and Ga-stabilized LLZO

Günther J. Redhammer,^{a*} Gerold Tippelt^a and Daniel Rettenwander^b

Received 16 July 2021

Accepted 18 November 2021

Edited by M. Gardiner, Australian National University, Australia

Keywords: solid-state electrolyte; LLZO; hydrothermal degradation; crystal structure; structure analysis; garnet; lattice expansion.

CCDC references: 2122845; 2122844; 2122843; 2122842

Supporting information: this article has supporting information at journals.iucr.org/c

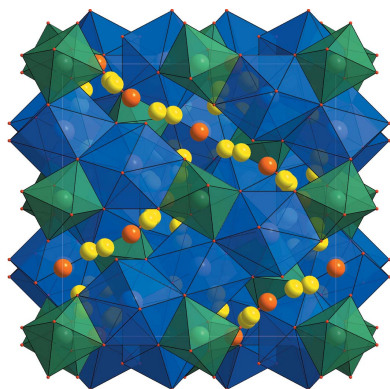
^aChemistry and Physics of Materials, University of Salzburg, Jakob Haringerstrasse 2A, 5020 Salzburg, Austria, and

^bDepartment of Materials Science and Engineering, NTNU Norwegian University of Science and Technology, Trondheim, Norway. *Correspondence e-mail: guenther.redhammer@sbg.ac.at

Single crystals of an Li-stuffed, Al- and Ga-stabilized garnet-type solid-state electrolyte material, $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO), have been analysed using single-crystal X-ray diffraction to determine the pristine structural state immediately after synthesis *via* ceramic sintering techniques. Hydrothermal treatment at 150 °C for 28 d induces a phase transition in the Al-stabilized compound from the commonly observed cubic $Ia\bar{3}d$ structure to the acentric $I\bar{4}3d$ subtype. Li^{I} ions at the interstitial octahedrally (4 + 2-fold) coordinated 48e site are most easily extracted and Al^{III} ions order onto the tetrahedral 12a site. Deep hydration induces a distinct depletion of Li^{I} at this site, while the second tetrahedral site, 12b, suffers only minor Li^{I} loss. Charge balance is maintained by the incorporation of H^{I} , which is bonded to an O atom. Hydration of Ga-stabilized LLZO induces similar effects, with complete depletion of Li^{I} at the 48e site. The $\text{Li}^{\text{I}}/\text{H}^{\text{I}}$ exchange not only leads to a distinct increase in the unit-cell size, but also alters some bonding topology, which is discussed here.

1. Introduction

The garnet family, $\text{X}_3\text{Y}_2\text{Z}_3\text{O}_{12}$, has been well described mineralogically and crystallographically in recent decades (Novak & Gibbs, 1971), and is of interest to a range of scientists from the fields of geoscience and technology, due to its thermodynamic stability in a variety of geological environments and its flexible structure, which can host ~60 different chemical elements as major and minor components (Geiger, 2013; Baxter *et al.*, 2013). Furthermore, the so-called Li-stuffed garnets, *e.g.* $\text{Li}_4\text{La}_3\text{Zr}_2\text{Li}_3\text{O}_{12}$, or as sum formula, $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO), have raised particular interest as promising materials for use as solid-state electrolytes in all solid-state Li batteries due to their superior Li-ion conductivity (Cussen, 2010; Wang *et al.*, 2020; Murugan *et al.*, 2007; Samson *et al.*, 2019). Pure end-member LLZO is tetragonal, has the space group $I4_1/acd$ (Awaka *et al.*, 2009) and has distinctly lower Li-ion conductivities. The high Li-ion conductivity is associated with the ‘standard’ cubic garnet structure with $Ia\bar{3}d$ symmetry. The latter can be stabilized by various aliovalent substitutions, *e.g.* by small amounts of Al^{III} , which – in the first experiments – entered the structure as a contaminant from the corundum crucibles during synthesis (Geiger *et al.*, 2011; Buschmann *et al.*, 2011). The incorporation of Ga^{III} into LLZO also increases the Li-ion conductivity, but induces a reduction of the symmetry to $I\bar{4}3d$ (Rettenwander *et al.*, 2016; Wagner *et al.*, 2016a; Robben *et al.*, 2016), *i.e.* the space group of hydrogarnet $\text{Ca}_3\text{Al}_2(\text{O}_4\text{H}_4)_3$ (Lager *et al.*, 1987). A stabilization of the cubic structure for nominally



OPEN ACCESS

pure LLZO is also possible by the uptake of H^I , which raises a question about LLZO stability in hydrous environments (Larraz *et al.*, 2013). Several studies have investigated the role of Li^I/H^I exchange under different environmental conditions and found that LLZO-type materials are distinctly unstable in the presence of moisture (Ma *et al.*, 2015; Galven *et al.*, 2011, 2012, 2013; Larraz *et al.*, 2015; Orera *et al.*, 2016; Liu *et al.*, 2019). Surfaces quickly degrade with the formation of $LiOH$ and Li_2CO_3 , and an increase in unit-cell parameters is observed as Li^I/H^I exchange progresses. Until now, only a few studies have systematically investigated the mechanisms behind this structural degradation. In recent studies, we have shown, using diffraction methods, that significant Li^I is especially lost from the interstitial sites of the structure in Al^{III} -, Ga^{III} - and Ta^V -substituted LLZOs during ageing at room temperature under high humidity (Hiebl *et al.*, 2019; Redhammer *et al.*, 2021a,b). In this article, we report on the deep hydration of Al- and Ga-substituted LLZO using hydrothermal treatment of single-crystalline material.

2. Experimental methodology

2.1. Synthesis and aging of material

Single crystals of Al- and Ga-stabilized LLZO were obtained using a solid-state ceramic sintering method, which has been described in detail elsewhere (Rettenwander *et al.*, 2016; Wagner *et al.*, 2016a). In brief, Li_2CO_3 (with an excess of 10%), La_2O_3 , ZrO_2 and Al_2O_3 or Ga_2O_3 were carefully mixed in the required stoichiometric proportions for the nominal compositions $Li_{6.55}La_3Zr_2Al_{0.15}O_{12}$ (Al15-LLZO) and $Li_{5.8}La_3Zr_2Ga_{0.4}O_{12}$ (Ga40-LLZO). The mixtures were pressed into pellets and preheated at 850 °C for 4 h for decarbonatization. The samples were subsequently milled in a high-energy ball mill under alcohol using ZrO_2 balls, then dried, pelletized and sintered at 1230 °C for 6 h. This yielded a dense ceramic consisting of large individual crystallites of up to 150 μm . Structural refinements were carried out on the fresh LLZOs within 24 h of synthesis to assess the unaltered structural state. Parts of the pellets were crushed carefully and aged in a 45 ml Teflon-lined autoclave (25 mg sample and 250 ml distilled water) at 150 °C for a period of 28 d. The pH value of the liquid, in which the crystals were submerged, was measured after the experiment; the pH value was ~ 13 for both compositions. The hydrated single LLZO crystallites were then filtered off and the remaining liquid was left to evaporate. The resulting precipitate was identified as Li_2CO_3 using powder diffraction (PXRD), *i.e.* proving that Li^I was extracted from the LLZO material.

2.2. Refinement

Information on data collection and refinement results is given in Table 1. Indexing the diffraction data for pristine Al-LLZO yields the space-group symmetry $Ia\bar{3}d$. Refining the structure with framework cations and O atoms results in only two strong residual electron-density peaks at the 24d and 96h positions. Assuming that Li atoms occupy only these two

positions, then there must be a distinct overpopulation at the 24d site. Thus, Al^{III} is assigned to the 24d site and its content was fixed using the chemical composition calculated from energy dispersive X-ray (EDX) analysis on a similar material synthesized using an identical experimental setup (Rettenwander *et al.*, 2016). The Li content was allowed to refine freely.

For pristine Ga-stabilized LLZO, indexing of the diffraction data yields the space-group symmetry $I\bar{4}3d$. Three different sites are identified from residual electron-density maps for the Li^I ions: at Wyckoff positions 12a, 12b and 48e. It is evident that Ga^{III} must be located at the 12a position, as the 12a site becomes distinctly overpopulated when refined with only Li^I . In subsequent refinements, both the Li1 and Li2 sites are assumed to be fully occupied and the electron density is modelled with $Li + Ga = 1$. The result is that Ga^{III} almost exclusively resides at the 12a position. Refinement of the anisotropic atomic displacement parameters (adps) is possible for all atoms using the same strategy as that applied by Wagner *et al.* (2016a,b). The data of the hydrothermally treated Ga-LLZO sample can also be indexed using $I\bar{4}3d$ symmetry when the model for untreated material is used as the starting point. The Li1 site is again assumed to be fully occupied and its electron density was modelled with $Li + Ga = 1$. This approach is considered valid as the resultant Ga^{III} content is similar (albeit slightly higher) to that obtained for the untreated sample. The Li2 and, in particular, the Li3 sites are distinctly depleted in Li and no anisotropic atomic displacement refinement is possible. Thus, the isotropic adps are adjusted and fixed to the U_{eq} value refined for the Li1 site; anisotropic adps could be obtained for Li1. Protons are located close to the O1 atom using residual electron-density maps. Fixing the U_{eq} value of hydrogen yields reliable occupation factors for this site and an almost charge-balanced chemical formula (with a slight surplus of 0.35 negative charges).

For deeply hydrated Al-LLZO, indexing of data yields a change in symmetry from $Ia\bar{3}d$ to acentric $I\bar{4}3d$. The structure of this compound is refined using the model of the Ga-stabilized LLZO, as described above for the La-, Zr- and the two O-atom positions. The electron densities at Li1 and Li2 were modelled first with only Li^+ ions. In this case, the Li1 position is distinctly overpopulated, while the occupation of the Li2 position is low, and there is no indication that the Li3 position is occupied at all. Consequently, all Al^{III} is assigned to the Li1 site and its occupation is fixed to the value used in the unaltered sample, consistent with the assumption that no Al left the structure during hydration. Refinement of the anisotropic adps is not possible for the Li1 site, and the isotropic adp is very small, so the isotropic adp of Li1 was adjusted in such a way that it has a similar value to the U_{eq} value of the Li2 site (where anisotropic adp refinements were possible) and fixed as such in subsequent refinements. Two distinct residual electron-density peaks are identified in residual electron-density maps: one high ($2.5 e \text{ \AA}^{-3}$), very close to the Zr-atom position, and another at $\sim 0.8 \text{ \AA}$ from the O1 atom. This latter (x, y, z) position is close to the proposed H-atom positions

Table 1
Experimental details.

For all structures: $Z = 8$. Experiments were carried out at 298 K with Mo $K\alpha$ radiation using a Bruker SMART APEX diffractometer. Absorption was corrected for by multi-scan methods (APEX2; Bruker, 2012). **LLZO-Al15-pristine** = fresh sample of Al-doped LLZO, measured directly after the end of the synthesis. **LLZO-Al15-hydro-150C** = Al-doped LLZO aged hydrothermally at 150 °C, **LLZO-Ga40-pristine** = fresh sample of Ga-doped LLZO, measured directly after the end of the synthesis and **LLZO-Ga40-hydro-150C** = Ga-doped LLZO aged hydrothermally at 150 °C.

	LLZO-Al15-pristine	LLZO-Al15-hydro-150C	LLZO-Ga40-pristine	LLZO-Ga40-hydro-150C
Crystal data				
Chemical formula	$\text{Al}_{0.15}\text{La}_{2.95}\text{Li}_{5.73}\text{O}_{12}\text{Zr}_2$	$\text{Al}_{0.15}\text{H}_{5.52}\text{La}_{2.88}\text{Li}_{1.64}\text{O}_{12}\text{Zr}_{1.95}$	$\text{Ga}_{0.28}\text{La}_{2.94}\text{Li}_{6.44}\text{O}_{12.00}\text{Zr}_{2.00}$	$\text{Ga}_{0.26}\text{H}_{3.90}\text{La}_{2.96}\text{Li}_{1.99}\text{O}_{12}\text{Zr}_2$
M_r	827.89	790.95	847.67	821.46
Crystal system, space group	Cubic, $Ia\bar{3}d$	Cubic, $I\bar{4}3d$	Cubic, $I\bar{4}3d$	Cubic, $I\bar{4}3d$
a (Å)	12.9637 (2)	13.0738 (2)	12.9669 (2)	13.06720 (12)
V (Å ³)	2178.65 (10)	2234.63 (10)	2180.26 (10)	2231.25 (6)
μ (mm ⁻¹)	13.24	12.61	13.88	13.57
Crystal size (mm)	0.12 × 0.11 × 0.07	0.13 × 0.12 × 0.08	0.13 × 0.13 × 0.10	0.12 × 0.11 × 0.09
Data collection				
T_{min} , T_{max}	0.22, 0.39	0.21, 0.36	0.19, 0.25	0.21, 0.36
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33130, 455, 441	34201, 819, 819	35033, 1054, 1045	35657, 918, 915
R_{int}	0.029	0.026	0.038	0.028
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.840	0.804	0.884	0.838
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.016, 0.032, 1.51	0.013, 0.029, 1.27	0.013, 0.026, 1.29	0.018, 0.037, 1.12
No. of reflections	455	819	1054	918
No. of parameters	25	44	48	43
No. of restraints	0	1	2	3
H-atom treatment	–	Only H-atom coordinates refined	–	Only H-atom coordinates refined
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.71, –0.44	0.58, –0.51	0.53, –0.65	0.54, –0.52
Absolute structure	–	Refined as an inversion twin	Refined as an inversion twin	Refined as an inversion twin
Absolute structure parameter	–	0.50 (3)	0.50 (4)	0.99944 (15)

Computer programs: APEX2 (Bruker, 2012), SIR2014 (Burla *et al.*, 2012), SHELXL2014 (Sheldrick, 2015), ORTEP-3 for Windows (Farrugia, 2012) and WinGX (Farrugia, 2012).

given by Larraz *et al.* (2013) and Orera *et al.* (2016). Hence, this residual density is assigned to the H atom, which is bonded to the O1 atom. Independent refinement of the x , y and z positions, and the occupation of the H atom is possible, whereas the isotropic adp had to be fixed. A residual density close to Zr can be explained by positional disorder at this site, similar to that reported for deeply hydrated Ta-substituted LLZO, which also transformed to the $I\bar{4}3d$ structure. However, there is a marked decrease in the reliability factors associated with the refinements when Zr^{IV} disorder is applied, *e.g.* there is no sign of another site close to O2 that would allow for another H atom to be bonded to the O2 atom. Furthermore, no reliable residual electron-density peaks can be detected.

Two additional crystals were hydrated in the same way and both were then analysed; the results are consistent with those reported in the tables and below.

3. Results and discussion

In the pristine state, Al-LLZO shows the typical garnet structure with $Ia\bar{3}d$ symmetry. La^{III} occupies the eightfold-coordinated $24c$ site with two symmetrically independent La–O bond lengths (see Table 2). A slight deficit in the La^{III} ion site occupation is observed, which is in line with previous

studies (Hiebl *et al.*, 2019; Rettenwander *et al.*, 2016; Wagner *et al.*, 2016a,b). The Zr^{IV} ions are located at the $16a$ position with a regular sixfold oxygen coordination and a bond length of

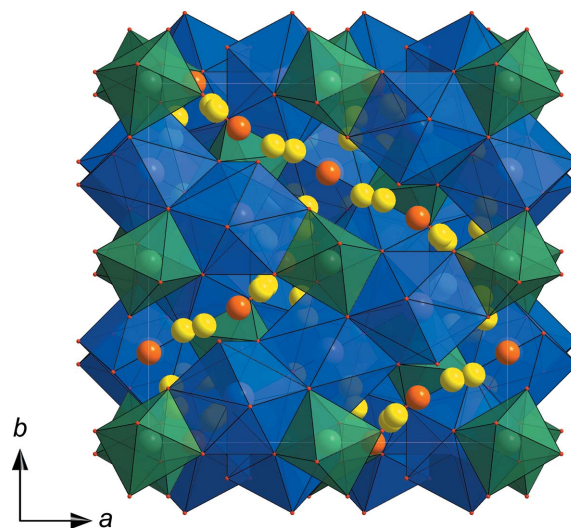


Figure 1
The crystal structure of Al-stabilized LLZO (space group $Ia\bar{3}d$) in a polyhedral format. LaO_8 sites are in light blue and ZrO_6 octahedra in sea green, whereas the Li1 (orange) and Li2 sites (yellow) are shown as spheres only for clarity and to highlight their diffusion pathway.

2.076 (16) Å. As depicted in Fig. 1, the garnet structure comprises an integrated framework constructed of edge-sharing octahedral and dodecahedral sites, in which the Li atoms are located at both the regular 24*d* tetrahedral site (Li1) and at the interstitial 96*h* position (Li2), often denoted to have a distorted octahedral coordination [Li2—O distances range between 1.854 (15) and 2.646 (14) Å, with the average of the four smaller bond lengths being 2.085 Å]. Al^{III} substitutes into the 24*d* position and the four equivalent Li—O lengths are 1.9044 (17) Å; both the 24*d* and the 96*h* positions show distinct vacancies.

The hydrothermally altered sample of Al-LLZO shows additional Bragg peaks of type *k* = odd and *l* = odd that obey *Ia* $\bar{3}$ *d* symmetry. Calculated precession images of the *hk0* plane for unaltered and altered Al-LLZO are compared in Fig. 2, where some Bragg peaks that obey *Ia* $\bar{3}$ *d* symmetry are marked. Indexing of the observed data definitively yield the space-group symmetry $\bar{I}43d$, in accordance with the findings of Larraz *et al.* (2013) and Orera *et al.* (2016) for Li¹/H¹⁻

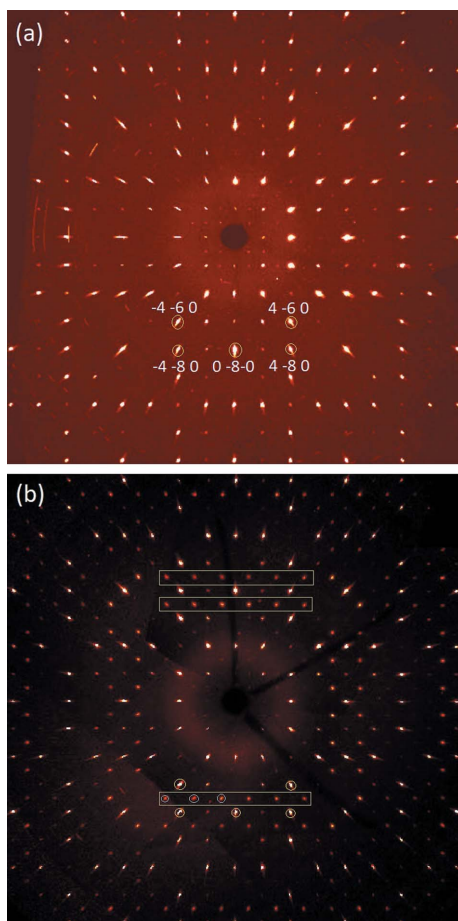


Figure 2
Reconstructed precession images of the *hk0* plane of (a) a single crystal of Al-stabilized LLZO directly after synthesis with some selected Bragg reflections indexed and (b) a single crystal after hydrothermal alteration at 150 °C for 28 d. Note the presence of sharp superstructure reflections, which obey *Ia* $\bar{3}$ *d* symmetry. In part (b), the yellow encircled Bragg reflections are the same as in part (a), while the blue encircled reflections in the rectangular box correspond (from left to right) to the $\bar{5}70$, $\bar{3}70$, $\bar{1}70$, ... Bragg reflections.

Table 2
Selected geometric parameters (Å).

LLZO-Al15-pristine			
La1—O1 ⁱ	2.5110 (17)	Li2—O1	1.854 (15)
La1—O1	2.5951 (17)	Li2—O1 ^{vii}	2.085 (14)
Zr1—O1 ⁱⁱ	2.1076 (16)	Li2—O1 ^{vi}	2.159 (15)
Li1—Li2 ⁱⁱⁱ	1.616 (14)	Li2—O1 ^{viii}	2.242 (14)
Li1—O1 ^{iv}	1.9044 (17)	Li2—Li2 ^{viii}	2.46 (2)
Li1—Li2 ^v	2.367 (14)	Li2—O1 ^{ix}	2.646 (14)
Li2—Li2 ^{vi}	0.79 (3)		
LLZO-Al15-hydro-150C			
La1—O1 ⁱ	2.506 (3)	Zr1B—O2 ^{xii}	2.06 (3)
La1—O1	2.518 (3)	Zr1B—O2 ^{iv}	2.10 (3)
La1—O2 ^x	2.544 (3)	Zr1B—O1 ⁱⁱ	2.14 (3)
La1—O2 ⁱ	2.607 (3)	Zr1B—O1 ^{xiv}	2.19 (3)
Zr1A—O1 ^{xi}	2.007 (4)	Zr1B—O1 ^{xi}	2.36 (3)
Zr1A—O2 ^{xiii}	2.217 (4)	Li1—O1 ^{xv}	1.998 (3)
Zr1B—O2 ^{xiii}	1.85 (3)	Li2—O2 ^{xvi}	1.976 (3)
LLZO-Ga40-pristine			
La1—O2 ^{xiii}	2.4935 (19)	Li2—O2 ^{xvi}	1.9246 (19)
La1—O1 ⁱ	2.5264 (19)	Li2—Li3 ^{xviii}	2.340 (9)
La1—O2 ⁱ	2.587 (2)	Li3—O1	1.878 (14)
La1—O1 ^{xvii}	2.5975 (19)	Li3—O1 ^{vii}	2.075 (8)
Zr1—O2 ^{xiii}	2.0823 (18)	Li3—O2 ⁱ	2.108 (9)
Zr1—O1 ⁱⁱ	2.1346 (18)	Li3—O1 ^{viii}	2.229 (8)
Li1—Li3 ⁱⁱⁱ	1.645 (8)	Li3—Li3 ^{vii}	2.513 (13)
Li1—O1 ^{xv}	1.8941 (18)	Li3—O2 ^{vii}	2.639 (8)
LLZO-Ga40-hydro-150C			
La1—O1 ⁱ	2.514 (3)	Li1—Li3 ⁱⁱⁱ	1.5 (2)
La1—O1 ^{xvii}	2.525 (3)	Li1—O1 ^{xv}	1.987 (4)
La1—O2 ^{xiii}	2.539 (4)	Li2—O2 ^{xvi}	1.982 (4)
La1—O2 ⁱ	2.603 (4)	Li2—Li3 ^{xviii}	3.2 (2)
Zr1—O1 ⁱⁱ	2.031 (3)	Li3—O1 ^{vii}	2.4 (2)
Zr1—O2 ^{xiii}	2.187 (4)	Li3—Li3 ^{viii}	2.6 (4)

Symmetry codes: (i) *z*, *x*, *y*; (ii) $x - \frac{1}{4}$, $z - \frac{1}{4}$, $y - \frac{1}{4}$; (iii) $-z + \frac{3}{4}$, $y - \frac{1}{4}$, $-x + \frac{1}{4}$; (iv) *z*, $-x$, $-y + \frac{1}{2}$; (v) $-y + \frac{1}{2}$, $z - \frac{1}{2}$, *x*; (vi) $-x + \frac{1}{4}$, $z - \frac{1}{4}$, $y + \frac{1}{4}$; (vii) $y - \frac{1}{4}$, $-x + \frac{1}{4}$, $-z + \frac{3}{4}$; (viii) $-y + \frac{1}{4}$, $x + \frac{1}{4}$, $-z + \frac{3}{4}$; (ix) *y*, $-z + \frac{1}{2}$, $x + \frac{1}{2}$; (x) $-x$, $y - \frac{1}{2}$, $-z + \frac{1}{2}$; (xi) $z - \frac{1}{4}$, $y - \frac{1}{4}$, $x - \frac{1}{4}$; (xii) $-y + \frac{1}{2}$, *z*, $-x$; (xiii) $-x$, $-y + \frac{1}{2}$, *z*; (xiv) $y - \frac{1}{4}$, $x - \frac{1}{4}$, $z - \frac{1}{4}$; (xv) $-z + \frac{3}{4}$, $-y + \frac{1}{4}$, $x + \frac{1}{4}$; (xvi) $x + \frac{3}{4}$, $-z + \frac{1}{4}$, $-y + \frac{3}{4}$; (xvii) *x*, $-y$, $-z + \frac{1}{2}$; (xviii) $y + \frac{3}{4}$, $-x + \frac{1}{4}$, $-z + \frac{3}{4}$.

exchanged LLZO. The symmetry reduction is associated with several rearrangements in the structural architecture. The oxygen site at 96*h* in *Ia* $\bar{3}$ *d* splits into two different 48*e* positions, *i.e.* O1 and O2, in $\bar{I}43d$, thus allowing for two different sets of Zr—O and four different La—O bond lengths. The Zr^{IV} ion shifts from (0, 0, 0) with site symmetry $\bar{3}$ (*Ia* $\bar{3}$ *d*) to the 16*c* position (*x*, *x*, *x*) with site symmetry 3 ($\bar{I}43d$). Some positional disorder is observed at the Zr position, where around 20% of the Zr^{IV} is displaced to a general 48*e* position, with a Zr—Zr offset of ~0.39 (3) Å. Free refinement of the site occupancies of these two Zr positions total 1.96 Zr^{IV} atoms per formula unit, *i.e.* very close to the expected value of 2.0. Whereas in *Ia* $\bar{3}$ *d*, the six Zr—O bond lengths are equivalent to a value of 2.1076 (16) Å. In the hydrothermally altered structure, Zr^{IV} is in a very distorted octahedral environment at 16*c*, with Zr1A—O1^{xi} bond lengths of 2.007 (4) Å (×3), and Zr1A—O2^{xiii} of 2.217 (4) Å (×3) (see Table 2 for symmetry codes). For the general position, the Zr1B—O bonds range between 1.85 (3) and 2.36 (3) Å (Table 2). It is interesting to note that a similar behaviour was found during hydrothermal alteration of Li₆La₃ZrTaO₁₂ (LLZTO). Pristine LLZTO shows *Ia* $\bar{3}$ *d* space-group symmetry but deep hydration induces

a symmetry reduction to $\bar{I}43d$. A disorder at the Zr/Ta site is also observed in hydrated LLZTO similar to that in hydrated Al-stabilized LLZO in this study. It would appear that the symmetry reduction, induced by Li^1/H^1 exchange, causes a large distortion of the O-atom environment around the 16c position and induces some positional disorder.

The regular 24d tetrahedral site of the $Ia\bar{3}d$ garnet structure splits into two different sites, 12a (Li1) and 12b (Li2), upon symmetry reduction to $\bar{I}43d$. Al^{III} is ordered onto the 12a (Li1) site but a distinct number of vacancies are observed on both sites. While ~ 4.5 apfu Li^1 occupy the interstitial 96h position in the pristine state, this position (Li3 at 48e) is completely unoccupied in the deeply hydrated form, *i.e.* all the Li^1 ions have vacated the interstitial octahedral site.

Recently, Redhammer *et al.* (2021b) observed a progressive increase of the tetrahedral site (24d and 12a) occupation in Al-stabilized LLZO during continuous Li^1/H^1 exchange in a humid atmosphere and under mild hydrothermal conditions. The shift and ordering of Li^1 from the interstitial site to the regular tetrahedral site, and the preference of Li^1 and Al^{III} for the 12a position, are described as triggers for the symmetry reduction from $Ia\bar{3}d$ to $\bar{I}43d$ (Redhammer *et al.*, 2021b). A study of the structure of the deeply hydrated samples here shows that, after complete recovery of Li^1 from the interstitial site, the tetrahedral 12a and 12b sites also take part in the Li^1/H^1 exchange. When compared to the data of Redhammer *et al.* (2021b), it is obvious that, in this study, more Li^1 is extracted from the 12a site [~ 1.4 to 0.64 (2) apfu], but there is only a moderate change in site occupation at 12b [~ 1.1 to 0.82 (2) apfu]. As Li^1 is extracted from the structure, H^1 is incorporated and bonds with the O1 atom. The Li^1 ions in the 12a tetrahedron are thus coordinated by four OH groups, with the O—H vector pointing towards the empty Li3 site (compare with Fig. 3). The proposed position of H^1 is in line with that found by Orera *et al.* (2016) for pure undoped LLZO based on neutron diffraction on polycrystalline powders. Refinements indicate that the deeply hydrated Al-LLZO has a composition of $\text{La}_{2.88}\text{Zr}_{1.95}\text{Al}_{0.15}\text{Li}_{1.64}\text{H}_{5.52}\text{O}_{12}$. It is also worth noting that a significantly lower number of La^{III} ions are found at the 24d site, so it would appear that La^{III} also leaves the structure under hydrothermal conditions. This is in line with the observations of Redhammer *et al.* (2021a,b), who observed an instability of LLZO powders in highly humid air, with decomposition of LLZO, leading to the formation of lanthanite $\text{La}_2(\text{CO}_3)_3 \cdot 8\text{H}_2\text{O}$ within ~ 30 d of exposure.

The Li^1/H^1 exchange is accompanied by a large increase in the *a* unit-cell parameter from 12.9637 (2) to 13.0738 (2) Å, which is among the largest values yet recorded for hydrated LLZO, *cf.* 13.06245 (4) Å at 77 K for hydrated LLZO with an $\text{Li}_{2.3}\text{H}_{4.7}\text{La}_3\text{Zr}_2\text{O}_{12}$ composition (Orera *et al.*, 2016) or 13.0530 (8) Å for $\text{Li}_{3.08}\text{H}_{3.52}\text{La}_3\text{Zr}_2\text{O}_{12}\text{Ta}_{0.4}$ (Yow *et al.*, 2016). A replacement of stronger Li—O bonds by weaker O—H bonds and the creation of a large number of vacant sites, especially around the empty 48e (Li3) site, both require more space and are considered responsible for the lattice expansion.

Pristine unaltered Ga-stabilized LLZO shows $\bar{I}43d$ symmetry. A section of this crystal structure is illustrated in Fig. 3,

together with that of the hydrothermally treated sample. Both the tetrahedrally coordinated 12a and 12b positions appear to be fully occupied, with the Ga^{III} ions ordered onto the 12a position. In contrast to the Li-stuffed garnets with $Ia\bar{3}d$ symmetry, the decreased number of vacancies at the regular tetrahedral sites are considered to be a characteristic feature of the $\bar{I}43d$ garnet structure. The 48e interstitial site [Li3 in Fig. 3(a)] is occupied by 3.71 Li^1 apfu, equivalent to being $\sim 62\%$ full. All of the tetrahedral faces of the fourfold oxygen coordination around the Li1 and Li2 sites are shared with neighbouring Li3 sites, with interatomic contacts of 1.645 (8) (Li1—Li3) and 2.340 (9) Å (Li2—Li3), thereby forming a three-dimensional network that is responsible for the good Li-ion conductivity in this compound. The dodecahedral site has a small number of vacancies, while the regular octahedral positions are fully occupied with Zr^{IV} , resulting in a com-

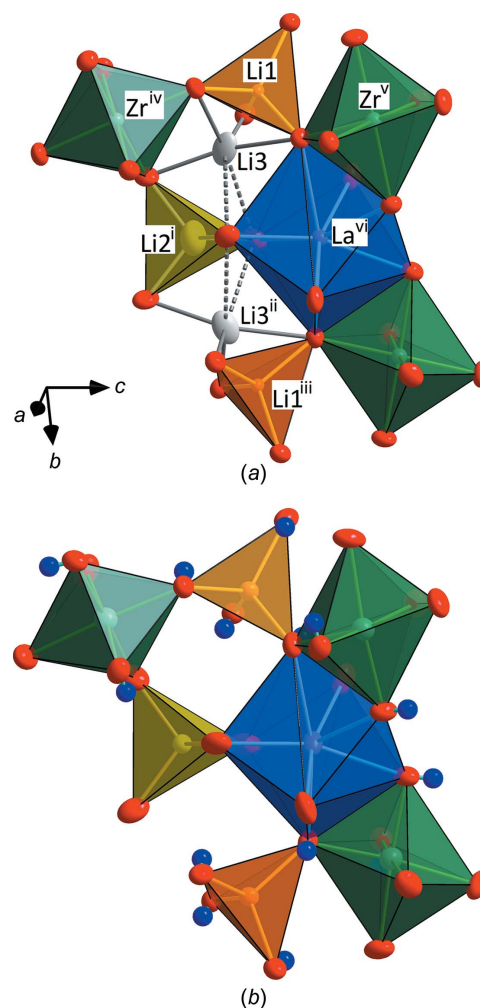


Figure 3
Polyhedral representations of part of the crystal structure of Ga-stabilized LLZO (space group $\bar{I}43d$) in the (a) pristine and (b) hydrothermally altered state viewed on the $(12, \bar{6}, 3)$ plane. LaO_8 sites are in light blue, ZrO_6 octahedra in green and Li1, Li2 and Li3 sites in orange, yellow and grey, respectively. The dashed grey bonds around the Li3 site are the two most distant. [Symmetry codes: (i) $-z + \frac{3}{4}, -y + \frac{1}{4}, x - \frac{3}{4}$; (ii) $-z + 1, -x + \frac{1}{2}, y$; (iii) $-x + 1, -y + \frac{1}{2}, z$; (iv) $-x + \frac{1}{2}, y, -z$; (v) $-x + \frac{1}{2}, -y, z + \frac{1}{2}$; (vi) $-z + \frac{3}{4}, -y + \frac{1}{4}, x + \frac{1}{4}$]

position of $\text{La}_{2.94}\text{Zr}_{2.00}\text{Ga}_{0.28}\text{Li}_{6.43}\text{O}_{12}$ for the unaltered Ga-stabilized LLZO material.

A smaller and larger set of La–O1/O2 bonds are observed at the dodecahedral site [2.4935 (19)–2.5264 (19) and 2.587 (2)–2.5975 (19) Å] and the octahedron is regular with two independent Zr–O bonds ranging between 2.0823 (18) and 2.1346 (18) Å. Therefore, the octahedra are much less distorted than those in the altered Al-LLZO with the same symmetry (Table 2). The Li1 (12a) site, which hosts Ga^{III} , is slightly smaller than the Li2 (12b) site, whereas the Li3 site, as in Al-LLZO, shows a very distorted 4 + 2-fold coordination, with bond lengths between 1.878 (4) and 2.639 (8) Å; the average of the four shorter bonds is 2.073 Å, *i.e.* slightly smaller than in the pristine Al-LLZO [see Fig. 3(a)].

As in Al-LLZO, hydrothermal treatment of Ga-LLZO induces $\text{Li}^{\text{I}}/\text{H}^{\text{I}}$ exchange. Again, a large increase of the lattice parameter to 13.06720 (12) Å is close to the value in hydrated Al-LLZO, suggesting that values around 13.07 Å represent an upper limit for lattice-parameter increase due to hydration. From site-occupation refinements, very minor Li^{I} ions are found at the interstitial 48e position, *i.e.* this site is almost completely depleted. One key difference with Al-LLZO is that no Li^{I} is lost from the 12a position. It seems that Ga^{III} ions pin Li^{I} at this site. However, Li^{I} ions are extracted from the 12b site where the amount of Li^{I} is reduced from 1.49 apfu in the pristine to 0.50 apfu in the altered sample. Protons are again located close to the O1 atom [Fig. 3(b)], giving rise to a fully hydrated $\text{Li}(\text{OH})_4$ coordination around the 12a site. Some differences to Al-LLZO are, however, evident: there is no significant reduction in the La-site occupation and no residual electron density is observed close to the Zr^{IV} ions, *i.e.* there is no indication of disorder at the 16c position in altered Ga-LLZO. Nevertheless, the ZrO_6 octahedron is much more distorted in the altered sample, with Zr–O bond lengths ranging between 2.03 (3) and 2.187 (4) Å; the difference between the two independent Zr–O bonds increases with prolonged $\text{Li}^{\text{I}}/\text{H}^{\text{I}}$ exchange. This was outlined by Redhammer *et al.* (2021b) and the data of this study fit the extrapolated trends observed there. A distinct alteration is also observed within the coordination sphere of the 24d site due to H^{I} incorporation. The most prominent effects include the reduction of the longer La1–O1^{xvii} distance by ~0.073 Å, as well as changes in the three other La–O bond lengths. In addition, Li1–O1^{xv} and Li2–O2^{xvi} are extended in the altered sample (see Table 2).

References

Awaka, J., Kijima, N., Hayakawa, H. & Akimoto, J. (2009). *J. Solid State Chem.* **182**, 2046–2052.
 Baxter, E. F., Caddick, M. J. & Ague, J. J. (2013). *Elements*, **9**, 415–419.
 Bruker (2012). *APEX2, SAINT and SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., Giacovazzo, C., Mallamo, M., Mazzone, A., Polidori, G. & Spagna, R. (2012). *J. Appl. Cryst.* **45**, 357–361.
 Buschmann, H., Dölle, J., Berendts, S., Kuhn, A., Bottke, P., Wilkening, M., Heitjans, P., Senyshyn, A., Ehrenberg, H., Lotnyk, A., Duppel, V., Kienle, L. & Janek, J. (2011). *Phys. Chem. Chem. Phys.* **13**, 19378–19392.
 Cussen, E. (2010). *Functional Oxides*, edited by D. W. Bruce, D. O'Hare & R. I. Walton, pp. 119–202. London: John Wiley & Sons Ltd.
 Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
 Galven, C., Dittmer, J., Suard, E., Le Berre, F. & Crosnier-Lopez, M.-P. (2012). *Chem. Mater.* **24**, 3335–3345.
 Galven, C., Fourquet, J.-L., Crosnier-Lopez, M.-P. & Le Berre, F. (2011). *Chem. Mater.* **23**, 1892–1900.
 Galven, C., Suard, E., Mounier, D., Crosnier-Lopez, M.-P. & Le Berre, F. (2013). *J. Mater. Res.* **28**, 2147–2153.
 Geiger, C. A. (2013). *Elements*, **9**, 447–452.
 Geiger, C. A., Alekseev, E., Lazic, B., Fisch, M., Armbruster, T., Langner, R., Fechtelkord, M., Kim, N., Pettke, T. & Weppner, W. (2011). *Inorg. Chem.* **50**, 1089–1097.
 Hiebl, C., Young, D., Wagner, R., Wilkening, H. M. R., Redhammer, G. J. & Rettenwander, D. (2019). *J. Phys. Chem. C*, **123**, 1094–1098.
 Lager, G. A., Armbruster, T. & Faber, J. (1987). *Am. Mineral.* **72**, 756–765.
 Larraz, G., Orera, A. & Sanjuán, M. L. (2013). *J. Mater. Chem. A*, **1**, 11419–11428.
 Larraz, G., Orera, A., Sanz, J., Sobrados, I., Diez-Gómez, V. & Sanjuán, M. L. (2015). *J. Mater. Chem. A*, **3**, 5683–5691.
 Liu, X., Chen, Y., Hood, Z. D., Ma, C., Yu, S., Sharafi, A., Wang, H., An, K., Sakamoto, J., Siegel, D. J., Cheng, Y., Jalarvo, N. H. & Chi, M. (2019). *Energy Environ. Sci.* **12**, 945–951.
 Ma, C., Rangasamy, E., Liang, C., Sakamoto, J., More, K. L. & Chi, M. (2015). *Angew. Chem. Int. Ed.* **54**, 129–133.
 Murugan, R., Thangadurai, V. & Weppner, W. (2007). *Angew. Chem. Int. Ed.* **46**, 7778–7781.
 Novak, G. A. & Gibbs, G. V. (1971). *Am. Mineral.* **56**, 791–825.
 Orera, A., Larraz, G., Rodríguez-Velamazán, J. A., Campo, J. & Sanjuán, M. L. (2016). *Inorg. Chem.* **55**, 1324–1332.
 Redhammer, G. J., Badami, P., Meven, M., Ganschow, S., Berendts, S., Tippelt, G. & Rettenwander, D. (2021a). *Appl. Mater. Interfaces*, **13**, 350–359.
 Redhammer, G. J., Tippelt, G., Portenkirchner, A. & Rettenwander, D. (2021b). *Crystals*, **11**, 721.
 Rettenwander, D., Redhammer, G., Preishuber-Pflügl, F., Cheng, L., Miara, L., Wagner, R., Welzl, A., Suard, E., Doeff, M. M., Wilkening, M., Fleig, J. & Amthauer, G. (2016). *Chem. Mater.* **28**, 2384–2392.
 Robben, L., Merzlyakova, E., Heitjans, P. & Gesing, T. M. (2016). *Acta Cryst. E* **72**, 287–289.
 Samson, A. J., Hofstetter, K., Bag, S. & Thangadurai, V. (2019). *Energy Environ. Sci.* **12**, 2957–2975.
 Sheldrick, G. M. (2015). *Acta Cryst. C* **71**, 3–8.
 Wagner, R., Redhammer, G. J., Rettenwander, D., Senyshyn, A., Schmidt, W., Wilkening, M. & Amthauer, G. (2016a). *Chem. Mater.* **28**, 1861–1871.
 Wagner, R., Redhammer, G. J., Rettenwander, D., Tippelt, G., Welzl, A., Taibl, S., Fleig, J., Franz, A., Lottermoser, W. & Amthauer, G. (2016b). *Chem. Mater.* **28**, 5943–5951.
 Wang, C., Fu, K., Kammampata, S. P., McOwen, D. W., Samson, A. J., Zhang, L., Hitz, G. T., Nolan, A. M., Wachsman, E. D., Mo, Y., Thangadurai, V. & Hu, L. (2020). *Chem. Rev.* **120**, 4257–4300.
 Yow, Z. F., Oh, Y. L., Gu, W. Y., Rao, R. P. & Adams, S. (2016). *Solid State Ionics*, **292**, 122–129.

supporting information

Acta Cryst. (2022). C78, 1-6 [https://doi.org/10.1107/S2053229621012250]

Deep hydration of an $\text{Li}_{7-3x}\text{La}_3\text{Zr}_2\text{M}^{\text{III}}_x\text{O}_{12}$ solid-state electrolyte material: a case study on Al- and Ga-stabilized LLZO

Günther J. Redhammer, Gerold Tippelt and Daniel Rettenwander

Computing details

For all structures, data collection: *APEX2* (Bruker, 2012); cell refinement: *APEX2* (Bruker, 2012); data reduction: *APEX2* (Bruker, 2012); program(s) used to solve structure: *SIR2014* (Burla *et al.*, 2012); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

(LLZO-Al15-pristine)

Crystal data

$\text{Al}_{0.15}\text{La}_{2.95}\text{Li}_{5.73}\text{O}_{12}\text{Zr}_2$

$M_r = 827.89$

Cubic, $Ia\bar{3}d$

Hall symbol: -I 4bd 2c 3

$a = 12.9637(2) \text{ \AA}$

$V = 2178.65(10) \text{ \AA}^3$

$Z = 8$

$F(000) = 2906$

$D_x = 5.048 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 33130 reflections

$\theta = 3.9\text{--}36.6^\circ$

$\mu = 13.24 \text{ mm}^{-1}$

$T = 298 \text{ K}$

Cuboid, colorless

$0.12 \times 0.11 \times 0.07 \text{ mm}$

Data collection

Bruker SMART APEX
diffractometer

Graphite monochromator

rotation, ω -scans at 4 different φ positions

Absorption correction: multi-scan

(*APEX2*; Bruker, 2012)

$T_{\text{min}} = 0.22$, $T_{\text{max}} = 0.39$

33130 measured reflections

455 independent reflections

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

$R_{\text{int}} = 0.029$

$\theta_{\text{max}} = 36.6^\circ$, $\theta_{\text{min}} = 3.9^\circ$

$h = -21 \rightarrow 21$

$k = -21 \rightarrow 21$

$l = -21 \rightarrow 21$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.016$

$wR(F^2) = 0.032$

$S = 1.51$

455 reflections

25 parameters

0 restraints

0 constraints

$w = 1/[\sigma^2(F_o^2) + (0.0044P)^2 + 13.2478P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.71 \text{ e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.44 \text{ e \AA}^{-3}$

Extinction correction: SHELXL2014

(Sheldrick, 2015),

$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00041 (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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
La1	0.125	0	0.25	0.00857 (8)	0.983 (3)
Zr1	0	0	0	0.00669 (12)	
O1	0.09999 (13)	0.19604 (13)	0.28188 (13)	0.0117 (3)	
Li1	0.375	0	0.25	0.022 (6)	0.47 (6)
Al1	0.375	0	0.25	0.022 (5)	0.05
Li2	0.0961 (10)	0.1880 (11)	0.4246 (11)	0.023 (4)*	0.36 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.01087 (11)	0.00742 (9)	0.00742 (9)	0	0	0.00134 (7)
Zr1	0.00669 (12)	0.00669 (12)	0.00669 (12)	0.00008 (8)	0.00008 (8)	0.00008 (8)
O1	0.0092 (6)	0.0120 (7)	0.0140 (7)	-0.0016 (5)	0.0003 (5)	0.0004 (5)
Li1	0.009 (9)	0.029 (12)	0.029 (12)	0	0	0
Al1	0.009 (15)	0.029 (9)	0.029 (9)	0	0	0

Geometric parameters (\AA , $^\circ$)

La1—O1 ⁱ	2.5110 (17)	O1—Zr1 ^{xv}	2.1076 (16)
La1—O1 ⁱⁱ	2.5110 (17)	O1—Li2 ^v	2.159 (15)
La1—O1 ⁱⁱⁱ	2.5110 (17)	O1—Li2 ^{xxii}	2.242 (14)
La1—O1 ^{iv}	2.5110 (17)	O1—La1 ^{xx}	2.5110 (17)
La1—O1	2.5951 (17)	O1—Li2 ^x	2.646 (14)
La1—O1 ^v	2.5952 (17)	Li1—Li2 ^{xi}	1.616 (14)
La1—O1 ^{vi}	2.5952 (17)	Li1—Li2 ^{viii}	1.616 (14)
La1—O1 ^{vii}	2.5952 (17)	Li1—Li2 ⁱ	1.616 (14)
La1—Li2 ^{viii}	2.992 (14)	Li1—Li2 ⁱⁱⁱ	1.616 (14)
La1—Li2 ^{ix}	2.992 (14)	Li1—O1 ^{viii}	1.9044 (17)
La1—Li2 ^x	2.992 (14)	Li1—O1 ⁱⁱⁱ	1.9044 (17)
La1—Li2 ^{xi}	2.992 (14)	Li1—O1 ^{xi}	1.9044 (17)
Zr1—O1 ^{xii}	2.1076 (16)	Li1—O1 ⁱ	1.9044 (17)
Zr1—O1 ^{vii}	2.1076 (16)	Li1—Li2 ^{xxiii}	2.367 (14)
Zr1—O1 ^{xiii}	2.1076 (16)	Li1—Li2 ^{xxiv}	2.367 (14)
Zr1—O1 ⁱⁱ	2.1076 (16)	Li1—Li2 ^{xxv}	2.367 (14)
Zr1—O1 ^{xiv}	2.1076 (16)	Li1—Li2 ^{xxvi}	2.367 (14)
Zr1—O1 ^{xv}	2.1076 (16)	Li2—Li2 ^v	0.79 (3)
Zr1—Li2 ^{ix}	2.906 (15)	Li2—Al1 ^{xx}	1.616 (14)
Zr1—Li2 ^{xvi}	2.906 (15)	Li2—Li1 ^{xx}	1.616 (14)
Zr1—Li2 ^{xvii}	2.906 (15)	Li2—O1 ^{xxii}	2.085 (14)

Zr1—Li2 ^{xviii}	2.906 (15)	Li2—O1 ^v	2.159 (15)
Zr1—Li2 ^{xix}	2.906 (15)	Li2—O1 ^{xxi}	2.242 (14)
Zr1—Li2 ^{vi}	2.906 (15)	Li2—Al1 ^{xxvii}	2.367 (14)
O1—Li2	1.854 (15)	Li2—Li1 ^{xxvii}	2.367 (14)
O1—Al1 ^{xx}	1.9044 (17)	Li2—Li2 ^{xxii}	2.46 (2)
O1—Li1 ^{xx}	1.9044 (17)	Li2—Li2 ^{xxi}	2.46 (2)
O1—Li2 ^{xxi}	2.085 (14)	Li2—O1 ^{xxviii}	2.646 (14)
O1 ⁱ —La1—O1 ⁱⁱ	111.62 (8)	Li1 ^{xx} —O1—La1 ^{xx}	93.43 (7)
O1 ⁱ —La1—O1 ⁱⁱⁱ	71.83 (8)	Li2 ^{xxi} —O1—La1 ^{xx}	80.6 (4)
O1 ⁱⁱ —La1—O1 ⁱⁱⁱ	160.65 (7)	Zr1 ^{xv} —O1—La1 ^{xx}	103.01 (7)
O1 ⁱ —La1—O1 ^{iv}	160.65 (7)	Li2 ^v —O1—La1 ^{xx}	164.2 (4)
O1 ⁱⁱ —La1—O1 ^{iv}	71.83 (8)	Li2 ^{xxii} —O1—La1 ^{xx}	77.8 (4)
O1 ⁱⁱⁱ —La1—O1 ^{iv}	111.62 (8)	Li2—O1—La1	96.1 (5)
O1 ⁱ —La1—O1	68.90 (7)	Al1 ^{xx} —O1—La1	123.07 (7)
O1 ⁱⁱ —La1—O1	73.03 (6)	Li1 ^{xx} —O1—La1	123.07 (7)
O1 ⁱⁱⁱ —La1—O1	124.22 (3)	Li2 ^{xxi} —O1—La1	170.6 (4)
O1 ^{iv} —La1—O1	95.13 (5)	Zr1 ^{xv} —O1—La1	100.28 (6)
O1 ⁱ —La1—O1 ^v	95.13 (5)	Li2 ^v —O1—La1	89.0 (4)
O1 ⁱⁱ —La1—O1 ^v	124.22 (3)	Li2 ^{xxii} —O1—La1	85.3 (4)
O1 ⁱⁱⁱ —La1—O1 ^v	73.03 (6)	La1 ^{xx} —O1—La1	102.03 (6)
O1 ^{iv} —La1—O1 ^v	68.90 (7)	Li2—O1—Li2 ^x	78.6 (7)
O1—La1—O1 ^v	72.77 (8)	Al1 ^{xx} —O1—Li2 ^x	60.1 (3)
O1 ⁱ —La1—O1 ^{vi}	124.22 (3)	Li1 ^{xx} —O1—Li2 ^x	60.1 (3)
O1 ⁱⁱ —La1—O1 ^{vi}	95.13 (5)	Li2 ^{xxi} —O1—Li2 ^x	102.4 (4)
O1 ⁱⁱⁱ —La1—O1 ^{vi}	68.90 (7)	Zr1 ^{xv} —O1—Li2 ^x	169.9 (3)
O1 ^{iv} —La1—O1 ^{vi}	73.03 (6)	Li2 ^v —O1—Li2 ^x	94.4 (3)
O1—La1—O1 ^{vi}	165.64 (7)	Li2 ^{xxii} —O1—Li2 ^x	16.0 (6)
O1 ^v —La1—O1 ^{vi}	109.12 (7)	La1 ^{xx} —O1—Li2 ^x	79.2 (3)
O1 ⁱ —La1—O1 ^{vii}	73.03 (6)	La1—O1—Li2 ^x	69.6 (3)
O1 ⁱⁱ —La1—O1 ^{vii}	68.90 (7)	Li2 ^{xi} —Li1—Li2 ^{viii}	133.1 (10)
O1 ⁱⁱⁱ —La1—O1 ^{vii}	95.13 (5)	Li2 ^{xi} —Li1—Li2 ⁱ	99.1 (4)
O1 ^{iv} —La1—O1 ^{vii}	124.22 (3)	Li2 ^{viii} —Li1—Li2 ⁱ	99.1 (4)
O1—La1—O1 ^{vii}	109.12 (7)	Li2 ^{xi} —Li1—Li2 ⁱⁱⁱ	99.1 (4)
O1 ^v —La1—O1 ^{vii}	165.64 (7)	Li2 ^{viii} —Li1—Li2 ⁱⁱⁱ	99.1 (4)
O1 ^{vi} —La1—O1 ^{vii}	72.77 (8)	Li2 ⁱ —Li1—Li2 ⁱⁱⁱ	133.1 (10)
O1 ⁱ —La1—Li2 ^{viii}	43.4 (3)	Li2 ^{xi} —Li1—O1 ^{viii}	163.6 (5)
O1 ⁱⁱ —La1—Li2 ^{viii}	147.5 (3)	Li2 ^{viii} —Li1—O1 ^{viii}	62.9 (5)
O1 ⁱⁱⁱ —La1—Li2 ^{viii}	47.1 (3)	Li2 ⁱ —Li1—O1 ^{viii}	78.7 (5)
O1 ^{iv} —La1—Li2 ^{viii}	124.3 (3)	Li2 ⁱⁱⁱ —Li1—O1 ^{viii}	72.1 (5)
O1—La1—Li2 ^{viii}	77.2 (3)	Li2 ^{xi} —Li1—O1 ⁱⁱⁱ	72.1 (5)
O1 ^v —La1—Li2 ^{viii}	56.0 (3)	Li2 ^{viii} —Li1—O1 ⁱⁱⁱ	78.7 (5)
O1 ^{vi} —La1—Li2 ^{viii}	116.0 (3)	Li2 ⁱ —Li1—O1 ⁱⁱⁱ	163.6 (5)
O1 ^{vii} —La1—Li2 ^{viii}	110.0 (3)	Li2 ⁱⁱⁱ —Li1—O1 ⁱⁱⁱ	62.9 (5)
O1 ⁱ —La1—Li2 ^{ix}	147.5 (3)	O1 ^{viii} —Li1—O1 ⁱⁱⁱ	113.69 (5)
O1 ⁱⁱ —La1—Li2 ^{ix}	43.4 (3)	Li2 ^{xi} —Li1—O1 ^{xi}	62.9 (5)
O1 ⁱⁱⁱ —La1—Li2 ^{ix}	124.3 (3)	Li2 ^{viii} —Li1—O1 ^{xi}	163.6 (5)
O1 ^{iv} —La1—Li2 ^{ix}	47.1 (3)	Li2 ⁱ —Li1—O1 ^{xi}	72.1 (5)

O1—La1—Li2 ^{ix}	110.0 (3)	Li2 ⁱⁱⁱ —Li1—O1 ^{xi}	78.7 (5)
O1 ^v —La1—Li2 ^{ix}	116.0 (3)	O1 ^{viii} —Li1—O1 ^{xi}	101.32 (10)
O1 ^{vi} —La1—Li2 ^{ix}	56.0 (3)	O1 ⁱⁱⁱ —Li1—O1 ^{xi}	113.69 (5)
O1 ^{vii} —La1—Li2 ^{ix}	77.2 (3)	Li2 ^{xi} —Li1—O1 ⁱ	78.7 (5)
Li2 ^{viii} —La1—Li2 ^{ix}	168.0 (6)	Li2 ^{viii} —Li1—O1 ⁱ	72.1 (5)
O1 ⁱ —La1—Li2 ^x	124.3 (3)	Li2 ⁱ —Li1—O1 ⁱ	62.9 (5)
O1 ⁱⁱ —La1—Li2 ^x	47.1 (3)	Li2 ⁱⁱⁱ —Li1—O1 ⁱ	163.6 (5)
O1 ⁱⁱⁱ —La1—Li2 ^x	147.5 (3)	O1 ^{viii} —Li1—O1 ⁱ	113.69 (6)
O1 ^{iv} —La1—Li2 ^x	43.4 (3)	O1 ⁱⁱⁱ —Li1—O1 ⁱ	101.32 (10)
O1—La1—Li2 ^x	56.0 (3)	O1 ^{xi} —Li1—O1 ⁱ	113.69 (5)
O1 ^v —La1—Li2 ^x	77.2 (3)	Li2 ^{xi} —Li1—Li2 ^{xxiii}	7.0 (9)
O1 ^{vi} —La1—Li2 ^x	110.0 (3)	Li2 ^{viii} —Li1—Li2 ^{xxiii}	135.9 (7)
O1 ^{vii} —La1—Li2 ^x	116.0 (3)	Li2 ⁱ —Li1—Li2 ^{xxiii}	92.1 (7)
Li2 ^{viii} —La1—Li2 ^x	122.0 (5)	Li2 ⁱⁱⁱ —Li1—Li2 ^{xxiii}	103.8 (7)
Li2 ^{ix} —La1—Li2 ^x	59.4 (5)	O1 ^{viii} —Li1—Li2 ^{xxiii}	160.7 (4)
O1 ⁱ —La1—Li2 ^{xi}	47.1 (3)	O1 ⁱⁱⁱ —Li1—Li2 ^{xxiii}	79.0 (4)
O1 ⁱⁱ —La1—Li2 ^{xi}	124.3 (3)	O1 ^{xi} —Li1—Li2 ^{xxiii}	59.6 (4)
O1 ⁱⁱⁱ —La1—Li2 ^{xi}	43.4 (3)	O1 ⁱ —Li1—Li2 ^{xxiii}	75.7 (3)
O1 ^{iv} —La1—Li2 ^{xi}	147.5 (3)	Li2 ^{xi} —Li1—Li2 ^{xxiv}	135.9 (7)
O1—La1—Li2 ^{xi}	116.0 (3)	Li2 ^{viii} —Li1—Li2 ^{xxiv}	7.0 (9)
O1 ^v —La1—Li2 ^{xi}	110.0 (3)	Li2 ⁱ —Li1—Li2 ^{xxiv}	103.8 (7)
O1 ^{vi} —La1—Li2 ^{xi}	77.2 (3)	Li2 ⁱⁱⁱ —Li1—Li2 ^{xxiv}	92.1 (7)
O1 ^{vii} —La1—Li2 ^{xi}	56.0 (3)	O1 ^{viii} —Li1—Li2 ^{xxiv}	59.6 (4)
Li2 ^{viii} —La1—Li2 ^{xi}	59.4 (5)	O1 ⁱⁱⁱ —Li1—Li2 ^{xxiv}	75.7 (3)
Li2 ^{ix} —La1—Li2 ^{xi}	122.0 (5)	O1 ^{xi} —Li1—Li2 ^{xxiv}	160.7 (4)
Li2 ^x —La1—Li2 ^{xi}	168.0 (6)	O1 ⁱ —Li1—Li2 ^{xxiv}	79.0 (4)
O1 ^{xii} —Zr1—O1 ^{vii}	180.00 (13)	Li2 ^{xxiii} —Li1—Li2 ^{xxiv}	139.6 (7)
O1 ^{xii} —Zr1—O1 ^{xiii}	86.55 (7)	Li2 ^{xi} —Li1—Li2 ^{xxv}	103.8 (7)
O1 ^{vii} —Zr1—O1 ^{xiii}	93.45 (7)	Li2 ^{viii} —Li1—Li2 ^{xxv}	92.1 (7)
O1 ^{xii} —Zr1—O1 ⁱⁱ	93.45 (7)	Li2 ⁱ —Li1—Li2 ^{xxv}	7.0 (9)
O1 ^{vii} —Zr1—O1 ⁱⁱ	86.55 (7)	Li2 ⁱⁱⁱ —Li1—Li2 ^{xxv}	135.9 (7)
O1 ^{xiii} —Zr1—O1 ⁱⁱ	180.00 (13)	O1 ^{viii} —Li1—Li2 ^{xxv}	75.7 (4)
O1 ^{xii} —Zr1—O1 ^{xiv}	86.55 (7)	O1 ⁱⁱⁱ —Li1—Li2 ^{xxv}	160.7 (4)
O1 ^{vii} —Zr1—O1 ^{xiv}	93.45 (7)	O1 ^{xi} —Li1—Li2 ^{xxv}	79.0 (4)
O1 ^{xiii} —Zr1—O1 ^{xiv}	86.55 (7)	O1 ⁱ —Li1—Li2 ^{xxv}	59.6 (4)
O1 ⁱⁱ —Zr1—O1 ^{xiv}	93.45 (7)	Li2 ^{xxiii} —Li1—Li2 ^{xxv}	96.8 (2)
O1 ^{xii} —Zr1—O1 ^{xv}	93.45 (7)	Li2 ^{xxiv} —Li1—Li2 ^{xxv}	96.8 (2)
O1 ^{vii} —Zr1—O1 ^{xv}	86.55 (7)	Li2 ^{xi} —Li1—Li2 ^{xxvi}	92.1 (7)
O1 ^{xiii} —Zr1—O1 ^{xv}	93.45 (7)	Li2 ^{viii} —Li1—Li2 ^{xxvi}	103.8 (7)
O1 ⁱⁱ —Zr1—O1 ^{xv}	86.55 (7)	Li2 ⁱ —Li1—Li2 ^{xxvi}	135.9 (7)
O1 ^{xiv} —Zr1—O1 ^{xv}	180.00 (9)	Li2 ⁱⁱⁱ —Li1—Li2 ^{xxvi}	7.0 (9)
O1 ^{xii} —Zr1—Li2 ^{ix}	93.0 (3)	O1 ^{viii} —Li1—Li2 ^{xxvi}	79.0 (4)
O1 ^{vii} —Zr1—Li2 ^{ix}	87.0 (3)	O1 ⁱⁱⁱ —Li1—Li2 ^{xxvi}	59.6 (4)
O1 ^{xiii} —Zr1—Li2 ^{ix}	134.2 (3)	O1 ^{xi} —Li1—Li2 ^{xxvi}	75.7 (3)
O1 ⁱⁱ —Zr1—Li2 ^{ix}	45.8 (3)	O1 ⁱ —Li1—Li2 ^{xxvi}	160.7 (4)
O1 ^{xiv} —Zr1—Li2 ^{ix}	47.8 (3)	Li2 ^{xxiii} —Li1—Li2 ^{xxvi}	96.8 (2)
O1 ^{xv} —Zr1—Li2 ^{ix}	132.2 (3)	Li2 ^{xxiv} —Li1—Li2 ^{xxvi}	96.8 (2)
O1 ^{xii} —Zr1—Li2 ^{xxvi}	87.0 (3)	Li2 ^{xxv} —Li1—Li2 ^{xxvi}	139.6 (7)

O1 ^{vii} —Zr1—Li2 ^{xvi}	93.0 (3)	Li2 ^v —Li2—Al1 ^{xx}	158 (3)
O1 ^{xiii} —Zr1—Li2 ^{xvi}	45.8 (3)	Li2 ^v —Li2—Li1 ^{xx}	158 (3)
O1 ⁱⁱ —Zr1—Li2 ^{xvi}	134.2 (3)	Al1 ^{xx} —Li2—Li1 ^{xx}	0
O1 ^{xiv} —Zr1—Li2 ^{xvi}	132.2 (3)	Li2 ^v —Li2—O1	101.9 (17)
O1 ^{xv} —Zr1—Li2 ^{xvi}	47.8 (3)	Al1 ^{xx} —Li2—O1	66.2 (5)
Li2 ^{ix} —Zr1—Li2 ^{xvi}	180.0 (7)	Li1 ^{xx} —Li2—O1	66.2 (5)
O1 ^{xii} —Zr1—Li2 ^{xvii}	134.2 (3)	Li2 ^v —Li2—O1 ^{xxii}	141 (3)
O1 ^{vii} —Zr1—Li2 ^{xvii}	45.8 (3)	Al1 ^{xx} —Li2—O1 ^{xxii}	60.4 (4)
O1 ^{xiii} —Zr1—Li2 ^{xvii}	47.8 (3)	Li1 ^{xx} —Li2—O1 ^{xxii}	60.4 (4)
O1 ⁱⁱ —Zr1—Li2 ^{xvii}	132.2 (3)	O1—Li2—O1 ^{xxii}	108.0 (7)
O1 ^{xiv} —Zr1—Li2 ^{xvii}	93.0 (3)	Li2 ^v —Li2—O1 ^v	57.2 (15)
O1 ^{xv} —Zr1—Li2 ^{xvii}	87.0 (3)	Al1 ^{xx} —Li2—O1 ^v	140.1 (8)
Li2 ^{ix} —Zr1—Li2 ^{xvii}	119.82 (4)	Li1 ^{xx} —Li2—O1 ^v	140.1 (8)
Li2 ^{xvi} —Zr1—Li2 ^{xvii}	60.18 (4)	O1—Li2—O1 ^v	99.9 (6)
O1 ^{xii} —Zr1—Li2 ^{xviii}	45.8 (3)	O1 ^{xxii} —Li2—O1 ^v	92.6 (6)
O1 ^{vii} —Zr1—Li2 ^{xviii}	134.2 (3)	Li2 ^v —Li2—O1 ^{xxi}	112.5 (10)
O1 ^{xiii} —Zr1—Li2 ^{xviii}	132.2 (3)	Al1 ^{xx} —Li2—O1 ^{xxi}	56.4 (4)
O1 ⁱⁱ —Zr1—Li2 ^{xviii}	47.8 (3)	Li1 ^{xx} —Li2—O1 ^{xxi}	56.4 (4)
O1 ^{xiv} —Zr1—Li2 ^{xviii}	87.0 (3)	O1—Li2—O1 ^{xxi}	101.8 (7)
O1 ^{xv} —Zr1—Li2 ^{xviii}	93.0 (3)	O1 ^{xxii} —Li2—O1 ^{xxi}	85.7 (5)
Li2 ^{ix} —Zr1—Li2 ^{xviii}	60.18 (4)	O1 ^v —Li2—O1 ^{xxi}	157.6 (7)
Li2 ^{xvi} —Zr1—Li2 ^{xviii}	119.82 (4)	Li2 ^v —Li2—Al1 ^{xxvii}	14.6 (19)
Li2 ^{xvii} —Zr1—Li2 ^{xviii}	180.0 (6)	Al1 ^{xx} —Li2—Al1 ^{xxvii}	170.3 (9)
O1 ^{xii} —Zr1—Li2 ^{xix}	47.8 (3)	Li1 ^{xx} —Li2—Al1 ^{xxvii}	170.3 (9)
O1 ^{vii} —Zr1—Li2 ^{xix}	132.2 (3)	O1—Li2—Al1 ^{xxvii}	114.1 (6)
O1 ^{xiii} —Zr1—Li2 ^{xix}	93.0 (3)	O1 ^{xxii} —Li2—Al1 ^{xxvii}	126.4 (7)
O1 ⁱⁱ —Zr1—Li2 ^{xix}	87.0 (3)	O1 ^v —Li2—Al1 ^{xxvii}	49.5 (3)
O1 ^{xiv} —Zr1—Li2 ^{xix}	134.2 (3)	O1 ^{xxi} —Li2—Al1 ^{xxvii}	115.1 (6)
O1 ^{xv} —Zr1—Li2 ^{xix}	45.8 (3)	Li2 ^v —Li2—Li1 ^{xxvii}	14.6 (19)
Li2 ^{ix} —Zr1—Li2 ^{xix}	119.82 (4)	Al1 ^{xx} —Li2—Li1 ^{xxvii}	170.3
Li2 ^{xvi} —Zr1—Li2 ^{xix}	60.18 (4)	Li1 ^{xx} —Li2—Li1 ^{xxvii}	170.3 (9)
Li2 ^{xvii} —Zr1—Li2 ^{xix}	119.82 (4)	O1—Li2—Li1 ^{xxvii}	114.1 (6)
Li2 ^{xviii} —Zr1—Li2 ^{xix}	60.18 (4)	O1 ^{xxii} —Li2—Li1 ^{xxvii}	126.4 (7)
O1 ^{xii} —Zr1—Li2 ^{vi}	132.2 (3)	O1 ^v —Li2—Li1 ^{xxvii}	49.5 (3)
O1 ^{vii} —Zr1—Li2 ^{vi}	47.8 (3)	O1 ^{xxi} —Li2—Li1 ^{xxvii}	115.1 (6)
O1 ^{xiii} —Zr1—Li2 ^{vi}	87.0 (3)	Al1 ^{xxvii} —Li2—Li1 ^{xxvii}	0
O1 ⁱⁱ —Zr1—Li2 ^{vi}	93.0 (3)	Li2 ^v —Li2—Li2 ^{xxii}	150.2 (6)
O1 ^{xiv} —Zr1—Li2 ^{vi}	45.8 (3)	Al1 ^{xx} —Li2—Li2 ^{xxii}	40.45 (19)
O1 ^{xv} —Zr1—Li2 ^{vi}	134.2 (3)	Li1 ^{xx} —Li2—Li2 ^{xxii}	40.45 (19)
Li2 ^{ix} —Zr1—Li2 ^{vi}	60.18 (4)	O1—Li2—Li2 ^{xxii}	60.7 (7)
Li2 ^{xvi} —Zr1—Li2 ^{vi}	119.82 (4)	O1 ^{xxii} —Li2—Li2 ^{xxii}	47.3 (4)
Li2 ^{xvii} —Zr1—Li2 ^{vi}	60.18 (4)	O1 ^v —Li2—Li2 ^{xxii}	99.7 (8)
Li2 ^{xviii} —Zr1—Li2 ^{vi}	119.82 (4)	O1 ^{xxi} —Li2—Li2 ^{xxii}	95.5 (4)
Li2 ^{xix} —Zr1—Li2 ^{vi}	180.0 (8)	Al1 ^{xxvii} —Li2—Li2 ^{xxii}	148.9 (8)
Li2—O1—Al1 ^{xx}	50.9 (4)	Li1 ^{xxvii} —Li2—Li2 ^{xxii}	148.9 (8)
Li2—O1—Li1 ^{xx}	50.9 (4)	Li2 ^v —Li2—Li2 ^{xxi}	118 (3)
Al1 ^{xx} —O1—Li1 ^{xx}	0	Al1 ^{xx} —Li2—Li2 ^{xxi}	40.45 (19)
Li2—O1—Li2 ^{xxi}	77.1 (6)	Li1 ^{xx} —Li2—Li2 ^{xxi}	40.45 (19)

Al1 ^{xx} —O1—Li2 ^{xxi}	47.5 (4)	O1—Li2—Li2 ^{xxi}	55.7 (7)
Li1 ^{xx} —O1—Li2 ^{xxi}	47.5 (4)	O1 ^{xxii} —Li2—Li2 ^{xxi}	99.8 (4)
Li2—O1—Zr1 ^{xv}	103.8 (4)	O1 ^v —Li2—Li2 ^{xxi}	155.1 (10)
Al1 ^{xx} —O1—Zr1 ^{xv}	129.08 (9)	O1 ^{xxi} —Li2—Li2 ^{xxi}	46.1 (4)
Li1 ^{xx} —O1—Zr1 ^{xv}	129.08 (9)	Al1 ^{xxvii} —Li2—Li2 ^{xxi}	130.9 (8)
Li2 ^{xxi} —O1—Zr1 ^{xv}	87.8 (4)	Li1 ^{xxvii} —Li2—Li2 ^{xxi}	130.9 (8)
Li2—O1—Li2 ^v	20.9 (7)	Li2 ^{xxii} —Li2—Li2 ^{xxi}	74.1 (6)
Al1 ^{xx} —O1—Li2 ^v	70.9 (4)	Li2 ^v —Li2—O1 ^{xxviii}	51.5 (9)
Li1 ^{xx} —O1—Li2 ^v	70.9 (4)	Al1 ^{xx} —Li2—O1 ^{xxviii}	130.2 (7)
Li2 ^{xxi} —O1—Li2 ^v	86.72 (8)	Li1 ^{xx} —Li2—O1 ^{xxviii}	130.2 (7)
Zr1 ^{xv} —O1—Li2 ^v	85.9 (4)	O1—Li2—O1 ^{xxviii}	146.7 (7)
Li2—O1—Li2 ^{xxii}	73.1 (6)	O1 ^{xxii} —Li2—O1 ^{xxviii}	105.0 (6)
Al1 ^{xx} —O1—Li2 ^{xxii}	45.0 (4)	O1 ^v —Li2—O1 ^{xxviii}	82.5 (5)
Li1 ^{xx} —O1—Li2 ^{xxii}	45.0 (4)	O1 ^{xxi} —Li2—O1 ^{xxviii}	76.4 (4)
Li2 ^{xxi} —O1—Li2 ^{xxii}	86.5 (6)	Al1 ^{xxvii} —Li2—O1 ^{xxviii}	44.2 (2)
Zr1 ^{xv} —O1—Li2 ^{xxii}	174.0 (4)	Li1 ^{xxvii} —Li2—O1 ^{xxviii}	44.2 (2)
Li2 ^v —O1—Li2 ^{xxii}	92.0 (7)	Li2 ^{xxii} —Li2—O1 ^{xxviii}	152.1 (9)
Li2—O1—La1 ^{xx}	144.1 (4)	Li2 ^{xxi} —Li2—O1 ^{xxviii}	114.5 (8)
Al1 ^{xx} —O1—La1 ^{xx}	93.43 (7)		

Symmetry codes: (i) z, x, y ; (ii) $-z+1/4, -y+1/4, -x+1/4$; (iii) $z, -x, -y+1/2$; (iv) $-z+1/4, y-1/4, x+1/4$; (v) $-x+1/4, z-1/4, y+1/4$; (vi) $x, -y, -z+1/2$; (vii) $-x+1/4, -z+1/4, -y+1/4$; (viii) $-z+3/4, -y+1/4, x+1/4$; (ix) $z-1/2, -x, y$; (x) $z-1/2, x, -y+1/2$; (xi) $-z+3/4, y-1/4, -x+1/4$; (xii) $x-1/4, z-1/4, y-1/4$; (xiii) $z-1/4, y-1/4, x-1/4$; (xiv) $y-1/4, x-1/4, z-1/4$; (xv) $-y+1/4, -x+1/4, -z+1/4$; (xvi) $-z+1/2, x, -y$; (xvii) $y, z-1/2, -x$; (xviii) $-y, -z+1/2, x$; (xix) $-x, y, z-1/2$; (xx) y, z, x ; (xxi) $-y+1/4, x+1/4, -z+3/4$; (xxii) $y-1/4, -x+1/4, -z+3/4$; (xxiii) $-y+1/2, z-1/2, x$; (xxiv) $-y+1/2, -z+1/2, -x+1/2$; (xxv) $y+1/4, -x+1/4, z-1/4$; (xxvi) $y+1/4, x-1/4, -z+3/4$; (xxvii) $-y+1/4, x-1/4, z+1/4$; (xxviii) $y, -z+1/2, x+1/2$.

(LLZO-Al15-hydro-150C)

Crystal data

Al_{0.15}H_{5.52}La_{2.88}Li_{1.64}O₁₂Zr_{1.95}
M_r = 790.95
 Cubic, *I*43*d*
 Hall symbol: I -4bd 2c 3
a = 13.0738 (2) Å
V = 2234.63 (10) Å³
Z = 8
F(000) = 2804.4

D_x = 4.707 Mg m⁻³
 Mo *K*α radiation, λ = 0.71073 Å
 Cell parameters from 34201 reflections
 θ = 3.8–34.9°
 μ = 12.61 mm⁻¹
T = 298 K
 Cuboid, colorless
 0.13 × 0.12 × 0.08 mm

Data collection

Bruker SMART APEX
 diffractometer
 Graphite monochromator
 rotation, ω-scans at 4 different φ positions
 Absorption correction: multi-scan
 (APEX2; Bruker, 2012)
T_{min} = 0.21, *T_{max}* = 0.36
 34201 measured reflections

819 independent reflections
 819 reflections with *I* > 2σ(*I*)
R_{int} = 0.026
 θ_{max} = 34.9°, θ_{min} = 3.8°
h = -21→21
k = -21→21
l = -21→21

Refinement

Refinement on *F*²
 Least-squares matrix: full
R[*F*² > 2σ(*F*²)] = 0.013
wR(*F*²) = 0.029

S = 1.27
 819 reflections
 44 parameters
 1 restraint

0 constraints
 Hydrogen site location: difference Fourier map
 Only H-atom coordinates refined
 $w = 1/[\sigma^2(F_o^2) + 15.2822P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.57 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.51 \text{ e } \text{\AA}^{-3}$

Extinction correction: SHELXL2014
 (Sheldrick, 2015),
 $F_c^* = kFc[1 + 0.001x\lambda^3/\sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.00083 (5)
 Absolute structure: Refined as an inversion
 twin.
 Absolute structure parameter: 0.50 (3)

Special details

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

Refinement. Refined as a 2-component inversion twin.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
La1	0.11936 (3)	0	0.25	0.01005 (9)	0.961 (10)
Zr1A	-0.01161 (12)	-0.01161 (12)	-0.01161 (12)	0.0069 (4)	0.79 (2)
Zr1B	-0.0073 (15)	0.006 (3)	0.013 (2)	0.024 (5)*	0.061 (6)
O1	0.0970 (2)	0.1899 (2)	0.2733 (3)	0.0132 (6)	
O2	0.0335 (3)	0.4452 (3)	0.1429 (2)	0.0149 (7)	
Li1	0.375	0	0.25	0.016*	0.62 (6)
Al1	0.375	0	0.25	0.016*	0.1
Li2	0.875	0	0.25	0.017 (9)	0.47 (9)
H1	0.098 (6)	0.180 (6)	0.323 (7)	0.025*	0.92 (17)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.00938 (13)	0.00852 (14)	0.01224 (15)	0	0	0.00403 (8)
Zr1A	0.0069 (4)	0.0069 (4)	0.0069 (4)	0.0000 (2)	0.0000 (2)	0.0000 (2)
O1	0.0112 (12)	0.0115 (13)	0.0169 (15)	0.0014 (9)	-0.0002 (10)	0.0028 (10)
O2	0.0193 (15)	0.0142 (13)	0.0110 (14)	0.0028 (10)	0.0005 (10)	0.0038 (10)
Li2	0.012 (14)	0.020 (12)	0.020 (12)	0	0	0

Geometric parameters (\AA , $^\circ$)

La1—O1 ⁱ	2.506 (3)	O1—Li1 ^{viii}	1.998 (3)
La1—O1 ⁱⁱ	2.506 (3)	O1—Zr1A ^{vii}	2.007 (4)
La1—O1	2.518 (3)	O1—Zr1B ^{xv}	2.14 (3)
La1—O1 ⁱⁱⁱ	2.518 (3)	O1—Zr1B ^{vii}	2.19 (3)
La1—O2 ^{iv}	2.544 (3)	O1—Zr1B ^{xvi}	2.36 (3)
La1—O2 ^v	2.544 (3)	O1—La1 ^{viii}	2.506 (3)
La1—O2 ⁱ	2.607 (3)	O1—H1	0.66 (9)
La1—O2 ⁱⁱ	2.607 (3)	O2—Zr1B ^{iv}	1.85 (3)
La1—Li2 ^{vi}	3.1947 (4)	O2—Li2 ^{xvii}	1.976 (3)
La1—Li1	3.3422 (4)	O2—Zr1B ^{xviii}	2.06 (3)

La1—Zr1A ^{vii}	3.487 (2)	O2—Zr1B ^{xix}	2.10 (3)
La1—H1	2.55 (8)	O2—Zr1A ^{iv}	2.217 (4)
Zr1A—Zr1B ^{viii}	0.39 (3)	O2—La1 ^{iv}	2.544 (3)
Zr1A—Zr1B ⁱ	0.39 (3)	O2—La1 ^{viii}	2.607 (3)
Zr1A—O1 ^{ix}	2.007 (4)	Li1—O1 ^{xx}	1.998 (3)
Zr1A—O1 ^x	2.007 (4)	Li1—O1 ⁱⁱ	1.998 (3)
Zr1A—O1 ^{xi}	2.007 (4)	Li1—O1 ⁱ	1.998 (3)
Zr1A—O2 ^{xii}	2.217 (4)	Li1—O1 ^{xxi}	1.998 (3)
Zr1A—O2 ^{iv}	2.217 (4)	Li1—La1 ^{xxii}	3.3422 (4)
Zr1A—O2 ⁱⁱ	2.217 (4)	Li1—Zr1B ^{xxiii}	3.54 (3)
Zr1A—La1 ^{xi}	3.487 (2)	Li1—Zr1B ^{xxiv}	3.54 (3)
Zr1A—La1 ^{ix}	3.487 (2)	Li1—Zr1B ^{vii}	3.54 (3)
Zr1A—La1 ^x	3.487 (2)	Li1—Zr1B ^{xii}	3.54 (3)
Zr1A—Li1 ^{xiii}	3.5953 (5)	Li1—Zr1A ^{xxv}	3.5953 (5)
Zr1B—Zr1B ^{viii}	0.32 (5)	Li1—Zr1A ^{xxiii}	3.5953 (5)
Zr1B—Zr1B ⁱ	0.32 (5)	Li2—O2 ^{xxvi}	1.976 (3)
Zr1B—O2 ^{iv}	1.85 (3)	Li2—O2 ^{xxvii}	1.976 (3)
Zr1B—O2 ^{xii}	2.06 (3)	Li2—O2 ^{xxviii}	1.976 (3)
Zr1B—O2 ⁱⁱ	2.10 (3)	Li2—O2 ^{xxix}	3.1947 (4)
Zr1B—O1 ^x	2.14 (3)	Li2—La1 ^{xxii}	3.1947 (4)
Zr1B—O1 ^{xi}	2.19 (3)	Li2—Zr1B ^{xxx}	3.46 (3)
Zr1B—O1 ^{ix}	2.36 (3)	Li2—Zr1B ^{xxii}	3.46 (3)
Zr1B—Li2 ^{vi}	3.47 (3)	Li2—Zr1B ^{xxix}	3.46 (3)
Zr1B—La1 ^{viii}	3.49 (4)	Li2—Zr1B ^{xxxi}	3.46 (3)
Zr1B—Li1 ^{xiv}	3.54 (3)		
O1—Al1 ^{viii}	1.998 (3)		
O1 ⁱ —La1—O1 ⁱⁱ	73.10 (16)	O1 ^{xi} —Zr1B—La1	94.1 (12)
O1 ⁱ —La1—O1	68.42 (15)	O1 ^{ix} —Zr1B—La1	136.1 (13)
O1 ⁱⁱ —La1—O1	123.66 (7)	Li2 ^{vi} —Zr1B—La1	54.4 (5)
O1 ⁱ —La1—O1 ⁱⁱⁱ	123.66 (7)	La1 ^{viii} —Zr1B—La1	69.7 (6)
O1 ⁱⁱ —La1—O1 ⁱⁱⁱ	68.42 (15)	Zr1B ^{viii} —Zr1B—Li1 ^{xiv}	108 (10)
O1—La1—O1 ⁱⁱⁱ	166.67 (15)	Zr1B ⁱ —Zr1B—Li1 ^{xiv}	160 (6)
O1 ⁱ —La1—O2 ^{iv}	108.41 (9)	O2 ^{iv} —Zr1B—Li1 ^{xiv}	74.0 (10)
O1 ⁱⁱ —La1—O2 ^{iv}	161.19 (8)	O2 ^{xii} —Zr1B—Li1 ^{xiv}	87.5 (13)
O1—La1—O2 ^{iv}	72.41 (10)	O2 ⁱⁱ —Zr1B—Li1 ^{xiv}	163.1 (15)
O1 ⁱⁱⁱ —La1—O2 ^{iv}	96.88 (11)	O1 ^x —Zr1B—Li1 ^{xiv}	30.1 (6)
O1 ⁱ —La1—O2 ^v	161.19 (8)	O1 ^{xi} —Zr1B—Li1 ^{xiv}	97.9 (5)
O1 ⁱⁱ —La1—O2 ^v	108.41 (9)	O1 ^{ix} —Zr1B—Li1 ^{xiv}	105.7 (10)
O1—La1—O2 ^v	96.88 (11)	Li2 ^{vi} —Zr1B—Li1 ^{xiv}	69.7 (5)
O1 ⁱⁱⁱ —La1—O2 ^v	72.41 (10)	La1 ^{viii} —Zr1B—Li1 ^{xiv}	68.9 (7)
O2 ^{iv} —La1—O2 ^v	76.42 (15)	La1—Zr1B—Li1 ^{xiv}	118.2 (9)
O1 ⁱ —La1—O2 ⁱ	97.31 (11)	Al1 ^{viii} —O1—Li1 ^{viii}	0
O1 ⁱⁱ —La1—O2 ⁱ	71.54 (10)	Al1 ^{viii} —O1—Zr1A ^{vii}	127.71 (18)
O1—La1—O2 ⁱ	74.30 (10)	Li1 ^{viii} —O1—Zr1A ^{vii}	127.71 (18)
O1 ⁱⁱⁱ —La1—O2 ⁱ	107.34 (10)	Al1 ^{viii} —O1—Zr1B ^{xv}	117.5 (10)
O2 ^{iv} —La1—O2 ⁱ	125.74 (7)	Li1 ^{viii} —O1—Zr1B ^{xv}	117.5 (10)
O2 ^v —La1—O2 ⁱ	66.49 (14)	Zr1A ^{vii} —O1—Zr1B ^{xv}	10.2 (9)

O1 ⁱ —La1—O2 ⁱⁱ	71.54 (10)	All ^{viii} —O1—Zr1B ^{vii}	121.3 (8)
O1 ⁱⁱ —La1—O2 ⁱⁱ	97.31 (11)	Li1 ^{viii} —O1—Zr1B ^{vii}	121.3 (8)
O1—La1—O2 ⁱⁱ	107.34 (10)	Zr1A ^{vii} —O1—Zr1B ^{vii}	9.5 (8)
O1 ⁱⁱⁱ —La1—O2 ⁱⁱ	74.30 (10)	Zr1B ^{xv} —O1—Zr1B ^{vii}	8.5 (11)
O2 ^{iv} —La1—O2 ⁱⁱ	66.49 (14)	All ^{viii} —O1—Zr1B ^{xvi}	123.4 (5)
O2 ^v —La1—O2 ⁱⁱ	125.74 (7)	Li1 ^{viii} —O1—Zr1B ^{xvi}	123.4 (5)
O2 ⁱ —La1—O2 ⁱⁱ	166.47 (14)	Zr1A ^{vii} —O1—Zr1B ^{xvi}	4.3 (4)
O1 ⁱ —La1—Li2 ^{vi}	143.45 (8)	Zr1B ^{xv} —O1—Zr1B ^{xvi}	6.0 (8)
O1 ⁱⁱ —La1—Li2 ^{vi}	143.45 (8)	Zr1B ^{vii} —O1—Zr1B ^{xvi}	6.9 (12)
O1—La1—Li2 ^{vi}	83.33 (7)	All ^{viii} —O1—La1 ^{viii}	95.15 (12)
O1 ⁱⁱⁱ —La1—Li2 ^{vi}	83.33 (7)	Li1 ^{viii} —O1—La1 ^{viii}	95.15 (12)
O2 ^{iv} —La1—Li2 ^{vi}	38.21 (8)	Zr1A ^{vii} —O1—La1 ^{viii}	100.61 (15)
O2 ^v —La1—Li2 ^{vi}	38.21 (8)	Zr1B ^{xv} —O1—La1 ^{viii}	103.0 (8)
O2 ⁱ —La1—Li2 ^{vi}	96.77 (7)	Zr1B ^{vii} —O1—La1 ^{viii}	109.2 (8)
O2 ⁱⁱ —La1—Li2 ^{vi}	96.77 (7)	Zr1B ^{xvi} —O1—La1 ^{viii}	102.3 (8)
O1 ⁱ —La1—Li1	36.55 (8)	All ^{viii} —O1—La1	122.82 (15)
O1 ⁱⁱ —La1—Li1	36.55 (8)	Li1 ^{viii} —O1—La1	122.82 (15)
O1—La1—Li1	96.67 (7)	Zr1A ^{vii} —O1—La1	100.20 (13)
O1 ⁱⁱⁱ —La1—Li1	96.67 (7)	Zr1B ^{xv} —O1—La1	108.8 (8)
O2 ^{iv} —La1—Li1	141.79 (8)	Zr1B ^{vii} —O1—La1	101.1 (7)
O2 ^v —La1—Li1	141.79 (8)	Zr1B ^{xvi} —O1—La1	103.4 (8)
O2 ⁱ —La1—Li1	83.23 (7)	La1 ^{viii} —O1—La1	105.71 (13)
O2 ⁱⁱ —La1—Li1	83.23 (7)	All ^{viii} —O1—H1	56 (7)
Li2 ^{vi} —La1—Li1	180	Li1 ^{viii} —O1—H1	56 (7)
O1 ⁱ —La1—Zr1A ^{vii}	34.45 (8)	Zr1A ^{vii} —O1—H1	106 (7)
O1 ⁱⁱ —La1—Zr1A ^{vii}	96.17 (8)	Zr1B ^{xv} —O1—H1	101 (7)
O1—La1—Zr1A ^{vii}	34.50 (7)	Zr1B ^{vii} —O1—H1	97 (7)
O1 ⁱⁱⁱ —La1—Zr1A ^{vii}	158.08 (7)	Zr1B ^{xvi} —O1—H1	103 (7)
O2 ^{iv} —La1—Zr1A ^{vii}	94.29 (8)	La1 ^{viii} —O1—H1	149 (7)
O2 ^v —La1—Zr1A ^{vii}	128.79 (7)	La1—O1—H1	85 (7)
O2 ⁱ —La1—Zr1A ^{vii}	80.78 (8)	Zr1B ^{iv} —O2—Li2 ^{xvii}	129.6 (7)
O2 ⁱⁱ —La1—Zr1A ^{vii}	93.16 (8)	Zr1B ^{iv} —O2—Zr1B ^{xviii}	7.3 (16)
Li2 ^{vi} —La1—Zr1A ^{vii}	116.505 (14)	Li2 ^{xvii} —O2—Zr1B ^{xviii}	130.6 (8)
Li1—La1—Zr1A ^{vii}	63.495 (14)	Zr1B ^{iv} —O2—Zr1B ^{xix}	5.9 (9)
O1 ⁱ —La1—H1	74.9 (17)	Li2 ^{xvii} —O2—Zr1B ^{xix}	135.6 (10)
O1 ⁱⁱ —La1—H1	116 (2)	Zr1B ^{xviii} —O2—Zr1B ^{xix}	8.8 (12)
O1—La1—H1	15 (2)	Zr1B ^{iv} —O2—Zr1A ^{iv}	4.1 (5)
O1 ⁱⁱⁱ —La1—H1	160.1 (18)	Li2 ^{xvii} —O2—Zr1A ^{iv}	125.57 (17)
O2 ^{iv} —La1—H1	82 (2)	Zr1B ^{xviii} —O2—Zr1A ^{iv}	9.7 (9)
O2 ^v —La1—H1	88.1 (17)	Zr1B ^{xix} —O2—Zr1A ^{iv}	10.0 (9)
O2 ⁱ —La1—H1	60 (2)	Zr1B ^{iv} —O2—La1 ^{iv}	105.3 (10)
O2 ⁱⁱ —La1—H1	122 (2)	Li2 ^{xvii} —O2—La1 ^{iv}	89.03 (12)
Li2 ^{vi} —La1—H1	83.6 (18)	Zr1B ^{xviii} —O2—La1 ^{iv}	97.9 (10)
Li1—La1—H1	96.4 (18)	Zr1B ^{xix} —O2—La1 ^{iv}	104.4 (9)
Zr1A ^{vii} —La1—H1	40.8 (17)	Zr1A ^{iv} —O2—La1 ^{iv}	106.84 (13)
Zr1B ^{viii} —Zr1A—Zr1B ⁱ	49 (4)	Zr1B ^{iv} —O2—La1 ^{viii}	101.5 (11)
Zr1B ^{viii} —Zr1A—O1 ^{ix}	105 (4)	Li2 ^{xvii} —O2—La1 ^{viii}	122.70 (14)
Zr1B ⁱ —Zr1A—O1 ^{ix}	113 (5)	Zr1B ^{xviii} —O2—La1 ^{viii}	103.6 (8)

Zr1B ^{viii} —Zr1A—O1 ^x	113 (5)	Zr1B ^{xix} —O2—La1 ^{viii}	96.1 (9)
Zr1B ⁱ —Zr1A—O1 ^x	153 (3)	Zr1A ^{iv} —O2—La1 ^{viii}	104.74 (13)
O1 ^{ix} —Zr1A—O1 ^x	89.46 (17)	La1 ^{iv} —O2—La1 ^{viii}	102.04 (12)
Zr1B ^{viii} —Zr1A—O1 ^{xi}	153 (3)	O1 ^{xx} —Li1—O1 ⁱⁱ	116.26 (11)
Zr1B ⁱ —Zr1A—O1 ^{xi}	105 (4)	O1 ^{xx} —Li1—O1 ⁱ	116.26 (11)
O1 ^{ix} —Zr1A—O1 ^{xi}	89.46 (17)	O1 ⁱⁱ —Li1—O1 ⁱ	96.61 (19)
O1 ^x —Zr1A—O1 ^{xi}	89.46 (17)	O1 ^{xx} —Li1—O1 ^{xxi}	96.61 (19)
Zr1B ^{viii} —Zr1A—O2 ^{xii}	20 (3)	O1 ⁱⁱ —Li1—O1 ^{xxi}	116.26 (11)
Zr1B ⁱ —Zr1A—O2 ^{xii}	68 (4)	O1 ⁱ —Li1—O1 ^{xxi}	116.26 (11)
O1 ^{ix} —Zr1A—O2 ^{xii}	94.57 (13)	O1 ^{xx} —Li1—La1	131.70 (10)
O1 ^x —Zr1A—O2 ^{xii}	96.47 (13)	O1 ⁱⁱ —Li1—La1	48.30 (10)
O1 ^{xi} —Zr1A—O2 ^{xii}	172.9 (2)	O1 ⁱ —Li1—La1	48.30 (10)
Zr1B ^{viii} —Zr1A—O2 ^{iv}	68 (4)	O1 ^{xxi} —Li1—La1	131.70 (10)
Zr1B ⁱ —Zr1A—O2 ^{iv}	62 (4)	O1 ^{xx} —Li1—La1 ^{xxii}	48.30 (10)
O1 ^{ix} —Zr1A—O2 ^{iv}	172.9 (2)	O1 ⁱⁱ —Li1—La1 ^{xxii}	131.70 (10)
O1 ^x —Zr1A—O2 ^{iv}	94.57 (13)	O1 ⁱ —Li1—La1 ^{xxii}	131.70 (10)
O1 ^{xi} —Zr1A—O2 ^{iv}	96.47 (13)	O1 ^{xxi} —Li1—La1 ^{xxii}	48.30 (10)
O2 ^{xii} —Zr1A—O2 ^{iv}	79.14 (16)	La1—Li1—La1 ^{xxii}	180
Zr1B ^{viii} —Zr1A—O2 ⁱⁱ	62 (4)	O1 ^{xx} —Li1—Zr1B ^{xxiii}	132.5 (5)
Zr1B ⁱ —Zr1A—O2 ⁱⁱ	20 (3)	O1 ⁱⁱ —Li1—Zr1B ^{xxiii}	32.5 (5)
O1 ^{ix} —Zr1A—O2 ⁱⁱ	96.47 (13)	O1 ⁱ —Li1—Zr1B ^{xxiii}	104.9 (5)
O1 ^x —Zr1A—O2 ⁱⁱ	172.9 (2)	O1 ^{xxi} —Li1—Zr1B ^{xxiii}	84.9 (5)
O1 ^{xi} —Zr1A—O2 ⁱⁱ	94.57 (13)	La1—Li1—Zr1B ^{xxiii}	63.8 (5)
O2 ^{xii} —Zr1A—O2 ⁱⁱ	79.14 (16)	La1 ^{xxii} —Li1—Zr1B ^{xxiii}	116.2 (5)
O2 ^{iv} —Zr1A—O2 ⁱⁱ	79.14 (16)	O1 ^{xx} —Li1—Zr1B ^{xxiv}	32.5 (5)
Zr1B ^{viii} —Zr1A—La1 ^{xi}	150 (6)	O1 ⁱⁱ —Li1—Zr1B ^{xxiv}	84.9 (5)
Zr1B ⁱ —Zr1A—La1 ^{xi}	139 (6)	O1 ⁱ —Li1—Zr1B ^{xxiv}	132.5 (5)
O1 ^{ix} —Zr1A—La1 ^{xi}	95.88 (14)	O1 ^{xxi} —Li1—Zr1B ^{xxiv}	104.9 (5)
O1 ^x —Zr1A—La1 ^{xi}	44.94 (11)	La1—Li1—Zr1B ^{xxiv}	116.2 (5)
O1 ^{xi} —Zr1A—La1 ^{xi}	45.30 (10)	La1 ^{xxii} —Li1—Zr1B ^{xxiv}	63.8 (5)
O2 ^{xii} —Zr1A—La1 ^{xi}	139.67 (9)	Zr1B ^{xxiii} —Li1—Zr1B ^{xxiv}	101.2 (4)
O2 ^{iv} —Zr1A—La1 ^{xi}	91.13 (9)	O1 ^{xx} —Li1—Zr1B ^{vii}	84.9 (5)
O2 ⁱⁱ —Zr1A—La1 ^{xi}	137.69 (9)	O1 ⁱⁱ —Li1—Zr1B ^{vii}	104.9 (5)
Zr1B ^{viii} —Zr1A—La1 ^{ix}	139 (6)	O1 ⁱ —Li1—Zr1B ^{vii}	32.5 (5)
Zr1B ⁱ —Zr1A—La1 ^{ix}	110 (2)	O1 ^{xxi} —Li1—Zr1B ^{vii}	132.5 (5)
O1 ^{ix} —Zr1A—La1 ^{ix}	45.30 (10)	La1—Li1—Zr1B ^{vii}	63.8 (5)
O1 ^x —Zr1A—La1 ^{ix}	95.88 (14)	La1 ^{xxii} —Li1—Zr1B ^{vii}	116.2 (5)
O1 ^{xi} —Zr1A—La1 ^{ix}	44.94 (11)	Zr1B ^{xxiii} —Li1—Zr1B ^{vii}	127.7 (9)
O2 ^{xii} —Zr1A—La1 ^{ix}	137.69 (9)	Zr1B ^{xxiv} —Li1—Zr1B ^{vii}	101.2 (4)
O2 ^{iv} —Zr1A—La1 ^{ix}	139.67 (9)	O1 ^{xx} —Li1—Zr1B ^{xii}	104.9 (5)
O2 ⁱⁱ —Zr1A—La1 ^{ix}	91.13 (9)	O1 ⁱⁱ —Li1—Zr1B ^{xii}	132.5 (5)
La1 ^{xi} —Zr1A—La1 ^{ix}	70.09 (5)	O1 ⁱ —Li1—Zr1B ^{xii}	84.9 (5)
Zr1B ^{viii} —Zr1A—La1 ^x	110 (2)	O1 ^{xxi} —Li1—Zr1B ^{xii}	32.5 (5)
Zr1B ⁱ —Zr1A—La1 ^x	150 (6)	La1—Li1—Zr1B ^{xii}	116.2 (5)
O1 ^{ix} —Zr1A—La1 ^x	44.94 (11)	La1 ^{xxii} —Li1—Zr1B ^{xii}	63.8 (5)
O1 ^x —Zr1A—La1 ^x	45.30 (10)	Zr1B ^{xxiii} —Li1—Zr1B ^{xii}	101.2 (4)
O1 ^{xi} —Zr1A—La1 ^x	95.88 (14)	Zr1B ^{xxiv} —Li1—Zr1B ^{xii}	127.7 (9)
O2 ^{xii} —Zr1A—La1 ^x	91.13 (9)	Zr1B ^{vii} —Li1—Zr1B ^{xii}	101.2 (4)

O2 ^{iv} —Zr1A—La1 ^x	137.69 (9)	O1 ^{xx} —Li1—Zr1A ^{xxv}	26.21 (10)
O2 ⁱⁱ —Zr1A—La1 ^x	139.67 (9)	O1 ⁱⁱ —Li1—Zr1A ^{xxv}	90.93 (10)
La1 ^{xi} —Zr1A—La1 ^x	70.09 (5)	O1 ⁱ —Li1—Zr1A ^{xxv}	130.14 (9)
La1 ^{ix} —Zr1A—La1 ^x	70.09 (5)	O1 ^{xxi} —Li1—Zr1A ^{xxv}	103.67 (10)
Zr1B ^{viii} —Zr1A—Li1 ^{xiii}	127 (3)	La1—Li1—Zr1A ^{xxv}	119.79 (3)
Zr1B ⁱ —Zr1A—Li1 ^{xiii}	79 (4)	La1 ^{xxii} —Li1—Zr1A ^{xxv}	60.21 (3)
O1 ^{ix} —Zr1A—Li1 ^{xiii}	100.02 (10)	Zr1B ^{xxiii} —Li1—Zr1A ^{xxv}	107.3 (5)
O1 ^x —Zr1A—Li1 ^{xiii}	113.16 (12)	Zr1B ^{xxiv} —Li1—Zr1A ^{xxv}	6.2 (5)
O1 ^{xi} —Zr1A—Li1 ^{xiii}	26.09 (10)	Zr1B ^{vii} —Li1—Zr1A ^{xxv}	98.1 (5)
O2 ^{xii} —Zr1A—Li1 ^{xiii}	146.86 (13)	Zr1B ^{xii} —Li1—Zr1A ^{xxv}	123.8 (5)
O2 ^{iv} —Zr1A—Li1 ^{xiii}	83.83 (9)	O1 ^{xx} —Li1—Zr1A ^{xxiii}	130.14 (9)
O2 ⁱⁱ —Zr1A—Li1 ^{xiii}	69.81 (9)	O1 ⁱⁱ —Li1—Zr1A ^{xxiii}	26.21 (10)
La1 ^{xi} —Zr1A—Li1 ^{xiii}	68.24 (3)	O1 ⁱ —Li1—Zr1A ^{xxiii}	103.67 (10)
La1 ^{ix} —Zr1A—Li1 ^{xiii}	56.29 (2)	O1 ^{xxi} —Li1—Zr1A ^{xxiii}	90.93 (10)
La1 ^x —Zr1A—Li1 ^{xiii}	120.04 (7)	La1—Li1—Zr1A ^{xxiii}	60.21 (3)
Zr1B ^{viii} —Zr1B—Zr1B ⁱ	60.00 (6)	La1 ^{xxii} —Li1—Zr1A ^{xxiii}	119.79 (3)
Zr1B ^{viii} —Zr1B—O2 ^{iv}	138 (5)	Zr1B ^{xxiii} —Li1—Zr1A ^{xxiii}	6.2 (5)
Zr1B ⁱ —Zr1B—O2 ^{iv}	126 (9)	Zr1B ^{xxiv} —Li1—Zr1A ^{xxiii}	98.1 (5)
Zr1B ^{viii} —Zr1B—O2 ^{xii}	47 (7)	Zr1B ^{vii} —Li1—Zr1A ^{xxiii}	123.8 (5)
Zr1B ⁱ —Zr1B—O2 ^{xii}	93 (9)	Zr1B ^{xii} —Li1—Zr1A ^{xxiii}	107.3 (5)
O2 ^{iv} —Zr1B—O2 ^{xii}	92.3 (15)	Zr1A ^{xxv} —Li1—Zr1A ^{xxiii}	104.29 (3)
Zr1B ^{viii} —Zr1B—O2 ⁱⁱ	78 (9)	O2 ^{xxvi} —Li2—O2 ^{xxvii}	111.48 (10)
Zr1B ⁱ —Zr1B—O2 ⁱⁱ	36 (5)	O2 ^{xxvi} —Li2—O2 ^{xvii}	111.48 (10)
O2 ^{iv} —Zr1B—O2 ⁱⁱ	90.9 (12)	O2 ^{xxvii} —Li2—O2 ^{xvii}	105.53 (19)
O2 ^{xii} —Zr1B—O2 ⁱⁱ	85.5 (5)	O2 ^{xxvi} —Li2—O2 ^{xxviii}	105.53 (19)
Zr1B ^{viii} —Zr1B—O1 ^x	95 (9)	O2 ^{xxvii} —Li2—O2 ^{xxviii}	111.48 (10)
Zr1B ⁱ —Zr1B—O1 ^x	130 (4)	O2 ^{xvii} —Li2—O2 ^{xxviii}	111.48 (10)
O2 ^{iv} —Zr1B—O1 ^x	101.9 (13)	O2 ^{xxvi} —Li2—La1 ^{xxix}	127.23 (9)
O2 ^{xii} —Zr1B—O1 ^x	97.3 (16)	O2 ^{xxvii} —Li2—La1 ^{xxix}	52.77 (9)
O2 ⁱⁱ —Zr1B—O1 ^x	166.7 (19)	O2 ^{xvii} —Li2—La1 ^{xxix}	52.77 (9)
Zr1B ^{viii} —Zr1B—O1 ^{xi}	119 (7)	O2 ^{xxviii} —Li2—La1 ^{xxix}	127.23 (9)
Zr1B ⁱ —Zr1B—O1 ^{xi}	77 (9)	O2 ^{xxvi} —Li2—La1 ^{xxii}	52.77 (9)
O2 ^{iv} —Zr1B—O1 ^{xi}	102.2 (13)	O2 ^{xxvii} —Li2—La1 ^{xxii}	127.23 (9)
O2 ^{xii} —Zr1B—O1 ^{xi}	165.4 (18)	O2 ^{xvii} —Li2—La1 ^{xxii}	127.23 (9)
O2 ⁱⁱ —Zr1B—O1 ^{xi}	92.7 (16)	O2 ^{xxviii} —Li2—La1 ^{xxii}	52.77 (9)
O1 ^x —Zr1B—O1 ^{xi}	81.4 (6)	La1 ^{xxix} —Li2—La1 ^{xxii}	180
Zr1B ^{viii} —Zr1B—O1 ^{ix}	44 (4)	O2 ^{xxvi} —Li2—Zr1B ^{xxx}	125.3 (7)
Zr1B ⁱ —Zr1B—O1 ^{ix}	54 (7)	O2 ^{xxvii} —Li2—Zr1B ^{xxx}	24.3 (5)
O2 ^{iv} —Zr1B—O1 ^{ix}	178.7 (12)	O2 ^{xvii} —Li2—Zr1B ^{xxx}	112.0 (5)
O2 ^{xii} —Zr1B—O1 ^{ix}	89.0 (11)	O2 ^{xxviii} —Li2—Zr1B ^{xxx}	87.6 (4)
O2 ⁱⁱ —Zr1B—O1 ^{ix}	89.6 (12)	La1 ^{xxix} —Li2—Zr1B ^{xxx}	63.6 (4)
O1 ^x —Zr1B—O1 ^{ix}	77.5 (10)	La1 ^{xxii} —Li2—Zr1B ^{xxx}	116.4 (4)
O1 ^{xi} —Zr1B—O1 ^{ix}	76.6 (11)	O2 ^{xxvi} —Li2—Zr1B ^{xxii}	24.3 (5)
Zr1B ^{viii} —Zr1B—Li2 ^{vi}	164 (6)	O2 ^{xxvii} —Li2—Zr1B ^{xxii}	87.6 (4)
Zr1B ⁱ —Zr1B—Li2 ^{vi}	126 (10)	O2 ^{xvii} —Li2—Zr1B ^{xxii}	125.3 (7)
O2 ^{iv} —Zr1B—Li2 ^{vi}	26.1 (4)	O2 ^{xxviii} —Li2—Zr1B ^{xxii}	112.0 (5)
O2 ^{xii} —Zr1B—Li2 ^{vi}	117.1 (14)	La1 ^{xxix} —Li2—Zr1B ^{xxii}	116.4 (4)
O2 ⁱⁱ —Zr1B—Li2 ^{vi}	100.0 (11)	La1 ^{xxii} —Li2—Zr1B ^{xxii}	63.6 (4)

O1 ^x —Zr1B—Li2 ^{vi}	90.3 (7)	Zr1B ^{xxx} —Li2—Zr1B ^{xxii}	101.4 (3)
O1 ^{xi} —Zr1B—Li2 ^{vi}	77.4 (7)	O2 ^{xxvi} —Li2—Zr1B ^{xxix}	87.6 (4)
O1 ^{ix} —Zr1B—Li2 ^{vi}	152.6 (9)	O2 ^{xxvii} —Li2—Zr1B ^{xxix}	112.0 (5)
Zr1B ^{viii} —Zr1B—La1 ^{viii}	93 (8)	O2 ^{xxviii} —Li2—Zr1B ^{xxix}	24.3 (5)
Zr1B ⁱ —Zr1B—La1 ^{viii}	125 (4)	O2 ^{xxviii} —Li2—Zr1B ^{xxix}	125.3 (7)
O2 ^{iv} —Zr1B—La1 ^{viii}	47.1 (9)	La1 ^{xxix} —Li2—Zr1B ^{xxix}	63.6 (4)
O2 ^{xii} —Zr1B—La1 ^{viii}	46.3 (8)	La1 ^{xxii} —Li2—Zr1B ^{xxix}	116.4 (4)
O2 ⁱⁱ —Zr1B—La1 ^{viii}	95.3 (9)	Zr1B ^{xxx} —Li2—Zr1B ^{xxix}	127.3 (8)
O1 ^x —Zr1B—La1 ^{viii}	95.9 (13)	Zr1B ^{xxii} —Li2—Zr1B ^{xxix}	101.4 (3)
O1 ^{xi} —Zr1B—La1 ^{viii}	148.2 (12)	O2 ^{xxvi} —Li2—Zr1B ^{xxxi}	112.0 (5)
O1 ^{ix} —Zr1B—La1 ^{viii}	134.1 (12)	O2 ^{xxvii} —Li2—Zr1B ^{xxxi}	125.3 (7)
Li2 ^{vi} —Zr1B—La1 ^{viii}	70.9 (7)	O2 ^{xxviii} —Li2—Zr1B ^{xxxi}	87.6 (4)
Zr1B ^{viii} —Zr1B—La1	118 (6)	O2 ^{xxviii} —Li2—Zr1B ^{xxxi}	24.3 (5)
Zr1B ⁱ —Zr1B—La1	82 (8)	La1 ^{xxix} —Li2—Zr1B ^{xxxi}	116.4 (4)
O2 ^{iv} —Zr1B—La1	44.2 (7)	La1 ^{xxii} —Li2—Zr1B ^{xxxi}	63.6 (4)
O2 ^{xii} —Zr1B—La1	95.2 (8)	Zr1B ^{xxx} —Li2—Zr1B ^{xxxi}	101.4 (3)
O2 ⁱⁱ —Zr1B—La1	47.5 (6)	Zr1B ^{xxii} —Li2—Zr1B ^{xxxi}	127.3 (8)
O1 ^x —Zr1B—La1	144.4 (12)	Zr1B ^{xxix} —Li2—Zr1B ^{xxxi}	101.4 (3)

Symmetry codes: (i) z, x, y ; (ii) $z, -x, -y+1/2$; (iii) $x, -y, -z+1/2$; (iv) $-x, -y+1/2, z$; (v) $-x, y-1/2, -z+1/2$; (vi) $x-1, y, z$; (vii) $y+1/4, x+1/4, z+1/4$; (viii) y, z, x ; (ix) $z-1/4, y-1/4, x-1/4$; (x) $x-1/4, z-1/4, y-1/4$; (xi) $y-1/4, x-1/4, z-1/4$; (xii) $-y+1/2, z, -x$; (xiii) $-y, z-1/2, -x+1/2$; (xiv) $z-1/2, -x+1/2, -y$; (xv) $x+1/4, z+1/4, y+1/4$; (xvi) $z+1/4, y+1/4, x+1/4$; (xvii) $-x+1, -y+1/2, z$; (xviii) $-z, -x+1/2, y$; (xix) $-y, -z+1/2, x$; (xx) $-z+3/4, -y+1/4, x+1/4$; (xxi) $-z+3/4, y-1/4, -x+1/4$; (xxii) $-x+3/4, z-1/4, -y+1/4$; (xxiii) $y+1/4, -x-1/4, -z+1/4$; (xxiv) $-y+1/2, -z, x+1/2$; (xxv) $-x+1/2, -y, z+1/2$; (xxvi) $x+3/4, z-1/4, y-1/4$; (xxvii) $-x+1, y-1/2, -z+1/2$; (xxviii) $x+3/4, -z+1/4, -y+3/4$; (xxix) $x+1, y, z$; (xxx) $x+1, -y, -z+1/2$; (xxxi) $-x+3/4, -z+1/4, y+1/4$.

(LLZO-Ga40-pristine)

Crystal data

Ga_{0.28}La_{2.94}Li_{6.44}O_{12.00}Zr_{2.00}
 $M_r = 847.67$
 Cubic, $I\bar{4}3d$
 Hall symbol: I -4bd 2c 3
 $a = 12.9669$ (2) Å
 $V = 2180.26$ (10) Å³
 $Z = 8$
 $F(000) = 2974.7$

$D_x = 5.165$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 35033 reflections
 $\theta = 3.9\text{--}38.9^\circ$
 $\mu = 13.88$ mm⁻¹
 $T = 298$ K
 Cuboid, colorless
 0.13 × 0.13 × 0.10 mm

Data collection

Bruker SMART APEX
 diffractometer
 Graphite monochromator
 rotation, ω -scans at 4 different φ positions
 Absorption correction: multi-scan
 (APEX2; Bruker, 2012)
 $T_{\min} = 0.19, T_{\max} = 0.25$
 35033 measured reflections

1054 independent reflections
 1045 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.038$
 $\theta_{\max} = 38.9^\circ, \theta_{\min} = 3.9^\circ$
 $h = -22 \rightarrow 22$
 $k = -22 \rightarrow 22$
 $l = -22 \rightarrow 22$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.013$
 $wR(F^2) = 0.026$
 $S = 1.29$
 1054 reflections

48 parameters
 2 restraints
 0 constraints
 $w = 1/[\sigma^2(F_o^2) + (0.0079P)^2 + 2.531P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.53 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.65 \text{ e } \text{\AA}^{-3}$
 Extinction correction: SHELXL2014
 (Sheldrick, 2015),
 $F_c^* = kF_c [1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00103 (4)
 Absolute structure: Refined as an inversion
 twin.
 Absolute structure parameter: 0.50 (4)

Special details

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

Refinement. Refined as a 2-component inversion twin.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
La1	0.11966 (2)	0	0.25	0.00584 (5)	0.9814 (19)
Zr1	0.00014 (2)	0.00014 (2)	0.00014 (2)	0.00502 (8)	
O1	0.09727 (14)	0.19681 (14)	0.27989 (14)	0.0087 (3)	
O2	0.03322 (15)	0.44478 (16)	0.14725 (13)	0.0105 (3)	
Li1	0.375	0	0.25	0.0038 (5)	0.818 (3)
Ga1	0.375	0	0.25	0.0038 (5)	0.182 (3)
Li2	0.875	0	0.25	0.021 (3)	0.995 (3)
Ga2	0.875	0	0.25	0.021 (3)	0.005 (3)
Li3	0.0971 (7)	0.1868 (6)	0.4268 (6)	0.014 (2)	0.62 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.00591 (7)	0.00574 (8)	0.00587 (8)	0	0	0.00065 (5)
Zr1	0.00502 (8)	0.00502 (8)	0.00502 (8)	0.00015 (6)	0.00015 (6)	0.00015 (6)
O1	0.0079 (7)	0.0087 (7)	0.0095 (7)	-0.0008 (6)	0.0013 (5)	-0.0002 (6)
O2	0.0134 (8)	0.0122 (8)	0.0059 (7)	0.0021 (6)	-0.0003 (5)	0.0009 (6)
Li1	0.0043 (8)	0.0035 (6)	0.0035 (6)	0	0	0
Ga1	0.0043 (8)	0.0035 (6)	0.0035 (6)	0	0	0
Li2	0.013 (4)	0.025 (4)	0.025 (4)	0	0	0
Ga2	0.013 (4)	0.025 (4)	0.025 (4)	0	0	0
Li3	0.022 (4)	0.014 (4)	0.007 (3)	-0.005 (3)	0.004 (3)	0.001 (2)

Geometric parameters (\AA , $^\circ$)

La1—O2 ⁱ	2.4935 (19)	O2—Li3 ^{xv}	2.108 (9)
La1—O2 ⁱⁱ	2.4935 (19)	O2—La1 ⁱ	2.4936 (19)
La1—O1 ⁱⁱⁱ	2.5264 (19)	O2—La1 ^{xv}	2.587 (2)
La1—O1 ^{iv}	2.5264 (19)	O2—Li3 ^{xvi}	2.639 (8)
La1—O2 ⁱⁱⁱ	2.587 (2)	Li1—Li3 ^{vii}	1.645 (8)
La1—O2 ^{iv}	2.587 (2)	Li1—Li3 ^{vi}	1.645 (8)
La1—O1 ^v	2.5975 (19)	Li1—Li3 ⁱⁱⁱ	1.645 (8)
La1—O1	2.5976 (19)	Li1—Li3 ^{iv}	1.645 (8)

La1—Li3 ^{vi}	3.037 (8)	Li1—O1 ^{vi}	1.8941 (18)
La1—Li3 ^{vii}	3.037 (8)	Li1—O1 ^{iv}	1.8941 (18)
La1—Ga2 ^{viii}	3.1725 (2)	Li1—O1 ⁱⁱⁱ	1.8941 (18)
La1—Li2 ^{viii}	3.1725 (2)	Li1—O1 ^{vii}	1.8941 (18)
Zr1—O2 ^{ix}	2.0823 (18)	Li1—La1 ^{xx}	3.3109 (2)
Zr1—O2 ^{iv}	2.0823 (18)	Li2—O2 ^{xxi}	1.9246 (19)
Zr1—O2 ⁱ	2.0823 (18)	Li2—O2 ^{xxii}	1.9246 (19)
Zr1—O1 ^x	2.1346 (18)	Li2—O2 ^{xxiii}	1.9246 (19)
Zr1—O1 ^{xi}	2.1346 (18)	Li2—O2 ^{xix}	1.9246 (19)
Zr1—O1 ^{xii}	2.1346 (18)	Li2—Li3 ^{xxiv}	2.340 (9)
Zr1—Li3 ^{xiii}	2.890 (8)	Li2—Li3 ^{xxv}	2.340 (9)
Zr1—Li3 ^v	2.890 (8)	Li2—Li3 ^{xxvi}	2.340 (9)
Zr1—Li3 ^{xiv}	2.890 (8)	Li2—Li3 ^{xxvii}	2.340 (9)
Zr1—Li3 ^x	3.140 (7)	Li2—La1 ^{xx}	3.1726 (2)
Zr1—Li3 ^{xi}	3.140 (7)	Li2—La1 ^{xxviii}	3.1726 (2)
Zr1—Li3 ^{xii}	3.140 (7)	Li3—Ga1 ^{xv}	1.645 (8)
O1—Ga1 ^{xv}	1.8941 (18)	Li3—Li1 ^{xv}	1.645 (8)
O1—Li1 ^{xv}	1.8941 (18)	Li3—O1 ^{xviii}	2.075 (8)
O1—Li3	1.909 (8)	Li3—O2 ⁱⁱⁱ	2.108 (9)
O1—Li3 ^{xvi}	2.075 (8)	Li3—O1 ^{xvi}	2.229 (8)
O1—Zr1 ^{xvii}	2.1346 (18)	Li3—Ga2 ^{xxix}	2.340 (9)
O1—Li3 ^{xviii}	2.229 (8)	Li3—Li2 ^{xxix}	2.340 (9)
O1—La1 ^{xv}	2.5264 (19)	Li3—Li3 ^{xvi}	2.513 (13)
O2—Ga2 ^{xix}	1.9247 (19)	Li3—Li3 ^{xviii}	2.513 (13)
O2—Li2 ^{xix}	1.9247 (19)	Li3—O2 ^{xviii}	2.639 (8)
O2—Zr1 ⁱ	2.0823 (18)	Li3—Zr1 ^v	2.890 (8)
O2 ⁱ —La1—O2 ⁱⁱ	74.68 (9)	Li3 ^{xv} —O2—La1 ⁱ	161.4 (2)
O2 ⁱ —La1—O1 ⁱⁱⁱ	111.38 (5)	Ga2 ^{xix} —O2—La1 ^{xv}	124.19 (9)
O2 ⁱⁱ —La1—O1 ⁱⁱⁱ	160.56 (5)	Li2 ^{xix} —O2—La1 ^{xv}	124.19 (9)
O2 ⁱ —La1—O1 ^{iv}	160.56 (5)	Zr1 ⁱ —O2—La1 ^{xv}	100.00 (7)
O2 ⁱⁱ —La1—O1 ^{iv}	111.38 (5)	Li3 ^{xv} —O2—La1 ^{xv}	90.4 (2)
O1 ⁱⁱⁱ —La1—O1 ^{iv}	69.36 (8)	La1 ⁱ —O2—La1 ^{xv}	102.82 (7)
O2 ⁱ —La1—O2 ⁱⁱⁱ	125.72 (4)	Ga2 ^{xix} —O2—Li3 ^{xvi}	59.26 (19)
O2 ⁱⁱ —La1—O2 ⁱⁱⁱ	68.66 (8)	Li2 ^{xix} —O2—Li3 ^{xvi}	59.26 (19)
O1 ⁱⁱⁱ —La1—O2 ⁱⁱⁱ	94.00 (6)	Zr1 ⁱ —O2—Li3 ^{xvi}	170.9 (2)
O1 ^{iv} —La1—O2 ⁱⁱⁱ	72.71 (6)	Li3 ^{xv} —O2—Li3 ^{xvi}	94.3 (2)
O2 ⁱ —La1—O2 ^{iv}	68.66 (8)	La1 ⁱ —O2—Li3 ^{xvi}	78.05 (18)
O2 ⁱⁱ —La1—O2 ^{iv}	125.72 (4)	La1 ^{xv} —O2—Li3 ^{xvi}	71.06 (19)
O1 ⁱⁱⁱ —La1—O2 ^{iv}	72.71 (6)	Li3 ^{vii} —Li1—Li3 ^{vi}	131.8 (5)
O1 ^{iv} —La1—O2 ^{iv}	94.00 (6)	Li3 ^{vii} —Li1—Li3 ⁱⁱⁱ	99.6 (2)
O2 ⁱⁱⁱ —La1—O2 ^{iv}	164.10 (8)	Li3 ^{vi} —Li1—Li3 ⁱⁱⁱ	99.6 (2)
O2 ⁱ —La1—O1 ^v	96.52 (6)	Li3 ^{vii} —Li1—Li3 ^{iv}	99.6 (2)
O2 ⁱⁱ —La1—O1 ^v	73.06 (6)	Li3 ^{vi} —Li1—Li3 ^{iv}	99.6 (2)
O1 ⁱⁱⁱ —La1—O1 ^v	122.80 (4)	Li3 ⁱⁱⁱ —Li1—Li3 ^{iv}	131.8 (5)
O1 ^{iv} —La1—O1 ^v	69.03 (8)	Li3 ^{vii} —Li1—O1 ^{vi}	163.0 (3)
O2 ⁱⁱⁱ —La1—O1 ^v	108.95 (5)	Li3 ^{vi} —Li1—O1 ^{vi}	64.8 (3)
O2 ^{iv} —La1—O1 ^v	72.92 (5)	Li3 ⁱⁱⁱ —Li1—O1 ^{vi}	77.7 (3)

O2 ⁱ —La1—O1	73.06 (6)	Li3 ^{iv} —Li1—O1 ^{vi}	71.4 (3)
O2 ⁱⁱ —La1—O1	96.52 (6)	Li3 ^{vii} —Li1—O1 ^{iv}	71.4 (3)
O1 ⁱⁱⁱ —La1—O1	69.03 (8)	Li3 ^{vi} —Li1—O1 ^{iv}	77.7 (3)
O1 ^{iv} —La1—O1	122.80 (4)	Li3 ⁱⁱⁱ —Li1—O1 ^{iv}	163.0 (3)
O2 ⁱⁱⁱ —La1—O1	72.92 (5)	Li3 ^{iv} —Li1—O1 ^{iv}	64.8 (3)
O2 ^{iv} —La1—O1	108.95 (5)	O1 ^{vi} —Li1—O1 ^{iv}	115.09 (6)
O1 ^v —La1—O1	167.16 (8)	Li3 ^{vii} —Li1—O1 ⁱⁱⁱ	77.7 (3)
O2 ⁱ —La1—Li3 ^{vi}	146.61 (16)	Li3 ^{vi} —Li1—O1 ⁱⁱⁱ	71.4 (3)
O2 ⁱⁱ —La1—Li3 ^{vi}	123.17 (17)	Li3 ⁱⁱⁱ —Li1—O1 ⁱⁱⁱ	64.8 (3)
O1 ⁱⁱⁱ —La1—Li3 ^{vi}	42.58 (16)	Li3 ^{iv} —Li1—O1 ⁱⁱⁱ	163.0 (3)
O1 ^{iv} —La1—Li3 ^{vi}	46.12 (15)	O1 ^{vi} —Li1—O1 ⁱⁱⁱ	115.09 (6)
O2 ⁱⁱⁱ —La1—Li3 ^{vi}	55.27 (17)	O1 ^{iv} —Li1—O1 ⁱⁱⁱ	98.74 (12)
O2 ^{iv} —La1—Li3 ^{vi}	109.23 (16)	Li3 ^{vii} —Li1—O1 ^{vii}	64.8 (3)
O1 ^v —La1—Li3 ^{vi}	115.09 (16)	Li3 ^{vi} —Li1—O1 ^{vii}	163.0 (3)
O1—La1—Li3 ^{vi}	76.72 (16)	Li3 ⁱⁱⁱ —Li1—O1 ^{vii}	71.4 (3)
O2 ⁱ —La1—Li3 ^{vii}	123.17 (17)	Li3 ^{iv} —Li1—O1 ^{vii}	77.7 (3)
O2 ⁱⁱ —La1—Li3 ^{vii}	146.61 (16)	O1 ^{vi} —Li1—O1 ^{vii}	98.74 (12)
O1 ⁱⁱⁱ —La1—Li3 ^{vii}	46.12 (15)	O1 ^{iv} —Li1—O1 ^{vii}	115.09 (6)
O1 ^{iv} —La1—Li3 ^{vii}	42.58 (16)	O1 ⁱⁱⁱ —Li1—O1 ^{vii}	115.09 (6)
O2 ⁱⁱⁱ —La1—Li3 ^{vii}	109.23 (16)	Li3 ^{vii} —Li1—La1 ^{xx}	114.1 (3)
O2 ^{iv} —La1—Li3 ^{vii}	55.27 (17)	Li3 ^{vi} —Li1—La1 ^{xx}	114.1 (3)
O1 ^v —La1—Li3 ^{vii}	76.72 (15)	Li3 ⁱⁱⁱ —Li1—La1 ^{xx}	65.9 (3)
O1—La1—Li3 ^{vii}	115.09 (16)	Li3 ^{iv} —Li1—La1 ^{xx}	65.9 (3)
Li3 ^{vi} —La1—Li3 ^{vii}	59.3 (3)	O1 ^{vi} —Li1—La1 ^{xx}	49.37 (6)
O2 ⁱ —La1—Ga2 ^{viii}	37.34 (4)	O1 ^{iv} —Li1—La1 ^{xx}	130.63 (6)
O2 ⁱⁱ —La1—Ga2 ^{viii}	37.34 (4)	O1 ⁱⁱⁱ —Li1—La1 ^{xx}	130.63 (6)
O1 ⁱⁱⁱ —La1—Ga2 ^{viii}	145.32 (4)	O1 ^{vii} —Li1—La1 ^{xx}	49.37 (6)
O1 ^{iv} —La1—Ga2 ^{viii}	145.32 (4)	Li3 ^{vii} —Li1—La1	65.9 (3)
O2 ⁱⁱⁱ —La1—Ga2 ^{viii}	97.95 (4)	Li3 ^{vi} —Li1—La1	65.9 (3)
O2 ^{iv} —La1—Ga2 ^{viii}	97.95 (4)	Li3 ⁱⁱⁱ —Li1—La1	114.1 (3)
O1 ^v —La1—Ga2 ^{viii}	83.58 (4)	Li3 ^{iv} —Li1—La1	114.1 (3)
O1—La1—Ga2 ^{viii}	83.58 (4)	O1 ^{vi} —Li1—La1	130.63 (6)
Li3 ^{vi} —La1—Ga2 ^{viii}	150.36 (16)	O1 ^{iv} —Li1—La1	49.37 (6)
Li3 ^{vii} —La1—Ga2 ^{viii}	150.36 (16)	O1 ⁱⁱⁱ —Li1—La1	49.37 (6)
O2 ⁱ —La1—Li2 ^{viii}	37.34 (4)	O1 ^{vii} —Li1—La1	130.63 (6)
O2 ⁱⁱ —La1—Li2 ^{viii}	37.34 (4)	La1 ^{xx} —Li1—La1	180
O1 ⁱⁱⁱ —La1—Li2 ^{viii}	145.32 (4)	O2 ^{xxi} —Li2—O2 ^{xxii}	112.48 (6)
O1 ^{iv} —La1—Li2 ^{viii}	145.32 (4)	O2 ^{xxi} —Li2—O2 ^{xxiii}	103.61 (12)
O2 ⁱⁱⁱ —La1—Li2 ^{viii}	97.95 (4)	O2 ^{xxii} —Li2—O2 ^{xxiii}	112.48 (6)
O2 ^{iv} —La1—Li2 ^{viii}	97.95 (4)	O2 ^{xxi} —Li2—O2 ^{xix}	112.48 (6)
O1 ^v —La1—Li2 ^{viii}	83.58 (4)	O2 ^{xxii} —Li2—O2 ^{xix}	103.60 (12)
O1—La1—Li2 ^{viii}	83.58 (4)	O2 ^{xxiii} —Li2—O2 ^{xix}	112.48 (6)
Li3 ^{vi} —La1—Li2 ^{viii}	150.36 (16)	O2 ^{xxi} —Li2—Li3 ^{xxiv}	161.7 (2)
Li3 ^{vii} —La1—Li2 ^{viii}	150.36 (16)	O2 ^{xxii} —Li2—Li3 ^{xxiv}	79.8 (2)
Ga2 ^{viii} —La1—Li2 ^{viii}	0	O2 ^{xxiii} —Li2—Li3 ^{xxiv}	58.3 (2)
O2 ^{ix} —Zr1—O2 ^{iv}	86.98 (8)	O2 ^{xix} —Li2—Li3 ^{xxiv}	75.8 (2)
O2 ^{ix} —Zr1—O2 ⁱ	86.98 (8)	O2 ^{xxi} —Li2—Li3 ^{xxv}	58.3 (2)
O2 ^{iv} —Zr1—O2 ⁱ	86.98 (8)	O2 ^{xxii} —Li2—Li3 ^{xxv}	75.8 (2)

O2 ^{ix} —Zr1—O1 ^x	94.92 (8)	O2 ^{xxiii} —Li2—Li3 ^{xxv}	161.7 (2)
O2 ^{iv} —Zr1—O1 ^x	177.97 (8)	O2 ^{xix} —Li2—Li3 ^{xxv}	79.8 (2)
O2 ⁱ —Zr1—O1 ^x	92.40 (7)	Li3 ^{xxiv} —Li2—Li3 ^{xxv}	140.0 (4)
O2 ^{ix} —Zr1—O1 ^{xi}	92.40 (7)	O2 ^{xxi} —Li2—Li3 ^{xxvi}	75.8 (2)
O2 ^{iv} —Zr1—O1 ^{xi}	94.92 (8)	O2 ^{xxii} —Li2—Li3 ^{xxvi}	161.7 (2)
O2 ⁱ —Zr1—O1 ^{xi}	177.97 (8)	O2 ^{xxiii} —Li2—Li3 ^{xxvi}	79.8 (2)
O1 ^x —Zr1—O1 ^{xi}	85.72 (7)	O2 ^{xix} —Li2—Li3 ^{xxvi}	58.3 (2)
O2 ^{ix} —Zr1—O1 ^{xii}	177.97 (8)	Li3 ^{xxiv} —Li2—Li3 ^{xxvi}	96.73 (13)
O2 ^{iv} —Zr1—O1 ^{xii}	92.40 (7)	Li3 ^{xxv} —Li2—Li3 ^{xxvi}	96.73 (13)
O2 ⁱ —Zr1—O1 ^{xii}	94.92 (8)	O2 ^{xxi} —Li2—Li3 ^{xxvii}	79.8 (2)
O1 ^x —Zr1—O1 ^{xii}	85.72 (7)	O2 ^{xxii} —Li2—Li3 ^{xxvii}	58.3 (2)
O1 ^{xi} —Zr1—O1 ^{xii}	85.72 (7)	O2 ^{xxiii} —Li2—Li3 ^{xxvii}	75.8 (2)
O2 ^{ix} —Zr1—Li3 ^{xiii}	46.76 (18)	O2 ^{xix} —Li2—Li3 ^{xxvii}	161.7 (2)
O2 ^{iv} —Zr1—Li3 ^{xiii}	94.45 (17)	Li3 ^{xxiv} —Li2—Li3 ^{xxvii}	96.73 (13)
O2 ⁱ —Zr1—Li3 ^{xiii}	133.42 (18)	Li3 ^{xxv} —Li2—Li3 ^{xxvii}	96.73 (13)
O1 ^x —Zr1—Li3 ^{xiii}	87.38 (16)	Li3 ^{xxvi} —Li2—Li3 ^{xxvii}	140.0 (4)
O1 ^{xi} —Zr1—Li3 ^{xiii}	45.80 (18)	O2 ^{xxi} —Li2—La1 ^{xx}	51.80 (6)
O1 ^{xii} —Zr1—Li3 ^{xiii}	131.42 (18)	O2 ^{xxii} —Li2—La1 ^{xx}	128.20 (6)
O2 ^{ix} —Zr1—Li3 ^v	133.42 (18)	O2 ^{xxiii} —Li2—La1 ^{xx}	51.80 (6)
O2 ^{iv} —Zr1—Li3 ^v	46.76 (18)	O2 ^{xix} —Li2—La1 ^{xx}	128.20 (6)
O2 ⁱ —Zr1—Li3 ^v	94.45 (17)	Li3 ^{xxiv} —Li2—La1 ^{xx}	110.0 (2)
O1 ^x —Zr1—Li3 ^v	131.42 (18)	Li3 ^{xxv} —Li2—La1 ^{xx}	110.0 (2)
O1 ^{xi} —Zr1—Li3 ^v	87.38 (16)	Li3 ^{xxvi} —Li2—La1 ^{xx}	70.0 (2)
O1 ^{xii} —Zr1—Li3 ^v	45.80 (18)	Li3 ^{xxvii} —Li2—La1 ^{xx}	70.0 (2)
Li3 ^{xiii} —Zr1—Li3 ^v	119.81 (2)	O2 ^{xxi} —Li2—La1 ^{xxviii}	128.20 (6)
O2 ^{ix} —Zr1—Li3 ^{xiv}	94.45 (17)	O2 ^{xxii} —Li2—La1 ^{xxviii}	51.80 (6)
O2 ^{iv} —Zr1—Li3 ^{xiv}	133.42 (18)	O2 ^{xxiii} —Li2—La1 ^{xxviii}	128.20 (6)
O2 ⁱ —Zr1—Li3 ^{xiv}	46.76 (18)	O2 ^{xix} —Li2—La1 ^{xxviii}	51.80 (6)
O1 ^x —Zr1—Li3 ^{xiv}	45.80 (18)	Li3 ^{xxiv} —Li2—La1 ^{xxviii}	70.0 (2)
O1 ^{xi} —Zr1—Li3 ^{xiv}	131.42 (18)	Li3 ^{xxv} —Li2—La1 ^{xxviii}	70.0 (2)
O1 ^{xii} —Zr1—Li3 ^{xiv}	87.38 (16)	Li3 ^{xxvi} —Li2—La1 ^{xxviii}	110.0 (2)
Li3 ^{xiii} —Zr1—Li3 ^{xiv}	119.81 (2)	Li3 ^{xxvii} —Li2—La1 ^{xxviii}	110.0 (2)
Li3 ^v —Zr1—Li3 ^{xiv}	119.81 (2)	La1 ^{xx} —Li2—La1 ^{xxviii}	180
O2 ^{ix} —Zr1—Li3 ^x	59.62 (16)	Ga1 ^{xv} —Li3—Li1 ^{xv}	0
O2 ^{iv} —Zr1—Li3 ^x	145.12 (16)	Ga1 ^{xv} —Li3—O1	63.9 (3)
O2 ⁱ —Zr1—Li3 ^x	81.85 (16)	Li1 ^{xv} —Li3—O1	63.9 (3)
O1 ^x —Zr1—Li3 ^x	36.53 (16)	Ga1 ^{xv} —Li3—O1 ^{xviii}	59.9 (3)
O1 ^{xi} —Zr1—Li3 ^x	96.18 (16)	Li1 ^{xv} —Li3—O1 ^{xviii}	59.9 (3)
O1 ^{xii} —Zr1—Li3 ^x	121.32 (16)	O1—Li3—O1 ^{xviii}	106.6 (4)
Li3 ^{xiii} —Zr1—Li3 ^x	70.8 (3)	Ga1 ^{xv} —Li3—O2 ⁱⁱⁱ	138.8 (5)
Li3 ^v —Zr1—Li3 ^x	166.5 (3)	Li1 ^{xv} —Li3—O2 ⁱⁱⁱ	138.8 (5)
Li3 ^{xiv} —Zr1—Li3 ^x	49.0 (3)	O1—Li3—O2 ⁱⁱⁱ	100.0 (4)
O2 ^{ix} —Zr1—Li3 ^{xi}	81.85 (16)	O1 ^{xviii} —Li3—O2 ⁱⁱⁱ	93.4 (3)
O2 ^{iv} —Zr1—Li3 ^{xi}	59.62 (16)	Ga1 ^{xv} —Li3—O1 ^{xvi}	56.1 (3)
O2 ⁱ —Zr1—Li3 ^{xi}	145.12 (16)	Li1 ^{xv} —Li3—O1 ^{xvi}	56.1 (3)
O1 ^x —Zr1—Li3 ^{xi}	121.32 (16)	O1—Li3—O1 ^{xvi}	100.9 (4)
O1 ^{xi} —Zr1—Li3 ^{xi}	36.53 (16)	O1 ^{xviii} —Li3—O1 ^{xvi}	83.7 (3)
O1 ^{xii} —Zr1—Li3 ^{xi}	96.18 (16)	O2 ⁱⁱⁱ —Li3—O1 ^{xvi}	158.8 (4)

Li3 ^{xiii} —Zr1—Li3 ^{xi}	49.0 (3)	Gal ^{xv} —Li3—Ga2 ^{xxix}	169.9 (5)
Li3 ^v —Zr1—Li3 ^{xi}	70.8 (3)	Li1 ^{xv} —Li3—Ga2 ^{xxix}	169.9 (5)
Li3 ^{xiv} —Zr1—Li3 ^{xi}	166.5 (3)	O1—Li3—Ga2 ^{xxix}	115.3 (4)
Li3 ^x —Zr1—Li3 ^{xi}	119.11 (5)	O1 ^{xviii} —Li3—Ga2 ^{xxix}	127.8 (4)
O2 ^{ix} —Zr1—Li3 ^{xii}	145.12 (16)	O2 ⁱⁱⁱ —Li3—Ga2 ^{xxix}	50.9 (2)
O2 ^{iv} —Zr1—Li3 ^{xii}	81.85 (16)	O1 ^{xvi} —Li3—Ga2 ^{xxix}	115.7 (4)
O2 ⁱ —Zr1—Li3 ^{xii}	59.62 (16)	Gal ^{xv} —Li3—Li2 ^{xxix}	169.9 (5)
O1 ^x —Zr1—Li3 ^{xii}	96.18 (16)	Li1 ^{xv} —Li3—Li2 ^{xxix}	169.9 (5)
O1 ^{xi} —Zr1—Li3 ^{xii}	121.32 (16)	O1—Li3—Li2 ^{xxix}	115.3 (4)
O1 ^{xii} —Zr1—Li3 ^{xii}	36.53 (16)	O1 ^{xviii} —Li3—Li2 ^{xxix}	127.8 (4)
Li3 ^{xiii} —Zr1—Li3 ^{xii}	166.5 (3)	O2 ⁱⁱⁱ —Li3—Li2 ^{xxix}	50.9 (2)
Li3 ^v —Zr1—Li3 ^{xii}	49.0 (3)	O1 ^{xvi} —Li3—Li2 ^{xxix}	115.7 (4)
Li3 ^{xiv} —Zr1—Li3 ^{xii}	70.8 (3)	Ga2 ^{xxix} —Li3—Li2 ^{xxix}	0
Li3 ^x —Zr1—Li3 ^{xii}	119.11 (5)	Gal ^{xv} —Li3—Li3 ^{xvi}	40.21 (10)
Li3 ^{xi} —Zr1—Li3 ^{xii}	119.11 (5)	Li1 ^{xv} —Li3—Li3 ^{xvi}	40.21 (10)
Gal ^{xv} —O1—Li1 ^{xv}	0	O1—Li3—Li3 ^{xvi}	53.9 (3)
Gal ^{xv} —O1—Li3	51.3 (3)	O1 ^{xviii} —Li3—Li3 ^{xvi}	99.0 (3)
Li1 ^{xv} —O1—Li3	51.3 (3)	O2 ⁱⁱⁱ —Li3—Li3 ^{xvi}	153.4 (5)
Gal ^{xv} —O1—Li3 ^{xvi}	48.7 (2)	O1 ^{xvi} —Li3—Li3 ^{xvi}	47.0 (2)
Li1 ^{xv} —O1—Li3 ^{xvi}	48.7 (2)	Ga2 ^{xxix} —Li3—Li3 ^{xvi}	130.4 (4)
Li3—O1—Li3 ^{xvi}	78.1 (3)	Li2 ^{xxix} —Li3—Li3 ^{xvi}	130.4 (4)
Gal ^{xv} —O1—Zr1 ^{xvii}	128.17 (10)	Gal ^{xv} —Li3—Li3 ^{xviii}	40.21 (10)
Li1 ^{xv} —O1—Zr1 ^{xvii}	128.17 (10)	Li1 ^{xv} —Li3—Li3 ^{xviii}	40.21 (10)
Li3—O1—Zr1 ^{xvii}	101.7 (3)	O1—Li3—Li3 ^{xviii}	58.7 (3)
Li3 ^{xvi} —O1—Zr1 ^{xvii}	86.7 (2)	O1 ^{xviii} —Li3—Li3 ^{xviii}	48.0 (2)
Gal ^{xv} —O1—Li3 ^{xviii}	46.1 (2)	O2 ⁱⁱⁱ —Li3—Li3 ^{xviii}	98.6 (5)
Li1 ^{xv} —O1—Li3 ^{xviii}	46.1 (2)	O1 ^{xvi} —Li3—Li3 ^{xviii}	95.0 (2)
Li3—O1—Li3 ^{xviii}	74.3 (3)	Ga2 ^{xxix} —Li3—Li3 ^{xviii}	149.1 (5)
Li3 ^{xvi} —O1—Li3 ^{xviii}	88.4 (4)	Li2 ^{xxix} —Li3—Li3 ^{xviii}	149.1 (5)
Zr1 ^{xvii} —O1—Li3 ^{xviii}	174.3 (2)	Li3 ^{xvi} —Li3—Li3 ^{xviii}	73.4 (3)
Gal ^{xv} —O1—La1 ^{xv}	95.95 (7)	Gal ^{xv} —Li3—O2 ^{xviii}	130.3 (4)
Li1 ^{xv} —O1—La1 ^{xv}	95.95 (7)	Li1 ^{xv} —Li3—O2 ^{xviii}	130.3 (4)
Li3—O1—La1 ^{xv}	147.0 (3)	O1—Li3—O2 ^{xviii}	148.4 (4)
Li3 ^{xvi} —O1—La1 ^{xv}	82.0 (2)	O1 ^{xviii} —Li3—O2 ^{xviii}	104.4 (3)
Zr1 ^{xvii} —O1—La1 ^{xv}	103.10 (7)	O2 ⁱⁱⁱ —Li3—O2 ^{xviii}	84.0 (3)
Li3 ^{xviii} —O1—La1 ^{xv}	79.11 (19)	O1 ^{xvi} —Li3—O2 ^{xviii}	76.5 (2)
Gal ^{xv} —O1—La1	121.96 (8)	Ga2 ^{xxix} —Li3—O2 ^{xviii}	44.98 (15)
Li1 ^{xv} —O1—La1	121.96 (8)	Li2 ^{xxix} —Li3—O2 ^{xviii}	44.98 (15)
Li3—O1—La1	94.7 (3)	Li3 ^{xvi} —Li3—O2 ^{xviii}	115.1 (4)
Li3 ^{xvi} —O1—La1	170.6 (2)	Li3 ^{xviii} —Li3—O2 ^{xviii}	152.2 (5)
Zr1 ^{xvii} —O1—La1	100.81 (7)	Gal ^{xv} —Li3—Zr1 ^v	102.6 (4)
Li3 ^{xviii} —O1—La1	83.8 (2)	Li1 ^{xv} —Li3—Zr1 ^v	102.6 (4)
La1 ^{xv} —O1—La1	101.62 (6)	O1—Li3—Zr1 ^v	112.6 (3)
Ga2 ^{xix} —O2—Li2 ^{xix}	0	O1 ^{xviii} —Li3—Zr1 ^v	47.50 (17)
Ga2 ^{xix} —O2—Zr1 ⁱ	129.42 (11)	O2 ⁱⁱⁱ —Li3—Zr1 ^v	46.02 (16)
Li2 ^{xix} —O2—Zr1 ⁱ	129.42 (11)	O1 ^{xvi} —Li3—Zr1 ^v	126.1 (3)
Ga2 ^{xix} —O2—Li3 ^{xv}	70.8 (2)	Ga2 ^{xxix} —Li3—Zr1 ^v	87.0 (2)
Li2 ^{xix} —O2—Li3 ^{xv}	70.8 (2)	Li2 ^{xxix} —Li3—Zr1 ^v	87.0 (2)

Zr1 ⁱ —O2—Li3 ^{xv}	87.2 (2)	Li3 ^{xvi} —Li3—Zr1 ^v	142.5 (4)
Ga2 ^{xix} —O2—La1 ⁱ	90.85 (7)	Li3 ^{xviii} —Li3—Zr1 ^v	70.7 (3)
Li2 ^{xix} —O2—La1 ⁱ	90.85 (7)	O2 ^{xviii} —Li3—Zr1 ^v	92.8 (2)
Zr1 ⁱ —O2—La1 ⁱ	103.05 (8)		

Symmetry codes: (i) $-x, -y+1/2, z$; (ii) $-x, y-1/2, -z+1/2$; (iii) z, x, y ; (iv) $z, -x, -y+1/2$; (v) $x, -y, -z+1/2$; (vi) $-z+3/4, -y+1/4, x+1/4$; (vii) $-z+3/4, y-1/4, -x+1/4$; (viii) $x-1, y, z$; (ix) $-y+1/2, z, -x$; (x) $x-1/4, z-1/4, y-1/4$; (xi) $z-1/4, y-1/4, x-1/4$; (xii) $y-1/4, x-1/4, z-1/4$; (xiii) $-z+1/2, x, -y$; (xiv) $-y, -z+1/2, x$; (xv) y, z, x ; (xvi) $-y+1/4, x+1/4, -z+3/4$; (xvii) $y+1/4, x+1/4, z+1/4$; (xviii) $y-1/4, -x+1/4, -z+3/4$; (xix) $-x+1, -y+1/2, z$; (xx) $-x+3/4, z-1/4, -y+1/4$; (xxi) $x+3/4, z-1/4, y-1/4$; (xxii) $-x+1, y-1/2, -z+1/2$; (xxiii) $x+3/4, -z+1/4, -y+3/4$; (xxiv) $y+3/4, -x+1/4, -z+3/4$; (xxv) $y+3/4, x-1/4, z-1/4$; (xxvi) $-y+1, -z+1/2, x$; (xxvii) $-y+1, z-1/2, -x+1/2$; (xxviii) $x+1, y, z$; (xxix) $-y+1/4, x-3/4, -z+3/4$.

(LLZO-Ga40-hydro-150C)

Crystal data

Ga_{0.26}H_{3.90}La_{2.96}Li_{1.99}O₁₂Zr₂
 $M_r = 821.46$
 Cubic, $I\bar{4}3d$
 Hall symbol: I -4bd 2c 3
 $a = 13.06720$ (12) Å
 $V = 2231.25$ (6) Å³
 $Z = 8$
 $F(000) = 2901.2$

$D_x = 4.891$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 35657 reflections
 $\theta = 3.8\text{--}36.6^\circ$
 $\mu = 13.57$ mm⁻¹
 $T = 298$ K
 Cuboid, colorless
 $0.12 \times 0.11 \times 0.09$ mm

Data collection

Bruker SMART APEX
 diffractometer
 Graphite monochromator
 rotation, ω -scans at 4 different ϕ positions
 Absorption correction: multi-scan
 (APEX2; Bruker, 2012)
 $T_{\min} = 0.21, T_{\max} = 0.36$
 35657 measured reflections

918 independent reflections
 915 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$
 $\theta_{\max} = 36.6^\circ, \theta_{\min} = 3.8^\circ$
 $h = -21 \rightarrow 21$
 $k = -21 \rightarrow 21$
 $l = -21 \rightarrow 21$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.018$
 $wR(F^2) = 0.037$
 $S = 1.12$
 918 reflections
 43 parameters
 3 restraints
 0 constraints
 Hydrogen site location: difference Fourier map
 Only H-atom coordinates refined

$w = 1/[\sigma^2(F_o^2) + (0.0072P)^2 + 28.9201P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.54$ e Å⁻³
 $\Delta\rho_{\min} = -0.52$ e Å⁻³
 Extinction correction: SHELXL2014
 (Sheldrick, 2015),
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.00055 (4)
 Absolute structure: Refined as an inversion
 twin.
 Absolute structure parameter: 0.99944 (15)

Special details

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

Refinement. Refined as a 2-component inversion twin.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
La1	0.11790 (3)	0	0.25	0.00993 (9)	0.986 (4)
Zr1	-0.01020 (3)	-0.01020 (3)	-0.01020 (3)	0.01011 (17)	
O1	0.0963 (3)	0.1906 (3)	0.2735 (3)	0.0106 (6)	
O2	0.0339 (3)	0.4448 (3)	0.1420 (3)	0.0138 (6)	
Li1	0.375	0	0.25	0.0068 (7)	0.824 (3)
Ga1	0.375	0	0.25	0.0068 (7)	0.176 (3)
Li2	0.875	0	0.25	0.007*	0.34 (5)
Li3	0.070 (16)	0.283 (15)	0.457 (16)	0.01*	0.04 (3)
H1	0.104 (11)	0.183 (10)	0.321 (8)	0.025*	0.65 (19)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.00856 (14)	0.00800 (14)	0.01322 (16)	0	0	0.00411 (10)
Zr1	0.01011 (17)	0.01011 (17)	0.01011 (17)	-0.00033 (13)	-0.00033 (13)	-0.00033 (13)
O1	0.0076 (11)	0.0106 (13)	0.0135 (14)	-0.0005 (10)	-0.0005 (10)	0.0019 (10)
O2	0.0191 (15)	0.0128 (14)	0.0095 (13)	0.0025 (11)	0.0030 (10)	0.0032 (11)
Li1	0.0055 (13)	0.0075 (10)	0.0075 (10)	0	0	0
Ga1	0.0055 (13)	0.0075 (10)	0.0075 (10)	0	0	0

Geometric parameters (\AA , $^\circ$)

La1—Li3 ⁱ	2.5 (2)	O2—La1 ^{xvi}	2.603 (4)
La1—Li3 ⁱⁱ	2.5 (2)	Li1—Li3 ⁱⁱⁱ	1.5 (2)
La1—O1 ⁱⁱⁱ	2.514 (3)	Li1—Li3 ⁱⁱ	1.5 (2)
La1—O1 ^{iv}	2.514 (3)	Li1—Li3 ^{iv}	1.5 (2)
La1—O1 ^v	2.525 (3)	Li1—Li3 ⁱ	1.5 (2)
La1—O1	2.525 (3)	Li1—O1 ⁱ	1.987 (4)
La1—O2 ^{vi}	2.539 (4)	Li1—O1 ^{iv}	1.987 (4)
La1—O2 ^{vii}	2.539 (4)	Li1—O1 ⁱⁱⁱ	1.987 (4)
La1—O2 ⁱⁱⁱ	2.603 (4)	Li1—O1 ⁱⁱ	1.987 (4)
La1—O2 ^{iv}	2.603 (4)	Li1—La1 ^{xx}	3.3596 (4)
La1—Li3 ^{viii}	2.7 (2)	Li1—Zr1 ^{xxi}	3.5997 (1)
La1—Li3 ^{ix}	2.7 (2)	Li1—Zr1 ^{xxii}	3.5997 (1)
Zr1—O1 ^x	2.031 (3)	Li2—O2 ^{xxiii}	1.982 (4)
Zr1—O1 ^{xi}	2.031 (3)	Li2—O2 ^{xxiv}	1.982 (4)
Zr1—O1 ^{viii}	2.031 (3)	Li2—O2 ^{xxv}	1.982 (4)
Zr1—O2 ^{iv}	2.187 (4)	Li2—O2 ^{xix}	1.982 (4)
Zr1—O2 ^{xii}	2.187 (4)	Li2—La1 ^{xx}	3.1740 (4)
Zr1—O2 ^{vi}	2.187 (4)	Li2—La1 ^{xxvi}	3.1740 (4)
Zr1—Li3 ^{xiii}	2.9 (2)	Li2—Li3 ^{xxvii}	3.2 (2)
Zr1—Li3 ^{xiv}	2.9 (2)	Li2—Li3 ^{xxviii}	3.2 (2)
Zr1—Li3 ^{vii}	2.9 (2)	Li2—Li3 ^{xxix}	3.2 (2)
Zr1—La1 ^{xi}	3.5178 (5)	Li2—Li3 ^{xxx}	3.2 (2)
Zr1—La1 ^{xv}	3.5178 (5)	Li3—O1 ^{xviii}	0.9 (2)

Zr1—La1 ^x	3.5178 (5)	Li3—Ga1 ^{xvi}	1.5 (2)
O1—Li3 ^{ix}	0.9 (2)	Li3—Li1 ^{xvi}	1.5 (2)
O1—Ga1 ^{xvi}	1.987 (4)	Li3—Li3 ^{vi}	2.0 (4)
O1—Li1 ^{xvi}	1.987 (4)	Li3—O1 ^{ix}	2.4 (2)
O1—Zr1 ^{xvii}	2.031 (3)	Li3—La1 ^{xxxi}	2.5 (2)
O1—Li3 ^{xviii}	2.4 (2)	Li3—Li3 ^{xviii}	2.6 (4)
O1—La1 ^{xvi}	2.514 (3)	Li3—Li3 ^{ix}	2.6 (4)
O2—Li2 ^{xix}	1.982 (4)	Li3—La1 ^{xviii}	2.7 (2)
O2—Zr1 ^{vi}	2.187 (4)	Li3—Zr1 ^{xxxii}	2.9 (2)
O2—La1 ^{vi}	2.539 (4)	Li3—Li2 ^{xxxiii}	3.2 (2)
Li3 ⁱ —La1—Li3 ⁱⁱ	48 (9)	Li3 ⁱⁱ —Li1—Li3 ⁱ	86 (10)
Li3 ⁱ —La1—O1 ⁱⁱⁱ	57 (5)	Li3 ^{iv} —Li1—Li3 ⁱ	122 (10)
Li3 ⁱⁱ —La1—O1 ⁱⁱⁱ	20 (5)	Li3 ⁱⁱⁱ —Li1—O1 ⁱ	24 (8)
Li3 ⁱ —La1—O1 ^{iv}	20 (5)	Li3 ⁱⁱ —Li1—O1 ⁱ	140 (8)
Li3 ⁱⁱ —La1—O1 ^{iv}	57 (5)	Li3 ^{iv} —Li1—O1 ⁱ	87 (8)
O1 ⁱⁱⁱ —La1—O1 ^{iv}	72.06 (16)	Li3 ⁱ —Li1—O1 ⁱ	102 (8)
Li3 ⁱ —La1—O1 ^v	89 (5)	Li3 ⁱⁱⁱ —Li1—O1 ^{iv}	140 (8)
Li3 ⁱⁱ —La1—O1 ^v	103 (5)	Li3 ⁱⁱ —Li1—O1 ^{iv}	87 (8)
O1 ⁱⁱⁱ —La1—O1 ^v	123.13 (7)	Li3 ^{iv} —Li1—O1 ^{iv}	102 (8)
O1 ^{iv} —La1—O1 ^v	68.54 (15)	Li3 ⁱ —Li1—O1 ^{iv}	24 (8)
Li3 ⁱ —La1—O1	103 (5)	O1 ⁱ —Li1—O1 ^{iv}	116.47 (11)
Li3 ⁱⁱ —La1—O1	89 (5)	Li3 ⁱⁱⁱ —Li1—O1 ⁱⁱⁱ	102 (8)
O1 ⁱⁱⁱ —La1—O1	68.54 (15)	Li3 ⁱⁱ —Li1—O1 ⁱⁱⁱ	24 (8)
O1 ^{iv} —La1—O1	123.13 (7)	Li3 ^{iv} —Li1—O1 ⁱⁱⁱ	140 (8)
O1 ^v —La1—O1	167.17 (15)	Li3 ⁱ —Li1—O1 ⁱⁱⁱ	87 (8)
Li3 ⁱ —La1—O2 ^{vi}	165 (5)	O1 ⁱ —Li1—O1 ⁱⁱⁱ	116.47 (11)
Li3 ⁱⁱ —La1—O2 ^{vi}	118 (5)	O1 ^{iv} —Li1—O1 ⁱⁱⁱ	96.2 (2)
O1 ⁱⁱⁱ —La1—O2 ^{vi}	108.54 (10)	Li3 ⁱⁱⁱ —Li1—O1 ⁱⁱ	87 (8)
O1 ^{iv} —La1—O2 ^{vi}	161.05 (10)	Li3 ⁱⁱ —Li1—O1 ⁱⁱ	102 (8)
O1 ^v —La1—O2 ^{vi}	97.21 (12)	Li3 ^{iv} —Li1—O1 ⁱⁱ	24 (8)
O1—La1—O2 ^{vi}	72.54 (11)	Li3 ⁱ —Li1—O1 ⁱⁱ	140 (8)
Li3 ⁱ —La1—O2 ^{vii}	118 (5)	O1 ⁱ —Li1—O1 ⁱⁱ	96.2 (2)
Li3 ⁱⁱ —La1—O2 ^{vii}	165 (5)	O1 ^{iv} —Li1—O1 ⁱⁱ	116.47 (11)
O1 ⁱⁱⁱ —La1—O2 ^{vii}	161.05 (10)	O1 ⁱⁱⁱ —Li1—O1 ⁱⁱ	116.47 (11)
O1 ^{iv} —La1—O2 ^{vii}	108.54 (10)	Li3 ⁱⁱⁱ —Li1—La1	137 (8)
O1 ^v —La1—O2 ^{vii}	72.54 (11)	Li3 ⁱⁱ —Li1—La1	43 (8)
O1—La1—O2 ^{vii}	97.21 (12)	Li3 ^{iv} —Li1—La1	137 (8)
O2 ^{vi} —La1—O2 ^{vii}	77.23 (18)	Li3 ⁱ —Li1—La1	43 (8)
Li3 ⁱ —La1—O2 ⁱⁱⁱ	64 (5)	O1 ⁱ —Li1—La1	131.89 (10)
Li3 ⁱⁱ —La1—O2 ⁱⁱⁱ	102 (5)	O1 ^{iv} —Li1—La1	48.11 (10)
O1 ⁱⁱⁱ —La1—O2 ⁱⁱⁱ	96.82 (12)	O1 ⁱⁱⁱ —Li1—La1	48.11 (10)
O1 ^{iv} —La1—O2 ⁱⁱⁱ	71.66 (11)	O1 ⁱⁱ —Li1—La1	131.89 (10)
O1 ^v —La1—O2 ⁱⁱⁱ	107.49 (10)	Li3 ⁱⁱⁱ —Li1—La1 ^{xx}	43 (8)
O1—La1—O2 ⁱⁱⁱ	74.13 (11)	Li3 ⁱⁱ —Li1—La1 ^{xx}	137 (8)
O2 ^{vi} —La1—O2 ⁱⁱⁱ	126.12 (8)	Li3 ^{iv} —Li1—La1 ^{xx}	43 (8)
O2 ^{vii} —La1—O2 ⁱⁱⁱ	66.40 (16)	Li3 ⁱ —Li1—La1 ^{xx}	137 (8)
Li3 ⁱ —La1—O2 ^{iv}	102 (5)	O1 ⁱ —Li1—La1 ^{xx}	48.11 (10)

Li3 ⁱⁱ —La1—O2 ^{iv}	64 (5)	O1 ^{iv} —Li1—La1 ^{xx}	131.89 (10)
O1 ⁱⁱⁱ —La1—O2 ^{iv}	71.66 (11)	O1 ⁱⁱⁱ —Li1—La1 ^{xx}	131.89 (10)
O1 ^{iv} —La1—O2 ^{iv}	96.82 (12)	O1 ⁱⁱ —Li1—La1 ^{xx}	48.11 (10)
O1 ^v —La1—O2 ^{iv}	74.13 (11)	La1—Li1—La1 ^{xx}	180
O1—La1—O2 ^{iv}	107.49 (10)	Li3 ⁱⁱⁱ —Li1—Zr1 ^{xxi}	50 (8)
O2 ^{vi} —La1—O2 ^{iv}	66.40 (16)	Li3 ⁱⁱ —Li1—Zr1 ^{xxi}	152 (8)
O2 ^{vii} —La1—O2 ^{iv}	126.12 (8)	Li3 ^{iv} —Li1—Zr1 ^{xxi}	85 (8)
O2 ⁱⁱⁱ —La1—O2 ^{iv}	166.09 (15)	Li3 ⁱ —Li1—Zr1 ^{xxi}	80 (8)
Li3 ⁱ —La1—Li3 ^{viii}	108 (9)	O1 ⁱ —Li1—Zr1 ^{xxi}	26.66 (10)
Li3 ⁱⁱ —La1—Li3 ^{viii}	117 (2)	O1 ^{iv} —Li1—Zr1 ^{xxi}	90.62 (10)
O1 ⁱⁱⁱ —La1—Li3 ^{viii}	136 (5)	O1 ⁱⁱⁱ —Li1—Zr1 ^{xxi}	130.13 (10)
O1 ^{iv} —La1—Li3 ^{viii}	88 (4)	O1 ⁱⁱ —Li1—Zr1 ^{xxi}	103.79 (10)
O1 ^v —La1—Li3 ^{viii}	19 (4)	La1—Li1—Zr1 ^{xxi}	119.390 (8)
O1—La1—Li3 ^{viii}	148 (4)	La1 ^{xx} —Li1—Zr1 ^{xxi}	60.610 (8)
O2 ^{vi} —La1—Li3 ^{viii}	79 (4)	Li3 ⁱⁱⁱ —Li1—Zr1 ^{xxii}	152 (8)
O2 ^{vii} —La1—Li3 ^{viii}	63 (5)	Li3 ⁱⁱ —Li1—Zr1 ^{xxii}	85 (8)
O2 ⁱⁱⁱ —La1—Li3 ^{viii}	114 (4)	Li3 ^{iv} —Li1—Zr1 ^{xxii}	80 (8)
O2 ^{iv} —La1—Li3 ^{viii}	72 (4)	Li3 ⁱ —Li1—Zr1 ^{xxii}	50 (8)
Li3 ⁱ —La1—Li3 ^{ix}	117 (2)	O1 ⁱ —Li1—Zr1 ^{xxii}	130.13 (10)
Li3 ⁱⁱ —La1—Li3 ^{ix}	108 (9)	O1 ^{iv} —Li1—Zr1 ^{xxii}	26.66 (10)
O1 ⁱⁱⁱ —La1—Li3 ^{ix}	88 (4)	O1 ⁱⁱⁱ —Li1—Zr1 ^{xxii}	103.79 (10)
O1 ^{iv} —La1—Li3 ^{ix}	136 (5)	O1 ⁱⁱ —Li1—Zr1 ^{xxii}	90.62 (10)
O1 ^v —La1—Li3 ^{ix}	148 (4)	La1—Li1—Zr1 ^{xxii}	60.610 (8)
O1—La1—Li3 ^{ix}	19 (4)	La1 ^{xx} —Li1—Zr1 ^{xxii}	119.390 (8)
O2 ^{vi} —La1—Li3 ^{ix}	63 (5)	Zr1 ^{xxi} —Li1—Zr1 ^{xxii}	103.936 (7)
O2 ^{vii} —La1—Li3 ^{ix}	79 (4)	O2 ^{xxiii} —Li2—O2 ^{xxiv}	111.13 (11)
O2 ⁱⁱⁱ —La1—Li3 ^{ix}	72 (4)	O2 ^{xxiii} —Li2—O2 ^{xxv}	106.2 (2)
O2 ^{iv} —La1—Li3 ^{ix}	114 (4)	O2 ^{xxiv} —Li2—O2 ^{xxv}	111.13 (11)
Li3 ^{viii} —La1—Li3 ^{ix}	131 (9)	O2 ^{xxiii} —Li2—O2 ^{xix}	111.13 (11)
O1 ^x —Zr1—O1 ^{xi}	88.64 (15)	O2 ^{xxiv} —Li2—O2 ^{xix}	106.2 (2)
O1 ^x —Zr1—O1 ^{viii}	88.64 (15)	O2 ^{xxv} —Li2—O2 ^{xix}	111.13 (11)
O1 ^{xi} —Zr1—O1 ^{viii}	88.64 (15)	O2 ^{xxiii} —Li2—La1 ^{xx}	53.10 (10)
O1 ^x —Zr1—O2 ^{iv}	173.91 (17)	O2 ^{xxiv} —Li2—La1 ^{xx}	126.90 (10)
O1 ^{xi} —Zr1—O2 ^{iv}	96.82 (14)	O2 ^{xxv} —Li2—La1 ^{xx}	53.10 (10)
O1 ^{viii} —Zr1—O2 ^{iv}	94.15 (14)	O2 ^{xix} —Li2—La1 ^{xx}	126.90 (10)
O1 ^x —Zr1—O2 ^{xii}	96.82 (14)	O2 ^{xxiii} —Li2—La1 ^{xxvi}	126.90 (10)
O1 ^{xi} —Zr1—O2 ^{xii}	94.15 (14)	O2 ^{xxiv} —Li2—La1 ^{xxvi}	53.10 (10)
O1 ^{viii} —Zr1—O2 ^{xii}	173.91 (17)	O2 ^{xxv} —Li2—La1 ^{xxvi}	126.90 (10)
O2 ^{iv} —Zr1—O2 ^{xii}	80.15 (16)	O2 ^{xix} —Li2—La1 ^{xxvi}	53.10 (10)
O1 ^x —Zr1—O2 ^{vi}	94.15 (14)	La1 ^{xx} —Li2—La1 ^{xxvi}	180
O1 ^{xi} —Zr1—O2 ^{vi}	173.91 (17)	O2 ^{xxiii} —Li2—Li3 ^{xxvii}	169 (4)
O1 ^{viii} —Zr1—O2 ^{vi}	96.82 (14)	O2 ^{xxiv} —Li2—Li3 ^{xxvii}	76 (4)
O2 ^{iv} —Zr1—O2 ^{vi}	80.15 (16)	O2 ^{xxv} —Li2—Li3 ^{xxvii}	78 (4)
O2 ^{xii} —Zr1—O2 ^{vi}	80.15 (16)	O2 ^{xix} —Li2—Li3 ^{xxvii}	58 (4)
O1 ^x —Zr1—Li3 ^{xiii}	89 (4)	La1 ^{xx} —Li2—Li3 ^{xxvii}	130 (4)
O1 ^{xi} —Zr1—Li3 ^{xiii}	3 (4)	La1 ^{xxvi} —Li2—Li3 ^{xxvii}	50 (4)
O1 ^{viii} —Zr1—Li3 ^{xiii}	92 (4)	O2 ^{xxiii} —Li2—Li3 ^{xxviii}	58 (4)
O2 ^{iv} —Zr1—Li3 ^{xiii}	96 (4)	O2 ^{xxiv} —Li2—Li3 ^{xxviii}	169 (4)

O2 ^{xii} —Zr1—Li3 ^{xiii}	91 (4)	O2 ^{xxv} —Li2—Li3 ^{xxviii}	76 (4)
O2 ^{vi} —Zr1—Li3 ^{xiii}	171 (4)	O2 ^{xix} —Li2—Li3 ^{xxviii}	78 (4)
O1 ^x —Zr1—Li3 ^{xiv}	3 (4)	La1 ^{xx} —Li2—Li3 ^{xxviii}	50 (4)
O1 ^{xi} —Zr1—Li3 ^{xiv}	92 (4)	La1 ^{xxvi} —Li2—Li3 ^{xxviii}	130 (4)
O1 ^{viii} —Zr1—Li3 ^{xiv}	89 (4)	Li3 ^{xxvii} —Li2—Li3 ^{xxviii}	115 (4)
O2 ^{iv} —Zr1—Li3 ^{xiv}	171 (4)	O2 ^{xxiii} —Li2—Li3 ^{xxix}	76 (4)
O2 ^{xii} —Zr1—Li3 ^{xiv}	96 (4)	O2 ^{xxiv} —Li2—Li3 ^{xxix}	78 (4)
O2 ^{vi} —Zr1—Li3 ^{xiv}	91 (4)	O2 ^{xxv} —Li2—Li3 ^{xxix}	58 (4)
Li3 ^{xiii} —Zr1—Li3 ^{xiv}	92 (6)	O2 ^{xix} —Li2—Li3 ^{xxix}	169 (4)
O1 ^x —Zr1—Li3 ^{vii}	92 (4)	La1 ^{xx} —Li2—Li3 ^{xxix}	50 (4)
O1 ^{xi} —Zr1—Li3 ^{vii}	89 (4)	La1 ^{xxvi} —Li2—Li3 ^{xxix}	130 (4)
O1 ^{viii} —Zr1—Li3 ^{vii}	3 (4)	Li3 ^{xxvii} —Li2—Li3 ^{xxix}	115 (4)
O2 ^{iv} —Zr1—Li3 ^{vii}	91 (4)	Li3 ^{xxviii} —Li2—Li3 ^{xxix}	99 (7)
O2 ^{xii} —Zr1—Li3 ^{vii}	171 (4)	O2 ^{xxiii} —Li2—Li3 ^{xxx}	78 (4)
O2 ^{vi} —Zr1—Li3 ^{vii}	96 (4)	O2 ^{xxiv} —Li2—Li3 ^{xxx}	58 (4)
Li3 ^{xiii} —Zr1—Li3 ^{vii}	92 (6)	O2 ^{xxv} —Li2—Li3 ^{xxx}	169 (4)
Li3 ^{xiv} —Zr1—Li3 ^{vii}	92 (6)	O2 ^{xix} —Li2—Li3 ^{xxx}	76 (4)
O1 ^x —Zr1—La1 ^{xi}	94.85 (10)	La1 ^{xx} —Li2—Li3 ^{xxx}	130 (4)
O1 ^{xi} —Zr1—La1 ^{xi}	44.88 (10)	La1 ^{xxvi} —Li2—Li3 ^{xxx}	50 (4)
O1 ^{viii} —Zr1—La1 ^{xi}	44.58 (10)	Li3 ^{xxvii} —Li2—Li3 ^{xxx}	99 (7)
O2 ^{iv} —Zr1—La1 ^{xi}	90.93 (10)	Li3 ^{xxviii} —Li2—Li3 ^{xxx}	115 (4)
O2 ^{xii} —Zr1—La1 ^{xi}	136.97 (10)	Li3 ^{xxix} —Li2—Li3 ^{xxx}	115 (4)
O2 ^{vi} —Zr1—La1 ^{xi}	139.95 (10)	O1 ^{xviii} —Li3—Ga1 ^{xvi}	113 (10)
Li3 ^{xiii} —Zr1—La1 ^{xi}	48 (4)	O1 ^{xviii} —Li3—Li1 ^{xvi}	113 (10)
Li3 ^{xiv} —Zr1—La1 ^{xi}	97 (4)	Ga1 ^{xvi} —Li3—Li1 ^{xvi}	0
Li3 ^{vii} —Zr1—La1 ^{xi}	45 (4)	O1 ^{xviii} —Li3—Li3 ^{vi}	106 (10)
O1 ^x —Zr1—La1 ^{xv}	44.58 (10)	Ga1 ^{xvi} —Li3—Li3 ^{vi}	47 (8)
O1 ^{xi} —Zr1—La1 ^{xv}	94.85 (10)	Li1 ^{xvi} —Li3—Li3 ^{vi}	47 (8)
O1 ^{viii} —Zr1—La1 ^{xv}	44.88 (10)	O1 ^{xviii} —Li3—O1 ^{ix}	122 (10)
O2 ^{iv} —Zr1—La1 ^{xv}	136.97 (10)	Ga1 ^{xvi} —Li3—O1 ^{ix}	56 (7)
O2 ^{xii} —Zr1—La1 ^{xv}	139.95 (10)	Li1 ^{xvi} —Li3—O1 ^{ix}	56 (7)
O2 ^{vi} —Zr1—La1 ^{xv}	90.93 (10)	Li3 ^{vi} —Li3—O1 ^{ix}	20 (7)
Li3 ^{xiii} —Zr1—La1 ^{xv}	97 (4)	O1 ^{xviii} —Li3—La1 ^{xxxi}	81 (10)
Li3 ^{xiv} —Zr1—La1 ^{xv}	45 (4)	Ga1 ^{xvi} —Li3—La1 ^{xxxi}	113 (10)
Li3 ^{vii} —Zr1—La1 ^{xv}	48 (4)	Li1 ^{xvi} —Li3—La1 ^{xxxi}	113 (10)
La1 ^{xi} —Zr1—La1 ^{xv}	69.360 (12)	Li3 ^{vi} —Li3—La1 ^{xxxi}	66 (5)
O1 ^x —Zr1—La1 ^x	44.88 (10)	O1 ^{ix} —Li3—La1 ^{xxxi}	62 (5)
O1 ^{xi} —Zr1—La1 ^x	44.58 (10)	O1 ^{xviii} —Li3—Li3 ^{xviii}	89 (10)
O1 ^{viii} —Zr1—La1 ^x	94.85 (10)	Ga1 ^{xvi} —Li3—Li3 ^{xviii}	29 (5)
O2 ^{iv} —Zr1—La1 ^x	139.95 (10)	Li1 ^{xvi} —Li3—Li3 ^{xviii}	29 (5)
O2 ^{xii} —Zr1—La1 ^x	90.93 (10)	Li3 ^{vi} —Li3—Li3 ^{xviii}	67 (5)
O2 ^{vi} —Zr1—La1 ^x	136.97 (10)	O1 ^{ix} —Li3—Li3 ^{xviii}	81 (5)
Li3 ^{xiii} —Zr1—La1 ^x	45 (4)	La1 ^{xxxi} —Li3—Li3 ^{xviii}	127 (9)
Li3 ^{xiv} —Zr1—La1 ^x	48 (4)	O1 ^{xviii} —Li3—Li3 ^{ix}	135 (10)
Li3 ^{vii} —Zr1—La1 ^x	97 (4)	Ga1 ^{xvi} —Li3—Li3 ^{ix}	29 (5)
La1 ^{xi} —Zr1—La1 ^x	69.360 (12)	Li1 ^{xvi} —Li3—Li3 ^{ix}	29 (5)
La1 ^{xv} —Zr1—La1 ^x	69.360 (12)	Li3 ^{vi} —Li3—Li3 ^{ix}	67 (5)
Li3 ^{ix} —O1—Ga1 ^{xvi}	43 (10)	O1 ^{ix} —Li3—Li3 ^{ix}	66 (5)

Li3 ^{ix} —O1—Li1 ^{xvi}	43 (10)	La1 ^{xxx} —Li3—Li3 ^{ix}	127 (9)
Gal ^{xvi} —O1—Li1 ^{xvii}	0	Li3 ^{xviii} —Li3—Li3 ^{ix}	46 (10)
Li3 ^{ix} —O1—Zr1 ^{xvii}	170 (10)	O1 ^{xviii} —Li3—La1 ^{xviii}	71 (10)
Gal ^{xvi} —O1—Zr1 ^{xvii}	127.29 (18)	Gal ^{xvi} —Li3—La1 ^{xviii}	145 (10)
Li1 ^{xvi} —O1—Zr1 ^{xvii}	127.29 (18)	Li1 ^{xvi} —Li3—La1 ^{xviii}	145 (10)
Li3 ^{ix} —O1—Li3 ^{xviii}	54 (10)	Li3 ^{vi} —Li3—La1 ^{xviii}	168 (4)
Gal ^{xvi} —O1—Li3 ^{xviii}	38 (5)	O1 ^{ix} —Li3—La1 ^{xviii}	153 (9)
Li1 ^{xvi} —O1—Li3 ^{xviii}	38 (5)	La1 ^{xxx} —Li3—La1 ^{xviii}	102 (7)
Zr1 ^{xvii} —O1—Li3 ^{xviii}	117 (5)	Li3 ^{xviii} —Li3—La1 ^{xviii}	124 (10)
Li3 ^{ix} —O1—La1 ^{xvi}	79 (10)	Li3 ^{ix} —Li3—La1 ^{xviii}	124 (10)
Gal ^{xvi} —O1—La1 ^{xvi}	95.85 (13)	O1 ^{xviii} —Li3—Zr1 ^{xxxii}	7 (10)
Li1 ^{xvi} —O1—La1 ^{xvi}	95.85 (13)	Gal ^{xvi} —Li3—Zr1 ^{xxxii}	106 (10)
Zr1 ^{xvii} —O1—La1 ^{xvi}	100.89 (14)	Li1 ^{xvi} —Li3—Zr1 ^{xxxii}	106 (10)
Li3 ^{xviii} —O1—La1 ^{xvi}	61 (5)	Li3 ^{vi} —Li3—Zr1 ^{xxxii}	99 (10)
Li3 ^{ix} —O1—La1	89 (10)	O1 ^{ix} —Li3—Zr1 ^{xxxii}	116 (8)
Gal ^{xvi} —O1—La1	122.52 (15)	La1 ^{xxx} —Li3—Zr1 ^{xxxii}	81 (5)
Li1 ^{xvi} —O1—La1	122.52 (15)	Li3 ^{xviii} —Li3—Zr1 ^{xxxii}	84 (8)
Zr1 ^{xvii} —O1—La1	100.55 (13)	Li3 ^{ix} —Li3—Zr1 ^{xxxii}	129 (10)
Li3 ^{xviii} —O1—La1	142 (5)	La1 ^{xviii} —Li3—Zr1 ^{xxxii}	78 (5)
La1 ^{xvi} —O1—La1	105.20 (13)	O1 ^{xviii} —Li3—Li2 ^{xxxiii}	133 (10)
Li2 ^{xix} —O2—Zr1 ^{vi}	126.18 (19)	Gal ^{xvi} —Li3—Li2 ^{xxxiii}	113 (10)
Li2 ^{xix} —O2—La1 ^{vi}	88.28 (13)	Li1 ^{xvi} —Li3—Li2 ^{xxxiii}	113 (10)
Zr1 ^{vi} —O2—La1 ^{vi}	106.46 (15)	Li3 ^{vi} —Li3—Li2 ^{xxxiii}	113 (10)
Li2 ^{xix} —O2—La1 ^{xvi}	123.00 (16)	O1 ^{ix} —Li3—Li2 ^{xxxiii}	93 (6)
Zr1 ^{vi} —O2—La1 ^{xvi}	104.36 (15)	La1 ^{xxx} —Li3—Li2 ^{xxxiii}	90 (6)
La1 ^{vi} —O2—La1 ^{xvi}	102.25 (13)	Li3 ^{xviii} —Li3—Li2 ^{xxxiii}	131 (10)
Li3 ⁱⁱⁱ —Li1—Li3 ⁱⁱ	122 (10)	Li3 ^{ix} —Li3—Li2 ^{xxxiii}	87 (8)
Li3 ⁱⁱⁱ —Li1—Li3 ^{iv}	86 (10)	La1 ^{xviii} —Li3—Li2 ^{xxxiii}	65 (4)
Li3 ⁱⁱ —Li1—Li3 ^{iv}	122 (10)	Zr1 ^{xxxii} —Li3—Li2 ^{xxxiii}	140 (7)
Li3 ⁱⁱⁱ —Li1—Li3 ⁱ	122 (10)		

Symmetry codes: (i) $-z+3/4, -y+1/4, x+1/4$; (ii) $-z+3/4, y-1/4, -x+1/4$; (iii) z, x, y ; (iv) $z, -x, -y+1/2$; (v) $x, -y, -z+1/2$; (vi) $-x, -y+1/2, z$; (vii) $-x, y-1/2, -z+1/2$; (viii) $y-1/4, x-1/4, z-1/4$; (ix) $y-1/4, -x+1/4, -z+3/4$; (x) $x-1/4, z-1/4, y-1/4$; (xi) $z-1/4, y-1/4, x-1/4$; (xii) $-y+1/2, z, -x$; (xiii) $-z+1/2, -x, y-1/2$; (xiv) $y-1/2, -z+1/2, -x$; (xv) $-y-1/4, x-1/4, -z+1/4$; (xvi) y, z, x ; (xvii) $y+1/4, x+1/4, z+1/4$; (xviii) $-y+1/4, x+1/4, -z+3/4$; (xix) $-x+1, -y+1/2, z$; (xx) $-x+3/4, z-1/4, -y+1/4$; (xxi) $-x+1/2, -y, z+1/2$; (xxii) $y+1/4, -x-1/4, -z+1/4$; (xxiii) $x+3/4, z-1/4, y-1/4$; (xxiv) $-x+1, y-1/2, -z+1/2$; (xxv) $x+3/4, -z+1/4, -y+3/4$; (xxvi) $x+1, y, z$; (xxvii) $y+3/4, -x+1/4, -z+3/4$; (xxviii) $-y+1, -z+1/2, x$; (xxix) $-y+1, z-1/2, -x+1/2$; (xxx) $y+3/4, x-1/4, z-1/4$; (xxxi) $z-1/4, -y+1/4, -x+3/4$; (xxxii) $-x, y+1/2, -z+1/2$; (xxxiii) $-y+1/4, x-3/4, -z+3/4$.

supporting information

Acta Cryst. (2022). C78, 1-6 [https://doi.org/10.1107/S2053229621012250]

Deep hydration of an $\text{Li}_{7-3x}\text{La}_3\text{Zr}_2\text{M}^{\text{III}}_x\text{O}_{12}$ solid-state electrolyte material: a case study on Al- and Ga-stabilized LLZO

Günther J. Redhammer, Gerold Tippelt and Daniel Rettenwander

Computing details

For all structures, data collection: *APEX2* (Bruker, 2012); cell refinement: *APEX2* (Bruker, 2012); data reduction: *APEX2* (Bruker, 2012); program(s) used to solve structure: *SIR2014* (Burla *et al.*, 2012); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

(LLZO-Al15-pristine)

Crystal data

$\text{Al}_{0.15}\text{La}_{2.95}\text{Li}_{5.73}\text{O}_{12}\text{Zr}_2$
 $M_r = 827.89$
 Cubic, $Ia\bar{3}d$
 Hall symbol: -I 4bd 2c 3
 $a = 12.9637(2) \text{ \AA}$
 $V = 2178.65(10) \text{ \AA}^3$
 $Z = 8$
 $F(000) = 2906$

$D_x = 5.048 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 33130 reflections
 $\theta = 3.9\text{--}36.6^\circ$
 $\mu = 13.24 \text{ mm}^{-1}$
 $T = 298 \text{ K}$
 Cuboid, colorless
 $0.12 \times 0.11 \times 0.07 \text{ mm}$

Data collection

Bruker SMART APEX
 diffractometer
 Graphite monochromator
 rotation, ω -scans at 4 different φ positions
 Absorption correction: multi-scan
 (APEX2; Bruker, 2012)
 $T_{\min} = 0.22$, $T_{\max} = 0.39$
 33130 measured reflections

455 independent reflections
 441 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
 $\theta_{\max} = 36.6^\circ$, $\theta_{\min} = 3.9^\circ$
 $h = -21 \rightarrow 21$
 $k = -21 \rightarrow 21$
 $l = -21 \rightarrow 21$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.016$
 $wR(F^2) = 0.032$
 $S = 1.51$
 455 reflections
 25 parameters
 0 restraints
 0 constraints

$w = 1/[\sigma^2(F_o^2) + (0.0044P)^2 + 13.2478P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.71 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.44 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL2014
 (Sheldrick, 2015),
 $F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.00041 (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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
La1	0.125	0	0.25	0.00857 (8)	0.983 (3)
Zr1	0	0	0	0.00669 (12)	
O1	0.09999 (13)	0.19604 (13)	0.28188 (13)	0.0117 (3)	
Li1	0.375	0	0.25	0.022 (6)	0.47 (6)
Al1	0.375	0	0.25	0.022 (5)	0.05
Li2	0.0961 (10)	0.1880 (11)	0.4246 (11)	0.023 (4)*	0.36 (2)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.01087 (11)	0.00742 (9)	0.00742 (9)	0	0	0.00134 (7)
Zr1	0.00669 (12)	0.00669 (12)	0.00669 (12)	0.00008 (8)	0.00008 (8)	0.00008 (8)
O1	0.0092 (6)	0.0120 (7)	0.0140 (7)	-0.0016 (5)	0.0003 (5)	0.0004 (5)
Li1	0.009 (9)	0.029 (12)	0.029 (12)	0	0	0
Al1	0.009 (15)	0.029 (9)	0.029 (9)	0	0	0

Geometric parameters (\AA , $^\circ$)

La1—O1 ⁱ	2.5110 (17)	O1—Zr1 ^{xv}	2.1076 (16)
La1—O1 ⁱⁱ	2.5110 (17)	O1—Li2 ^v	2.159 (15)
La1—O1 ⁱⁱⁱ	2.5110 (17)	O1—Li2 ^{xxii}	2.242 (14)
La1—O1 ^{iv}	2.5110 (17)	O1—La1 ^{xx}	2.5110 (17)
La1—O1	2.5951 (17)	O1—Li2 ^x	2.646 (14)
La1—O1 ^v	2.5952 (17)	Li1—Li2 ^{xi}	1.616 (14)
La1—O1 ^{vi}	2.5952 (17)	Li1—Li2 ^{viii}	1.616 (14)
La1—O1 ^{vii}	2.5952 (17)	Li1—Li2 ⁱ	1.616 (14)
La1—Li2 ^{viii}	2.992 (14)	Li1—Li2 ⁱⁱⁱ	1.616 (14)
La1—Li2 ^{ix}	2.992 (14)	Li1—O1 ^{viii}	1.9044 (17)
La1—Li2 ^x	2.992 (14)	Li1—O1 ⁱⁱⁱ	1.9044 (17)
La1—Li2 ^{xi}	2.992 (14)	Li1—O1 ^{xi}	1.9044 (17)
Zr1—O1 ^{xii}	2.1076 (16)	Li1—O1 ⁱ	1.9044 (17)
Zr1—O1 ^{vii}	2.1076 (16)	Li1—Li2 ^{xxiii}	2.367 (14)
Zr1—O1 ^{xiii}	2.1076 (16)	Li1—Li2 ^{xxiv}	2.367 (14)
Zr1—O1 ⁱⁱ	2.1076 (16)	Li1—Li2 ^{xxv}	2.367 (14)
Zr1—O1 ^{xiv}	2.1076 (16)	Li1—Li2 ^{xxvi}	2.367 (14)
Zr1—O1 ^{xv}	2.1076 (16)	Li2—Li2 ^v	0.79 (3)
Zr1—Li2 ^{ix}	2.906 (15)	Li2—Al1 ^{xx}	1.616 (14)
Zr1—Li2 ^{xvi}	2.906 (15)	Li2—Li1 ^{xx}	1.616 (14)
Zr1—Li2 ^{xvii}	2.906 (15)	Li2—O1 ^{xxii}	2.085 (14)

Zr1—Li2 ^{xviii}	2.906 (15)	Li2—O1 ^v	2.159 (15)
Zr1—Li2 ^{xix}	2.906 (15)	Li2—O1 ^{xxi}	2.242 (14)
Zr1—Li2 ^{vi}	2.906 (15)	Li2—Al1 ^{xxvii}	2.367 (14)
O1—Li2	1.854 (15)	Li2—Li1 ^{xxvii}	2.367 (14)
O1—Al1 ^{xx}	1.9044 (17)	Li2—Li2 ^{xxii}	2.46 (2)
O1—Li1 ^{xx}	1.9044 (17)	Li2—Li2 ^{xxi}	2.46 (2)
O1—Li2 ^{xxi}	2.085 (14)	Li2—O1 ^{xxviii}	2.646 (14)
O1 ⁱ —La1—O1 ⁱⁱ	111.62 (8)	Li1 ^{xx} —O1—La1 ^{xx}	93.43 (7)
O1 ⁱ —La1—O1 ⁱⁱⁱ	71.83 (8)	Li2 ^{xxi} —O1—La1 ^{xx}	80.6 (4)
O1 ⁱⁱ —La1—O1 ⁱⁱⁱ	160.65 (7)	Zr1 ^{xv} —O1—La1 ^{xx}	103.01 (7)
O1 ⁱ —La1—O1 ^{iv}	160.65 (7)	Li2 ^v —O1—La1 ^{xx}	164.2 (4)
O1 ⁱⁱ —La1—O1 ^{iv}	71.83 (8)	Li2 ^{xxii} —O1—La1 ^{xx}	77.8 (4)
O1 ⁱⁱⁱ —La1—O1 ^{iv}	111.62 (8)	Li2—O1—La1	96.1 (5)
O1 ⁱ —La1—O1	68.90 (7)	Al1 ^{xx} —O1—La1	123.07 (7)
O1 ⁱⁱ —La1—O1	73.03 (6)	Li1 ^{xx} —O1—La1	123.07 (7)
O1 ⁱⁱⁱ —La1—O1	124.22 (3)	Li2 ^{xxi} —O1—La1	170.6 (4)
O1 ^{iv} —La1—O1	95.13 (5)	Zr1 ^{xv} —O1—La1	100.28 (6)
O1 ⁱ —La1—O1 ^v	95.13 (5)	Li2 ^v —O1—La1	89.0 (4)
O1 ⁱⁱ —La1—O1 ^v	124.22 (3)	Li2 ^{xxii} —O1—La1	85.3 (4)
O1 ⁱⁱⁱ —La1—O1 ^v	73.03 (6)	La1 ^{xx} —O1—La1	102.03 (6)
O1 ^{iv} —La1—O1 ^v	68.90 (7)	Li2—O1—Li2 ^x	78.6 (7)
O1—La1—O1 ^v	72.77 (8)	Al1 ^{xx} —O1—Li2 ^x	60.1 (3)
O1 ⁱ —La1—O1 ^{vi}	124.22 (3)	Li1 ^{xx} —O1—Li2 ^x	60.1 (3)
O1 ⁱⁱ —La1—O1 ^{vi}	95.13 (5)	Li2 ^{xxi} —O1—Li2 ^x	102.4 (4)
O1 ⁱⁱⁱ —La1—O1 ^{vi}	68.90 (7)	Zr1 ^{xv} —O1—Li2 ^x	169.9 (3)
O1 ^{iv} —La1—O1 ^{vi}	73.03 (6)	Li2 ^v —O1—Li2 ^x	94.4 (3)
O1—La1—O1 ^{vi}	165.64 (7)	Li2 ^{xxii} —O1—Li2 ^x	16.0 (6)
O1 ^v —La1—O1 ^{vi}	109.12 (7)	La1 ^{xx} —O1—Li2 ^x	79.2 (3)
O1 ⁱ —La1—O1 ^{vii}	73.03 (6)	La1—O1—Li2 ^x	69.6 (3)
O1 ⁱⁱ —La1—O1 ^{vii}	68.90 (7)	Li2 ^{xi} —Li1—Li2 ^{viii}	133.1 (10)
O1 ⁱⁱⁱ —La1—O1 ^{vii}	95.13 (5)	Li2 ^{xi} —Li1—Li2 ⁱ	99.1 (4)
O1 ^{iv} —La1—O1 ^{vii}	124.22 (3)	Li2 ^{viii} —Li1—Li2 ⁱ	99.1 (4)
O1—La1—O1 ^{vii}	109.12 (7)	Li2 ^{xi} —Li1—Li2 ⁱⁱⁱ	99.1 (4)
O1 ^v —La1—O1 ^{vii}	165.64 (7)	Li2 ^{viii} —Li1—Li2 ⁱⁱⁱ	99.1 (4)
O1 ^{vi} —La1—O1 ^{vii}	72.77 (8)	Li2 ⁱ —Li1—Li2 ⁱⁱⁱ	133.1 (10)
O1 ⁱ —La1—Li2 ^{viii}	43.4 (3)	Li2 ^{xi} —Li1—O1 ^{viii}	163.6 (5)
O1 ⁱⁱ —La1—Li2 ^{viii}	147.5 (3)	Li2 ^{viii} —Li1—O1 ^{viii}	62.9 (5)
O1 ⁱⁱⁱ —La1—Li2 ^{viii}	47.1 (3)	Li2 ⁱ —Li1—O1 ^{viii}	78.7 (5)
O1 ^{iv} —La1—Li2 ^{viii}	124.3 (3)	Li2 ⁱⁱⁱ —Li1—O1 ^{viii}	72.1 (5)
O1—La1—Li2 ^{viii}	77.2 (3)	Li2 ^{xi} —Li1—O1 ⁱⁱⁱ	72.1 (5)
O1 ^v —La1—Li2 ^{viii}	56.0 (3)	Li2 ^{viii} —Li1—O1 ⁱⁱⁱ	78.7 (5)
O1 ^{vi} —La1—Li2 ^{viii}	116.0 (3)	Li2 ⁱ —Li1—O1 ⁱⁱⁱ	163.6 (5)
O1 ^{vii} —La1—Li2 ^{viii}	110.0 (3)	Li2 ⁱⁱⁱ —Li1—O1 ⁱⁱⁱ	62.9 (5)
O1 ⁱ —La1—Li2 ^{ix}	147.5 (3)	O1 ^{viii} —Li1—O1 ⁱⁱⁱ	113.69 (5)
O1 ⁱⁱ —La1—Li2 ^{ix}	43.4 (3)	Li2 ^{xi} —Li1—O1 ^{xi}	62.9 (5)
O1 ⁱⁱⁱ —La1—Li2 ^{ix}	124.3 (3)	Li2 ^{viii} —Li1—O1 ^{xi}	163.6 (5)
O1 ^{iv} —La1—Li2 ^{ix}	47.1 (3)	Li2 ⁱ —Li1—O1 ^{xi}	72.1 (5)

O1—La1—Li2 ^{ix}	110.0 (3)	Li2 ⁱⁱⁱ —Li1—O1 ^{xi}	78.7 (5)
O1 ^v —La1—Li2 ^{ix}	116.0 (3)	O1 ^{viii} —Li1—O1 ^{xi}	101.32 (10)
O1 ^{vi} —La1—Li2 ^{ix}	56.0 (3)	O1 ⁱⁱⁱ —Li1—O1 ^{xi}	113.69 (5)
O1 ^{vii} —La1—Li2 ^{ix}	77.2 (3)	Li2 ^{xi} —Li1—O1 ⁱ	78.7 (5)
Li2 ^{viii} —La1—Li2 ^{ix}	168.0 (6)	Li2 ^{viii} —Li1—O1 ⁱ	72.1 (5)
O1 ⁱ —La1—Li2 ^x	124.3 (3)	Li2 ⁱ —Li1—O1 ⁱ	62.9 (5)
O1 ⁱⁱ —La1—Li2 ^x	47.1 (3)	Li2 ⁱⁱⁱ —Li1—O1 ⁱ	163.6 (5)
O1 ⁱⁱⁱ —La1—Li2 ^x	147.5 (3)	O1 ^{viii} —Li1—O1 ⁱ	113.69 (6)
O1 ^{iv} —La1—Li2 ^x	43.4 (3)	O1 ⁱⁱⁱ —Li1—O1 ⁱ	101.32 (10)
O1—La1—Li2 ^x	56.0 (3)	O1 ^{xi} —Li1—O1 ⁱ	113.69 (5)
O1 ^v —La1—Li2 ^x	77.2 (3)	Li2 ^{xi} —Li1—Li2 ^{xxiii}	7.0 (9)
O1 ^{vi} —La1—Li2 ^x	110.0 (3)	Li2 ^{viii} —Li1—Li2 ^{xxiii}	135.9 (7)
O1 ^{vii} —La1—Li2 ^x	116.0 (3)	Li2 ⁱ —Li1—Li2 ^{xxiii}	92.1 (7)
Li2 ^{viii} —La1—Li2 ^x	122.0 (5)	Li2 ⁱⁱⁱ —Li1—Li2 ^{xxiii}	103.8 (7)
Li2 ^{ix} —La1—Li2 ^x	59.4 (5)	O1 ^{viii} —Li1—Li2 ^{xxiii}	160.7 (4)
O1 ⁱ —La1—Li2 ^{xi}	47.1 (3)	O1 ⁱⁱⁱ —Li1—Li2 ^{xxiii}	79.0 (4)
O1 ⁱⁱ —La1—Li2 ^{xi}	124.3 (3)	O1 ^{xi} —Li1—Li2 ^{xxiii}	59.6 (4)
O1 ⁱⁱⁱ —La1—Li2 ^{xi}	43.4 (3)	O1 ⁱ —Li1—Li2 ^{xxiii}	75.7 (3)
O1 ^{iv} —La1—Li2 ^{xi}	147.5 (3)	Li2 ^{xi} —Li1—Li2 ^{xxiv}	135.9 (7)
O1—La1—Li2 ^{xi}	116.0 (3)	Li2 ^{viii} —Li1—Li2 ^{xxiv}	7.0 (9)
O1 ^v —La1—Li2 ^{xi}	110.0 (3)	Li2 ⁱ —Li1—Li2 ^{xxiv}	103.8 (7)
O1 ^{vi} —La1—Li2 ^{xi}	77.2 (3)	Li2 ⁱⁱⁱ —Li1—Li2 ^{xxiv}	92.1 (7)
O1 ^{vii} —La1—Li2 ^{xi}	56.0 (3)	O1 ^{viii} —Li1—Li2 ^{xxiv}	59.6 (4)
Li2 ^{viii} —La1—Li2 ^{xi}	59.4 (5)	O1 ⁱⁱⁱ —Li1—Li2 ^{xxiv}	75.7 (3)
Li2 ^{ix} —La1—Li2 ^{xi}	122.0 (5)	O1 ^{xi} —Li1—Li2 ^{xxiv}	160.7 (4)
Li2 ^x —La1—Li2 ^{xi}	168.0 (6)	O1 ⁱ —Li1—Li2 ^{xxiv}	79.0 (4)
O1 ^{xii} —Zr1—O1 ^{vii}	180.00 (13)	Li2 ^{xxiii} —Li1—Li2 ^{xxiv}	139.6 (7)
O1 ^{xii} —Zr1—O1 ^{xiii}	86.55 (7)	Li2 ^{xi} —Li1—Li2 ^{xxv}	103.8 (7)
O1 ^{vii} —Zr1—O1 ^{xiii}	93.45 (7)	Li2 ^{viii} —Li1—Li2 ^{xxv}	92.1 (7)
O1 ^{xii} —Zr1—O1 ⁱⁱ	93.45 (7)	Li2 ⁱ —Li1—Li2 ^{xxv}	7.0 (9)
O1 ^{vii} —Zr1—O1 ⁱⁱ	86.55 (7)	Li2 ⁱⁱⁱ —Li1—Li2 ^{xxv}	135.9 (7)
O1 ^{xiii} —Zr1—O1 ⁱⁱ	180.00 (13)	O1 ^{viii} —Li1—Li2 ^{xxv}	75.7 (4)
O1 ^{xii} —Zr1—O1 ^{xiv}	86.55 (7)	O1 ⁱⁱⁱ —Li1—Li2 ^{xxv}	160.7 (4)
O1 ^{vii} —Zr1—O1 ^{xiv}	93.45 (7)	O1 ^{xi} —Li1—Li2 ^{xxv}	79.0 (4)
O1 ^{xiii} —Zr1—O1 ^{xiv}	86.55 (7)	O1 ⁱ —Li1—Li2 ^{xxv}	59.6 (4)
O1 ⁱⁱ —Zr1—O1 ^{xiv}	93.45 (7)	Li2 ^{xxiii} —Li1—Li2 ^{xxv}	96.8 (2)
O1 ^{xii} —Zr1—O1 ^{xv}	93.45 (7)	Li2 ^{xxiv} —Li1—Li2 ^{xxv}	96.8 (2)
O1 ^{vii} —Zr1—O1 ^{xv}	86.55 (7)	Li2 ^{xi} —Li1—Li2 ^{xxvi}	92.1 (7)
O1 ^{xiii} —Zr1—O1 ^{xv}	93.45 (7)	Li2 ^{viii} —Li1—Li2 ^{xxvi}	103.8 (7)
O1 ⁱⁱ —Zr1—O1 ^{xv}	86.55 (7)	Li2 ⁱ —Li1—Li2 ^{xxvi}	135.9 (7)
O1 ^{xiv} —Zr1—O1 ^{xv}	180.00 (9)	Li2 ⁱⁱⁱ —Li1—Li2 ^{xxvi}	7.0 (9)
O1 ^{xii} —Zr1—Li2 ^{ix}	93.0 (3)	O1 ^{viii} —Li1—Li2 ^{xxvi}	79.0 (4)
O1 ^{vii} —Zr1—Li2 ^{ix}	87.0 (3)	O1 ⁱⁱⁱ —Li1—Li2 ^{xxvi}	59.6 (4)
O1 ^{xiii} —Zr1—Li2 ^{ix}	134.2 (3)	O1 ^{xi} —Li1—Li2 ^{xxvi}	75.7 (3)
O1 ⁱⁱ —Zr1—Li2 ^{ix}	45.8 (3)	O1 ⁱ —Li1—Li2 ^{xxvi}	160.7 (4)
O1 ^{xiv} —Zr1—Li2 ^{ix}	47.8 (3)	Li2 ^{xxiii} —Li1—Li2 ^{xxvi}	96.8 (2)
O1 ^{xv} —Zr1—Li2 ^{ix}	132.2 (3)	Li2 ^{xxiv} —Li1—Li2 ^{xxvi}	96.8 (2)
O1 ^{xii} —Zr1—Li2 ^{xxvi}	87.0 (3)	Li2 ^{xxv} —Li1—Li2 ^{xxvi}	139.6 (7)

O1 ^{vii} —Zr1—Li2 ^{xvi}	93.0 (3)	Li2 ^v —Li2—Al1 ^{xx}	158 (3)
O1 ^{xiii} —Zr1—Li2 ^{xvi}	45.8 (3)	Li2 ^v —Li2—Li1 ^{xx}	158 (3)
O1 ⁱⁱ —Zr1—Li2 ^{xvi}	134.2 (3)	Al1 ^{xx} —Li2—Li1 ^{xx}	0
O1 ^{xiv} —Zr1—Li2 ^{xvi}	132.2 (3)	Li2 ^v —Li2—O1	101.9 (17)
O1 ^{xv} —Zr1—Li2 ^{xvi}	47.8 (3)	Al1 ^{xx} —Li2—O1	66.2 (5)
Li2 ^{ix} —Zr1—Li2 ^{xvi}	180.0 (7)	Li1 ^{xx} —Li2—O1	66.2 (5)
O1 ^{xii} —Zr1—Li2 ^{xvii}	134.2 (3)	Li2 ^v —Li2—O1 ^{xxii}	141 (3)
O1 ^{vii} —Zr1—Li2 ^{xvii}	45.8 (3)	Al1 ^{xx} —Li2—O1 ^{xxii}	60.4 (4)
O1 ^{xiii} —Zr1—Li2 ^{xvii}	47.8 (3)	Li1 ^{xx} —Li2—O1 ^{xxii}	60.4 (4)
O1 ⁱⁱ —Zr1—Li2 ^{xvii}	132.2 (3)	O1—Li2—O1 ^{xxii}	108.0 (7)
O1 ^{xiv} —Zr1—Li2 ^{xvii}	93.0 (3)	Li2 ^v —Li2—O1 ^v	57.2 (15)
O1 ^{xv} —Zr1—Li2 ^{xvii}	87.0 (3)	Al1 ^{xx} —Li2—O1 ^v	140.1 (8)
Li2 ^{ix} —Zr1—Li2 ^{xvii}	119.82 (4)	Li1 ^{xx} —Li2—O1 ^v	140.1 (8)
Li2 ^{xvi} —Zr1—Li2 ^{xvii}	60.18 (4)	O1—Li2—O1 ^v	99.9 (6)
O1 ^{xii} —Zr1—Li2 ^{xviii}	45.8 (3)	O1 ^{xxii} —Li2—O1 ^v	92.6 (6)
O1 ^{vii} —Zr1—Li2 ^{xviii}	134.2 (3)	Li2 ^v —Li2—O1 ^{xxi}	112.5 (10)
O1 ^{xiii} —Zr1—Li2 ^{xviii}	132.2 (3)	Al1 ^{xx} —Li2—O1 ^{xxi}	56.4 (4)
O1 ⁱⁱ —Zr1—Li2 ^{xviii}	47.8 (3)	Li1 ^{xx} —Li2—O1 ^{xxi}	56.4 (4)
O1 ^{xiv} —Zr1—Li2 ^{xviii}	87.0 (3)	O1—Li2—O1 ^{xxi}	101.8 (7)
O1 ^{xv} —Zr1—Li2 ^{xviii}	93.0 (3)	O1 ^{xxii} —Li2—O1 ^{xxi}	85.7 (5)
Li2 ^{ix} —Zr1—Li2 ^{xviii}	60.18 (4)	O1 ^v —Li2—O1 ^{xxi}	157.6 (7)
Li2 ^{xvi} —Zr1—Li2 ^{xviii}	119.82 (4)	Li2 ^v —Li2—Al1 ^{xxvii}	14.6 (19)
Li2 ^{xvii} —Zr1—Li2 ^{xviii}	180.0 (6)	Al1 ^{xx} —Li2—Al1 ^{xxvii}	170.3 (9)
O1 ^{xii} —Zr1—Li2 ^{xix}	47.8 (3)	Li1 ^{xx} —Li2—Al1 ^{xxvii}	170.3 (9)
O1 ^{vii} —Zr1—Li2 ^{xix}	132.2 (3)	O1—Li2—Al1 ^{xxvii}	114.1 (6)
O1 ^{xiii} —Zr1—Li2 ^{xix}	93.0 (3)	O1 ^{xxii} —Li2—Al1 ^{xxvii}	126.4 (7)
O1 ⁱⁱ —Zr1—Li2 ^{xix}	87.0 (3)	O1 ^v —Li2—Al1 ^{xxvii}	49.5 (3)
O1 ^{xiv} —Zr1—Li2 ^{xix}	134.2 (3)	O1 ^{xxi} —Li2—Al1 ^{xxvii}	115.1 (6)
O1 ^{xv} —Zr1—Li2 ^{xix}	45.8 (3)	Li2 ^v —Li2—Li1 ^{xxvii}	14.6 (19)
Li2 ^{ix} —Zr1—Li2 ^{xix}	119.82 (4)	Al1 ^{xx} —Li2—Li1 ^{xxvii}	170.3
Li2 ^{xvi} —Zr1—Li2 ^{xix}	60.18 (4)	Li1 ^{xx} —Li2—Li1 ^{xxvii}	170.3 (9)
Li2 ^{xvii} —Zr1—Li2 ^{xix}	119.82 (4)	O1—Li2—Li1 ^{xxvii}	114.1 (6)
Li2 ^{xviii} —Zr1—Li2 ^{xix}	60.18 (4)	O1 ^{xxii} —Li2—Li1 ^{xxvii}	126.4 (7)
O1 ^{xii} —Zr1—Li2 ^{vi}	132.2 (3)	O1 ^v —Li2—Li1 ^{xxvii}	49.5 (3)
O1 ^{vii} —Zr1—Li2 ^{vi}	47.8 (3)	O1 ^{xxi} —Li2—Li1 ^{xxvii}	115.1 (6)
O1 ^{xiii} —Zr1—Li2 ^{vi}	87.0 (3)	Al1 ^{xxvii} —Li2—Li1 ^{xxvii}	0
O1 ⁱⁱ —Zr1—Li2 ^{vi}	93.0 (3)	Li2 ^v —Li2—Li2 ^{xxii}	150.2 (6)
O1 ^{xiv} —Zr1—Li2 ^{vi}	45.8 (3)	Al1 ^{xx} —Li2—Li2 ^{xxii}	40.45 (19)
O1 ^{xv} —Zr1—Li2 ^{vi}	134.2 (3)	Li1 ^{xx} —Li2—Li2 ^{xxii}	40.45 (19)
Li2 ^{ix} —Zr1—Li2 ^{vi}	60.18 (4)	O1—Li2—Li2 ^{xxii}	60.7 (7)
Li2 ^{xvi} —Zr1—Li2 ^{vi}	119.82 (4)	O1 ^{xxii} —Li2—Li2 ^{xxii}	47.3 (4)
Li2 ^{xvii} —Zr1—Li2 ^{vi}	60.18 (4)	O1 ^v —Li2—Li2 ^{xxii}	99.7 (8)
Li2 ^{xviii} —Zr1—Li2 ^{vi}	119.82 (4)	O1 ^{xxi} —Li2—Li2 ^{xxii}	95.5 (4)
Li2 ^{xix} —Zr1—Li2 ^{vi}	180.0 (8)	Al1 ^{xxvii} —Li2—Li2 ^{xxii}	148.9 (8)
Li2—O1—Al1 ^{xx}	50.9 (4)	Li1 ^{xxvii} —Li2—Li2 ^{xxii}	148.9 (8)
Li2—O1—Li1 ^{xx}	50.9 (4)	Li2 ^v —Li2—Li2 ^{xxi}	118 (3)
Al1 ^{xx} —O1—Li1 ^{xx}	0	Al1 ^{xx} —Li2—Li2 ^{xxi}	40.45 (19)
Li2—O1—Li2 ^{xxi}	77.1 (6)	Li1 ^{xx} —Li2—Li2 ^{xxi}	40.45 (19)

Al1 ^{xx} —O1—Li2 ^{xxi}	47.5 (4)	O1—Li2—Li2 ^{xxi}	55.7 (7)
Li1 ^{xx} —O1—Li2 ^{xxi}	47.5 (4)	O1 ^{xxii} —Li2—Li2 ^{xxi}	99.8 (4)
Li2—O1—Zr1 ^{xv}	103.8 (4)	O1 ^v —Li2—Li2 ^{xxi}	155.1 (10)
Al1 ^{xx} —O1—Zr1 ^{xv}	129.08 (9)	O1 ^{xxi} —Li2—Li2 ^{xxi}	46.1 (4)
Li1 ^{xx} —O1—Zr1 ^{xv}	129.08 (9)	Al1 ^{xxvii} —Li2—Li2 ^{xxi}	130.9 (8)
Li2 ^{xxi} —O1—Zr1 ^{xv}	87.8 (4)	Li1 ^{xxvii} —Li2—Li2 ^{xxi}	130.9 (8)
Li2—O1—Li2 ^v	20.9 (7)	Li2 ^{xxii} —Li2—Li2 ^{xxi}	74.1 (6)
Al1 ^{xx} —O1—Li2 ^v	70.9 (4)	Li2 ^v —Li2—O1 ^{xxviii}	51.5 (9)
Li1 ^{xx} —O1—Li2 ^v	70.9 (4)	Al1 ^{xx} —Li2—O1 ^{xxviii}	130.2 (7)
Li2 ^{xxi} —O1—Li2 ^v	86.72 (8)	Li1 ^{xx} —Li2—O1 ^{xxviii}	130.2 (7)
Zr1 ^{xv} —O1—Li2 ^v	85.9 (4)	O1—Li2—O1 ^{xxviii}	146.7 (7)
Li2—O1—Li2 ^{xxii}	73.1 (6)	O1 ^{xxii} —Li2—O1 ^{xxviii}	105.0 (6)
Al1 ^{xx} —O1—Li2 ^{xxii}	45.0 (4)	O1 ^v —Li2—O1 ^{xxviii}	82.5 (5)
Li1 ^{xx} —O1—Li2 ^{xxii}	45.0 (4)	O1 ^{xxi} —Li2—O1 ^{xxviii}	76.4 (4)
Li2 ^{xxi} —O1—Li2 ^{xxii}	86.5 (6)	Al1 ^{xxvii} —Li2—O1 ^{xxviii}	44.2 (2)
Zr1 ^{xv} —O1—Li2 ^{xxii}	174.0 (4)	Li1 ^{xxvii} —Li2—O1 ^{xxviii}	44.2 (2)
Li2 ^v —O1—Li2 ^{xxii}	92.0 (7)	Li2 ^{xxii} —Li2—O1 ^{xxviii}	152.1 (9)
Li2—O1—La1 ^{xx}	144.1 (4)	Li2 ^{xxi} —Li2—O1 ^{xxviii}	114.5 (8)
Al1 ^{xx} —O1—La1 ^{xx}	93.43 (7)		

Symmetry codes: (i) z, x, y ; (ii) $-z+1/4, -y+1/4, -x+1/4$; (iii) $z, -x, -y+1/2$; (iv) $-z+1/4, y-1/4, x+1/4$; (v) $-x+1/4, z-1/4, y+1/4$; (vi) $x, -y, -z+1/2$; (vii) $-x+1/4, -z+1/4, -y+1/4$; (viii) $-z+3/4, -y+1/4, x+1/4$; (ix) $z-1/2, -x, y$; (x) $z-1/2, x, -y+1/2$; (xi) $-z+3/4, y-1/4, -x+1/4$; (xii) $x-1/4, z-1/4, y-1/4$; (xiii) $z-1/4, y-1/4, x-1/4$; (xiv) $y-1/4, x-1/4, z-1/4$; (xv) $-y+1/4, -x+1/4, -z+1/4$; (xvi) $-z+1/2, x, -y$; (xvii) $y, z-1/2, -x$; (xviii) $-y, -z+1/2, x$; (xix) $-x, y, z-1/2$; (xx) y, z, x ; (xxi) $-y+1/4, x+1/4, -z+3/4$; (xxii) $y-1/4, -x+1/4, -z+3/4$; (xxiii) $-y+1/2, z-1/2, x$; (xxiv) $-y+1/2, -z+1/2, -x+1/2$; (xxv) $y+1/4, -x+1/4, z-1/4$; (xxvi) $y+1/4, x-1/4, -z+3/4$; (xxvii) $-y+1/4, x-1/4, z+1/4$; (xxviii) $y, -z+1/2, x+1/2$.

(LLZO-Al15-hydro-150C)

Crystal data

Al_{0.15}H_{5.52}La_{2.88}Li_{1.64}O₁₂Zr_{1.95}
M_r = 790.95
 Cubic, *I*43*d*
 Hall symbol: I -4bd 2c 3
a = 13.0738 (2) Å
V = 2234.63 (10) Å³
Z = 8
F(000) = 2804.4

D_x = 4.707 Mg m⁻³
 Mo *K*α radiation, λ = 0.71073 Å
 Cell parameters from 34201 reflections
 θ = 3.8–34.9°
 μ = 12.61 mm⁻¹
T = 298 K
 Cuboid, colorless
 0.13 × 0.12 × 0.08 mm

Data collection

Bruker SMART APEX
 diffractometer
 Graphite monochromator
 rotation, ω-scans at 4 different φ positions
 Absorption correction: multi-scan
 (APEX2; Bruker, 2012)
T_{min} = 0.21, *T_{max}* = 0.36
 34201 measured reflections

819 independent reflections
 819 reflections with *I* > 2σ(*I*)
R_{int} = 0.026
 θ_{max} = 34.9°, θ_{min} = 3.8°
h = -21→21
k = -21→21
l = -21→21

Refinement

Refinement on *F*²
 Least-squares matrix: full
R[*F*² > 2σ(*F*²)] = 0.013
wR(*F*²) = 0.029

S = 1.27
 819 reflections
 44 parameters
 1 restraint

0 constraints
 Hydrogen site location: difference Fourier map
 Only H-atom coordinates refined
 $w = 1/[\sigma^2(F_o^2) + 15.2822P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.57 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.51 \text{ e } \text{\AA}^{-3}$

Extinction correction: SHELXL2014
 (Sheldrick, 2015),
 $F_c^* = kFc[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.00083 (5)
 Absolute structure: Refined as an inversion
 twin.
 Absolute structure parameter: 0.50 (3)

Special details

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

Refinement. Refined as a 2-component inversion twin.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
La1	0.11936 (3)	0	0.25	0.01005 (9)	0.961 (10)
Zr1A	-0.01161 (12)	-0.01161 (12)	-0.01161 (12)	0.0069 (4)	0.79 (2)
Zr1B	-0.0073 (15)	0.006 (3)	0.013 (2)	0.024 (5)*	0.061 (6)
O1	0.0970 (2)	0.1899 (2)	0.2733 (3)	0.0132 (6)	
O2	0.0335 (3)	0.4452 (3)	0.1429 (2)	0.0149 (7)	
Li1	0.375	0	0.25	0.016*	0.62 (6)
Al1	0.375	0	0.25	0.016*	0.1
Li2	0.875	0	0.25	0.017 (9)	0.47 (9)
H1	0.098 (6)	0.180 (6)	0.323 (7)	0.025*	0.92 (17)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.00938 (13)	0.00852 (14)	0.01224 (15)	0	0	0.00403 (8)
Zr1A	0.0069 (4)	0.0069 (4)	0.0069 (4)	0.0000 (2)	0.0000 (2)	0.0000 (2)
O1	0.0112 (12)	0.0115 (13)	0.0169 (15)	0.0014 (9)	-0.0002 (10)	0.0028 (10)
O2	0.0193 (15)	0.0142 (13)	0.0110 (14)	0.0028 (10)	0.0005 (10)	0.0038 (10)
Li2	0.012 (14)	0.020 (12)	0.020 (12)	0	0	0

Geometric parameters (\AA , $^\circ$)

La1—O1 ⁱ	2.506 (3)	O1—Li1 ^{viii}	1.998 (3)
La1—O1 ⁱⁱ	2.506 (3)	O1—Zr1A ^{vii}	2.007 (4)
La1—O1	2.518 (3)	O1—Zr1B ^{xv}	2.14 (3)
La1—O1 ⁱⁱⁱ	2.518 (3)	O1—Zr1B ^{vii}	2.19 (3)
La1—O2 ^{iv}	2.544 (3)	O1—Zr1B ^{xvi}	2.36 (3)
La1—O2 ^v	2.544 (3)	O1—La1 ^{viii}	2.506 (3)
La1—O2 ⁱ	2.607 (3)	O1—H1	0.66 (9)
La1—O2 ⁱⁱ	2.607 (3)	O2—Zr1B ^{iv}	1.85 (3)
La1—Li2 ^{vi}	3.1947 (4)	O2—Li2 ^{xvii}	1.976 (3)
La1—Li1	3.3422 (4)	O2—Zr1B ^{xviii}	2.06 (3)

La1—Zr1A ^{vii}	3.487 (2)	O2—Zr1B ^{xix}	2.10 (3)
La1—H1	2.55 (8)	O2—Zr1A ^{iv}	2.217 (4)
Zr1A—Zr1B ^{viii}	0.39 (3)	O2—La1 ^{iv}	2.544 (3)
Zr1A—Zr1B ⁱ	0.39 (3)	O2—La1 ^{viii}	2.607 (3)
Zr1A—O1 ^{ix}	2.007 (4)	Li1—O1 ^{xx}	1.998 (3)
Zr1A—O1 ^x	2.007 (4)	Li1—O1 ⁱⁱ	1.998 (3)
Zr1A—O1 ^{xi}	2.007 (4)	Li1—O1 ⁱ	1.998 (3)
Zr1A—O2 ^{xii}	2.217 (4)	Li1—O1 ^{xxi}	1.998 (3)
Zr1A—O2 ^{iv}	2.217 (4)	Li1—La1 ^{xxii}	3.3422 (4)
Zr1A—O2 ⁱⁱ	2.217 (4)	Li1—Zr1B ^{xxiii}	3.54 (3)
Zr1A—La1 ^{xi}	3.487 (2)	Li1—Zr1B ^{xxiv}	3.54 (3)
Zr1A—La1 ^{ix}	3.487 (2)	Li1—Zr1B ^{vii}	3.54 (3)
Zr1A—La1 ^x	3.487 (2)	Li1—Zr1B ^{xii}	3.54 (3)
Zr1A—Li1 ^{xiii}	3.5953 (5)	Li1—Zr1A ^{xxv}	3.5953 (5)
Zr1B—Zr1B ^{viii}	0.32 (5)	Li1—Zr1A ^{xxiii}	3.5953 (5)
Zr1B—Zr1B ⁱ	0.32 (5)	Li2—O2 ^{xxvi}	1.976 (3)
Zr1B—O2 ^{iv}	1.85 (3)	Li2—O2 ^{xxvii}	1.976 (3)
Zr1B—O2 ^{xii}	2.06 (3)	Li2—O2 ^{xxviii}	1.976 (3)
Zr1B—O2 ⁱⁱ	2.10 (3)	Li2—O2 ^{xxix}	3.1947 (4)
Zr1B—O1 ^x	2.14 (3)	Li2—La1 ^{xxii}	3.1947 (4)
Zr1B—O1 ^{xi}	2.19 (3)	Li2—Zr1B ^{xxx}	3.46 (3)
Zr1B—O1 ^{ix}	2.36 (3)	Li2—Zr1B ^{xxii}	3.46 (3)
Zr1B—Li2 ^{vi}	3.47 (3)	Li2—Zr1B ^{xxix}	3.46 (3)
Zr1B—La1 ^{viii}	3.49 (4)	Li2—Zr1B ^{xxxi}	3.46 (3)
Zr1B—Li1 ^{xiv}	3.54 (3)		
O1—Al1 ^{viii}	1.998 (3)		
O1 ⁱ —La1—O1 ⁱⁱ	73.10 (16)	O1 ^{xi} —Zr1B—La1	94.1 (12)
O1 ⁱ —La1—O1	68.42 (15)	O1 ^{ix} —Zr1B—La1	136.1 (13)
O1 ⁱⁱ —La1—O1	123.66 (7)	Li2 ^{vi} —Zr1B—La1	54.4 (5)
O1 ⁱ —La1—O1 ⁱⁱⁱ	123.66 (7)	La1 ^{viii} —Zr1B—La1	69.7 (6)
O1 ⁱⁱ —La1—O1 ⁱⁱⁱ	68.42 (15)	Zr1B ^{viii} —Zr1B—Li1 ^{xiv}	108 (10)
O1—La1—O1 ⁱⁱⁱ	166.67 (15)	Zr1B ⁱ —Zr1B—Li1 ^{xiv}	160 (6)
O1 ⁱ —La1—O2 ^{iv}	108.41 (9)	O2 ^{iv} —Zr1B—Li1 ^{xiv}	74.0 (10)
O1 ⁱⁱ —La1—O2 ^{iv}	161.19 (8)	O2 ^{xii} —Zr1B—Li1 ^{xiv}	87.5 (13)
O1—La1—O2 ^{iv}	72.41 (10)	O2 ⁱⁱ —Zr1B—Li1 ^{xiv}	163.1 (15)
O1 ⁱⁱⁱ —La1—O2 ^{iv}	96.88 (11)	O1 ^x —Zr1B—Li1 ^{xiv}	30.1 (6)
O1 ⁱ —La1—O2 ^v	161.19 (8)	O1 ^{xi} —Zr1B—Li1 ^{xiv}	97.9 (5)
O1 ⁱⁱ —La1—O2 ^v	108.41 (9)	O1 ^{ix} —Zr1B—Li1 ^{xiv}	105.7 (10)
O1—La1—O2 ^v	96.88 (11)	Li2 ^{vi} —Zr1B—Li1 ^{xiv}	69.7 (5)
O1 ⁱⁱⁱ —La1—O2 ^v	72.41 (10)	La1 ^{viii} —Zr1B—Li1 ^{xiv}	68.9 (7)
O2 ^{iv} —La1—O2 ^v	76.42 (15)	La1—Zr1B—Li1 ^{xiv}	118.2 (9)
O1 ⁱ —La1—O2 ⁱ	97.31 (11)	Al1 ^{viii} —O1—Li1 ^{viii}	0
O1 ⁱⁱ —La1—O2 ⁱ	71.54 (10)	Al1 ^{viii} —O1—Zr1A ^{vii}	127.71 (18)
O1—La1—O2 ⁱ	74.30 (10)	Li1 ^{viii} —O1—Zr1A ^{vii}	127.71 (18)
O1 ⁱⁱⁱ —La1—O2 ⁱ	107.34 (10)	Al1 ^{viii} —O1—Zr1B ^{xv}	117.5 (10)
O2 ^{iv} —La1—O2 ⁱ	125.74 (7)	Li1 ^{viii} —O1—Zr1B ^{xv}	117.5 (10)
O2 ^v —La1—O2 ⁱ	66.49 (14)	Zr1A ^{vii} —O1—Zr1B ^{xv}	10.2 (9)

O1 ⁱ —La1—O2 ⁱⁱ	71.54 (10)	All ^{viii} —O1—Zr1B ^{vii}	121.3 (8)
O1 ⁱⁱ —La1—O2 ⁱⁱ	97.31 (11)	Li1 ^{viii} —O1—Zr1B ^{vii}	121.3 (8)
O1—La1—O2 ⁱⁱ	107.34 (10)	Zr1A ^{vii} —O1—Zr1B ^{vii}	9.5 (8)
O1 ⁱⁱⁱ —La1—O2 ⁱⁱ	74.30 (10)	Zr1B ^{xv} —O1—Zr1B ^{vii}	8.5 (11)
O2 ^{iv} —La1—O2 ⁱⁱ	66.49 (14)	All ^{viii} —O1—Zr1B ^{xvi}	123.4 (5)
O2 ^v —La1—O2 ⁱⁱ	125.74 (7)	Li1 ^{viii} —O1—Zr1B ^{xvi}	123.4 (5)
O2 ⁱ —La1—O2 ⁱⁱ	166.47 (14)	Zr1A ^{vii} —O1—Zr1B ^{xvi}	4.3 (4)
O1 ⁱ —La1—Li2 ^{vi}	143.45 (8)	Zr1B ^{xv} —O1—Zr1B ^{xvi}	6.0 (8)
O1 ⁱⁱ —La1—Li2 ^{vi}	143.45 (8)	Zr1B ^{vii} —O1—Zr1B ^{xvi}	6.9 (12)
O1—La1—Li2 ^{vi}	83.33 (7)	All ^{viii} —O1—La1 ^{viii}	95.15 (12)
O1 ⁱⁱⁱ —La1—Li2 ^{vi}	83.33 (7)	Li1 ^{viii} —O1—La1 ^{viii}	95.15 (12)
O2 ^{iv} —La1—Li2 ^{vi}	38.21 (8)	Zr1A ^{vii} —O1—La1 ^{viii}	100.61 (15)
O2 ^v —La1—Li2 ^{vi}	38.21 (8)	Zr1B ^{xv} —O1—La1 ^{viii}	103.0 (8)
O2 ⁱ —La1—Li2 ^{vi}	96.77 (7)	Zr1B ^{vii} —O1—La1 ^{viii}	109.2 (8)
O2 ⁱⁱ —La1—Li2 ^{vi}	96.77 (7)	Zr1B ^{xvi} —O1—La1 ^{viii}	102.3 (8)
O1 ⁱ —La1—Li1	36.55 (8)	All ^{viii} —O1—La1	122.82 (15)
O1 ⁱⁱ —La1—Li1	36.55 (8)	Li1 ^{viii} —O1—La1	122.82 (15)
O1—La1—Li1	96.67 (7)	Zr1A ^{vii} —O1—La1	100.20 (13)
O1 ⁱⁱⁱ —La1—Li1	96.67 (7)	Zr1B ^{xv} —O1—La1	108.8 (8)
O2 ^{iv} —La1—Li1	141.79 (8)	Zr1B ^{vii} —O1—La1	101.1 (7)
O2 ^v —La1—Li1	141.79 (8)	Zr1B ^{xvi} —O1—La1	103.4 (8)
O2 ⁱ —La1—Li1	83.23 (7)	La1 ^{viii} —O1—La1	105.71 (13)
O2 ⁱⁱ —La1—Li1	83.23 (7)	All ^{viii} —O1—H1	56 (7)
Li2 ^{vi} —La1—Li1	180	Li1 ^{viii} —O1—H1	56 (7)
O1 ⁱ —La1—Zr1A ^{vii}	34.45 (8)	Zr1A ^{vii} —O1—H1	106 (7)
O1 ⁱⁱ —La1—Zr1A ^{vii}	96.17 (8)	Zr1B ^{xv} —O1—H1	101 (7)
O1—La1—Zr1A ^{vii}	34.50 (7)	Zr1B ^{vii} —O1—H1	97 (7)
O1 ⁱⁱⁱ —La1—Zr1A ^{vii}	158.08 (7)	Zr1B ^{xvi} —O1—H1	103 (7)
O2 ^{iv} —La1—Zr1A ^{vii}	94.29 (8)	La1 ^{viii} —O1—H1	149 (7)
O2 ^v —La1—Zr1A ^{vii}	128.79 (7)	La1—O1—H1	85 (7)
O2 ⁱ —La1—Zr1A ^{vii}	80.78 (8)	Zr1B ^{iv} —O2—Li2 ^{xvii}	129.6 (7)
O2 ⁱⁱ —La1—Zr1A ^{vii}	93.16 (8)	Zr1B ^{iv} —O2—Zr1B ^{xviii}	7.3 (16)
Li2 ^{vi} —La1—Zr1A ^{vii}	116.505 (14)	Li2 ^{xvii} —O2—Zr1B ^{xviii}	130.6 (8)
Li1—La1—Zr1A ^{vii}	63.495 (14)	Zr1B ^{iv} —O2—Zr1B ^{xix}	5.9 (9)
O1 ⁱ —La1—H1	74.9 (17)	Li2 ^{xvii} —O2—Zr1B ^{xix}	135.6 (10)
O1 ⁱⁱ —La1—H1	116 (2)	Zr1B ^{xviii} —O2—Zr1B ^{xix}	8.8 (12)
O1—La1—H1	15 (2)	Zr1B ^{iv} —O2—Zr1A ^{iv}	4.1 (5)
O1 ⁱⁱⁱ —La1—H1	160.1 (18)	Li2 ^{xvii} —O2—Zr1A ^{iv}	125.57 (17)
O2 ^{iv} —La1—H1	82 (2)	Zr1B ^{xviii} —O2—Zr1A ^{iv}	9.7 (9)
O2 ^v —La1—H1	88.1 (17)	Zr1B ^{xix} —O2—Zr1A ^{iv}	10.0 (9)
O2 ⁱ —La1—H1	60 (2)	Zr1B ^{iv} —O2—La1 ^{iv}	105.3 (10)
O2 ⁱⁱ —La1—H1	122 (2)	Li2 ^{xvii} —O2—La1 ^{iv}	89.03 (12)
Li2 ^{vi} —La1—H1	83.6 (18)	Zr1B ^{xviii} —O2—La1 ^{iv}	97.9 (10)
Li1—La1—H1	96.4 (18)	Zr1B ^{xix} —O2—La1 ^{iv}	104.4 (9)
Zr1A ^{vii} —La1—H1	40.8 (17)	Zr1A ^{iv} —O2—La1 ^{iv}	106.84 (13)
Zr1B ^{viii} —Zr1A—Zr1B ⁱ	49 (4)	Zr1B ^{iv} —O2—La1 ^{viii}	101.5 (11)
Zr1B ^{viii} —Zr1A—O1 ^{ix}	105 (4)	Li2 ^{xvii} —O2—La1 ^{viii}	122.70 (14)
Zr1B ⁱ —Zr1A—O1 ^{ix}	113 (5)	Zr1B ^{xviii} —O2—La1 ^{viii}	103.6 (8)

Zr1B ^{viii} —Zr1A—O1 ^x	113 (5)	Zr1B ^{xix} —O2—La1 ^{viii}	96.1 (9)
Zr1B ⁱ —Zr1A—O1 ^x	153 (3)	Zr1A ^{iv} —O2—La1 ^{viii}	104.74 (13)
O1 ^{ix} —Zr1A—O1 ^x	89.46 (17)	La1 ^{iv} —O2—La1 ^{viii}	102.04 (12)
Zr1B ^{viii} —Zr1A—O1 ^{xi}	153 (3)	O1 ^{xx} —Li1—O1 ⁱⁱ	116.26 (11)
Zr1B ⁱ —Zr1A—O1 ^{xi}	105 (4)	O1 ^{xx} —Li1—O1 ⁱ	116.26 (11)
O1 ^{ix} —Zr1A—O1 ^{xi}	89.46 (17)	O1 ⁱⁱ —Li1—O1 ⁱ	96.61 (19)
O1 ^x —Zr1A—O1 ^{xi}	89.46 (17)	O1 ^{xx} —Li1—O1 ^{xxi}	96.61 (19)
Zr1B ^{viii} —Zr1A—O2 ^{xii}	20 (3)	O1 ⁱⁱ —Li1—O1 ^{xxi}	116.26 (11)
Zr1B ⁱ —Zr1A—O2 ^{xii}	68 (4)	O1 ⁱ —Li1—O1 ^{xxi}	116.26 (11)
O1 ^{ix} —Zr1A—O2 ^{xii}	94.57 (13)	O1 ^{xx} —Li1—La1	131.70 (10)
O1 ^x —Zr1A—O2 ^{xii}	96.47 (13)	O1 ⁱⁱ —Li1—La1	48.30 (10)
O1 ^{xi} —Zr1A—O2 ^{xii}	172.9 (2)	O1 ⁱ —Li1—La1	48.30 (10)
Zr1B ^{viii} —Zr1A—O2 ^{iv}	68 (4)	O1 ^{xxi} —Li1—La1	131.70 (10)
Zr1B ⁱ —Zr1A—O2 ^{iv}	62 (4)	O1 ^{xx} —Li1—La1 ^{xxii}	48.30 (10)
O1 ^{ix} —Zr1A—O2 ^{iv}	172.9 (2)	O1 ⁱⁱ —Li1—La1 ^{xxii}	131.70 (10)
O1 ^x —Zr1A—O2 ^{iv}	94.57 (13)	O1 ⁱ —Li1—La1 ^{xxii}	131.70 (10)
O1 ^{xi} —Zr1A—O2 ^{iv}	96.47 (13)	O1 ^{xxi} —Li1—La1 ^{xxii}	48.30 (10)
O2 ^{xii} —Zr1A—O2 ^{iv}	79.14 (16)	La1—Li1—La1 ^{xxii}	180
Zr1B ^{viii} —Zr1A—O2 ⁱⁱ	62 (4)	O1 ^{xx} —Li1—Zr1B ^{xxiii}	132.5 (5)
Zr1B ⁱ —Zr1A—O2 ⁱⁱ	20 (3)	O1 ⁱⁱ —Li1—Zr1B ^{xxiii}	32.5 (5)
O1 ^{ix} —Zr1A—O2 ⁱⁱ	96.47 (13)	O1 ⁱ —Li1—Zr1B ^{xxiii}	104.9 (5)
O1 ^x —Zr1A—O2 ⁱⁱ	172.9 (2)	O1 ^{xxi} —Li1—Zr1B ^{xxiii}	84.9 (5)
O1 ^{xi} —Zr1A—O2 ⁱⁱ	94.57 (13)	La1—Li1—Zr1B ^{xxiii}	63.8 (5)
O2 ^{xii} —Zr1A—O2 ⁱⁱ	79.14 (16)	La1 ^{xxii} —Li1—Zr1B ^{xxiii}	116.2 (5)
O2 ^{iv} —Zr1A—O2 ⁱⁱ	79.14 (16)	O1 ^{xx} —Li1—Zr1B ^{xxiv}	32.5 (5)
Zr1B ^{viii} —Zr1A—La1 ^{xi}	150 (6)	O1 ⁱⁱ —Li1—Zr1B ^{xxiv}	84.9 (5)
Zr1B ⁱ —Zr1A—La1 ^{xi}	139 (6)	O1 ⁱ —Li1—Zr1B ^{xxiv}	132.5 (5)
O1 ^{ix} —Zr1A—La1 ^{xi}	95.88 (14)	O1 ^{xxi} —Li1—Zr1B ^{xxiv}	104.9 (5)
O1 ^x —Zr1A—La1 ^{xi}	44.94 (11)	La1—Li1—Zr1B ^{xxiv}	116.2 (5)
O1 ^{xi} —Zr1A—La1 ^{xi}	45.30 (10)	La1 ^{xxii} —Li1—Zr1B ^{xxiv}	63.8 (5)
O2 ^{xii} —Zr1A—La1 ^{xi}	139.67 (9)	Zr1B ^{xxiii} —Li1—Zr1B ^{xxiv}	101.2 (4)
O2 ^{iv} —Zr1A—La1 ^{xi}	91.13 (9)	O1 ^{xx} —Li1—Zr1B ^{vii}	84.9 (5)
O2 ⁱⁱ —Zr1A—La1 ^{xi}	137.69 (9)	O1 ⁱⁱ —Li1—Zr1B ^{vii}	104.9 (5)
Zr1B ^{viii} —Zr1A—La1 ^{ix}	139 (6)	O1 ⁱ —Li1—Zr1B ^{vii}	32.5 (5)
Zr1B ⁱ —Zr1A—La1 ^{ix}	110 (2)	O1 ^{xxi} —Li1—Zr1B ^{vii}	132.5 (5)
O1 ^{ix} —Zr1A—La1 ^{ix}	45.30 (10)	La1—Li1—Zr1B ^{vii}	63.8 (5)
O1 ^x —Zr1A—La1 ^{ix}	95.88 (14)	La1 ^{xxii} —Li1—Zr1B ^{vii}	116.2 (5)
O1 ^{xi} —Zr1A—La1 ^{ix}	44.94 (11)	Zr1B ^{xxiii} —Li1—Zr1B ^{vii}	127.7 (9)
O2 ^{xii} —Zr1A—La1 ^{ix}	137.69 (9)	Zr1B ^{xxiv} —Li1—Zr1B ^{vii}	101.2 (4)
O2 ^{iv} —Zr1A—La1 ^{ix}	139.67 (9)	O1 ^{xx} —Li1—Zr1B ^{xii}	104.9 (5)
O2 ⁱⁱ —Zr1A—La1 ^{ix}	91.13 (9)	O1 ⁱⁱ —Li1—Zr1B ^{xii}	132.5 (5)
La1 ^{xi} —Zr1A—La1 ^{ix}	70.09 (5)	O1 ⁱ —Li1—Zr1B ^{xii}	84.9 (5)
Zr1B ^{viii} —Zr1A—La1 ^x	110 (2)	O1 ^{xxi} —Li1—Zr1B ^{xii}	32.5 (5)
Zr1B ⁱ —Zr1A—La1 ^x	150 (6)	La1—Li1—Zr1B ^{xii}	116.2 (5)
O1 ^{ix} —Zr1A—La1 ^x	44.94 (11)	La1 ^{xxii} —Li1—Zr1B ^{xii}	63.8 (5)
O1 ^x —Zr1A—La1 ^x	45.30 (10)	Zr1B ^{xxiii} —Li1—Zr1B ^{xii}	101.2 (4)
O1 ^{xi} —Zr1A—La1 ^x	95.88 (14)	Zr1B ^{xxiv} —Li1—Zr1B ^{xii}	127.7 (9)
O2 ^{xii} —Zr1A—La1 ^x	91.13 (9)	Zr1B ^{vii} —Li1—Zr1B ^{xii}	101.2 (4)

O2 ^{iv} —Zr1A—La1 ^x	137.69 (9)	O1 ^{xx} —Li1—Zr1A ^{xxv}	26.21 (10)
O2 ⁱⁱ —Zr1A—La1 ^x	139.67 (9)	O1 ⁱⁱ —Li1—Zr1A ^{xxv}	90.93 (10)
La1 ^{xi} —Zr1A—La1 ^x	70.09 (5)	O1 ⁱ —Li1—Zr1A ^{xxv}	130.14 (9)
La1 ^{ix} —Zr1A—La1 ^x	70.09 (5)	O1 ^{xxi} —Li1—Zr1A ^{xxv}	103.67 (10)
Zr1B ^{viii} —Zr1A—Li1 ^{xiii}	127 (3)	La1—Li1—Zr1A ^{xxv}	119.79 (3)
Zr1B ⁱ —Zr1A—Li1 ^{xiii}	79 (4)	La1 ^{xxii} —Li1—Zr1A ^{xxv}	60.21 (3)
O1 ^{ix} —Zr1A—Li1 ^{xiii}	100.02 (10)	Zr1B ^{xxiii} —Li1—Zr1A ^{xxv}	107.3 (5)
O1 ^x —Zr1A—Li1 ^{xiii}	113.16 (12)	Zr1B ^{xxiv} —Li1—Zr1A ^{xxv}	6.2 (5)
O1 ^{xi} —Zr1A—Li1 ^{xiii}	26.09 (10)	Zr1B ^{vii} —Li1—Zr1A ^{xxv}	98.1 (5)
O2 ^{xii} —Zr1A—Li1 ^{xiii}	146.86 (13)	Zr1B ^{xii} —Li1—Zr1A ^{xxv}	123.8 (5)
O2 ^{iv} —Zr1A—Li1 ^{xiii}	83.83 (9)	O1 ^{xx} —Li1—Zr1A ^{xxiii}	130.14 (9)
O2 ⁱⁱ —Zr1A—Li1 ^{xiii}	69.81 (9)	O1 ⁱⁱ —Li1—Zr1A ^{xxiii}	26.21 (10)
La1 ^{xi} —Zr1A—Li1 ^{xiii}	68.24 (3)	O1 ⁱ —Li1—Zr1A ^{xxiii}	103.67 (10)
La1 ^{ix} —Zr1A—Li1 ^{xiii}	56.29 (2)	O1 ^{xxi} —Li1—Zr1A ^{xxiii}	90.93 (10)
La1 ^x —Zr1A—Li1 ^{xiii}	120.04 (7)	La1—Li1—Zr1A ^{xxiii}	60.21 (3)
Zr1B ^{viii} —Zr1B—Zr1B ⁱ	60.00 (6)	La1 ^{xxii} —Li1—Zr1A ^{xxiii}	119.79 (3)
Zr1B ^{viii} —Zr1B—O2 ^{iv}	138 (5)	Zr1B ^{xxiii} —Li1—Zr1A ^{xxiii}	6.2 (5)
Zr1B ⁱ —Zr1B—O2 ^{iv}	126 (9)	Zr1B ^{xxiv} —Li1—Zr1A ^{xxiii}	98.1 (5)
Zr1B ^{viii} —Zr1B—O2 ^{xii}	47 (7)	Zr1B ^{vii} —Li1—Zr1A ^{xxiii}	123.8 (5)
Zr1B ⁱ —Zr1B—O2 ^{xii}	93 (9)	Zr1B ^{xii} —Li1—Zr1A ^{xxiii}	107.3 (5)
O2 ^{iv} —Zr1B—O2 ^{xii}	92.3 (15)	Zr1A ^{xxv} —Li1—Zr1A ^{xxiii}	104.29 (3)
Zr1B ^{viii} —Zr1B—O2 ⁱⁱ	78 (9)	O2 ^{xxvi} —Li2—O2 ^{xxvii}	111.48 (10)
Zr1B ⁱ —Zr1B—O2 ⁱⁱ	36 (5)	O2 ^{xxvi} —Li2—O2 ^{xvii}	111.48 (10)
O2 ^{iv} —Zr1B—O2 ⁱⁱ	90.9 (12)	O2 ^{xxvii} —Li2—O2 ^{xvii}	105.53 (19)
O2 ^{xii} —Zr1B—O2 ⁱⁱ	85.5 (5)	O2 ^{xxvi} —Li2—O2 ^{xxviii}	105.53 (19)
Zr1B ^{viii} —Zr1B—O1 ^x	95 (9)	O2 ^{xxvii} —Li2—O2 ^{xxviii}	111.48 (10)
Zr1B ⁱ —Zr1B—O1 ^x	130 (4)	O2 ^{xvii} —Li2—O2 ^{xxviii}	111.48 (10)
O2 ^{iv} —Zr1B—O1 ^x	101.9 (13)	O2 ^{xxvi} —Li2—La1 ^{xxix}	127.23 (9)
O2 ^{xii} —Zr1B—O1 ^x	97.3 (16)	O2 ^{xxvii} —Li2—La1 ^{xxix}	52.77 (9)
O2 ⁱⁱ —Zr1B—O1 ^x	166.7 (19)	O2 ^{xvii} —Li2—La1 ^{xxix}	52.77 (9)
Zr1B ^{viii} —Zr1B—O1 ^{xi}	119 (7)	O2 ^{xxviii} —Li2—La1 ^{xxix}	127.23 (9)
Zr1B ⁱ —Zr1B—O1 ^{xi}	77 (9)	O2 ^{xxvi} —Li2—La1 ^{xxii}	52.77 (9)
O2 ^{iv} —Zr1B—O1 ^{xi}	102.2 (13)	O2 ^{xxvii} —Li2—La1 ^{xxii}	127.23 (9)
O2 ^{xii} —Zr1B—O1 ^{xi}	165.4 (18)	O2 ^{xvii} —Li2—La1 ^{xxii}	127.23 (9)
O2 ⁱⁱ —Zr1B—O1 ^{xi}	92.7 (16)	O2 ^{xxviii} —Li2—La1 ^{xxii}	52.77 (9)
O1 ^x —Zr1B—O1 ^{xi}	81.4 (6)	La1 ^{xxix} —Li2—La1 ^{xxii}	180
Zr1B ^{viii} —Zr1B—O1 ^{ix}	44 (4)	O2 ^{xxvi} —Li2—Zr1B ^{xxx}	125.3 (7)
Zr1B ⁱ —Zr1B—O1 ^{ix}	54 (7)	O2 ^{xxvii} —Li2—Zr1B ^{xxx}	24.3 (5)
O2 ^{iv} —Zr1B—O1 ^{ix}	178.7 (12)	O2 ^{xvii} —Li2—Zr1B ^{xxx}	112.0 (5)
O2 ^{xii} —Zr1B—O1 ^{ix}	89.0 (11)	O2 ^{xxviii} —Li2—Zr1B ^{xxx}	87.6 (4)
O2 ⁱⁱ —Zr1B—O1 ^{ix}	89.6 (12)	La1 ^{xxix} —Li2—Zr1B ^{xxx}	63.6 (4)
O1 ^x —Zr1B—O1 ^{ix}	77.5 (10)	La1 ^{xxii} —Li2—Zr1B ^{xxx}	116.4 (4)
O1 ^{xi} —Zr1B—O1 ^{ix}	76.6 (11)	O2 ^{xxvi} —Li2—Zr1B ^{xxii}	24.3 (5)
Zr1B ^{viii} —Zr1B—Li2 ^{vi}	164 (6)	O2 ^{xxvii} —Li2—Zr1B ^{xxii}	87.6 (4)
Zr1B ⁱ —Zr1B—Li2 ^{vi}	126 (10)	O2 ^{xvii} —Li2—Zr1B ^{xxii}	125.3 (7)
O2 ^{iv} —Zr1B—Li2 ^{vi}	26.1 (4)	O2 ^{xxviii} —Li2—Zr1B ^{xxii}	112.0 (5)
O2 ^{xii} —Zr1B—Li2 ^{vi}	117.1 (14)	La1 ^{xxix} —Li2—Zr1B ^{xxii}	116.4 (4)
O2 ⁱⁱ —Zr1B—Li2 ^{vi}	100.0 (11)	La1 ^{xxii} —Li2—Zr1B ^{xxii}	63.6 (4)

O1 ^x —Zr1B—Li2 ^{vi}	90.3 (7)	Zr1B ^{xxx} —Li2—Zr1B ^{xxii}	101.4 (3)
O1 ^{xi} —Zr1B—Li2 ^{vi}	77.4 (7)	O2 ^{xxvi} —Li2—Zr1B ^{xxix}	87.6 (4)
O1 ^{ix} —Zr1B—Li2 ^{vi}	152.6 (9)	O2 ^{xxvii} —Li2—Zr1B ^{xxix}	112.0 (5)
Zr1B ^{viii} —Zr1B—La1 ^{viii}	93 (8)	O2 ^{xxviii} —Li2—Zr1B ^{xxix}	24.3 (5)
Zr1B ⁱ —Zr1B—La1 ^{viii}	125 (4)	O2 ^{xxviii} —Li2—Zr1B ^{xxix}	125.3 (7)
O2 ^{iv} —Zr1B—La1 ^{viii}	47.1 (9)	La1 ^{xxix} —Li2—Zr1B ^{xxix}	63.6 (4)
O2 ^{xii} —Zr1B—La1 ^{viii}	46.3 (8)	La1 ^{xxii} —Li2—Zr1B ^{xxix}	116.4 (4)
O2 ⁱⁱ —Zr1B—La1 ^{viii}	95.3 (9)	Zr1B ^{xxx} —Li2—Zr1B ^{xxix}	127.3 (8)
O1 ^x —Zr1B—La1 ^{viii}	95.9 (13)	Zr1B ^{xxii} —Li2—Zr1B ^{xxix}	101.4 (3)
O1 ^{xi} —Zr1B—La1 ^{viii}	148.2 (12)	O2 ^{xxvi} —Li2—Zr1B ^{xxxi}	112.0 (5)
O1 ^{ix} —Zr1B—La1 ^{viii}	134.1 (12)	O2 ^{xxvii} —Li2—Zr1B ^{xxxi}	125.3 (7)
Li2 ^{vi} —Zr1B—La1 ^{viii}	70.9 (7)	O2 ^{xxviii} —Li2—Zr1B ^{xxxi}	87.6 (4)
Zr1B ^{viii} —Zr1B—La1	118 (6)	O2 ^{xxviii} —Li2—Zr1B ^{xxxi}	24.3 (5)
Zr1B ⁱ —Zr1B—La1	82 (8)	La1 ^{xxix} —Li2—Zr1B ^{xxxi}	116.4 (4)
O2 ^{iv} —Zr1B—La1	44.2 (7)	La1 ^{xxii} —Li2—Zr1B ^{xxxi}	63.6 (4)
O2 ^{xii} —Zr1B—La1	95.2 (8)	Zr1B ^{xxx} —Li2—Zr1B ^{xxxi}	101.4 (3)
O2 ⁱⁱ —Zr1B—La1	47.5 (6)	Zr1B ^{xxii} —Li2—Zr1B ^{xxxi}	127.3 (8)
O1 ^x —Zr1B—La1	144.4 (12)	Zr1B ^{xxix} —Li2—Zr1B ^{xxxi}	101.4 (3)

Symmetry codes: (i) z, x, y ; (ii) $z, -x, -y+1/2$; (iii) $x, -y, -z+1/2$; (iv) $-x, -y+1/2, z$; (v) $-x, y-1/2, -z+1/2$; (vi) $x-1, y, z$; (vii) $y+1/4, x+1/4, z+1/4$; (viii) y, z, x ; (ix) $z-1/4, y-1/4, x-1/4$; (x) $x-1/4, z-1/4, y-1/4$; (xi) $y-1/4, x-1/4, z-1/4$; (xii) $-y+1/2, z, -x$; (xiii) $-y, z-1/2, -x+1/2$; (xiv) $z-1/2, -x+1/2, -y$; (xv) $x+1/4, z+1/4, y+1/4$; (xvi) $z+1/4, y+1/4, x+1/4$; (xvii) $-x+1, -y+1/2, z$; (xviii) $-z, -x+1/2, y$; (xix) $-y, -z+1/2, x$; (xx) $-z+3/4, -y+1/4, x+1/4$; (xxi) $-z+3/4, y-1/4, -x+1/4$; (xxii) $-x+3/4, z-1/4, -y+1/4$; (xxiii) $y+1/4, -x-1/4, -z+1/4$; (xxiv) $-y+1/2, -z, x+1/2$; (xxv) $-x+1/2, -y, z+1/2$; (xxvi) $x+3/4, z-1/4, y-1/4$; (xxvii) $-x+1, y-1/2, -z+1/2$; (xxviii) $x+3/4, -z+1/4, -y+3/4$; (xxix) $x+1, y, z$; (xxx) $x+1, -y, -z+1/2$; (xxxi) $-x+3/4, -z+1/4, y+1/4$.

(LLZO-Ga40-pristine)

Crystal data

Ga_{0.28}La_{2.94}Li_{6.44}O_{12.00}Zr_{2.00}
 $M_r = 847.67$
 Cubic, $I\bar{4}3d$
 Hall symbol: I -4bd 2c 3
 $a = 12.9669$ (2) Å
 $V = 2180.26$ (10) Å³
 $Z = 8$
 $F(000) = 2974.7$

$D_x = 5.165$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 35033 reflections
 $\theta = 3.9\text{--}38.9^\circ$
 $\mu = 13.88$ mm⁻¹
 $T = 298$ K
 Cuboid, colorless
 0.13 × 0.13 × 0.10 mm

Data collection

Bruker SMART APEX
 diffractometer
 Graphite monochromator
 rotation, ω -scans at 4 different φ positions
 Absorption correction: multi-scan
 (APEX2; Bruker, 2012)
 $T_{\min} = 0.19, T_{\max} = 0.25$
 35033 measured reflections

1054 independent reflections
 1045 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.038$
 $\theta_{\max} = 38.9^\circ, \theta_{\min} = 3.9^\circ$
 $h = -22 \rightarrow 22$
 $k = -22 \rightarrow 22$
 $l = -22 \rightarrow 22$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.013$
 $wR(F^2) = 0.026$
 $S = 1.29$
 1054 reflections

48 parameters
 2 restraints
 0 constraints
 $w = 1/[\sigma^2(F_o^2) + (0.0079P)^2 + 2.531P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.53 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.65 \text{ e } \text{\AA}^{-3}$
 Extinction correction: SHELXL2014
 (Sheldrick, 2015),
 $F_c^* = kF_c [1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00103 (4)
 Absolute structure: Refined as an inversion
 twin.
 Absolute structure parameter: 0.50 (4)

Special details

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

Refinement. Refined as a 2-component inversion twin.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
La1	0.11966 (2)	0	0.25	0.00584 (5)	0.9814 (19)
Zr1	0.00014 (2)	0.00014 (2)	0.00014 (2)	0.00502 (8)	
O1	0.09727 (14)	0.19681 (14)	0.27989 (14)	0.0087 (3)	
O2	0.03322 (15)	0.44478 (16)	0.14725 (13)	0.0105 (3)	
Li1	0.375	0	0.25	0.0038 (5)	0.818 (3)
Ga1	0.375	0	0.25	0.0038 (5)	0.182 (3)
Li2	0.875	0	0.25	0.021 (3)	0.995 (3)
Ga2	0.875	0	0.25	0.021 (3)	0.005 (3)
Li3	0.0971 (7)	0.1868 (6)	0.4268 (6)	0.014 (2)	0.62 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.00591 (7)	0.00574 (8)	0.00587 (8)	0	0	0.00065 (5)
Zr1	0.00502 (8)	0.00502 (8)	0.00502 (8)	0.00015 (6)	0.00015 (6)	0.00015 (6)
O1	0.0079 (7)	0.0087 (7)	0.0095 (7)	-0.0008 (6)	0.0013 (5)	-0.0002 (6)
O2	0.0134 (8)	0.0122 (8)	0.0059 (7)	0.0021 (6)	-0.0003 (5)	0.0009 (6)
Li1	0.0043 (8)	0.0035 (6)	0.0035 (6)	0	0	0
Ga1	0.0043 (8)	0.0035 (6)	0.0035 (6)	0	0	0
Li2	0.013 (4)	0.025 (4)	0.025 (4)	0	0	0
Ga2	0.013 (4)	0.025 (4)	0.025 (4)	0	0	0
Li3	0.022 (4)	0.014 (4)	0.007 (3)	-0.005 (3)	0.004 (3)	0.001 (2)

Geometric parameters (\AA , $^\circ$)

La1—O2 ⁱ	2.4935 (19)	O2—Li3 ^{xv}	2.108 (9)
La1—O2 ⁱⁱ	2.4935 (19)	O2—La1 ⁱ	2.4936 (19)
La1—O1 ⁱⁱⁱ	2.5264 (19)	O2—La1 ^{xv}	2.587 (2)
La1—O1 ^{iv}	2.5264 (19)	O2—Li3 ^{xvi}	2.639 (8)
La1—O2 ⁱⁱⁱ	2.587 (2)	Li1—Li3 ^{vii}	1.645 (8)
La1—O2 ^{iv}	2.587 (2)	Li1—Li3 ^{vi}	1.645 (8)
La1—O1 ^v	2.5975 (19)	Li1—Li3 ⁱⁱⁱ	1.645 (8)
La1—O1	2.5976 (19)	Li1—Li3 ^{iv}	1.645 (8)

La1—Li3 ^{vi}	3.037 (8)	Li1—O1 ^{vi}	1.8941 (18)
La1—Li3 ^{vii}	3.037 (8)	Li1—O1 ^{iv}	1.8941 (18)
La1—Ga2 ^{viii}	3.1725 (2)	Li1—O1 ⁱⁱⁱ	1.8941 (18)
La1—Li2 ^{viii}	3.1725 (2)	Li1—O1 ^{vii}	1.8941 (18)
Zr1—O2 ^{ix}	2.0823 (18)	Li1—La1 ^{xx}	3.3109 (2)
Zr1—O2 ^{iv}	2.0823 (18)	Li2—O2 ^{xxi}	1.9246 (19)
Zr1—O2 ⁱ	2.0823 (18)	Li2—O2 ^{xxii}	1.9246 (19)
Zr1—O1 ^x	2.1346 (18)	Li2—O2 ^{xxiii}	1.9246 (19)
Zr1—O1 ^{xi}	2.1346 (18)	Li2—O2 ^{xix}	1.9246 (19)
Zr1—O1 ^{xii}	2.1346 (18)	Li2—Li3 ^{xxiv}	2.340 (9)
Zr1—Li3 ^{xiii}	2.890 (8)	Li2—Li3 ^{xxv}	2.340 (9)
Zr1—Li3 ^v	2.890 (8)	Li2—Li3 ^{xxvi}	2.340 (9)
Zr1—Li3 ^{xiv}	2.890 (8)	Li2—Li3 ^{xxvii}	2.340 (9)
Zr1—Li3 ^x	3.140 (7)	Li2—La1 ^{xx}	3.1726 (2)
Zr1—Li3 ^{xi}	3.140 (7)	Li2—La1 ^{xxviii}	3.1726 (2)
Zr1—Li3 ^{xii}	3.140 (7)	Li3—Ga1 ^{xv}	1.645 (8)
O1—Ga1 ^{xv}	1.8941 (18)	Li3—Li1 ^{xv}	1.645 (8)
O1—Li1 ^{xv}	1.8941 (18)	Li3—O1 ^{xviii}	2.075 (8)
O1—Li3	1.909 (8)	Li3—O2 ⁱⁱⁱ	2.108 (9)
O1—Li3 ^{xvi}	2.075 (8)	Li3—O1 ^{xvi}	2.229 (8)
O1—Zr1 ^{xvii}	2.1346 (18)	Li3—Ga2 ^{xxix}	2.340 (9)
O1—Li3 ^{xviii}	2.229 (8)	Li3—Li2 ^{xxix}	2.340 (9)
O1—La1 ^{xv}	2.5264 (19)	Li3—Li3 ^{xvi}	2.513 (13)
O2—Ga2 ^{xix}	1.9247 (19)	Li3—Li3 ^{xviii}	2.513 (13)
O2—Li2 ^{xix}	1.9247 (19)	Li3—O2 ^{xviii}	2.639 (8)
O2—Zr1 ⁱ	2.0823 (18)	Li3—Zr1 ^v	2.890 (8)
O2 ⁱ —La1—O2 ⁱⁱ	74.68 (9)	Li3 ^{xv} —O2—La1 ⁱ	161.4 (2)
O2 ⁱ —La1—O1 ⁱⁱⁱ	111.38 (5)	Ga2 ^{xix} —O2—La1 ^{xv}	124.19 (9)
O2 ⁱⁱ —La1—O1 ⁱⁱⁱ	160.56 (5)	Li2 ^{xix} —O2—La1 ^{xv}	124.19 (9)
O2 ⁱ —La1—O1 ^{iv}	160.56 (5)	Zr1 ⁱ —O2—La1 ^{xv}	100.00 (7)
O2 ⁱⁱ —La1—O1 ^{iv}	111.38 (5)	Li3 ^{xv} —O2—La1 ^{xv}	90.4 (2)
O1 ⁱⁱⁱ —La1—O1 ^{iv}	69.36 (8)	La1 ⁱ —O2—La1 ^{xv}	102.82 (7)
O2 ⁱ —La1—O2 ⁱⁱⁱ	125.72 (4)	Ga2 ^{xix} —O2—Li3 ^{xvi}	59.26 (19)
O2 ⁱⁱ —La1—O2 ⁱⁱⁱ	68.66 (8)	Li2 ^{xix} —O2—Li3 ^{xvi}	59.26 (19)
O1 ⁱⁱⁱ —La1—O2 ⁱⁱⁱ	94.00 (6)	Zr1 ⁱ —O2—Li3 ^{xvi}	170.9 (2)
O1 ^{iv} —La1—O2 ⁱⁱⁱ	72.71 (6)	Li3 ^{xv} —O2—Li3 ^{xvi}	94.3 (2)
O2 ⁱ —La1—O2 ^{iv}	68.66 (8)	La1 ⁱ —O2—Li3 ^{xvi}	78.05 (18)
O2 ⁱⁱ —La1—O2 ^{iv}	125.72 (4)	La1 ^{xv} —O2—Li3 ^{xvi}	71.06 (19)
O1 ⁱⁱⁱ —La1—O2 ^{iv}	72.71 (6)	Li3 ^{vii} —Li1—Li3 ^{vi}	131.8 (5)
O1 ^{iv} —La1—O2 ^{iv}	94.00 (6)	Li3 ^{vii} —Li1—Li3 ⁱⁱⁱ	99.6 (2)
O2 ⁱⁱⁱ —La1—O2 ^{iv}	164.10 (8)	Li3 ^{vi} —Li1—Li3 ⁱⁱⁱ	99.6 (2)
O2 ⁱ —La1—O1 ^v	96.52 (6)	Li3 ^{vii} —Li1—Li3 ^{iv}	99.6 (2)
O2 ⁱⁱ —La1—O1 ^v	73.06 (6)	Li3 ^{vi} —Li1—Li3 ^{iv}	99.6 (2)
O1 ⁱⁱⁱ —La1—O1 ^v	122.80 (4)	Li3 ⁱⁱⁱ —Li1—Li3 ^{iv}	131.8 (5)
O1 ^{iv} —La1—O1 ^v	69.03 (8)	Li3 ^{vii} —Li1—O1 ^{vi}	163.0 (3)
O2 ⁱⁱⁱ —La1—O1 ^v	108.95 (5)	Li3 ^{vi} —Li1—O1 ^{vi}	64.8 (3)
O2 ^{iv} —La1—O1 ^v	72.92 (5)	Li3 ⁱⁱⁱ —Li1—O1 ^{vi}	77.7 (3)

O2 ⁱ —La1—O1	73.06 (6)	Li3 ^{iv} —Li1—O1 ^{vi}	71.4 (3)
O2 ⁱⁱ —La1—O1	96.52 (6)	Li3 ^{vii} —Li1—O1 ^{iv}	71.4 (3)
O1 ⁱⁱⁱ —La1—O1	69.03 (8)	Li3 ^{vi} —Li1—O1 ^{iv}	77.7 (3)
O1 ^{iv} —La1—O1	122.80 (4)	Li3 ⁱⁱⁱ —Li1—O1 ^{iv}	163.0 (3)
O2 ⁱⁱⁱ —La1—O1	72.92 (5)	Li3 ^{iv} —Li1—O1 ^{iv}	64.8 (3)
O2 ^{iv} —La1—O1	108.95 (5)	O1 ^{vi} —Li1—O1 ^{iv}	115.09 (6)
O1 ^v —La1—O1	167.16 (8)	Li3 ^{vii} —Li1—O1 ⁱⁱⁱ	77.7 (3)
O2 ⁱ —La1—Li3 ^{vi}	146.61 (16)	Li3 ^{vi} —Li1—O1 ⁱⁱⁱ	71.4 (3)
O2 ⁱⁱ —La1—Li3 ^{vi}	123.17 (17)	Li3 ⁱⁱⁱ —Li1—O1 ⁱⁱⁱ	64.8 (3)
O1 ⁱⁱⁱ —La1—Li3 ^{vi}	42.58 (16)	Li3 ^{iv} —Li1—O1 ⁱⁱⁱ	163.0 (3)
O1 ^{iv} —La1—Li3 ^{vi}	46.12 (15)	O1 ^{vi} —Li1—O1 ⁱⁱⁱ	115.09 (6)
O2 ⁱⁱⁱ —La1—Li3 ^{vi}	55.27 (17)	O1 ^{iv} —Li1—O1 ⁱⁱⁱ	98.74 (12)
O2 ^{iv} —La1—Li3 ^{vi}	109.23 (16)	Li3 ^{vii} —Li1—O1 ^{vii}	64.8 (3)
O1 ^v —La1—Li3 ^{vi}	115.09 (16)	Li3 ^{vi} —Li1—O1 ^{vii}	163.0 (3)
O1—La1—Li3 ^{vi}	76.72 (16)	Li3 ⁱⁱⁱ —Li1—O1 ^{vii}	71.4 (3)
O2 ⁱ —La1—Li3 ^{vii}	123.17 (17)	Li3 ^{iv} —Li1—O1 ^{vii}	77.7 (3)
O2 ⁱⁱ —La1—Li3 ^{vii}	146.61 (16)	O1 ^{vi} —Li1—O1 ^{vii}	98.74 (12)
O1 ⁱⁱⁱ —La1—Li3 ^{vii}	46.12 (15)	O1 ^{iv} —Li1—O1 ^{vii}	115.09 (6)
O1 ^{iv} —La1—Li3 ^{vii}	42.58 (16)	O1 ⁱⁱⁱ —Li1—O1 ^{vii}	115.09 (6)
O2 ⁱⁱⁱ —La1—Li3 ^{vii}	109.23 (16)	Li3 ^{vii} —Li1—La1 ^{xx}	114.1 (3)
O2 ^{iv} —La1—Li3 ^{vii}	55.27 (17)	Li3 ^{vi} —Li1—La1 ^{xx}	114.1 (3)
O1 ^v —La1—Li3 ^{vii}	76.72 (15)	Li3 ⁱⁱⁱ —Li1—La1 ^{xx}	65.9 (3)
O1—La1—Li3 ^{vii}	115.09 (16)	Li3 ^{iv} —Li1—La1 ^{xx}	65.9 (3)
Li3 ^{vi} —La1—Li3 ^{vii}	59.3 (3)	O1 ^{vi} —Li1—La1 ^{xx}	49.37 (6)
O2 ⁱ —La1—Ga2 ^{viii}	37.34 (4)	O1 ^{iv} —Li1—La1 ^{xx}	130.63 (6)
O2 ⁱⁱ —La1—Ga2 ^{viii}	37.34 (4)	O1 ⁱⁱⁱ —Li1—La1 ^{xx}	130.63 (6)
O1 ⁱⁱⁱ —La1—Ga2 ^{viii}	145.32 (4)	O1 ^{vii} —Li1—La1 ^{xx}	49.37 (6)
O1 ^{iv} —La1—Ga2 ^{viii}	145.32 (4)	Li3 ^{vii} —Li1—La1	65.9 (3)
O2 ⁱⁱⁱ —La1—Ga2 ^{viii}	97.95 (4)	Li3 ^{vi} —Li1—La1	65.9 (3)
O2 ^{iv} —La1—Ga2 ^{viii}	97.95 (4)	Li3 ⁱⁱⁱ —Li1—La1	114.1 (3)
O1 ^v —La1—Ga2 ^{viii}	83.58 (4)	Li3 ^{iv} —Li1—La1	114.1 (3)
O1—La1—Ga2 ^{viii}	83.58 (4)	O1 ^{vi} —Li1—La1	130.63 (6)
Li3 ^{vi} —La1—Ga2 ^{viii}	150.36 (16)	O1 ^{iv} —Li1—La1	49.37 (6)
Li3 ^{vii} —La1—Ga2 ^{viii}	150.36 (16)	O1 ⁱⁱⁱ —Li1—La1	49.37 (6)
O2 ⁱ —La1—Li2 ^{viii}	37.34 (4)	O1 ^{vii} —Li1—La1	130.63 (6)
O2 ⁱⁱ —La1—Li2 ^{viii}	37.34 (4)	La1 ^{xx} —Li1—La1	180
O1 ⁱⁱⁱ —La1—Li2 ^{viii}	145.32 (4)	O2 ^{xxi} —Li2—O2 ^{xxii}	112.48 (6)
O1 ^{iv} —La1—Li2 ^{viii}	145.32 (4)	O2 ^{xxi} —Li2—O2 ^{xxiii}	103.61 (12)
O2 ⁱⁱⁱ —La1—Li2 ^{viii}	97.95 (4)	O2 ^{xxii} —Li2—O2 ^{xxiii}	112.48 (6)
O2 ^{iv} —La1—Li2 ^{viii}	97.95 (4)	O2 ^{xxi} —Li2—O2 ^{xix}	112.48 (6)
O1 ^v —La1—Li2 ^{viii}	83.58 (4)	O2 ^{xxii} —Li2—O2 ^{xix}	103.60 (12)
O1—La1—Li2 ^{viii}	83.58 (4)	O2 ^{xxiii} —Li2—O2 ^{xix}	112.48 (6)
Li3 ^{vi} —La1—Li2 ^{viii}	150.36 (16)	O2 ^{xxi} —Li2—Li3 ^{xxiv}	161.7 (2)
Li3 ^{vii} —La1—Li2 ^{viii}	150.36 (16)	O2 ^{xxii} —Li2—Li3 ^{xxiv}	79.8 (2)
Ga2 ^{viii} —La1—Li2 ^{viii}	0	O2 ^{xxiii} —Li2—Li3 ^{xxiv}	58.3 (2)
O2 ^{ix} —Zr1—O2 ^{iv}	86.98 (8)	O2 ^{xix} —Li2—Li3 ^{xxiv}	75.8 (2)
O2 ^{ix} —Zr1—O2 ⁱ	86.98 (8)	O2 ^{xxi} —Li2—Li3 ^{xxv}	58.3 (2)
O2 ^{iv} —Zr1—O2 ⁱ	86.98 (8)	O2 ^{xxii} —Li2—Li3 ^{xxv}	75.8 (2)

O2 ^{ix} —Zr1—O1 ^x	94.92 (8)	O2 ^{xxiii} —Li2—Li3 ^{xxv}	161.7 (2)
O2 ^{iv} —Zr1—O1 ^x	177.97 (8)	O2 ^{xix} —Li2—Li3 ^{xxv}	79.8 (2)
O2 ⁱ —Zr1—O1 ^x	92.40 (7)	Li3 ^{xxiv} —Li2—Li3 ^{xxv}	140.0 (4)
O2 ^{ix} —Zr1—O1 ^{xi}	92.40 (7)	O2 ^{xxi} —Li2—Li3 ^{xxvi}	75.8 (2)
O2 ^{iv} —Zr1—O1 ^{xi}	94.92 (8)	O2 ^{xxii} —Li2—Li3 ^{xxvi}	161.7 (2)
O2 ⁱ —Zr1—O1 ^{xi}	177.97 (8)	O2 ^{xxiii} —Li2—Li3 ^{xxvi}	79.8 (2)
O1 ^x —Zr1—O1 ^{xi}	85.72 (7)	O2 ^{xix} —Li2—Li3 ^{xxvi}	58.3 (2)
O2 ^{ix} —Zr1—O1 ^{xii}	177.97 (8)	Li3 ^{xxiv} —Li2—Li3 ^{xxvi}	96.73 (13)
O2 ^{iv} —Zr1—O1 ^{xii}	92.40 (7)	Li3 ^{xxv} —Li2—Li3 ^{xxvi}	96.73 (13)
O2 ⁱ —Zr1—O1 ^{xii}	94.92 (8)	O2 ^{xxi} —Li2—Li3 ^{xxvii}	79.8 (2)
O1 ^x —Zr1—O1 ^{xii}	85.72 (7)	O2 ^{xxii} —Li2—Li3 ^{xxvii}	58.3 (2)
O1 ^{xi} —Zr1—O1 ^{xii}	85.72 (7)	O2 ^{xxiii} —Li2—Li3 ^{xxvii}	75.8 (2)
O2 ^{ix} —Zr1—Li3 ^{xiii}	46.76 (18)	O2 ^{xix} —Li2—Li3 ^{xxvii}	161.7 (2)
O2 ^{iv} —Zr1—Li3 ^{xiii}	94.45 (17)	Li3 ^{xxiv} —Li2—Li3 ^{xxvii}	96.73 (13)
O2 ⁱ —Zr1—Li3 ^{xiii}	133.42 (18)	Li3 ^{xxv} —Li2—Li3 ^{xxvii}	96.73 (13)
O1 ^x —Zr1—Li3 ^{xiii}	87.38 (16)	Li3 ^{xxvi} —Li2—Li3 ^{xxvii}	140.0 (4)
O1 ^{xi} —Zr1—Li3 ^{xiii}	45.80 (18)	O2 ^{xxi} —Li2—La1 ^{xx}	51.80 (6)
O1 ^{xii} —Zr1—Li3 ^{xiii}	131.42 (18)	O2 ^{xxii} —Li2—La1 ^{xx}	128.20 (6)
O2 ^{ix} —Zr1—Li3 ^v	133.42 (18)	O2 ^{xxiii} —Li2—La1 ^{xx}	51.80 (6)
O2 ^{iv} —Zr1—Li3 ^v	46.76 (18)	O2 ^{xix} —Li2—La1 ^{xx}	128.20 (6)
O2 ⁱ —Zr1—Li3 ^v	94.45 (17)	Li3 ^{xxiv} —Li2—La1 ^{xx}	110.0 (2)
O1 ^x —Zr1—Li3 ^v	131.42 (18)	Li3 ^{xxv} —Li2—La1 ^{xx}	110.0 (2)
O1 ^{xi} —Zr1—Li3 ^v	87.38 (16)	Li3 ^{xxvi} —Li2—La1 ^{xx}	70.0 (2)
O1 ^{xii} —Zr1—Li3 ^v	45.80 (18)	Li3 ^{xxvii} —Li2—La1 ^{xx}	70.0 (2)
Li3 ^{xiii} —Zr1—Li3 ^v	119.81 (2)	O2 ^{xxi} —Li2—La1 ^{xxviii}	128.20 (6)
O2 ^{ix} —Zr1—Li3 ^{xiv}	94.45 (17)	O2 ^{xxii} —Li2—La1 ^{xxviii}	51.80 (6)
O2 ^{iv} —Zr1—Li3 ^{xiv}	133.42 (18)	O2 ^{xxiii} —Li2—La1 ^{xxviii}	128.20 (6)
O2 ⁱ —Zr1—Li3 ^{xiv}	46.76 (18)	O2 ^{xix} —Li2—La1 ^{xxviii}	51.80 (6)
O1 ^x —Zr1—Li3 ^{xiv}	45.80 (18)	Li3 ^{xxiv} —Li2—La1 ^{xxviii}	70.0 (2)
O1 ^{xi} —Zr1—Li3 ^{xiv}	131.42 (18)	Li3 ^{xxv} —Li2—La1 ^{xxviii}	70.0 (2)
O1 ^{xii} —Zr1—Li3 ^{xiv}	87.38 (16)	Li3 ^{xxvi} —Li2—La1 ^{xxviii}	110.0 (2)
Li3 ^{xiii} —Zr1—Li3 ^{xiv}	119.81 (2)	Li3 ^{xxvii} —Li2—La1 ^{xxviii}	110.0 (2)
Li3 ^v —Zr1—Li3 ^{xiv}	119.81 (2)	La1 ^{xx} —Li2—La1 ^{xxviii}	180
O2 ^{ix} —Zr1—Li3 ^x	59.62 (16)	Ga1 ^{xv} —Li3—Li1 ^{xv}	0
O2 ^{iv} —Zr1—Li3 ^x	145.12 (16)	Ga1 ^{xv} —Li3—O1	63.9 (3)
O2 ⁱ —Zr1—Li3 ^x	81.85 (16)	Li1 ^{xv} —Li3—O1	63.9 (3)
O1 ^x —Zr1—Li3 ^x	36.53 (16)	Ga1 ^{xv} —Li3—O1 ^{xviii}	59.9 (3)
O1 ^{xi} —Zr1—Li3 ^x	96.18 (16)	Li1 ^{xv} —Li3—O1 ^{xviii}	59.9 (3)
O1 ^{xii} —Zr1—Li3 ^x	121.32 (16)	O1—Li3—O1 ^{xviii}	106.6 (4)
Li3 ^{xiii} —Zr1—Li3 ^x	70.8 (3)	Ga1 ^{xv} —Li3—O2 ⁱⁱⁱ	138.8 (5)
Li3 ^v —Zr1—Li3 ^x	166.5 (3)	Li1 ^{xv} —Li3—O2 ⁱⁱⁱ	138.8 (5)
Li3 ^{xiv} —Zr1—Li3 ^x	49.0 (3)	O1—Li3—O2 ⁱⁱⁱ	100.0 (4)
O2 ^{ix} —Zr1—Li3 ^{xi}	81.85 (16)	O1 ^{xviii} —Li3—O2 ⁱⁱⁱ	93.4 (3)
O2 ^{iv} —Zr1—Li3 ^{xi}	59.62 (16)	Ga1 ^{xv} —Li3—O1 ^{xvi}	56.1 (3)
O2 ⁱ —Zr1—Li3 ^{xi}	145.12 (16)	Li1 ^{xv} —Li3—O1 ^{xvi}	56.1 (3)
O1 ^x —Zr1—Li3 ^{xi}	121.32 (16)	O1—Li3—O1 ^{xvi}	100.9 (4)
O1 ^{xi} —Zr1—Li3 ^{xi}	36.53 (16)	O1 ^{xviii} —Li3—O1 ^{xvi}	83.7 (3)
O1 ^{xii} —Zr1—Li3 ^{xi}	96.18 (16)	O2 ⁱⁱⁱ —Li3—O1 ^{xvi}	158.8 (4)

Li3 ^{xiii} —Zr1—Li3 ^{xi}	49.0 (3)	Gal ^{xv} —Li3—Ga2 ^{xxix}	169.9 (5)
Li3 ^v —Zr1—Li3 ^{xi}	70.8 (3)	Li1 ^{xv} —Li3—Ga2 ^{xxix}	169.9 (5)
Li3 ^{xiv} —Zr1—Li3 ^{xi}	166.5 (3)	O1—Li3—Ga2 ^{xxix}	115.3 (4)
Li3 ^x —Zr1—Li3 ^{xi}	119.11 (5)	O1 ^{xviii} —Li3—Ga2 ^{xxix}	127.8 (4)
O2 ^{ix} —Zr1—Li3 ^{xii}	145.12 (16)	O2 ⁱⁱⁱ —Li3—Ga2 ^{xxix}	50.9 (2)
O2 ^{iv} —Zr1—Li3 ^{xii}	81.85 (16)	O1 ^{xvi} —Li3—Ga2 ^{xxix}	115.7 (4)
O2 ⁱ —Zr1—Li3 ^{xii}	59.62 (16)	Gal ^{xv} —Li3—Li2 ^{xxix}	169.9 (5)
O1 ^x —Zr1—Li3 ^{xii}	96.18 (16)	Li1 ^{xv} —Li3—Li2 ^{xxix}	169.9 (5)
O1 ^{xi} —Zr1—Li3 ^{xii}	121.32 (16)	O1—Li3—Li2 ^{xxix}	115.3 (4)
O1 ^{xii} —Zr1—Li3 ^{xii}	36.53 (16)	O1 ^{xviii} —Li3—Li2 ^{xxix}	127.8 (4)
Li3 ^{xiii} —Zr1—Li3 ^{xii}	166.5 (3)	O2 ⁱⁱⁱ —Li3—Li2 ^{xxix}	50.9 (2)
Li3 ^v —Zr1—Li3 ^{xii}	49.0 (3)	O1 ^{xvi} —Li3—Li2 ^{xxix}	115.7 (4)
Li3 ^{xiv} —Zr1—Li3 ^{xii}	70.8 (3)	Ga2 ^{xxix} —Li3—Li2 ^{xxix}	0
Li3 ^x —Zr1—Li3 ^{xii}	119.11 (5)	Gal ^{xv} —Li3—Li3 ^{xvi}	40.21 (10)
Li3 ^{xi} —Zr1—Li3 ^{xii}	119.11 (5)	Li1 ^{xv} —Li3—Li3 ^{xvi}	40.21 (10)
Gal ^{xv} —O1—Li1 ^{xv}	0	O1—Li3—Li3 ^{xvi}	53.9 (3)
Gal ^{xv} —O1—Li3	51.3 (3)	O1 ^{xviii} —Li3—Li3 ^{xvi}	99.0 (3)
Li1 ^{xv} —O1—Li3	51.3 (3)	O2 ⁱⁱⁱ —Li3—Li3 ^{xvi}	153.4 (5)
Gal ^{xv} —O1—Li3 ^{xvi}	48.7 (2)	O1 ^{xvi} —Li3—Li3 ^{xvi}	47.0 (2)
Li1 ^{xv} —O1—Li3 ^{xvi}	48.7 (2)	Ga2 ^{xxix} —Li3—Li3 ^{xvi}	130.4 (4)
Li3—O1—Li3 ^{xvi}	78.1 (3)	Li2 ^{xxix} —Li3—Li3 ^{xvi}	130.4 (4)
Gal ^{xv} —O1—Zr1 ^{xvii}	128.17 (10)	Gal ^{xv} —Li3—Li3 ^{xviii}	40.21 (10)
Li1 ^{xv} —O1—Zr1 ^{xvii}	128.17 (10)	Li1 ^{xv} —Li3—Li3 ^{xviii}	40.21 (10)
Li3—O1—Zr1 ^{xvii}	101.7 (3)	O1—Li3—Li3 ^{xviii}	58.7 (3)
Li3 ^{xvi} —O1—Zr1 ^{xvii}	86.7 (2)	O1 ^{xviii} —Li3—Li3 ^{xviii}	48.0 (2)
Gal ^{xv} —O1—Li3 ^{xviii}	46.1 (2)	O2 ⁱⁱⁱ —Li3—Li3 ^{xviii}	98.6 (5)
Li1 ^{xv} —O1—Li3 ^{xviii}	46.1 (2)	O1 ^{xvi} —Li3—Li3 ^{xviii}	95.0 (2)
Li3—O1—Li3 ^{xviii}	74.3 (3)	Ga2 ^{xxix} —Li3—Li3 ^{xviii}	149.1 (5)
Li3 ^{xvi} —O1—Li3 ^{xviii}	88.4 (4)	Li2 ^{xxix} —Li3—Li3 ^{xviii}	149.1 (5)
Zr1 ^{xvii} —O1—Li3 ^{xviii}	174.3 (2)	Li3 ^{xvi} —Li3—Li3 ^{xviii}	73.4 (3)
Gal ^{xv} —O1—La1 ^{xv}	95.95 (7)	Gal ^{xv} —Li3—O2 ^{xviii}	130.3 (4)
Li1 ^{xv} —O1—La1 ^{xv}	95.95 (7)	Li1 ^{xv} —Li3—O2 ^{xviii}	130.3 (4)
Li3—O1—La1 ^{xv}	147.0 (3)	O1—Li3—O2 ^{xviii}	148.4 (4)
Li3 ^{xvi} —O1—La1 ^{xv}	82.0 (2)	O1 ^{xviii} —Li3—O2 ^{xviii}	104.4 (3)
Zr1 ^{xvii} —O1—La1 ^{xv}	103.10 (7)	O2 ⁱⁱⁱ —Li3—O2 ^{xviii}	84.0 (3)
Li3 ^{xviii} —O1—La1 ^{xv}	79.11 (19)	O1 ^{xvi} —Li3—O2 ^{xviii}	76.5 (2)
Gal ^{xv} —O1—La1	121.96 (8)	Ga2 ^{xxix} —Li3—O2 ^{xviii}	44.98 (15)
Li1 ^{xv} —O1—La1	121.96 (8)	Li2 ^{xxix} —Li3—O2 ^{xviii}	44.98 (15)
Li3—O1—La1	94.7 (3)	Li3 ^{xvi} —Li3—O2 ^{xviii}	115.1 (4)
Li3 ^{xvi} —O1—La1	170.6 (2)	Li3 ^{xviii} —Li3—O2 ^{xviii}	152.2 (5)
Zr1 ^{xvii} —O1—La1	100.81 (7)	Gal ^{xv} —Li3—Zr1 ^v	102.6 (4)
Li3 ^{xviii} —O1—La1	83.8 (2)	Li1 ^{xv} —Li3—Zr1 ^v	102.6 (4)
La1 ^{xv} —O1—La1	101.62 (6)	O1—Li3—Zr1 ^v	112.6 (3)
Ga2 ^{xix} —O2—Li2 ^{xix}	0	O1 ^{xviii} —Li3—Zr1 ^v	47.50 (17)
Ga2 ^{xix} —O2—Zr1 ⁱ	129.42 (11)	O2 ⁱⁱⁱ —Li3—Zr1 ^v	46.02 (16)
Li2 ^{xix} —O2—Zr1 ⁱ	129.42 (11)	O1 ^{xvi} —Li3—Zr1 ^v	126.1 (3)
Ga2 ^{xix} —O2—Li3 ^{xv}	70.8 (2)	Ga2 ^{xxix} —Li3—Zr1 ^v	87.0 (2)
Li2 ^{xix} —O2—Li3 ^{xv}	70.8 (2)	Li2 ^{xxix} —Li3—Zr1 ^v	87.0 (2)

Zr1 ⁱ —O2—Li3 ^{xv}	87.2 (2)	Li3 ^{xvi} —Li3—Zr1 ^v	142.5 (4)
Ga2 ^{xix} —O2—La1 ⁱ	90.85 (7)	Li3 ^{xviii} —Li3—Zr1 ^v	70.7 (3)
Li2 ^{xix} —O2—La1 ⁱ	90.85 (7)	O2 ^{xviii} —Li3—Zr1 ^v	92.8 (2)
Zr1 ⁱ —O2—La1 ⁱ	103.05 (8)		

Symmetry codes: (i) $-x, -y+1/2, z$; (ii) $-x, y-1/2, -z+1/2$; (iii) z, x, y ; (iv) $z, -x, -y+1/2$; (v) $x, -y, -z+1/2$; (vi) $-z+3/4, -y+1/4, x+1/4$; (vii) $-z+3/4, y-1/4, -x+1/4$; (viii) $x-1, y, z$; (ix) $-y+1/2, z, -x$; (x) $x-1/4, z-1/4, y-1/4$; (xi) $z-1/4, y-1/4, x-1/4$; (xii) $y-1/4, x-1/4, z-1/4$; (xiii) $-z+1/2, x, -y$; (xiv) $-y, -z+1/2, x$; (xv) y, z, x ; (xvi) $-y+1/4, x+1/4, -z+3/4$; (xvii) $y+1/4, x+1/4, z+1/4$; (xviii) $y-1/4, -x+1/4, -z+3/4$; (xix) $-x+1, -y+1/2, z$; (xx) $-x+3/4, z-1/4, -y+1/4$; (xxi) $x+3/4, z-1/4, y-1/4$; (xxii) $-x+1, y-1/2, -z+1/2$; (xxiii) $x+3/4, -z+1/4, -y+3/4$; (xxiv) $y+3/4, -x+1/4, -z+3/4$; (xxv) $y+3/4, x-1/4, z-1/4$; (xxvi) $-y+1, -z+1/2, x$; (xxvii) $-y+1, z-1/2, -x+1/2$; (xxviii) $x+1, y, z$; (xxix) $-y+1/4, x-3/4, -z+3/4$.

(LLZO-Ga40-hydro-150C)

Crystal data

Ga_{0.26}H_{3.90}La_{2.96}Li_{1.99}O₁₂Zr₂
 $M_r = 821.46$
 Cubic, $I\bar{4}3d$
 Hall symbol: I -4bd 2c 3
 $a = 13.06720$ (12) Å
 $V = 2231.25$ (6) Å³
 $Z = 8$
 $F(000) = 2901.2$

$D_x = 4.891$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 35657 reflections
 $\theta = 3.8\text{--}36.6^\circ$
 $\mu = 13.57$ mm⁻¹
 $T = 298$ K
 Cuboid, colorless
 0.12 × 0.11 × 0.09 mm

Data collection

Bruker SMART APEX
 diffractometer
 Graphite monochromator
 rotation, ω -scans at 4 different ϕ positions
 Absorption correction: multi-scan
 (APEX2; Bruker, 2012)
 $T_{\min} = 0.21, T_{\max} = 0.36$
 35657 measured reflections

918 independent reflections
 915 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.028$
 $\theta_{\max} = 36.6^\circ, \theta_{\min} = 3.8^\circ$
 $h = -21 \rightarrow 21$
 $k = -21 \rightarrow 21$
 $l = -21 \rightarrow 21$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.018$
 $wR(F^2) = 0.037$
 $S = 1.12$
 918 reflections
 43 parameters
 3 restraints
 0 constraints
 Hydrogen site location: difference Fourier map
 Only H-atom coordinates refined

$w = 1/[\sigma^2(F_o^2) + (0.0072P)^2 + 28.9201P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.54$ e Å⁻³
 $\Delta\rho_{\min} = -0.52$ e Å⁻³
 Extinction correction: SHELXL2014
 (Sheldrick, 2015),
 $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.00055 (4)
 Absolute structure: Refined as an inversion
 twin.
 Absolute structure parameter: 0.99944 (15)

Special details

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

Refinement. Refined as a 2-component inversion twin.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
La1	0.11790 (3)	0	0.25	0.00993 (9)	0.986 (4)
Zr1	-0.01020 (3)	-0.01020 (3)	-0.01020 (3)	0.01011 (17)	
O1	0.0963 (3)	0.1906 (3)	0.2735 (3)	0.0106 (6)	
O2	0.0339 (3)	0.4448 (3)	0.1420 (3)	0.0138 (6)	
Li1	0.375	0	0.25	0.0068 (7)	0.824 (3)
Ga1	0.375	0	0.25	0.0068 (7)	0.176 (3)
Li2	0.875	0	0.25	0.007*	0.34 (5)
Li3	0.070 (16)	0.283 (15)	0.457 (16)	0.01*	0.04 (3)
H1	0.104 (11)	0.183 (10)	0.321 (8)	0.025*	0.65 (19)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.00856 (14)	0.00800 (14)	0.01322 (16)	0	0	0.00411 (10)
Zr1	0.01011 (17)	0.01011 (17)	0.01011 (17)	-0.00033 (13)	-0.00033 (13)	-0.00033 (13)
O1	0.0076 (11)	0.0106 (13)	0.0135 (14)	-0.0005 (10)	-0.0005 (10)	0.0019 (10)
O2	0.0191 (15)	0.0128 (14)	0.0095 (13)	0.0025 (11)	0.0030 (10)	0.0032 (11)
Li1	0.0055 (13)	0.0075 (10)	0.0075 (10)	0	0	0
Ga1	0.0055 (13)	0.0075 (10)	0.0075 (10)	0	0	0

Geometric parameters (\AA , $^\circ$)

La1—Li3 ⁱ	2.5 (2)	O2—La1 ^{xvi}	2.603 (4)
La1—Li3 ⁱⁱ	2.5 (2)	Li1—Li3 ⁱⁱⁱ	1.5 (2)
La1—O1 ⁱⁱⁱ	2.514 (3)	Li1—Li3 ⁱⁱ	1.5 (2)
La1—O1 ^{iv}	2.514 (3)	Li1—Li3 ^{iv}	1.5 (2)
La1—O1 ^v	2.525 (3)	Li1—Li3 ⁱ	1.5 (2)
La1—O1	2.525 (3)	Li1—O1 ⁱ	1.987 (4)
La1—O2 ^{vi}	2.539 (4)	Li1—O1 ^{iv}	1.987 (4)
La1—O2 ^{vii}	2.539 (4)	Li1—O1 ⁱⁱⁱ	1.987 (4)
La1—O2 ⁱⁱⁱ	2.603 (4)	Li1—O1 ⁱⁱ	1.987 (4)
La1—O2 ^{iv}	2.603 (4)	Li1—La1 ^{xx}	3.3596 (4)
La1—Li3 ^{viii}	2.7 (2)	Li1—Zr1 ^{xxi}	3.5997 (1)
La1—Li3 ^{ix}	2.7 (2)	Li1—Zr1 ^{xxii}	3.5997 (1)
Zr1—O1 ^x	2.031 (3)	Li2—O2 ^{xxiii}	1.982 (4)
Zr1—O1 ^{xi}	2.031 (3)	Li2—O2 ^{xxiv}	1.982 (4)
Zr1—O1 ^{viii}	2.031 (3)	Li2—O2 ^{xxv}	1.982 (4)
Zr1—O2 ^{iv}	2.187 (4)	Li2—O2 ^{xix}	1.982 (4)
Zr1—O2 ^{xii}	2.187 (4)	Li2—La1 ^{xx}	3.1740 (4)
Zr1—O2 ^{vi}	2.187 (4)	Li2—La1 ^{xxvi}	3.1740 (4)
Zr1—Li3 ^{xiii}	2.9 (2)	Li2—Li3 ^{xxvii}	3.2 (2)
Zr1—Li3 ^{xiv}	2.9 (2)	Li2—Li3 ^{xxviii}	3.2 (2)
Zr1—Li3 ^{vii}	2.9 (2)	Li2—Li3 ^{xxix}	3.2 (2)
Zr1—La1 ^{xi}	3.5178 (5)	Li2—Li3 ^{xxx}	3.2 (2)
Zr1—La1 ^{xv}	3.5178 (5)	Li3—O1 ^{xviii}	0.9 (2)

Zr1—La1 ^x	3.5178 (5)	Li3—Ga1 ^{xvi}	1.5 (2)
O1—Li3 ^{ix}	0.9 (2)	Li3—Li1 ^{xvi}	1.5 (2)
O1—Ga1 ^{xvi}	1.987 (4)	Li3—Li3 ^{vi}	2.0 (4)
O1—Li1 ^{xvi}	1.987 (4)	Li3—O1 ^{ix}	2.4 (2)
O1—Zr1 ^{xvii}	2.031 (3)	Li3—La1 ^{xxxi}	2.5 (2)
O1—Li3 ^{xviii}	2.4 (2)	Li3—Li3 ^{xviii}	2.6 (4)
O1—La1 ^{xvi}	2.514 (3)	Li3—Li3 ^{ix}	2.6 (4)
O2—Li2 ^{xix}	1.982 (4)	Li3—La1 ^{xviii}	2.7 (2)
O2—Zr1 ^{vi}	2.187 (4)	Li3—Zr1 ^{xxxii}	2.9 (2)
O2—La1 ^{vi}	2.539 (4)	Li3—Li2 ^{xxxiii}	3.2 (2)
Li3 ⁱ —La1—Li3 ⁱⁱ	48 (9)	Li3 ⁱⁱ —Li1—Li3 ⁱ	86 (10)
Li3 ⁱ —La1—O1 ⁱⁱⁱ	57 (5)	Li3 ^{iv} —Li1—Li3 ⁱ	122 (10)
Li3 ⁱⁱ —La1—O1 ⁱⁱⁱ	20 (5)	Li3 ⁱⁱⁱ —Li1—O1 ⁱ	24 (8)
Li3 ⁱ —La1—O1 ^{iv}	20 (5)	Li3 ⁱⁱ —Li1—O1 ⁱ	140 (8)
Li3 ⁱⁱ —La1—O1 ^{iv}	57 (5)	Li3 ^{iv} —Li1—O1 ⁱ	87 (8)
O1 ⁱⁱⁱ —La1—O1 ^{iv}	72.06 (16)	Li3 ⁱ —Li1—O1 ⁱ	102 (8)
Li3 ⁱ —La1—O1 ^v	89 (5)	Li3 ⁱⁱⁱ —Li1—O1 ^{iv}	140 (8)
Li3 ⁱⁱ —La1—O1 ^v	103 (5)	Li3 ⁱⁱ —Li1—O1 ^{iv}	87 (8)
O1 ⁱⁱⁱ —La1—O1 ^v	123.13 (7)	Li3 ^{iv} —Li1—O1 ^{iv}	102 (8)
O1 ^{iv} —La1—O1 ^v	68.54 (15)	Li3 ⁱ —Li1—O1 ^{iv}	24 (8)
Li3 ⁱ —La1—O1	103 (5)	O1 ⁱ —Li1—O1 ^{iv}	116.47 (11)
Li3 ⁱⁱ —La1—O1	89 (5)	Li3 ⁱⁱⁱ —Li1—O1 ⁱⁱⁱ	102 (8)
O1 ⁱⁱⁱ —La1—O1	68.54 (15)	Li3 ⁱⁱ —Li1—O1 ⁱⁱⁱ	24 (8)
O1 ^{iv} —La1—O1	123.13 (7)	Li3 ^{iv} —Li1—O1 ⁱⁱⁱ	140 (8)
O1 ^v —La1—O1	167.17 (15)	Li3 ⁱ —Li1—O1 ⁱⁱⁱ	87 (8)
Li3 ⁱ —La1—O2 ^{vi}	165 (5)	O1 ⁱ —Li1—O1 ⁱⁱⁱ	116.47 (11)
Li3 ⁱⁱ —La1—O2 ^{vi}	118 (5)	O1 ^{iv} —Li1—O1 ⁱⁱⁱ	96.2 (2)
O1 ⁱⁱⁱ —La1—O2 ^{vi}	108.54 (10)	Li3 ⁱⁱⁱ —Li1—O1 ⁱⁱ	87 (8)
O1 ^{iv} —La1—O2 ^{vi}	161.05 (10)	Li3 ⁱⁱ —Li1—O1 ⁱⁱ	102 (8)
O1 ^v —La1—O2 ^{vi}	97.21 (12)	Li3 ^{iv} —Li1—O1 ⁱⁱ	24 (8)
O1—La1—O2 ^{vi}	72.54 (11)	Li3 ⁱ —Li1—O1 ⁱⁱ	140 (8)
Li3 ⁱ —La1—O2 ^{vii}	118 (5)	O1 ⁱ —Li1—O1 ⁱⁱ	96.2 (2)
Li3 ⁱⁱ —La1—O2 ^{vii}	165 (5)	O1 ^{iv} —Li1—O1 ⁱⁱ	116.47 (11)
O1 ⁱⁱⁱ —La1—O2 ^{vii}	161.05 (10)	O1 ⁱⁱⁱ —Li1—O1 ⁱⁱ	116.47 (11)
O1 ^{iv} —La1—O2 ^{vii}	108.54 (10)	Li3 ⁱⁱⁱ —Li1—La1	137 (8)
O1 ^v —La1—O2 ^{vii}	72.54 (11)	Li3 ⁱⁱ —Li1—La1	43 (8)
O1—La1—O2 ^{vii}	97.21 (12)	Li3 ^{iv} —Li1—La1	137 (8)
O2 ^{vi} —La1—O2 ^{vii}	77.23 (18)	Li3 ⁱ —Li1—La1	43 (8)
Li3 ⁱ —La1—O2 ⁱⁱⁱ	64 (5)	O1 ⁱ —Li1—La1	131.89 (10)
Li3 ⁱⁱ —La1—O2 ⁱⁱⁱ	102 (5)	O1 ^{iv} —Li1—La1	48.11 (10)
O1 ⁱⁱⁱ —La1—O2 ⁱⁱⁱ	96.82 (12)	O1 ⁱⁱⁱ —Li1—La1	48.11 (10)
O1 ^{iv} —La1—O2 ⁱⁱⁱ	71.66 (11)	O1 ⁱⁱ —Li1—La1	131.89 (10)
O1 ^v —La1—O2 ⁱⁱⁱ	107.49 (10)	Li3 ⁱⁱⁱ —Li1—La1 ^{xx}	43 (8)
O1—La1—O2 ⁱⁱⁱ	74.13 (11)	Li3 ⁱⁱ —Li1—La1 ^{xx}	137 (8)
O2 ^{vi} —La1—O2 ⁱⁱⁱ	126.12 (8)	Li3 ^{iv} —Li1—La1 ^{xx}	43 (8)
O2 ^{vii} —La1—O2 ⁱⁱⁱ	66.40 (16)	Li3 ⁱ —Li1—La1 ^{xx}	137 (8)
Li3 ⁱ —La1—O2 ^{iv}	102 (5)	O1 ⁱ —Li1—La1 ^{xx}	48.11 (10)

Li3 ⁱⁱ —La1—O2 ^{iv}	64 (5)	O1 ^{iv} —Li1—La1 ^{xx}	131.89 (10)
O1 ⁱⁱⁱ —La1—O2 ^{iv}	71.66 (11)	O1 ⁱⁱⁱ —Li1—La1 ^{xx}	131.89 (10)
O1 ^{iv} —La1—O2 ^{iv}	96.82 (12)	O1 ⁱⁱ —Li1—La1 ^{xx}	48.11 (10)
O1 ^v —La1—O2 ^{iv}	74.13 (11)	La1—Li1—La1 ^{xx}	180
O1—La1—O2 ^{iv}	107.49 (10)	Li3 ⁱⁱⁱ —Li1—Zr1 ^{xxi}	50 (8)
O2 ^{vi} —La1—O2 ^{iv}	66.40 (16)	Li3 ⁱⁱ —Li1—Zr1 ^{xxi}	152 (8)
O2 ^{vii} —La1—O2 ^{iv}	126.12 (8)	Li3 ^{iv} —Li1—Zr1 ^{xxi}	85 (8)
O2 ⁱⁱⁱ —La1—O2 ^{iv}	166.09 (15)	Li3 ⁱ —Li1—Zr1 ^{xxi}	80 (8)
Li3 ⁱ —La1—Li3 ^{viii}	108 (9)	O1 ⁱ —Li1—Zr1 ^{xxi}	26.66 (10)
Li3 ⁱⁱ —La1—Li3 ^{viii}	117 (2)	O1 ^{iv} —Li1—Zr1 ^{xxi}	90.62 (10)
O1 ⁱⁱⁱ —La1—Li3 ^{viii}	136 (5)	O1 ⁱⁱⁱ —Li1—Zr1 ^{xxi}	130.13 (10)
O1 ^{iv} —La1—Li3 ^{viii}	88 (4)	O1 ⁱⁱ —Li1—Zr1 ^{xxi}	103.79 (10)
O1 ^v —La1—Li3 ^{viii}	19 (4)	La1—Li1—Zr1 ^{xxi}	119.390 (8)
O1—La1—Li3 ^{viii}	148 (4)	La1 ^{xx} —Li1—Zr1 ^{xxi}	60.610 (8)
O2 ^{vi} —La1—Li3 ^{viii}	79 (4)	Li3 ⁱⁱⁱ —Li1—Zr1 ^{xxii}	152 (8)
O2 ^{vii} —La1—Li3 ^{viii}	63 (5)	Li3 ⁱⁱ —Li1—Zr1 ^{xxii}	85 (8)
O2 ⁱⁱⁱ —La1—Li3 ^{viii}	114 (4)	Li3 ^{iv} —Li1—Zr1 ^{xxii}	80 (8)
O2 ^{iv} —La1—Li3 ^{viii}	72 (4)	Li3 ⁱ —Li1—Zr1 ^{xxii}	50 (8)
Li3 ⁱ —La1—Li3 ^{ix}	117 (2)	O1 ⁱ —Li1—Zr1 ^{xxii}	130.13 (10)
Li3 ⁱⁱ —La1—Li3 ^{ix}	108 (9)	O1 ^{iv} —Li1—Zr1 ^{xxii}	26.66 (10)
O1 ⁱⁱⁱ —La1—Li3 ^{ix}	88 (4)	O1 ⁱⁱⁱ —Li1—Zr1 ^{xxii}	103.79 (10)
O1 ^{iv} —La1—Li3 ^{ix}	136 (5)	O1 ⁱⁱ —Li1—Zr1 ^{xxii}	90.62 (10)
O1 ^v —La1—Li3 ^{ix}	148 (4)	La1—Li1—Zr1 ^{xxii}	60.610 (8)
O1—La1—Li3 ^{ix}	19 (4)	La1 ^{xx} —Li1—Zr1 ^{xxii}	119.390 (8)
O2 ^{vi} —La1—Li3 ^{ix}	63 (5)	Zr1 ^{xxi} —Li1—Zr1 ^{xxii}	103.936 (7)
O2 ^{vii} —La1—Li3 ^{ix}	79 (4)	O2 ^{xxiii} —Li2—O2 ^{xxiv}	111.13 (11)
O2 ⁱⁱⁱ —La1—Li3 ^{ix}	72 (4)	O2 ^{xxiii} —Li2—O2 ^{xxv}	106.2 (2)
O2 ^{iv} —La1—Li3 ^{ix}	114 (4)	O2 ^{xxiv} —Li2—O2 ^{xxv}	111.13 (11)
Li3 ^{viii} —La1—Li3 ^{ix}	131 (9)	O2 ^{xxiii} —Li2—O2 ^{xix}	111.13 (11)
O1 ^x —Zr1—O1 ^{xi}	88.64 (15)	O2 ^{xxiv} —Li2—O2 ^{xix}	106.2 (2)
O1 ^x —Zr1—O1 ^{viii}	88.64 (15)	O2 ^{xxv} —Li2—O2 ^{xix}	111.13 (11)
O1 ^{xi} —Zr1—O1 ^{viii}	88.64 (15)	O2 ^{xxiii} —Li2—La1 ^{xx}	53.10 (10)
O1 ^x —Zr1—O2 ^{iv}	173.91 (17)	O2 ^{xxiv} —Li2—La1 ^{xx}	126.90 (10)
O1 ^{xi} —Zr1—O2 ^{iv}	96.82 (14)	O2 ^{xxv} —Li2—La1 ^{xx}	53.10 (10)
O1 ^{viii} —Zr1—O2 ^{iv}	94.15 (14)	O2 ^{xix} —Li2—La1 ^{xx}	126.90 (10)
O1 ^x —Zr1—O2 ^{xii}	96.82 (14)	O2 ^{xxiii} —Li2—La1 ^{xxvi}	126.90 (10)
O1 ^{xi} —Zr1—O2 ^{xii}	94.15 (14)	O2 ^{xxiv} —Li2—La1 ^{xxvi}	53.10 (10)
O1 ^{viii} —Zr1—O2 ^{xii}	173.91 (17)	O2 ^{xxv} —Li2—La1 ^{xxvi}	126.90 (10)
O2 ^{iv} —Zr1—O2 ^{xii}	80.15 (16)	O2 ^{xix} —Li2—La1 ^{xxvi}	53.10 (10)
O1 ^x —Zr1—O2 ^{vi}	94.15 (14)	La1 ^{xx} —Li2—La1 ^{xxvi}	180
O1 ^{xi} —Zr1—O2 ^{vi}	173.91 (17)	O2 ^{xxiii} —Li2—Li3 ^{xxvii}	169 (4)
O1 ^{viii} —Zr1—O2 ^{vi}	96.82 (14)	O2 ^{xxiv} —Li2—Li3 ^{xxvii}	76 (4)
O2 ^{iv} —Zr1—O2 ^{vi}	80.15 (16)	O2 ^{xxv} —Li2—Li3 ^{xxvii}	78 (4)
O2 ^{xii} —Zr1—O2 ^{vi}	80.15 (16)	O2 ^{xix} —Li2—Li3 ^{xxvii}	58 (4)
O1 ^x —Zr1—Li3 ^{xiii}	89 (4)	La1 ^{xx} —Li2—Li3 ^{xxvii}	130 (4)
O1 ^{xi} —Zr1—Li3 ^{xiii}	3 (4)	La1 ^{xxvi} —Li2—Li3 ^{xxvii}	50 (4)
O1 ^{viii} —Zr1—Li3 ^{xiii}	92 (4)	O2 ^{xxiii} —Li2—Li3 ^{xxviii}	58 (4)
O2 ^{iv} —Zr1—Li3 ^{xiii}	96 (4)	O2 ^{xxiv} —Li2—Li3 ^{xxviii}	169 (4)

O2 ^{xii} —Zr1—Li3 ^{xiii}	91 (4)	O2 ^{xxv} —Li2—Li3 ^{xxviii}	76 (4)
O2 ^{vi} —Zr1—Li3 ^{xiii}	171 (4)	O2 ^{xix} —Li2—Li3 ^{xxviii}	78 (4)
O1 ^x —Zr1—Li3 ^{xiv}	3 (4)	La1 ^{xx} —Li2—Li3 ^{xxviii}	50 (4)
O1 ^{xi} —Zr1—Li3 ^{xiv}	92 (4)	La1 ^{xxvi} —Li2—Li3 ^{xxviii}	130 (4)
O1 ^{viii} —Zr1—Li3 ^{xiv}	89 (4)	Li3 ^{xxvii} —Li2—Li3 ^{xxviii}	115 (4)
O2 ^{iv} —Zr1—Li3 ^{xiv}	171 (4)	O2 ^{xxiii} —Li2—Li3 ^{xxix}	76 (4)
O2 ^{xii} —Zr1—Li3 ^{xiv}	96 (4)	O2 ^{xxiv} —Li2—Li3 ^{xxix}	78 (4)
O2 ^{vi} —Zr1—Li3 ^{xiv}	91 (4)	O2 ^{xxv} —Li2—Li3 ^{xxix}	58 (4)
Li3 ^{xiii} —Zr1—Li3 ^{xiv}	92 (6)	O2 ^{xix} —Li2—Li3 ^{xxix}	169 (4)
O1 ^x —Zr1—Li3 ^{vii}	92 (4)	La1 ^{xx} —Li2—Li3 ^{xxix}	50 (4)
O1 ^{xi} —Zr1—Li3 ^{vii}	89 (4)	La1 ^{xxvi} —Li2—Li3 ^{xxix}	130 (4)
O1 ^{viii} —Zr1—Li3 ^{vii}	3 (4)	Li3 ^{xxvii} —Li2—Li3 ^{xxix}	115 (4)
O2 ^{iv} —Zr1—Li3 ^{vii}	91 (4)	Li3 ^{xxviii} —Li2—Li3 ^{xxix}	99 (7)
O2 ^{xii} —Zr1—Li3 ^{vii}	171 (4)	O2 ^{xxiii} —Li2—Li3 ^{xxx}	78 (4)
O2 ^{vi} —Zr1—Li3 ^{vii}	96 (4)	O2 ^{xxiv} —Li2—Li3 ^{xxx}	58 (4)
Li3 ^{xiii} —Zr1—Li3 ^{vii}	92 (6)	O2 ^{xxv} —Li2—Li3 ^{xxx}	169 (4)
Li3 ^{xiv} —Zr1—Li3 ^{vii}	92 (6)	O2 ^{xix} —Li2—Li3 ^{xxx}	76 (4)
O1 ^x —Zr1—La1 ^{xi}	94.85 (10)	La1 ^{xx} —Li2—Li3 ^{xxx}	130 (4)
O1 ^{xi} —Zr1—La1 ^{xi}	44.88 (10)	La1 ^{xxvi} —Li2—Li3 ^{xxx}	50 (4)
O1 ^{viii} —Zr1—La1 ^{xi}	44.58 (10)	Li3 ^{xxvii} —Li2—Li3 ^{xxx}	99 (7)
O2 ^{iv} —Zr1—La1 ^{xi}	90.93 (10)	Li3 ^{xxviii} —Li2—Li3 ^{xxx}	115 (4)
O2 ^{xii} —Zr1—La1 ^{xi}	136.97 (10)	Li3 ^{xxix} —Li2—Li3 ^{xxx}	115 (4)
O2 ^{vi} —Zr1—La1 ^{xi}	139.95 (10)	O1 ^{xviii} —Li3—Ga1 ^{xvi}	113 (10)
Li3 ^{xiii} —Zr1—La1 ^{xi}	48 (4)	O1 ^{xviii} —Li3—Li1 ^{xvi}	113 (10)
Li3 ^{xiv} —Zr1—La1 ^{xi}	97 (4)	Ga1 ^{xvi} —Li3—Li1 ^{xvi}	0
Li3 ^{vii} —Zr1—La1 ^{xi}	45 (4)	O1 ^{xviii} —Li3—Li3 ^{vi}	106 (10)
O1 ^x —Zr1—La1 ^{xv}	44.58 (10)	Ga1 ^{xvi} —Li3—Li3 ^{vi}	47 (8)
O1 ^{xi} —Zr1—La1 ^{xv}	94.85 (10)	Li1 ^{xvi} —Li3—Li3 ^{vi}	47 (8)
O1 ^{viii} —Zr1—La1 ^{xv}	44.88 (10)	O1 ^{xviii} —Li3—O1 ^{ix}	122 (10)
O2 ^{iv} —Zr1—La1 ^{xv}	136.97 (10)	Ga1 ^{xvi} —Li3—O1 ^{ix}	56 (7)
O2 ^{xii} —Zr1—La1 ^{xv}	139.95 (10)	Li1 ^{xvi} —Li3—O1 ^{ix}	56 (7)
O2 ^{vi} —Zr1—La1 ^{xv}	90.93 (10)	Li3 ^{vi} —Li3—O1 ^{ix}	20 (7)
Li3 ^{xiii} —Zr1—La1 ^{xv}	97 (4)	O1 ^{xviii} —Li3—La1 ^{xxxi}	81 (10)
Li3 ^{xiv} —Zr1—La1 ^{xv}	45 (4)	Ga1 ^{xvi} —Li3—La1 ^{xxxi}	113 (10)
Li3 ^{vii} —Zr1—La1 ^{xv}	48 (4)	Li1 ^{xvi} —Li3—La1 ^{xxxi}	113 (10)
La1 ^{xi} —Zr1—La1 ^{xv}	69.360 (12)	Li3 ^{vi} —Li3—La1 ^{xxxi}	66 (5)
O1 ^x —Zr1—La1 ^x	44.88 (10)	O1 ^{ix} —Li3—La1 ^{xxxi}	62 (5)
O1 ^{xi} —Zr1—La1 ^x	44.58 (10)	O1 ^{xviii} —Li3—Li3 ^{xviii}	89 (10)
O1 ^{viii} —Zr1—La1 ^x	94.85 (10)	Ga1 ^{xvi} —Li3—Li3 ^{xviii}	29 (5)
O2 ^{iv} —Zr1—La1 ^x	139.95 (10)	Li1 ^{xvi} —Li3—Li3 ^{xviii}	29 (5)
O2 ^{xii} —Zr1—La1 ^x	90.93 (10)	Li3 ^{vi} —Li3—Li3 ^{xviii}	67 (5)
O2 ^{vi} —Zr1—La1 ^x	136.97 (10)	O1 ^{ix} —Li3—Li3 ^{xviii}	81 (5)
Li3 ^{xiii} —Zr1—La1 ^x	45 (4)	La1 ^{xxxi} —Li3—Li3 ^{xviii}	127 (9)
Li3 ^{xiv} —Zr1—La1 ^x	48 (4)	O1 ^{xviii} —Li3—Li3 ^{ix}	135 (10)
Li3 ^{vii} —Zr1—La1 ^x	97 (4)	Ga1 ^{xvi} —Li3—Li3 ^{ix}	29 (5)
La1 ^{xi} —Zr1—La1 ^x	69.360 (12)	Li1 ^{xvi} —Li3—Li3 ^{ix}	29 (5)
La1 ^{xv} —Zr1—La1 ^x	69.360 (12)	Li3 ^{vi} —Li3—Li3 ^{ix}	67 (5)
Li3 ^{ix} —O1—Ga1 ^{xvi}	43 (10)	O1 ^{ix} —Li3—Li3 ^{ix}	66 (5)

Li3 ^{ix} —O1—Li1 ^{xvi}	43 (10)	La1 ^{xxx} —Li3—Li3 ^{ix}	127 (9)
Gal ^{xvi} —O1—Li1 ^{xvii}	0	Li3 ^{xviii} —Li3—Li3 ^{ix}	46 (10)
Li3 ^{ix} —O1—Zr1 ^{xvii}	170 (10)	O1 ^{xviii} —Li3—La1 ^{xviii}	71 (10)
Gal ^{xvi} —O1—Zr1 ^{xvii}	127.29 (18)	Gal ^{xvi} —Li3—La1 ^{xviii}	145 (10)
Li1 ^{xvi} —O1—Zr1 ^{xvii}	127.29 (18)	Li1 ^{xvi} —Li3—La1 ^{xviii}	145 (10)
Li3 ^{ix} —O1—Li3 ^{xviii}	54 (10)	Li3 ^{vi} —Li3—La1 ^{xviii}	168 (4)
Gal ^{xvi} —O1—Li3 ^{xviii}	38 (5)	O1 ^{ix} —Li3—La1 ^{xviii}	153 (9)
Li1 ^{xvi} —O1—Li3 ^{xviii}	38 (5)	La1 ^{xxx} —Li3—La1 ^{xviii}	102 (7)
Zr1 ^{xvii} —O1—Li3 ^{xviii}	117 (5)	Li3 ^{xviii} —Li3—La1 ^{xviii}	124 (10)
Li3 ^{ix} —O1—La1 ^{xvi}	79 (10)	Li3 ^{ix} —Li3—La1 ^{xviii}	124 (10)
Gal ^{xvi} —O1—La1 ^{xvi}	95.85 (13)	O1 ^{xviii} —Li3—Zr1 ^{xxxii}	7 (10)
Li1 ^{xvi} —O1—La1 ^{xvi}	95.85 (13)	Gal ^{xvi} —Li3—Zr1 ^{xxxii}	106 (10)
Zr1 ^{xvii} —O1—La1 ^{xvi}	100.89 (14)	Li1 ^{xvi} —Li3—Zr1 ^{xxxii}	106 (10)
Li3 ^{xviii} —O1—La1 ^{xvi}	61 (5)	Li3 ^{vi} —Li3—Zr1 ^{xxxii}	99 (10)
Li3 ^{ix} —O1—La1	89 (10)	O1 ^{ix} —Li3—Zr1 ^{xxxii}	116 (8)
Gal ^{xvi} —O1—La1	122.52 (15)	La1 ^{xxx} —Li3—Zr1 ^{xxxii}	81 (5)
Li1 ^{xvi} —O1—La1	122.52 (15)	Li3 ^{xviii} —Li3—Zr1 ^{xxxii}	84 (8)
Zr1 ^{xvii} —O1—La1	100.55 (13)	Li3 ^{ix} —Li3—Zr1 ^{xxxii}	129 (10)
Li3 ^{xviii} —O1—La1	142 (5)	La1 ^{xviii} —Li3—Zr1 ^{xxxii}	78 (5)
La1 ^{xvi} —O1—La1	105.20 (13)	O1 ^{xviii} —Li3—Li2 ^{xxxiii}	133 (10)
Li2 ^{xix} —O2—Zr1 ^{vi}	126.18 (19)	Gal ^{xvi} —Li3—Li2 ^{xxxiii}	113 (10)
Li2 ^{xix} —O2—La1 ^{vi}	88.28 (13)	Li1 ^{xvi} —Li3—Li2 ^{xxxiii}	113 (10)
Zr1 ^{vi} —O2—La1 ^{vi}	106.46 (15)	Li3 ^{vi} —Li3—Li2 ^{xxxiii}	113 (10)
Li2 ^{xix} —O2—La1 ^{xvi}	123.00 (16)	O1 ^{ix} —Li3—Li2 ^{xxxiii}	93 (6)
Zr1 ^{vi} —O2—La1 ^{xvi}	104.36 (15)	La1 ^{xxx} —Li3—Li2 ^{xxxiii}	90 (6)
La1 ^{vi} —O2—La1 ^{xvi}	102.25 (13)	Li3 ^{xviii} —Li3—Li2 ^{xxxiii}	131 (10)
Li3 ⁱⁱⁱ —Li1—Li3 ⁱⁱ	122 (10)	Li3 ^{ix} —Li3—Li2 ^{xxxiii}	87 (8)
Li3 ⁱⁱⁱ —Li1—Li3 ^{iv}	86 (10)	La1 ^{xviii} —Li3—Li2 ^{xxxiii}	65 (4)
Li3 ⁱⁱ —Li1—Li3 ^{iv}	122 (10)	Zr1 ^{xxxii} —Li3—Li2 ^{xxxiii}	140 (7)
Li3 ⁱⁱⁱ —Li1—Li3 ⁱ	122 (10)		

Symmetry codes: (i) $-z+3/4, -y+1/4, x+1/4$; (ii) $-z+3/4, y-1/4, -x+1/4$; (iii) z, x, y ; (iv) $z, -x, -y+1/2$; (v) $x, -y, -z+1/2$; (vi) $-x, -y+1/2, z$; (vii) $-x, y-1/2, -z+1/2$; (viii) $y-1/4, x-1/4, z-1/4$; (ix) $y-1/4, -x+1/4, -z+3/4$; (x) $x-1/4, z-1/4, y-1/4$; (xi) $z-1/4, y-1/4, x-1/4$; (xii) $-y+1/2, z, -x$; (xiii) $-z+1/2, -x, y-1/2$; (xiv) $y-1/2, -z+1/2, -x$; (xv) $-y-1/4, x-1/4, -z+1/4$; (xvi) y, z, x ; (xvii) $y+1/4, x+1/4, z+1/4$; (xviii) $-y+1/4, x+1/4, -z+3/4$; (xix) $-x+1, -y+1/2, z$; (xx) $-x+3/4, z-1/4, -y+1/4$; (xxi) $-x+1/2, -y, z+1/2$; (xxii) $y+1/4, -x-1/4, -z+1/4$; (xxiii) $x+3/4, z-1/4, y-1/4$; (xxiv) $-x+1, y-1/2, -z+1/2$; (xxv) $x+3/4, -z+1/4, -y+3/4$; (xxvi) $x+1, y, z$; (xxvii) $y+3/4, -x+1/4, -z+3/4$; (xxviii) $-y+1, -z+1/2, x$; (xxix) $-y+1, z-1/2, -x+1/2$; (xxx) $y+3/4, x-1/4, z-1/4$; (xxxi) $z-1/4, -y+1/4, -x+3/4$; (xxxii) $-x, y+1/2, -z+1/2$; (xxxiii) $-y+1/4, x-3/4, -z+3/4$.