Electronic stabilization by occupational disorder in the ternary bismuthide $Li_{3-x-y}In_xBi$ ($x \simeq 0.14$, $y \simeq 0.28$)

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Abstract

A ternary derivative of Li_3Bi with the composition $Li_{3-x-y}In_xBi$ ($x \simeq 0.14$, $y \simeq 0.28$) was produced by a mixed In+Bi flux approach. The crystal structure adopts space group $Fd\bar{3}m$ (No. 227) with a = 13.337 (4) Å and can be viewed as a 2×2×2 superstructure of the parent Li_3Bi phase, resulting from a partial ordering of Li and In in the tetrahedral voids of the Bi *fcc* packing. In addition to the Li/In substitutional disorder, partial occupation of some Li sites is observed. The Li deficiency develops to reduce the total electron count in the system, counteracting thereby the electron doping introduced by the In substitution. First-principle calculations confirm the electronic rationale of the observed disorder.

1. Introduction

Among the methods used for single crystal growth of intermetallic compounds, the so-called flux growth approach has gained notable recognition owing to its simplicity and adaptability (Kanatzidis *et al.*, 2005; Phelan *et al.*, 2012; Latturner, 2018; Wang *et al.*, 2020). Typically utilized fluxes encompass low-melting metals, such as Zn, Cd, Al, Ga, In, Sn, Pb, and Bi (Hu *et al.*, 2007; White *et al.*, 2015; Janka *et al.*, 2014; He *et al.*, 2012; Verchenko *et al.*, 2012; Childs *et al.*, 2019; Baranets & Bobev, 2019; Ovchinnikov, Darone *et al.*, 2018; Baranets, Darone *et al.*, 2019; Baranets, Voss *et al.*, 2019; Ovchinnikov & Bobev, 2019*a*; Motoyama *et al.*, 2018). In some cases, liquid alloys, in particular eutectic mixtures, or congruently melting compounds are utilized (Stojanovic & Latturner, 2007; Tucker *et al.*, 2012; Verchenko *et al.*, 2019; Rhodehouse *et al.*, 2018). When the elements employed as a flux constitute the structure of the targeted crystals, the term "self-flux" is commonly used. The advantage of the self-flux approach is that it allows growth of materials without contamination by foreign elements (Ye *et al.*, 1996; Ovchinnikov, Makongo *et al.*, 2018; Ovchinnikov & Bobev, 2020). Availability of large single crystals enables accurate measurements of intrinsic electronic, magnetic, and thermal properties and their anisotropy depending on the crystallographic direction.

Recently, we started employing metal fluxes for production of Li-containing intermetallic compounds, targeting materials with potentially interesting electrochemical properties (Ovchinnikov & Bobev, 2019*b*,*c*). Due to the high chemical reactivity and volatility of Li, such flux reactions require special care, e.g., slow heating rates and moderate annealing temperatures, in order to avoid Li losses due to side reactions with the reactor materials. Many of the compounds produced in the course of those synthetic attempts can be described as charge-balanced compositions and fall in the broad class of Zintl phases. Chemical bonding and stability of such materials can be rationalized utilizing a simple electron counting scheme (Nesper, 2014; Ovchinnikov & Bobev, 2019*d*).

In this contribution, we present synthesis, structural and *ab-initio* characterization of the ternary phase $Li_{3-x-y}In_xBi$ ($x \simeq 0.14$, $y \simeq 0.29$), grown from a mixed In+Bi flux. In contrast to $Ca_{11}In_xBi_{10-x}$, prepared by a similar method (Ovchinnikov & Bobev, 2018), $Li_{3-x-y}In_xBi$ does not exhibit any appreciable In/Bi mixing in the crystallographic sites. The In species substitute for Li instead, resulting in an increase of the total electron number, compensated by simultaneous vacancy formation in the Li substructure.

2. Experimental

2.1. Synthesis and crystallization

All weighning and mixing steps were perfomed in an argon-filled glovebox with controlled atmosphere. Single crystals of $Li_{3-x-y}In_xBi$ ($x \simeq 0.14$, $y \simeq 0.28$) with linear dimensions up to about 0.5 mm were grown employing a mixed In+Bi flux method. For this purpose, a mixture of Li, Bi, and In (Alfa, all with purity at least 99.9 wt. %) were mixed with the molar ratio 1:1:3, respectively, and loaded in a 2 ml alumina crucible topped with a piece of quartz wool. The crucible was sealed in an evacuated fused silica tube and heated up to 1073 K with a rate of 100 K/h, kept at this temperature for 12 h, and cooled down to 773 K with a rate of 5 K/h. At this point, the reaction tube was taken out from the furnace, inverted, and subjected to centrifugation. After opening the tube in the glovebox, black single crystals were found in the crucible and on the quartz wool. When left in the ambient atmosphere, the crystals deteriorate within hours. Powder X-ray diffraction measurements (PXRD) were conducted on a Rigaku Miniflex diffractometer (Cu Kα radiation, $\lambda = 1.5418$ Å) operating inside a nitrogen-filled glovebox to prevent degradation of the sample. Data were collected in a Θ–Θ scan mode within the 2Θ range 10–70° with a step size of 0.05° and 2 s/step acquisition time.

2.2. Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 1. A single crystal was selected under dry Parathone-N oil and cut to suitable dimensions with a scalpel. The crystal was mounted on a low-background plastic loop and immediately transferred onto a Bruker SMART CCD diffractometer equipped with monochromated Mo Kα radiation ($\lambda = 0.71073$ Å), where it was cooled down to 200 K in a nitrogen stream. The collected raw data were integrated using the *SAINT* software (Bruker, 2014). Semiempirical absorption correction was carried out with *SADABS* (Bruker, 2014). The crystal structure was solved by dual-space methods with *SHELXT* (Sheldrick, 2015*a*) and refined by full-matrix least squares methods on F^2 with *SHELXL* (Sheldrick, 2015*b*). Atomic coordinates were standardized using *STRUCTURE TIDY* (Gelato & Parthé, 1987).

3. Results and discussion

The powder X-ray diffraction pattern (PXRD) recorded from several ground single crystals is given in Fig. 1. Indexing of the most intense reflections readily yielded a face-centered cubic unit cell with $a \simeq 6.68$ Å. This lattice parameter is close to that of the binary Li bismuthide Li_3Bi, crystallizing in the *anti*-BiF_3 structure type (sometimes also called the Li_3Bi type, space group $Fm\overline{3}m$, Pearson code *cF*16, Ferro & Saccone, 2008). The relative intensities of the peaks were also consistent with the Li_3Bi model. However, a number of reflections could not be indexed with that unit cell or ascribed to any potential impurity phases. In fact, to assign integer *hkl* indices to all the observed reflections, a doubling of the unit cell parameter was necessary, suggesting that the studied compound may crystallize in a superstructure of Li_3Bi, which was confirmed by the subsequent X-ray diffraction measurement on a selected single crystal.

Single-crystal X-ray diffraction study (SCXRD) revealed a face-centered cubic unit cell with the lattice parameter $a = 13.337$ (4) Å (at $T = 200$ K). Analysis of the systematic extinctions suggested two possible space groups – $Fd\overline{3}$ (No. 203) and $Fd\overline{3}m$ (No. 227). Both options were tested and yielded indistinguishable structures. Therefore, the higher symmetry space group $Fd\overline{3}m$ was retained. At the structure solution step, the positions of the heavy atoms In and Bi were located. Four symmetry unique Li atoms were found by difference Fourier mapping.

The initial refinement produced a sizeable difference electron density hole in the position of the In atom. This issue can be resolved by treating the affected site as either underoccupied or mixed-occupied with a lighter element – Li in this case. It is worthwhile to note that the two models of disorder result in close In/Bi ratios and thus could not be distinguished by, e.g., energy-dispersive X-ray spectroscopy (EDX), conventionally employed for semi-quantitative determination of heavy elements. Nevertheless, we will demonstrate below using first-principle calculations that the model with mixed occupation is likely correct, due to electronic reasons. Mutual substitutions between Li and some p-elements, such as Ga, In, and Sn, have been frequently observed in other intermetallic compounds, including bismuthides (Fedorchuk *et al.*, 2011; Smetana *et al.*, 2010; Ovchinnikov & Bobev, 2019*b*; You & Bobev, 2010; Ovchinnikov & Bobev, 2019*c*; Sreeraj *et al.*, 2005; Ojwang & Bobev, 2018). The overall occupation factor for the discussed site was set to 1, resulting in the refined In/Li ratio of 0.577 (8)/0.423, respectively. For the sake of brevity, in the following discussion, this position will be referred to as In.

Two of the four symmetry unique Li sites (Li3 and Li4) also displayed considerable negative residual electron densities and unphysically large displacement parameters. Because of that, they were refined as partially occupied. At the final stage of the refinement, the Li1, Li2, In, and Bi atoms were refined anisotropically. To avoid correlations with the occupation factors, the isotropic displacement parameters of the deficient Li3 and Li4 sites were kept equal to the equivalent isotropic displacement parameter (U_{eq}) of the fully occupied Li2 position (since U_{eq} for another fully occupied Li site, Li1, was equal to that of Li2 within one standard uncertainty, the choice of the reference Li atom does not affect the results). The occupancies of both Li3 and Li4 refined to about 0.6.

The studied material with the refined composition $Li_{3-x-y}In_xBi$ ($x = 0.14$ (1), $y = 0.29$ (8)) is a Li-deficient substitutional derivative of the binary Li_3Bi phase, with a partial ordering of In and Li in the structure (Fig. 2). The Bi atoms form an almost perfect *fcc* packing with the octahedral voids occupied by Li atoms (Li2 and Li3). The tetrahedral voids accommodate In (≡ 0.577 (8)In+0.423Li) and Li (Li1 and Li4) in an alternating manner (Fig. 2a). To better visualize the arrangement of the In and Li atoms, it is convenient to break down the structure into separate building blocks.

The In and Li4 positions (Wyckoff sites 8*a* and 8*b*, respectively) are located in the vertices of two diamond-like frameworks. The Li3 atoms are situated in the midpoints of the lines connecting the adjacent nods of the former framework, while the Li2 species occupy the corresponding positions in the latter framework. In this representation, two interpenetrating *β*-cristobalite-type substructures arise – $In(Li3)_2$ and $(Li4)(Li2)_2$, which are in turn embedded in a three-dimensional $(Li1)_6Bi_4$ framework with an *anti*-Ag_2O_3-type structure (Fig. 2b).

The Li–Bi distances in the $(Li1)Bi_4$ tetrahedra measure 2×2.87 (1) Å and 2×2.92 (1) Å, whereas they are shorter in the $(Li4)Bi_4$ tetrahedra with the partially occupied Li4 site (4×2.7740 (6) Å), in accordance with the smaller effective atomic volume for the latter crystallographic position. The opposite trend is observed for the octahedrally coordinated Li positions, with $d_{Li–Bi} = 3.270$ (1) Å around the fully occupied Li2 and $d_{Li–Bi} = 3.4013$ (3) Å around the deficient Li3 site. In this case, owing to the larger volume of the octahedral voids, the atomic size factor is less important. Due to a higher bonding ionicity in the case of octahedral coordination, partial removal of Li reduces on average the electrostatic attraction between the centers of the octahedra and the anionic Bi species, resulting in the observed expansion of the o-ctahedra. Another reasoning could be the relatively short interatomic Li–In distances around Li1 ($d_{Li1–In} = 3.23$ (2) Å) and Li3 ($d_{Li1–In} = 2.8877$ (3) Å), similar to the bonding contacts in Li indides (Sun *et al.*, 2005; Chumak *et al.*, 2014). This suggests possible Li–In bonding interactions, which would result in higher effective coordination numbers of these two Li sites and hence longer distances to the surrounding atoms. Despite the discussed small differences, all Li–Bi inter-atomic separations in $Li_{3-x-y}In_xBi$ ($x \simeq 0.14$, $y \simeq 0.29$) are in good correspondence with the values reported for tetra-hedrally and octahedrally coordinated sites in other Li bismuthides (Pan *et al.*, 2006; Schäfer *et al.*, 2014; Ojwang & Bobev, 2018). The symmetry unique In–Bi contact around the mixed-occupied In site (≡ 0.577 (8)In+0.423Li) is 3.0013 (6) Å long, which is comparable to the Li–Bi distances in the $LiBi_4$ tetrahedra described above and is in good agreement with the literature data on the compounds with tetrahedral Bi environment of In atoms (Bobev & Sevov, 2002;

Sun *et al.*, 2006).

The crystal structure of $Li_{3-x-y}In_xBi$ (x = 0.14 (1), y = 0.29 (8)) is formally isopointal to that of $Li_{13}In_3$ (Stöhr *et al.*, 1978). However, the bonding interactions in the two materials are clearly distinct. In the idealized case of full electron transfer to the atoms of the most electronegative element, the latter phase can be considered an electron-short solid according to the notation $(Li^+)_{13}(In^{5-})_3(h^+)_2$, where *h* denotes an electron hole, whereas the former composition is essentially electron-balanced and can be classified as a Zintl phase: $(Li^+)_{2.57\,(8)}(In^{3+})_{0.14\,(1)}(Bi^{3-})(e^-)_{0.01\,(6)}$. From this description, it is evident that the observed Li deficiency is required to compensate for the increased electron number upon In substitution for Li. The refined charge-neutral composition corroborates the treatment of the In site as mixed-occupied with Li, rather as underoccupied, since in the latter case, the composition would be too Li-deficient, resulting in electron shortage of about 0.1 e^- per formula unit.

In order to examine the electronic structure of $Li_{3-x-y}In_xBi$, we conducted first-principle calculations on an idealized model with the composition $Li_{11}InBi_4$, where all deficient Li sites were treated as fully occupied, and the mixed In/Li position was considered to be pure In. The calculations were performed with the TB-LMTO-ASA code (Jepsen & Andersen, 2000), using the von Barth-Hedin implementation of the LDA exchange-correlation functional (Barth & Hedin, 1972) and a 16×16×16 *k*-point grid. Due to the close-packed character of the structure, introduction of empty spheres was not required. The electronic density of states is shown in Fig. 3a. In accordance with the formal notion $(Li^+)_{11}(In^{3+})(Bi^{3-})_4(e^-)_2$, the Fermi level ($E_F$) crosses a region of finite DOS, situated above a pseudogap. Within the rigid band approximation, the pseudogap would shift to E_F upon removal of 2 e^- per formula unit with respect to the idealized formula $Li_{11}InBi_4$. Such an electron-poorer situation would correspond, in particular, to the experimentally determined composition, as detailed in the formal electron accounting above. Chemical bonding in $Li_{11}InBi_4$ was investigated utilizing Crystal Orbital Hamilton Population analysis (COHP, Steinberg & Dronskowski, 2018). The Li–Bi contacts in the $LiBi_4$ tetrahedra were found to display bonding interactions below E_F (Fig. 3b). For the $LiBi_6$ octahedra, the Fermi level crosses a domain of antibonding character (Fig. 3b), whereas removal of two electrons per formula unit would place E_F at the top of the bonding states. However, shifting of the Fermi level would not change the magnitude of the interactions considerably, as for both $Li_{11}InBi_4$ and the electron-poorer composition, negative integrated COHP values remain around 0.4 and 0.2 eV/bond for the tetrahedra and octahedra, respectively. The lower value for the octahedral coordination is related to higher ionicity of bonding and hence reduced covalency (Ovchinnikov *et al.*, 2018). The situation is different for the In–Bi interaction (Fig. 3c), which appears to be drastically underoptimized due to the electron excess in $Li_{11}InBi_4$, with the Fermi level crossing a sizeable peak of antibonding character above the pseudogap. The corresponding –ICOHP value measures 1.1 eV/bond at E_F. Recuperation to the optimal electron count would eliminate electrons from the antibonding states and increase the –ICOHP number up to 1.7 eV/bond. Finally, the Li–In interactions (Fig. 3d) demonstrate a weakly bonding nature, similar to the Li–Bi contacts in terms of the –ICOHP magnitude. The occupied states above the pseudogap are antibonding, leading to slight underoptimization at E_F in $Li_{11}InBi_4$, whereas for the electron-poorer composition, the Li–In bonding would be essentially fully optimized.

In conclusion, it is evident that the charge-balanced composition, realized in $Li_{3-x-y}In_xBi$ ($x \simeq 0.14$, $y \simeq 0.29$) is pivotal for stabilization of the chemical bonding, especially for the strong covalent In–Bi interactions. Thus, the results of the first-principle calculations corroborate the simple rationale based on the electron accounting given above. Due to the presence of cationic vacancies in the structure, the new ternary phase $Li_{3-x-y}In_xBi$ may display some Li-ion mobility, which makes it interesting for future electrochemical studies.

Table 1

Experimental details

Crystal data	
Chemical formula	$BiIn_{0.14}Li_{2.56}$
M_r	243.34
Crystal system, space group	Cubic, $Fd\bar{3}m$
Temperature (K)	200
a (Å)	13.337 (4)
V (Å^3)	2373 (2)
Z	32
Radiation type	Mo $K\alpha$
μ (mm^{-1})	60.18
Crystal size (mm)	0.11 × 0.08 × 0.05
Data collection	
Diffractometer	CCD area detector
Absorption correction	Multi-scan
T_{min}, T_{max}	0.01, 0.06
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	2306, 177, 144
R_{int}	0.047
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.674
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.024, 0.053, 1.06
No. of reflections	177
No. of parameters	14
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.23, −0.76

Computer programs: Bruker *SMART* (Bruker, 2014), Bruker *SAINT* (Bruker, 2014), SHELXT (Sheldrick, 2015a), *SHELXL2014*/7 (Sheldrick, 2015b), *DIAMOND* (Brandenburg, 2014), *publCIF* (Westrip, 2010).

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Figure 1

Figure 1. Experimental (black) and calculated (red) PXRD patterns of ground $Li_{3-x-y}In_xBi$ crystals ($x \simeq 0.14$, $y \simeq 0.29$). Dashed lines indicate positions of the Bragg peaks in the *anti*-BiF_3-type subcell. Some intense superstructure reflections are marked with diamonds.

Figure 2

Figure 2. (a) Crystal structure of $Li_{3-x-y}In_xBi$ ($x \simeq 0.14$, $y \simeq 0.29$). Li, In, and Bi atoms are shown in orange, cyan, and blue, respectively. Li- and In-centered Bi tetrahedra are shown in green and blue, respectively. (b) Interpenetrating β-cristobalite-type $In(Li3)_2$ (blue) and $(Li4)(Li2)_2$ (red) frameworks embedded in an *anti*-Ag_2O_3-type $(Li1)_6Bi_4$ substructure (green tetrahedra). The unit cell is outlined in gray.

Figure 3

Figure 3. (a) Total and projected electronic densities of states (DOS) for the idealized $Li_{11}InBi_4$ model. (b-d) Crystal Orbital Hamilton Population curves (COHP) for selected interactions. Dashed lines denote integrated curves. The positions of the Fermi level for $Li_{11}InBi_4$ and the experimentally determined composition are marked with black dashed and dotted lines, respectively.

supporting information

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Alexander Ovchinnikov* and Svilen Bobev

Computing details

Data collection: Bruker *SMART* (Bruker, 2014); cell refinement: Bruker *SAINT* (Bruker, 2014); data reduction: Bruker *SAINT* (Bruker, 2014); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014*/7 (Sheldrick, 2015b); molecular graphics: *DIAMOND* (Brandenburg, 2014); software used to prepare material for publication: *publCIF* (Westrip, 2010).

(shelx)

Crystal data

$BiIn_{0.14}Li_{2.56}$
$M_r = 243.34$
Cubic, $Fd\bar{3}m$
$a = 13.337$ (4) Å
$V = 2373$ (2) Å^3
$Z = 32$
$F(000) = 3128$
$D_x = 5.450$ Mg m^{-3}

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 230 reflections
$\theta = 5.3$–$26.1°$
$\mu = 60.18$ mm^{-1}
$T = 200$ K
Irregular, black
$0.11 \times 0.08 \times 0.05$ mm

Data collection

CCD area detector diffractometer
Radiation source: sealed tube
phi and ω scans
Absorption correction: multi-scan
$T_{min} = 0.01$, $T_{max} = 0.06$
2306 measured reflections

177 independent reflections
144 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 28.6°$, $\theta_{min} = 2.7°$
$h = -17 \rightarrow 15$
$k = -12 \rightarrow 14$
$l = -17 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.053$
$S = 1.06$
177 reflections
14 parameters

0 restraints
$w = 1/[\sigma^2(F_o^2) + (0.0217P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.23$ e Å^{-3}
$\Delta\rho_{min} = -0.76$ e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Li1	0.3673 (16)	0.1250	0.1250	0.046 (8)	
Li2	0.5000	0.5000	0.5000	0.040 (13)	
Li3	0.0000	0.0000	0.0000	0.040*	0.63 (12)
Li4	0.3750	0.3750	0.3750	0.040*	0.57 (13)
In	0.1250	0.1250	0.1250	0.0207 (12)	0.577 (8)
Li5	0.1250	0.1250	0.1250	0.0207 (12)	0.423 (8)
Bi	0.25492 (2)	0.25492 (2)	0.25492 (2)	0.0222 (2)	

Atomic displacement parameters (Å^2) for (shelx)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Li1	0.021 (13)	0.058 (12)	0.058 (12)	0.000	0.000	−0.020 (13)
Li2	0.040 (13)	0.040 (13)	0.040 (13)	0.011 (14)	0.011 (14)	0.011 (14)
In	0.0207 (12)	0.0207 (12)	0.0207 (12)	0.000	0.000	0.000
Li5	0.0207 (12)	0.0207 (12)	0.0207 (12)	0.000	0.000	0.000
Bi	0.0222 (2)	0.0222 (2)	0.0222 (2)	0.00327 (14)	0.00327 (14)	0.00327 (14)

Geometric parameters (Å, º) for (shelx)

Li1—Li3^{i}	2.830 (12)	Li3—Bi^{i}	3.4013 (3)
Li1—Li3^{ii}	2.830 (12)	Li3—Bi^{xxxii}	3.4013 (3)
Li1—Bi	2.873 (11)	Li3—Bi^{ii}	3.4013 (3)
Li1—Bi^{iii}	2.873 (11)	Li3—Li3^{iii}	4.7155
Li1—Bi^{iv}	2.915 (13)	Li3—Li3^{xxxvii}	4.7155
Li1—Bi^{v}	2.915 (13)	Li3—Li3^{xxxviii}	4.7155 (7)
Li1—Li2^{vi}	2.948 (13)	Li3—Li3^{i}	4.7155 (7)
Li1—Li2^{vii}	2.948 (13)	Li4—Bi^{vi}	2.7740 (6)
Li1—In	3.23 (2)	Li4—Bi^{xxv}	2.7740 (6)
Li1—Li1^{viii}	3.3375 (13)	Li4—Bi^{xxvii}	2.7740 (6)
Li1—Li1^{ix}	3.3375 (13)	Li4—Bi	2.7740 (6)
Li1—Li1^{x}	3.3375 (13)	Li4—Li2^{vi}	2.8877 (3)
Li1—Li1^{xi}	3.3375 (13)	Li4—Li2^{xxv}	2.8877 (3)
Li1—Li4^{xii}	3.44 (2)	Li4—Li2^{xxvii}	2.8877 (3)
Li1—Li1^{xiii}	4.57 (3)	Li4—Li1^{xii}	3.44 (2)
Li1—Li1^{xiv}	4.57 (3)	Li4—Li1^{xxxix}	3.44 (2)
Li1—Li1^{xv}	4.57 (3)	Li4—Li1^{viii}	3.44 (2)
Li1—Li1^{xvi}	4.57 (3)	Li4—Li1^{xviii}	3.44 (2)
Li1—Li4	4.7166 (5)	Li4—Li1^{xxi}	3.44 (2)
Li2—Li4^{xvii}	2.8877 (3)	Li4—Li1^{x}	3.44 (2)
Li2—Li4	2.8877 (3)	Li4—Li1^{xvi}	4.7166 (9)
Li2—Li1^{xviii}	2.948 (13)	Li4—Li1^{xix}	4.7166 (5)
Li2—Li1^{xix}	2.948 (13)	Li4—Li1^{xv}	4.7166 (9)
Li2—Li1^{xii}	2.948 (13)	Li4—Li1^{xx}	4.7166 (9)
Li2—Li1^{xx}	2.948 (13)	Li4—Li1^{xxii}	4.7166 (9)
Li2—Li1^{xxi}	2.948 (13)	In—Li3^{iii}	2.8877 (3)
Li2—Li1^{xxii}	2.948 (13)	In—Li3^{i}	2.8877 (3)
Li2—Bi^{xxiii}	3.2701 (11)	In—Li3^{ii}	2.8877 (3)
Li2—Bi^{vi}	3.2701 (11)	In—Bi	3.0013 (6)

Li2—Bi^{xxiv}	3.2701 (3)	In—Bi^{iii}	3.0013 (6)
Li2—Bi^{xxv}	3.2701 (3)	In—Bi^{i}	3.0013 (6)
Li2—Bi^{xxvi}	3.2701 (3)	In—Bi^{ii}	3.0013 (6)
Li2—Bi^{xxvii}	3.2701 (3)	In—Li1^{ii}	3.23 (2)
Li2—Li2^{xxviii}	4.7155	In—Li1^{xv}	3.23 (2)
Li2—Li2^{vi}	4.7155	In—Li1^{xiii}	3.23 (2)
Li2—Li2^{xxv}	4.7155 (7)	Bi—Li1^{xv}	2.873 (11)
Li2—Li2^{xxix}	4.7155 (7)	Bi—Li1^{xvi}	2.873 (11)
Li2—Li2^{xxx}	4.7155 (7)	Bi—Li1^{x}	2.915 (13)
Li2—Li2^{xxvii}	4.7155 (7)	Bi—Li1^{xxxix}	2.915 (13)
Li3—Li1^{xxxi}	2.830 (12)	Bi—Li1^{viii}	2.915 (13)
Li3—Li1^{xiv}	2.830 (12)	Bi—Li2^{xxvii}	3.2701 (3)
Li3—Li1^{xxxii}	2.830 (12)	Bi—Li2^{vi}	3.2701 (11)
Li3—Li1^{ii}	2.830 (12)	Bi—Li2^{xxv}	3.2701 (3)
Li3—Li1^{xxxiii}	2.830 (12)	Bi—Li3^{i}	3.4012 (3)
Li3—Li1^{xiii}	2.830 (12)	Bi—Li3^{iii}	3.4012 (11)
Li3—Li5^{xxxiv}	2.8877 (3)	Bi—Li3^{ii}	3.4012 (3)
Li3—In^{xxxiv}	2.8877 (3)	Bi—Bi^{vi}	4.5299 (9)
Li3—In	2.8877 (3)	Bi—Bi^{xxv}	4.5299 (11)
Li3—Bi^{xxxv}	3.4013 (11)	Bi—Bi^{xxvii}	4.5299 (11)
Li3—Bi^{iii}	3.4013 (11)	Bi—Bi^{xl}	4.7173 (1)
Li3—Bi^{xxxvi}	3.4013 (3)	Bi—Bi^{iv}	4.7173 (7)

Li3^{i}—Li1—Li3^{ii}	112.9 (7)	Bi^{ii}—Li3—Li3^{iii}	46.116 (5)
Li3^{i}—Li1—Bi	73.2 (3)	Li1^{xxxi}—Li3—Li3^{xxxvii}	88.5 (3)
Li3^{ii}—Li1—Bi	73.2 (3)	Li1^{xiv}—Li3—Li3^{xxxvii}	91.5 (3)
Li3^{i}—Li1—Bi^{iii}	73.2 (3)	Li1^{xxxii}—Li3—Li3^{xxxvii}	33.6 (4)
Li3^{ii}—Li1—Bi^{iii}	73.2 (3)	Li1^{ii}—Li3—Li3^{xxxvii}	146.4 (4)
Bi—Li1—Bi^{iii}	117.1 (7)	Li1^{xxxiii}—Li3—Li3^{xxxvii}	88.5 (3)
Li3^{i}—Li1—Bi^{iv}	174.5 (7)	Li1^{xiii}—Li3—Li3^{xxxvii}	91.5 (3)
Li3^{ii}—Li1—Bi^{iv}	72.59 (4)	Li5^{xxxiv}—Li3—Li3^{xxxvii}	35.264 (8)
Bi—Li1—Bi^{iv}	109.18 (7)	In^{xxxiv}—Li3—Li3^{xxxvii}	35.264 (8)
Bi^{iii}—Li1—Bi^{iv}	109.18 (7)	In—Li3—Li3^{xxxvii}	144.736 (8)
Li3^{i}—Li1—Bi^{v}	72.59 (4)	Bi^{xxxv}—Li3—Li3^{xxxvii}	91.564 (7)
Li3^{ii}—Li1—Bi^{v}	174.5 (7)	Bi^{iii}—Li3—Li3^{xxxvii}	88.436 (7)
Bi—Li1—Bi^{v}	109.18 (7)	Bi^{xxxvi}—Li3—Li3^{xxxvii}	46.116 (5)
Bi^{iii}—Li1—Bi^{v}	109.18 (7)	Bi^{i}—Li3—Li3^{xxxvii}	133.884 (5)
Bi^{iv}—Li1—Bi^{v}	102.0 (6)	Bi^{xxxii}—Li3—Li3^{xxxvii}	46.116 (5)
Li3^{i}—Li1—Li2^{vi}	109.39 (4)	Bi^{ii}—Li3—Li3^{xxxvii}	133.884 (5)
Li3^{ii}—Li1—Li2^{vi}	109.39 (4)	Li3^{iii}—Li3—Li3^{xxxvii}	180.0
Bi—Li1—Li2^{vi}	68.35 (4)	Li1^{xxxi}—Li3—Li3^{xxxviii}	33.6 (4)
Bi^{iii}—Li1—Li2^{vi}	174.6 (7)	Li1^{xiv}—Li3—Li3^{xxxviii}	146.4 (4)
Bi^{iv}—Li1—Li2^{vi}	67.8 (3)	Li1^{xxxii}—Li3—Li3^{xxxviii}	88.5 (3)
Bi^{v}—Li1—Li2^{vi}	67.8 (3)	Li1^{ii}—Li3—Li3^{xxxviii}	91.5 (3)
Li3^{i}—Li1—Li2^{vii}	109.39 (4)	Li1^{xxxiii}—Li3—Li3^{xxxviii}	88.5 (3)
Li3^{ii}—Li1—Li2^{vii}	109.39 (4)	Li1^{xiii}—Li3—Li3^{xxxviii}	91.5 (3)
Bi—Li1—Li2^{vii}	174.6 (7)	Li5^{xxxiv}—Li3—Li3^{xxxviii}	35.264 (5)
Bi^{iii}—Li1—Li2^{vii}	68.35 (4)	In^{xxxiv}—Li3—Li3^{xxxviii}	35.264 (5)
Bi^{iv}—Li1—Li2^{vii}	67.8 (3)	In—Li3—Li3^{xxxviii}	144.736 (5)
Bi^{v}—Li1—Li2^{vii}	67.8 (3)	Bi^{xxxv}—Li3—Li3^{xxxviii}	46.116 (10)
Li2^{vi}—Li1—Li2^{vii}	106.2 (7)	Bi^{iii}—Li3—Li3^{xxxviii}	133.884 (11)

Li3^{i}—Li1—In	56.4 (4)
Li3^{ii}—Li1—In	56.4 (4)
Bi—Li1—In	58.5 (4)
Bi^{iii}—Li1—In	58.5 (4)
Bi^{iv}—Li1—In	129.0 (3)
Bi^{v}—Li1—In	129.0 (3)
Li2^{vi}—Li1—In	126.9 (3)
Li2^{vii}—Li1—In	126.9 (3)
Li3^{i}—Li1—Li1^{viii}	128.6 (7)
Li3^{ii}—Li1—Li1^{viii}	53.86 (19)
Bi—Li1—Li1^{viii}	55.4 (3)
Bi^{iii}—Li1—Li1^{viii}	126.88 (9)
Bi^{iv}—Li1—Li1^{viii}	54.2 (3)
Bi^{v}—Li1—Li1^{viii}	123.1 (2)
Li2^{vi}—Li1—Li1^{viii}	55.53 (15)
Li2^{vii}—Li1—Li1^{viii}	121.9 (7)
In—Li1—Li1^{viii}	91.8 (4)
Li3^{i}—Li1—Li1^{ix}	53.86 (19)
Li3^{ii}—Li1—Li1^{ix}	128.6 (7)
Bi—Li1—Li1^{ix}	126.88 (9)
Bi^{iii}—Li1—Li1^{ix}	55.4 (3)
Bi^{iv}—Li1—Li1^{ix}	123.1 (2)
Bi^{v}—Li1—Li1^{ix}	54.2 (3)
Li2^{vi}—Li1—Li1^{ix}	121.9 (7)
Li2^{vii}—Li1—Li1^{ix}	55.53 (15)
In—Li1—Li1^{ix}	91.8 (4)
Li1^{viii}—Li1—Li1^{ix}	176.5 (7)
Li3^{i}—Li1—Li1^{x}	53.86 (19)
Li3^{ii}—Li1—Li1^{x}	128.6 (7)
Bi—Li1—Li1^{x}	55.4 (3)
Bi^{iii}—Li1—Li1^{x}	126.88 (9)
Bi^{iv}—Li1—Li1^{x}	123.1 (2)
Bi^{v}—Li1—Li1^{x}	54.2 (3)
Li2^{vi}—Li1—Li1^{x}	55.53 (15)
Li2^{vii}—Li1—Li1^{x}	121.9 (7)
In—Li1—Li1^{x}	91.8 (4)
Li1^{viii}—Li1—Li1^{x}	93.5 (7)
Li1^{ix}—Li1—Li1^{x}	86.4 (7)
Li3^{i}—Li1—Li1^{xi}	128.6 (7)
Li3^{ii}—Li1—Li1^{xi}	53.86 (19)
Bi—Li1—Li1^{xi}	126.88 (9)
Bi^{iii}—Li1—Li1^{xi}	55.4 (3)
Bi^{iv}—Li1—Li1^{xi}	54.2 (3)
Bi^{v}—Li1—Li1^{xi}	123.1 (2)
Li2^{vi}—Li1—Li1^{xi}	121.9 (7)
Li2^{vii}—Li1—Li1^{xi}	55.53 (15)
In—Li1—Li1^{xi}	91.8 (4)
Li1^{viii}—Li1—Li1^{xi}	86.4 (7)
Li1^{ix}—Li1—Li1^{xi}	93.5 (7)
Li1^{x}—Li1—Li1^{xi}	176.5 (7)
Li3^{i}—Li1—Li4^{xii}	123.6 (4)
Bi^{xxxvi}—Li3—Li3^{xxxviii}	91.564 (7)
Bi^{i}—Li3—Li3^{xxxviii}	88.436 (7)
Bi^{xxxii}—Li3—Li3^{xxxviii}	46.116 (10)
Bi^{ii}—Li3—Li3^{xxxviii}	133.884 (10)
Li3^{iii}—Li3—Li3^{xxxviii}	120.000 (5)
Li3^{xxxvii}—Li3—Li3^{xxxviii}	60.000 (5)
Li1^{xxxi}—Li3—Li3^{i}	146.4 (4)
Li1^{xiv}—Li3—Li3^{i}	33.6 (4)
Li1^{xxxii}—Li3—Li3^{i}	91.5 (3)
Li1^{ii}—Li3—Li3^{i}	88.5 (3)
Li1^{xxxiii}—Li3—Li3^{i}	91.5 (3)
Li1^{xiii}—Li3—Li3^{i}	88.5 (3)
Li5^{xxxiv}—Li3—Li3^{i}	144.736 (5)
In^{xxxiv}—Li3—Li3^{i}	144.736 (5)
In—Li3—Li3^{i}	35.264 (5)
Bi^{xxxv}—Li3—Li3^{i}	133.884 (11)
Bi^{iii}—Li3—Li3^{i}	46.116 (10)
Bi^{xxxvi}—Li3—Li3^{i}	88.436 (7)
Bi^{i}—Li3—Li3^{i}	91.564 (7)
Bi^{xxxii}—Li3—Li3^{i}	133.884 (10)
Bi^{ii}—Li3—Li3^{i}	46.116 (10)
Li3^{iii}—Li3—Li3^{i}	60.000 (5)
Li3^{xxxvii}—Li3—Li3^{i}	120.000 (5)
Li3^{xxxviii}—Li3—Li3^{i}	180.0
Bi^{vi}—Li4—Bi^{xxv}	109.471 (9)
Bi^{vi}—Li4—Bi^{xxvii}	109.471 (9)
Bi^{xxv}—Li4—Bi^{xxvii}	109.471 (17)
Bi^{vi}—Li4—Bi	109.471 (18)
Bi^{xxv}—Li4—Bi	109.471 (8)
Bi^{xxvii}—Li4—Bi	109.471 (8)
Bi^{vi}—Li4—Li2	70.529 (17)
Bi^{xxv}—Li4—Li2	70.529 (8)
Bi^{xxvii}—Li4—Li2	70.529 (8)
Bi—Li4—Li2	180.0
Bi^{vi}—Li4—Li2^{vi}	180.0
Bi^{xxv}—Li4—Li2^{vi}	70.529 (9)
Bi^{xxvii}—Li4—Li2^{vi}	70.529 (9)
Bi—Li4—Li2^{vi}	70.529 (17)
Li2—Li4—Li2^{vi}	109.471 (17)
Bi^{vi}—Li4—Li2^{xxv}	70.529 (9)
Bi^{xxv}—Li4—Li2^{xxv}	180.0
Bi^{xxvii}—Li4—Li2^{xxv}	70.529 (17)
Bi—Li4—Li2^{xxv}	70.529 (9)
Li2—Li4—Li2^{xxv}	109.471 (9)
Li2^{vi}—Li4—Li2^{xxv}	109.471 (8)
Bi^{vi}—Li4—Li2^{xxvii}	70.529 (9)
Bi^{xxv}—Li4—Li2^{xxvii}	70.529 (17)
Bi^{xxvii}—Li4—Li2^{xxvii}	180.0
Bi—Li4—Li2^{xxvii}	70.529 (9)
Li2—Li4—Li2^{xxvii}	109.471 (9)
Li2^{vi}—Li4—Li2^{xxvii}	109.471 (8)

Li3^{ii}—Li1—Li4^{xii}	123.6 (4)
Bi—Li1—Li4^{xii}	121.5 (4)
Bi^{iii}—Li1—Li4^{xii}	121.5 (4)
Bi^{iv}—Li1—Li4^{xii}	51.0 (3)
Bi^{v}—Li1—Li4^{xii}	51.0 (3)
Li2^{vi}—Li1—Li4^{xii}	53.1 (3)
Li2^{vii}—Li1—Li4^{xii}	53.1 (3)
In—Li1—Li4^{xii}	180.0
Li1^{viii}—Li1—Li4^{xii}	88.2 (4)
Li1^{ix}—Li1—Li4^{xii}	88.2 (4)
Li1^{x}—Li1—Li4^{xii}	88.2 (4)
Li1^{xi}—Li1—Li4^{xii}	88.2 (4)
Li3^{i}—Li1—Li1^{xiii}	91.5 (3)
Li3^{ii}—Li1—Li1^{xiii}	36.14 (19)
Bi—Li1—Li1^{xiii}	93.3 (3)
Bi^{iii}—Li1—Li1^{xiii}	37.3 (2)
Bi^{iv}—Li1—Li1^{xiii}	93.3 (3)
Bi^{v}—Li1—Li1^{xiii}	146.48 (14)
Li2^{vi}—Li1—Li1^{xiii}	145.53 (15)
Li2^{vii}—Li1—Li1^{xiii}	91.4 (3)
In—Li1—Li1^{xiii}	45.000 (10)
Li1^{viii}—Li1—Li1^{xiii}	90.000 (1)
Li1^{ix}—Li1—Li1^{xiii}	92.5 (5)
Li1^{x}—Li1—Li1^{xiii}	136.7 (3)
Li1^{xi}—Li1—Li1^{xiii}	46.8 (4)
Li4^{xii}—Li1—Li1^{xiii}	135.000 (9)
Li3^{i}—Li1—Li1^{xiv}	36.14 (19)
Li3^{ii}—Li1—Li1^{xiv}	91.5 (3)
Bi—Li1—Li1^{xiv}	93.3 (3)
Bi^{iii}—Li1—Li1^{xiv}	37.3 (2)
Bi^{iv}—Li1—Li1^{xiv}	146.48 (14)
Bi^{v}—Li1—Li1^{xiv}	93.3 (3)
Li2^{vi}—Li1—Li1^{xiv}	145.53 (15)
Li2^{vii}—Li1—Li1^{xiv}	91.4 (3)
In—Li1—Li1^{xiv}	45.000 (10)
Li1^{viii}—Li1—Li1^{xiv}	136.7 (3)
Li1^{ix}—Li1—Li1^{xiv}	46.8 (4)
Li1^{x}—Li1—Li1^{xiv}	90.000 (1)
Li1^{xi}—Li1—Li1^{xiv}	92.5 (5)
Li4^{xii}—Li1—Li1^{xiv}	135.000 (9)
Li1^{xiii}—Li1—Li1^{xiv}	60.000 (11)
Li3^{i}—Li1—Li1^{xv}	91.5 (3)
Li3^{ii}—Li1—Li1^{xv}	36.14 (19)
Bi—Li1—Li1^{xv}	37.3 (2)
Bi^{iii}—Li1—Li1^{xv}	93.3 (3)
Bi^{iv}—Li1—Li1^{xv}	93.3 (3)
Bi^{v}—Li1—Li1^{xv}	146.48 (14)
Li2^{vi}—Li1—Li1^{xv}	91.4 (3)
Li2^{vii}—Li1—Li1^{xv}	145.53 (15)
In—Li1—Li1^{xv}	45.000 (9)
Li1^{viii}—Li1—Li1^{xv}	46.8 (4)
Li2^{xxv}—Li4—Li2^{xxvii}	109.471 (18)
Bi^{vi}—Li4—Li1^{xii}	125.264 (9)
Bi^{xxv}—Li4—Li1^{xii}	54.736 (8)
Bi^{xxvii}—Li4—Li1^{xii}	54.736 (8)
Bi—Li4—Li1^{xii}	125.264 (9)
Li2—Li4—Li1^{xii}	54.736 (8)
Li2^{vi}—Li4—Li1^{xii}	54.736 (8)
Li2^{xxv}—Li4—Li1^{xii}	125.264 (9)
Li2^{xxvii}—Li4—Li1^{xii}	125.264 (9)
Bi^{vi}—Li4—Li1^{xxxix}	54.736 (9)
Bi^{xxv}—Li4—Li1^{xxxix}	125.264 (8)
Bi^{xxvii}—Li4—Li1^{xxxix}	125.264 (8)
Bi—Li4—Li1^{xxxix}	54.736 (9)
Li2—Li4—Li1^{xxxix}	125.264 (8)
Li2^{vi}—Li4—Li1^{xxxix}	125.264 (8)
Li2^{xxv}—Li4—Li1^{xxxix}	54.736 (9)
Li2^{xxvii}—Li4—Li1^{xxxix}	54.736 (8)
Li1^{xii}—Li4—Li1^{xxxix}	180.0
Bi^{vi}—Li4—Li1^{viii}	125.264 (4)
Bi^{xxv}—Li4—Li1^{viii}	125.264 (4)
Bi^{xxvii}—Li4—Li1^{viii}	54.736 (4)
Bi—Li4—Li1^{viii}	54.736 (5)
Li2—Li4—Li1^{viii}	125.264 (4)
Li2^{vi}—Li4—Li1^{viii}	54.736 (5)
Li2^{xxv}—Li4—Li1^{viii}	54.736 (5)
Li2^{xxvii}—Li4—Li1^{viii}	125.264 (5)
Li1^{xii}—Li4—Li1^{viii}	90.0
Li1^{xxxix}—Li4—Li1^{viii}	90.000 (1)
Bi^{vi}—Li4—Li1^{xviii}	54.736 (5)
Bi^{xxv}—Li4—Li1^{xviii}	54.736 (4)
Bi^{xxvii}—Li4—Li1^{xviii}	125.264 (5)
Bi—Li4—Li1^{xviii}	125.264 (4)
Li2—Li4—Li1^{xviii}	54.736 (4)
Li2^{vi}—Li4—Li1^{xviii}	125.264 (4)
Li2^{xxv}—Li4—Li1^{xviii}	125.264 (4)
Li2^{xxvii}—Li4—Li1^{xviii}	54.736 (5)
Li1^{xii}—Li4—Li1^{xviii}	90.000 (1)
Li1^{xxxix}—Li4—Li1^{xviii}	90.000 (1)
Li1^{viii}—Li4—Li1^{xviii}	180.0
Bi^{vi}—Li4—Li1^{xxi}	54.736 (4)
Bi^{xxv}—Li4—Li1^{xxi}	125.264 (5)
Bi^{xxvii}—Li4—Li1^{xxi}	54.736 (4)
Bi—Li4—Li1^{xxi}	125.264 (4)
Li2—Li4—Li1^{xxi}	54.736 (4)
Li2^{vi}—Li4—Li1^{xxi}	125.264 (4)
Li2^{xxv}—Li4—Li1^{xxi}	54.736 (5)
Li2^{xxvii}—Li4—Li1^{xxi}	125.264 (4)
Li1^{xii}—Li4—Li1^{xxi}	90.000 (2)
Li1^{xxxix}—Li4—Li1^{xxi}	90.000 (1)
Li1^{viii}—Li4—Li1^{xxi}	90.0
Li1^{xviii}—Li4—Li1^{xxi}	90.000 (1)

Li1^{ix}—Li1—Li1^{xv}	136.7 (3)
Li1^{x}—Li1—Li1^{xv}	92.5 (5)
Li1^{xi}—Li1—Li1^{xv}	90.0
Li4^{xii}—Li1—Li1^{xv}	135.000 (9)
Li1^{xiii}—Li1—Li1^{xv}	60.000 (10)
Li1^{xiv}—Li1—Li1^{xv}	90.000 (19)
Li3^{i}—Li1—Li1^{xvi}	36.14 (19)
Li3^{ii}—Li1—Li1^{xvi}	91.5 (3)
Bi—Li1—Li1^{xvi}	37.3 (2)
Bi^{iii}—Li1—Li1^{xvi}	93.3 (3)
Bi^{iv}—Li1—Li1^{xvi}	146.48 (14)
Bi^{v}—Li1—Li1^{xvi}	93.3 (3)
Li2^{vi}—Li1—Li1^{xvi}	91.4 (3)
Li2^{vii}—Li1—Li1^{xvi}	145.53 (15)
In—Li1—Li1^{xvi}	45.000 (9)
Li1^{viii}—Li1—Li1^{xvi}	92.5 (5)
Li1^{ix}—Li1—Li1^{xvi}	90.0
Li1^{x}—Li1—Li1^{xvi}	46.8 (4)
Li1^{xi}—Li1—Li1^{xvi}	136.7 (3)
Li4^{xii}—Li1—Li1^{xvi}	135.000 (9)
Li1^{xiii}—Li1—Li1^{xvi}	90.000 (19)
Li1^{xiv}—Li1—Li1^{xvi}	60.000 (10)
Li1^{xv}—Li1—Li1^{xvi}	60.000 (10)
Li3^{i}—Li1—Li4	90.69 (13)
Li3^{ii}—Li1—Li4	90.69 (13)
Bi—Li1—Li4	32.70 (10)
Bi^{iii}—Li1—Li4	149.8 (6)
Bi^{iv}—Li1—Li4	89.21 (17)
Bi^{v}—Li1—Li4	89.21 (17)
Li2^{vi}—Li1—Li4	35.65 (7)
Li2^{vii}—Li1—Li4	141.9 (6)
In—Li1—Li4	91.2 (3)
Li1^{viii}—Li1—Li4	46.8 (4)
Li1^{ix}—Li1—Li4	133.1 (4)
Li1^{x}—Li1—Li4	46.8 (4)
Li1^{xi}—Li1—Li4	133.1 (4)
Li4^{xii}—Li1—Li4	88.8 (3)
Li1^{xiii}—Li1—Li4	121.0 (2)
Li1^{xiv}—Li1—Li4	121.0 (2)
Li1^{xv}—Li1—Li4	61.0 (2)
Li1^{xvi}—Li1—Li4	61.0 (2)
Li4^{xvii}—Li2—Li4	180.0
Li4^{xvii}—Li2—Li1^{xviii}	107.8 (3)
Li4—Li2—Li1^{xviii}	72.2 (3)
Li4^{xvii}—Li2—Li1^{xix}	72.2 (3)
Li4—Li2—Li1^{xix}	107.8 (3)
Li1^{xviii}—Li2—Li1^{xix}	68.9 (3)
Li4^{xvii}—Li2—Li1^{xii}	107.8 (3)
Li4—Li2—Li1^{xii}	72.2 (3)
Li1^{xviii}—Li2—Li1^{xii}	111.1 (3)
Li1^{xix}—Li2—Li1^{xii}	180.0
Bi^{vi}—Li4—Li1^{x}	125.264 (4)
Bi^{xxv}—Li4—Li1^{x}	54.736 (4)
Bi^{xxvii}—Li4—Li1^{x}	125.264 (4)
Bi—Li4—Li1^{x}	54.736 (5)
Li2—Li4—Li1^{x}	125.264 (4)
Li2^{vi}—Li4—Li1^{x}	54.736 (5)
Li2^{xxv}—Li4—Li1^{x}	125.264 (5)
Li2^{xxvii}—Li4—Li1^{x}	54.736 (5)
Li1^{xii}—Li4—Li1^{x}	90.0
Li1^{xxxix}—Li4—Li1^{x}	90.000 (2)
Li1^{viii}—Li4—Li1^{x}	90.000 (1)
Li1^{xviii}—Li4—Li1^{x}	90.0
Li1^{xxi}—Li4—Li1^{x}	180.0
Bi^{vi}—Li4—Li1^{xvi}	90.72 (15)
Bi^{xxv}—Li4—Li1^{xvi}	90.72 (15)
Bi^{xxvii}—Li4—Li1^{xvi}	143.5 (3)
Bi—Li4—Li1^{xvi}	34.0 (3)
Li2—Li4—Li1^{xvi}	146.0 (3)
Li2^{vi}—Li4—Li1^{xvi}	89.28 (15)
Li2^{xxv}—Li4—Li1^{xvi}	89.28 (15)
Li2^{xxvii}—Li4—Li1^{xvi}	36.5 (3)
Li1^{xii}—Li4—Li1^{xvi}	134.986 (10)
Li1^{xxxix}—Li4—Li1^{xvi}	45.014 (11)
Li1^{viii}—Li4—Li1^{xvi}	88.8 (3)
Li1^{xviii}—Li4—Li1^{xvi}	91.2 (3)
Li1^{xxi}—Li4—Li1^{xvi}	134.986 (10)
Li1^{x}—Li4—Li1^{xvi}	45.014 (10)
Bi^{vi}—Li4—Li1^{xix}	34.0 (3)
Bi^{xxv}—Li4—Li1^{xix}	90.72 (15)
Bi^{xxvii}—Li4—Li1^{xix}	90.72 (15)
Bi—Li4—Li1^{xix}	143.5 (3)
Li2—Li4—Li1^{xix}	36.5 (3)
Li2^{vi}—Li4—Li1^{xix}	146.0 (3)
Li2^{xxv}—Li4—Li1^{xix}	89.28 (15)
Li2^{xxvii}—Li4—Li1^{xix}	89.28 (15)
Li1^{xii}—Li4—Li1^{xix}	91.2 (3)
Li1^{xxxix}—Li4—Li1^{xix}	88.8 (3)
Li1^{viii}—Li4—Li1^{xix}	134.986 (6)
Li1^{xviii}—Li4—Li1^{xix}	45.014 (5)
Li1^{xxi}—Li4—Li1^{xix}	45.014 (6)
Li1^{x}—Li4—Li1^{xix}	134.986 (6)
Li1^{xvi}—Li4—Li1^{xix}	119.984 (9)
Bi^{vi}—Li4—Li1^{xv}	90.72 (15)
Bi^{xxv}—Li4—Li1^{xv}	143.5 (3)
Bi^{xxvii}—Li4—Li1^{xv}	90.72 (15)
Bi—Li4—Li1^{xv}	34.0 (3)
Li2—Li4—Li1^{xv}	146.0 (3)
Li2^{vi}—Li4—Li1^{xv}	89.28 (15)
Li2^{xxv}—Li4—Li1^{xv}	36.5 (3)
Li2^{xxvii}—Li4—Li1^{xv}	89.28 (15)
Li1^{xii}—Li4—Li1^{xv}	134.986 (11)

Li4^{xvii}—Li2—Li1^{xx}	72.2 (3)
Li4—Li2—Li1^{xx}	107.8 (3)
Li1^{xviii}—Li2—Li1^{xx}	180.0
Li1^{xix}—Li2—Li1^{xx}	111.1 (3)
Li1^{xii}—Li2—Li1^{xx}	68.9 (3)
Li4^{xvii}—Li2—Li1^{xxi}	107.8 (3)
Li4—Li2—Li1^{xxi}	72.2 (3)
Li1^{xviii}—Li2—Li1^{xxi}	111.1 (3)
Li1^{xix}—Li2—Li1^{xxi}	68.9 (3)
Li1^{xii}—Li2—Li1^{xxi}	111.1 (3)
Li1^{xx}—Li2—Li1^{xxi}	68.9 (3)
Li4^{xvii}—Li2—Li1^{xxii}	72.2 (3)
Li4—Li2—Li1^{xxii}	107.8 (3)
Li1^{xviii}—Li2—Li1^{xxii}	68.9 (3)
Li1^{xix}—Li2—Li1^{xxii}	111.1 (3)
Li1^{xii}—Li2—Li1^{xxii}	68.9 (3)
Li1^{xx}—Li2—Li1^{xxii}	111.1 (3)
Li1^{xxi}—Li2—Li1^{xxii}	180.0
Li4^{xvii}—Li2—Bi^{xxiii}	53.109 (11)
Li4—Li2—Bi^{xxiii}	126.891 (11)
Li1^{xviii}—Li2—Bi^{xxiii}	124.37 (18)
Li1^{xix}—Li2—Bi^{xxiii}	125.3 (3)
Li1^{xii}—Li2—Bi^{xxiii}	54.7 (3)
Li1^{xx}—Li2—Bi^{xxiii}	55.63 (18)
Li1^{xxi}—Li2—Bi^{xxiii}	124.37 (18)
Li1^{xxii}—Li2—Bi^{xxiii}	55.63 (18)
Li4^{xvii}—Li2—Bi^{vi}	126.891 (11)
Li4—Li2—Bi^{vi}	53.109 (11)
Li1^{xviii}—Li2—Bi^{vi}	55.63 (18)
Li1^{xix}—Li2—Bi^{vi}	54.7 (3)
Li1^{xii}—Li2—Bi^{vi}	125.3 (3)
Li1^{xx}—Li2—Bi^{vi}	124.37 (18)
Li1^{xxi}—Li2—Bi^{vi}	55.63 (18)
Li1^{xxii}—Li2—Bi^{vi}	124.37 (18)
Bi^{xxiii}—Li2—Bi^{vi}	180.000 (11)
Li4^{xvii}—Li2—Bi^{xxiv}	53.109 (9)
Li4—Li2—Bi^{xxiv}	126.891 (9)
Li1^{xviii}—Li2—Bi^{xxiv}	124.37 (18)
Li1^{xix}—Li2—Bi^{xxiv}	55.63 (18)
Li1^{xii}—Li2—Bi^{xxiv}	124.37 (18)
Li1^{xx}—Li2—Bi^{xxiv}	55.63 (18)
Li1^{xxi}—Li2—Bi^{xxiv}	54.7 (3)
Li1^{xxii}—Li2—Bi^{xxiv}	125.3 (3)
Bi^{xxiii}—Li2—Bi^{xxiv}	87.677 (12)
Bi^{vi}—Li2—Bi^{xxiv}	92.323 (12)
Li4^{xvii}—Li2—Bi^{xxv}	126.891 (9)
Li4—Li2—Bi^{xxv}	53.109 (9)
Li1^{xviii}—Li2—Bi^{xxv}	55.63 (18)
Li1^{xix}—Li2—Bi^{xxv}	124.37 (18)
Li1^{xii}—Li2—Bi^{xxv}	55.63 (18)
Li1^{xx}—Li2—Bi^{xxv}	124.37 (18)
Li1^{xxxix}—Li4—Li1^{xv}	45.014 (11)
Li1^{viii}—Li4—Li1^{xv}	45.014 (10)
Li1^{xviii}—Li4—Li1^{xv}	134.986 (11)
Li1^{xxi}—Li4—Li1^{xv}	91.2 (3)
Li1^{x}—Li4—Li1^{xv}	88.8 (3)
Li1^{xvi}—Li4—Li1^{xv}	58.0 (4)
Li1^{xix}—Li4—Li1^{xv}	119.984 (9)
Bi^{vi}—Li4—Li1^{xx}	90.72 (15)
Bi^{xxv}—Li4—Li1^{xx}	90.72 (15)
Bi^{xxvii}—Li4—Li1^{xx}	34.0 (3)
Bi—Li4—Li1^{xx}	143.5 (3)
Li2—Li4—Li1^{xx}	36.5 (3)
Li2^{vi}—Li4—Li1^{xx}	89.28 (15)
Li2^{xxv}—Li4—Li1^{xx}	89.28 (15)
Li2^{xxvii}—Li4—Li1^{xx}	146.0 (3)
Li1^{xii}—Li4—Li1^{xx}	45.014 (11)
Li1^{xxxix}—Li4—Li1^{xx}	134.986 (10)
Li1^{viii}—Li4—Li1^{xx}	88.8 (3)
Li1^{xviii}—Li4—Li1^{xx}	91.2 (3)
Li1^{xxi}—Li4—Li1^{xx}	45.014 (10)
Li1^{x}—Li4—Li1^{xx}	134.986 (11)
Li1^{xvi}—Li4—Li1^{xx}	177.5 (5)
Li1^{xix}—Li4—Li1^{xx}	62.0 (4)
Li1^{xv}—Li4—Li1^{xx}	119.984 (12)
Bi^{vi}—Li4—Li1^{xxii}	90.72 (15)
Bi^{xxv}—Li4—Li1^{xxii}	34.0 (3)
Bi^{xxvii}—Li4—Li1^{xxii}	90.72 (15)
Bi—Li4—Li1^{xxii}	143.5 (3)
Li2—Li4—Li1^{xxii}	36.5 (3)
Li2^{vi}—Li4—Li1^{xxii}	89.28 (15)
Li2^{xxv}—Li4—Li1^{xxii}	146.0 (3)
Li2^{xxvii}—Li4—Li1^{xxii}	89.28 (15)
Li1^{xii}—Li4—Li1^{xxii}	45.014 (11)
Li1^{xxxix}—Li4—Li1^{xxii}	134.986 (11)
Li1^{viii}—Li4—Li1^{xxii}	134.986 (11)
Li1^{xviii}—Li4—Li1^{xxii}	45.014 (10)
Li1^{xxi}—Li4—Li1^{xxii}	91.2 (3)
Li1^{x}—Li4—Li1^{xxii}	88.8 (3)
Li1^{xvi}—Li4—Li1^{xxii}	119.984 (12)
Li1^{xix}—Li4—Li1^{xxii}	62.0 (4)
Li1^{xv}—Li4—Li1^{xxii}	177.5 (5)
Li1^{xx}—Li4—Li1^{xxii}	62.0 (4)
Bi^{vi}—Li4—Li1	143.5 (3)
Bi^{xxv}—Li4—Li1	90.72 (15)
Bi^{xxvii}—Li4—Li1	90.72 (15)
Bi—Li4—Li1	34.0 (3)
Li2—Li4—Li1	146.0 (3)
Li2^{vi}—Li4—Li1	36.5 (3)
Li2^{xxv}—Li4—Li1	89.28 (15)
Li2^{xxvii}—Li4—Li1	89.28 (15)
Li1^{xii}—Li4—Li1	91.2 (3)

Li1^{xxi}—Li2—Bi^{xxv}	125.3 (3)
Li1^{xxii}—Li2—Bi^{xxv}	54.7 (3)
Bi^{xxiii}—Li2—Bi^{xxv}	92.323 (11)
Bi^{vi}—Li2—Bi^{xxv}	87.677 (12)
Bi^{xxiv}—Li2—Bi^{xxv}	180.000 (11)
Li4^{xvii}—Li2—Bi^{xxvi}	53.109 (9)
Li4—Li2—Bi^{xxvi}	126.891 (9)
Li1^{xviii}—Li2—Bi^{xxvi}	54.7 (3)
Li1^{xix}—Li2—Bi^{xxvi}	55.63 (18)
Li1^{xii}—Li2—Bi^{xxvi}	124.37 (18)
Li1^{xx}—Li2—Bi^{xxvi}	125.3 (3)
Li1^{xxi}—Li2—Bi^{xxvi}	124.37 (18)
Li1^{xxii}—Li2—Bi^{xxvi}	55.63 (18)
Bi^{xxiii}—Li2—Bi^{xxvi}	87.677 (12)
Bi^{vi}—Li2—Bi^{xxvi}	92.323 (12)
Bi^{xxiv}—Li2—Bi^{xxvi}	87.677 (11)
Bi^{xxv}—Li2—Bi^{xxvi}	92.323 (11)
Li4^{xvii}—Li2—Bi^{xxvii}	126.891 (9)
Li4—Li2—Bi^{xxvii}	53.109 (9)
Li1^{xviii}—Li2—Bi^{xxvii}	125.3 (3)
Li1^{xix}—Li2—Bi^{xxvii}	124.37 (18)
Li1^{xii}—Li2—Bi^{xxvii}	55.63 (18)
Li1^{xx}—Li2—Bi^{xxvii}	54.7 (3)
Li1^{xxi}—Li2—Bi^{xxvii}	55.63 (18)
Li1^{xxii}—Li2—Bi^{xxvii}	124.37 (18)
Bi^{xxiii}—Li2—Bi^{xxvii}	92.323 (12)
Bi^{vi}—Li2—Bi^{xxvii}	87.677 (12)
Bi^{xxiv}—Li2—Bi^{xxvii}	92.323 (11)
Bi^{xxv}—Li2—Bi^{xxvii}	87.677 (11)
Bi^{xxvi}—Li2—Bi^{xxvii}	180.0
Li4^{xvii}—Li2—Li2^{xxviii}	35.264 (8)
Li4—Li2—Li2^{xxviii}	144.736 (8)
Li1^{xviii}—Li2—Li2^{xxviii}	88.6 (3)
Li1^{xix}—Li2—Li2^{xxviii}	36.9 (3)
Li1^{xii}—Li2—Li2^{xxviii}	143.1 (3)
Li1^{xx}—Li2—Li2^{xxviii}	91.4 (3)
Li1^{xxi}—Li2—Li2^{xxviii}	88.6 (3)
Li1^{xxii}—Li2—Li2^{xxviii}	91.4 (3)
Bi^{xxiii}—Li2—Li2^{xxviii}	88.374 (8)
Bi^{vi}—Li2—Li2^{xxviii}	91.626 (8)
Bi^{xxiv}—Li2—Li2^{xxviii}	43.862 (6)
Bi^{xxv}—Li2—Li2^{xxviii}	136.138 (5)
Bi^{xxvi}—Li2—Li2^{xxviii}	43.862 (6)
Bi^{xxvii}—Li2—Li2^{xxviii}	136.138 (6)
Li4^{xvii}—Li2—Li2^{vi}	144.736 (8)
Li4—Li2—Li2^{vi}	35.264 (8)
Li1^{xviii}—Li2—Li2^{vi}	91.4 (3)
Li1^{xix}—Li2—Li2^{vi}	143.1 (3)
Li1^{xii}—Li2—Li2^{vi}	36.9 (3)
Li1^{xx}—Li2—Li2^{vi}	88.6 (3)
Li1^{xxi}—Li2—Li2^{vi}	91.4 (3)
Li1^{xxxix}—Li4—Li1	88.8 (3)
Li1^{viii}—Li4—Li1	45.014 (5)
Li1^{xviii}—Li4—Li1	134.986 (5)
Li1^{xxi}—Li4—Li1	134.986 (6)
Li1^{x}—Li4—Li1	45.014 (6)
Li1^{xvi}—Li4—Li1	58.0 (4)
Li1^{xix}—Li4—Li1	177.5 (5)
Li1^{xv}—Li4—Li1	58.0 (4)
Li1^{xx}—Li4—Li1	119.984 (8)
Li1^{xxii}—Li4—Li1	119.984 (8)
Li3—In—Li3^{iii}	109.471 (18)
Li3—In—Li3^{i}	109.471 (8)
Li3^{iii}—In—Li3^{i}	109.471 (9)
Li3—In—Li3^{ii}	109.471 (8)
Li3^{iii}—In—Li3^{ii}	109.471 (9)
Li3^{i}—In—Li3^{ii}	109.471 (17)
Li3—In—Bi	180.0
Li3^{iii}—In—Bi	70.529 (17)
Li3^{i}—In—Bi	70.529 (8)
Li3^{ii}—In—Bi	70.529 (8)
Li3—In—Bi^{iii}	70.529 (18)
Li3^{iii}—In—Bi^{iii}	180.0
Li3^{i}—In—Bi^{iii}	70.529 (9)
Li3^{ii}—In—Bi^{iii}	70.529 (9)
Bi—In—Bi^{iii}	109.471 (18)
Li3—In—Bi^{i}	70.529 (9)
Li3^{iii}—In—Bi^{i}	70.529 (9)
Li3^{i}—In—Bi^{i}	180.0
Li3^{ii}—In—Bi^{i}	70.529 (17)
Bi—In—Bi^{i}	109.471 (8)
Bi^{iii}—In—Bi^{i}	109.471 (9)
Li3—In—Bi^{ii}	70.529 (8)
Li3^{iii}—In—Bi^{ii}	70.529 (9)
Li3^{i}—In—Bi^{ii}	70.529 (17)
Li3^{ii}—In—Bi^{ii}	180.0
Bi—In—Bi^{ii}	109.471 (8)
Bi^{iii}—In—Bi^{ii}	109.471 (9)
Bi^{i}—In—Bi^{ii}	109.471 (17)
Li3—In—Li1	125.264 (9)
Li3^{iii}—In—Li1	125.264 (8)
Li3^{i}—In—Li1	54.736 (9)
Li3^{ii}—In—Li1	54.736 (9)
Bi—In—Li1	54.736 (9)
Bi^{iii}—In—Li1	54.736 (8)
Bi^{i}—In—Li1	125.264 (8)
Bi^{ii}—In—Li1	125.264 (8)
Li3—In—Li1^{ii}	54.736 (9)
Li3^{iii}—In—Li1^{ii}	54.736 (8)
Li3^{i}—In—Li1^{ii}	125.264 (9)
Li3^{ii}—In—Li1^{ii}	125.264 (9)
Bi—In—Li1^{ii}	125.264 (9)

Li1^{xxii}—Li2—Li2^{vi}	88.6 (3)
Bi^{xxiii}—Li2—Li2^{vi}	91.626 (8)
Bi^{vi}—Li2—Li2^{vi}	88.374 (8)
Bi^{xxiv}—Li2—Li2^{vi}	136.138 (6)
Bi^{xxv}—Li2—Li2^{vi}	43.862 (6)
Bi^{xxvi}—Li2—Li2^{vi}	136.138 (6)
Bi^{xxvii}—Li2—Li2^{vi}	43.862 (5)
Li2^{xxviii}—Li2—Li2^{vi}	180.0
Li4^{xvii}—Li2—Li2^{xxv}	144.736 (4)
Li4—Li2—Li2^{xxv}	35.264 (5)
Li1^{xviii}—Li2—Li2^{xxv}	91.4 (3)
Li1^{xix}—Li2—Li2^{xxv}	88.6 (3)
Li1^{xii}—Li2—Li2^{xxv}	91.4 (3)
Li1^{xx}—Li2—Li2^{xxv}	88.6 (3)
Li1^{xxi}—Li2—Li2^{xxv}	36.9 (3)
Li1^{xxii}—Li2—Li2^{xxv}	143.1 (3)
Bi^{xxiii}—Li2—Li2^{xxv}	136.138 (10)
Bi^{vi}—Li2—Li2^{xxv}	43.862 (10)
Bi^{xxiv}—Li2—Li2^{xxv}	91.626 (8)
Bi^{xxv}—Li2—Li2^{xxv}	88.374 (8)
Bi^{xxvi}—Li2—Li2^{xxv}	136.138 (10)
Bi^{xxvii}—Li2—Li2^{xxv}	43.862 (10)
Li2^{xxviii}—Li2—Li2^{xxv}	120.000 (5)
Li2^{vi}—Li2—Li2^{xxv}	60.000 (5)
Li4^{xvii}—Li2—Li2^{xxix}	35.264 (5)
Li4—Li2—Li2^{xxix}	144.736 (4)
Li1^{xviii}—Li2—Li2^{xxix}	88.6 (3)
Li1^{xix}—Li2—Li2^{xxix}	91.4 (3)
Li1^{xii}—Li2—Li2^{xxix}	88.6 (3)
Li1^{xx}—Li2—Li2^{xxix}	91.4 (3)
Li1^{xxi}—Li2—Li2^{xxix}	143.1 (3)
Li1^{xxii}—Li2—Li2^{xxix}	36.9 (3)
Bi^{xxiii}—Li2—Li2^{xxix}	43.862 (10)
Bi^{vi}—Li2—Li2^{xxix}	136.138 (10)
Bi^{xxiv}—Li2—Li2^{xxix}	88.374 (8)
Bi^{xxv}—Li2—Li2^{xxix}	91.626 (8)
Bi^{xxvi}—Li2—Li2^{xxix}	43.862 (10)
Bi^{xxvii}—Li2—Li2^{xxix}	136.138 (10)
Li2^{xxviii}—Li2—Li2^{xxix}	60.000 (5)
Li2^{vi}—Li2—Li2^{xxix}	120.000 (5)
Li2^{xxv}—Li2—Li2^{xxix}	180.0
Li4^{xvii}—Li2—Li2^{xxx}	35.264 (5)
Li4—Li2—Li2^{xxx}	144.736 (4)
Li1^{xviii}—Li2—Li2^{xxx}	143.1 (3)
Li1^{xix}—Li2—Li2^{xxx}	91.4 (3)
Li1^{xii}—Li2—Li2^{xxx}	88.6 (3)
Li1^{xx}—Li2—Li2^{xxx}	36.9 (3)
Li1^{xxi}—Li2—Li2^{xxx}	88.6 (3)
Li1^{xxii}—Li2—Li2^{xxx}	91.4 (3)
Bi^{xxiii}—Li2—Li2^{xxx}	43.862 (10)
Bi^{vi}—Li2—Li2^{xxx}	136.138 (10)
Bi^{iii}—In—Li1^{ii}	125.264 (8)
Bi^{i}—In—Li1^{ii}	54.736 (8)
Bi^{ii}—In—Li1^{ii}	54.736 (8)
Li1—In—Li1^{ii}	180.0
Li3—In—Li1^{xv}	125.264 (4)
Li3^{iii}—In—Li1^{xv}	54.736 (5)
Li3^{i}—In—Li1^{xv}	125.264 (5)
Li3^{ii}—In—Li1^{xv}	54.736 (5)
Bi—In—Li1^{xv}	54.736 (4)
Bi^{iii}—In—Li1^{xv}	125.264 (4)
Bi^{i}—In—Li1^{xv}	54.736 (5)
Bi^{ii}—In—Li1^{xv}	125.264 (4)
Li1—In—Li1^{xv}	90.0
Li1^{ii}—In—Li1^{xv}	90.000 (1)
Li3—In—Li1^{xiii}	54.736 (4)
Li3^{iii}—In—Li1^{xiii}	125.264 (4)
Li3^{i}—In—Li1^{xiii}	125.264 (4)
Li3^{ii}—In—Li1^{xiii}	54.736 (5)
Bi—In—Li1^{xiii}	125.264 (4)
Bi^{iii}—In—Li1^{xiii}	54.736 (5)
Bi^{i}—In—Li1^{xiii}	54.736 (5)
Bi^{ii}—In—Li1^{xiii}	125.264 (5)
Li1—In—Li1^{xiii}	90.0
Li1^{ii}—In—Li1^{xiii}	90.000 (1)
Li1^{xv}—In—Li1^{xiii}	90.0
Li4—Bi—Li1	113.3 (4)
Li4—Bi—Li1^{xv}	113.3 (4)
Li1—Bi—Li1^{xv}	105.4 (4)
Li4—Bi—Li1^{xvi}	113.3 (4)
Li1—Bi—Li1^{xvi}	105.4 (4)
Li1^{xv}—Bi—Li1^{xvi}	105.4 (4)
Li4—Bi—Li1^{x}	74.3 (3)
Li1—Bi—Li1^{x}	70.425 (9)
Li1^{xv}—Bi—Li1^{x}	172.4 (7)
Li1^{xvi}—Bi—Li1^{x}	70.424 (18)
Li4—Bi—Li1^{xxxix}	74.3 (3)
Li1—Bi—Li1^{xxxix}	172.4 (7)
Li1^{xv}—Bi—Li1^{xxxix}	70.424 (11)
Li1^{xvi}—Bi—Li1^{xxxix}	70.424 (11)
Li1^{x}—Bi—Li1^{xxxix}	113.0 (3)
Li4—Bi—Li1^{viii}	74.3 (3)
Li1—Bi—Li1^{viii}	70.425 (9)
Li1^{xv}—Bi—Li1^{viii}	70.424 (17)
Li1^{xvi}—Bi—Li1^{viii}	172.4 (7)
Li1^{x}—Bi—Li1^{viii}	113.0 (3)
Li1^{xxxix}—Bi—Li1^{viii}	113.0 (3)
Li4—Bi—In	180.00 (3)
Li1—Bi—In	66.7 (4)
Li1^{xv}—Bi—In	66.7 (4)
Li1^{xvi}—Bi—In	66.7 (4)
Li1^{x}—Bi—In	105.7 (3)

Bi^{xxiv}—Li2—Li2^{xxx}	43.862 (10)
Bi^{xxv}—Li2—Li2^{xxx}	136.138 (10)
Bi^{xxvi}—Li2—Li2^{xxx}	88.374 (8)
Bi^{xxvii}—Li2—Li2^{xxx}	91.626 (8)
Li2^{xxviii}—Li2—Li2^{xxx}	60.000 (5)
Li2^{vi}—Li2—Li2^{xxx}	120.000 (5)
Li2^{xxv}—Li2—Li2^{xxx}	120.000 (11)
Li2^{xxix}—Li2—Li2^{xxx}	60.000 (11)
Li4^{xvii}—Li2—Li2^{xxvii}	144.736 (5)
Li4—Li2—Li2^{xxvii}	35.264 (5)
Li1^{xviii}—Li2—Li2^{xxvii}	36.9 (3)
Li1^{xix}—Li2—Li2^{xxvii}	88.6 (3)
Li1^{xii}—Li2—Li2^{xxvii}	91.4 (3)
Li1^{xx}—Li2—Li2^{xxvii}	143.1 (3)
Li1^{xxi}—Li2—Li2^{xxvii}	91.4 (3)
Li1^{xxii}—Li2—Li2^{xxvii}	88.6 (3)
Bi^{xxiii}—Li2—Li2^{xxvii}	136.138 (10)
Bi^{vi}—Li2—Li2^{xxvii}	43.862 (10)
Bi^{xxiv}—Li2—Li2^{xxvii}	136.138 (10)
Bi^{xxv}—Li2—Li2^{xxvii}	43.862 (10)
Bi^{xxvi}—Li2—Li2^{xxvii}	91.626 (8)
Bi^{xxvii}—Li2—Li2^{xxvii}	88.374 (8)
Li2^{xxviii}—Li2—Li2^{xxvii}	120.000 (5)
Li2^{vi}—Li2—Li2^{xxvii}	60.000 (5)
Li2^{xxv}—Li2—Li2^{xxvii}	60.000 (11)
Li2^{xxix}—Li2—Li2^{xxvii}	120.000 (11)
Li2^{xxx}—Li2—Li2^{xxvii}	180.0
Li1^{xxxi}—Li3—Li1^{xiv}	180.0 (7)
Li1^{xxxi}—Li3—Li1^{xxxii}	107.7 (4)
Li1^{xiv}—Li3—Li1^{xxxii}	72.3 (4)
Li1^{xxxi}—Li3—Li1^{ii}	72.3 (4)
Li1^{xiv}—Li3—Li1^{ii}	107.7 (4)
Li1^{xxxii}—Li3—Li1^{ii}	180.0 (7)
Li1^{xxxi}—Li3—Li1^{xxxiii}	107.7 (4)
Li1^{xiv}—Li3—Li1^{xxxiii}	72.3 (4)
Li1^{xxxii}—Li3—Li1^{xxxiii}	107.7 (4)
Li1^{ii}—Li3—Li1^{xxxiii}	72.3 (4)
Li1^{xxxi}—Li3—Li1^{xiii}	72.3 (4)
Li1^{xiv}—Li3—Li1^{xiii}	107.7 (4)
Li1^{xxxii}—Li3—Li1^{xiii}	72.3 (4)
Li1^{ii}—Li3—Li1^{xiii}	107.7 (4)
Li1^{xxxiii}—Li3—Li1^{xiii}	180.0
Li1^{xxxi}—Li3—Li5^{xxxiv}	68.8 (4)
Li1^{xiv}—Li3—Li5^{xxxiv}	111.2 (4)
Li1^{xxxii}—Li3—Li5^{xxxiv}	68.8 (4)
Li1^{ii}—Li3—Li5^{xxxiv}	111.2 (4)
Li1^{xxxiii}—Li3—Li5^{xxxiv}	68.8 (4)
Li1^{xiii}—Li3—Li5^{xxxiv}	111.2 (4)
Li1^{xxxi}—Li3—In^{xxxiv}	68.8 (4)
Li1^{xiv}—Li3—In^{xxxiv}	111.2 (4)
Li1^{xxxii}—Li3—In^{xxxiv}	68.8 (4)
Li1^{xxxix}—Bi—In	105.7 (3)
Li1^{viii}—Bi—In	105.7 (3)
Li4—Bi—Li2^{xxvii}	56.361 (9)
Li1—Bi—Li2^{xxvii}	126.97 (15)
Li1^{xv}—Bi—Li2^{xxvii}	126.97 (15)
Li1^{xvi}—Bi—Li2^{xxvii}	56.9 (4)
Li1^{x}—Bi—Li2^{xxvii}	56.58 (16)
Li1^{xxxix}—Bi—Li2^{xxvii}	56.58 (16)
Li1^{viii}—Bi—Li2^{xxvii}	130.6 (3)
In—Bi—Li2^{xxvii}	123.639 (9)
Li4—Bi—Li2^{vi}	56.361 (12)
Li1—Bi—Li2^{vi}	56.9 (4)
Li1^{xv}—Bi—Li2^{vi}	126.97 (15)
Li1^{xvi}—Bi—Li2^{vi}	126.97 (15)
Li1^{x}—Bi—Li2^{vi}	56.58 (16)
Li1^{xxxix}—Bi—Li2^{vi}	130.6 (3)
Li1^{viii}—Bi—Li2^{vi}	56.58 (16)
In—Bi—Li2^{vi}	123.639 (12)
Li2^{xxvii}—Bi—Li2^{vi}	92.275 (11)
Li4—Bi—Li2^{xxv}	56.361 (9)
Li1—Bi—Li2^{xxv}	126.97 (15)
Li1^{xv}—Bi—Li2^{xxv}	56.9 (4)
Li1^{xvi}—Bi—Li2^{xxv}	126.97 (15)
Li1^{x}—Bi—Li2^{xxv}	130.6 (3)
Li1^{xxxix}—Bi—Li2^{xxv}	56.58 (16)
Li1^{viii}—Bi—Li2^{xxv}	56.58 (16)
In—Bi—Li2^{xxv}	123.639 (9)
Li2^{xxvii}—Bi—Li2^{xxv}	92.275 (11)
Li2^{vi}—Bi—Li2^{xxv}	92.275 (11)
Li4—Bi—Li3^{i}	126.827 (8)
Li1—Bi—Li3^{i}	52.80 (18)
Li1^{xv}—Bi—Li3^{i}	119.9 (4)
Li1^{xvi}—Bi—Li3^{i}	52.80 (18)
Li1^{x}—Bi—Li3^{i}	52.5 (3)
Li1^{xxxix}—Bi—Li3^{i}	123.20 (18)
Li1^{viii}—Bi—Li3^{i}	123.20 (18)
In—Bi—Li3^{i}	53.173 (8)
Li2^{xxvii}—Bi—Li3^{i}	89.934 (1)
Li2^{vi}—Bi—Li3^{i}	89.934 (1)
Li2^{xxv}—Bi—Li3^{i}	176.812 (15)
Li4—Bi—Li3^{iii}	126.827 (11)
Li1—Bi—Li3^{iii}	119.9 (4)
Li1^{xv}—Bi—Li3^{iii}	52.80 (18)
Li1^{xvi}—Bi—Li3^{iii}	52.80 (18)
Li1^{x}—Bi—Li3^{iii}	123.20 (18)
Li1^{xxxix}—Bi—Li3^{iii}	52.5 (3)
Li1^{viii}—Bi—Li3^{iii}	123.20 (18)
In—Bi—Li3^{iii}	53.173 (11)
Li2^{xxvii}—Bi—Li3^{iii}	89.934 (1)
Li2^{vi}—Bi—Li3^{iii}	176.812 (15)
Li2^{xxv}—Bi—Li3^{iii}	89.934 (1)

Li1^{ii}—Li3—In^{xxxiv}	111.2 (4)	Li3^{i}—Bi—Li3^{iii}	87.769 (11)
Li1^{xxxiii}—Li3—In^{xxxiv}	68.8 (4)	Li4—Bi—Li3^{ii}	126.827 (8)
Li1^{xiii}—Li3—In^{xxxiv}	111.2 (4)	Li1—Bi—Li3^{ii}	52.80 (18)
Li5^{xxxiv}—Li3—In^{xxxiv}	0.0	Li1^{xv}—Bi—Li3^{ii}	52.80 (18)
Li1^{xxxi}—Li3—In	111.2 (4)	Li1^{xvi}—Bi—Li3^{ii}	119.9 (4)
Li1^{xiv}—Li3—In	68.8 (4)	Li1^{x}—Bi—Li3^{ii}	123.20 (18)
Li1^{xxxii}—Li3—In	111.2 (4)	Li1^{xxxix}—Bi—Li3^{ii}	123.20 (18)
Li1^{ii}—Li3—In	68.8 (4)	Li1^{viii}—Bi—Li3^{ii}	52.5 (3)
Li1^{xxxiii}—Li3—In	111.2 (4)	In—Bi—Li3^{ii}	53.173 (8)
Li1^{xiii}—Li3—In	68.8 (4)	Li2^{xxvii}—Bi—Li3^{ii}	176.812 (16)
Li5^{xxxiv}—Li3—In	180.0	Li2^{vi}—Bi—Li3^{ii}	89.934 (1)
In^{xxxiv}—Li3—In	180.0	Li2^{xxv}—Bi—Li3^{ii}	89.934 (1)
Li1^{xxxi}—Li3—Bi^{xxxv}	53.96 (16)	Li3^{i}—Bi—Li3^{ii}	87.769 (11)
Li1^{xiv}—Li3—Bi^{xxxv}	126.04 (16)	Li3^{iii}—Bi—Li3^{ii}	87.769 (11)
Li1^{xxxii}—Li3—Bi^{xxxv}	125.1 (4)	Li4—Bi—Bi^{vi}	35.264 (9)
Li1^{ii}—Li3—Bi^{xxxv}	54.9 (4)	Li1—Bi—Bi^{vi}	148.5 (4)
Li1^{xxxiii}—Li3—Bi^{xxxv}	53.96 (16)	Li1^{xv}—Bi—Bi^{vi}	93.3 (3)
Li1^{xiii}—Li3—Bi^{xxxv}	126.04 (16)	Li1^{xvi}—Bi—Bi^{vi}	93.3 (3)
Li5^{xxxiv}—Li3—Bi^{xxxv}	56.299 (11)	Li1^{x}—Bi—Bi^{vi}	93.3 (3)
In^{xxxiv}—Li3—Bi^{xxxv}	56.299 (11)	Li1^{xxxix}—Bi—Bi^{vi}	39.0 (3)
In—Li3—Bi^{xxxv}	123.701 (11)	Li1^{viii}—Bi—Bi^{vi}	93.3 (3)
Li1^{xxxi}—Li3—Bi^{iii}	126.04 (16)	In—Bi—Bi^{vi}	144.736 (8)
Li1^{xiv}—Li3—Bi^{iii}	53.96 (16)	Li2^{xxvii}—Bi—Bi^{vi}	46.161 (6)
Li1^{xxxii}—Li3—Bi^{iii}	54.9 (4)	Li2^{vi}—Bi—Bi^{vi}	91.625 (8)
Li1^{ii}—Li3—Bi^{iii}	125.1 (4)	Li2^{xxv}—Bi—Bi^{vi}	46.161 (6)
Li1^{xxxiii}—Li3—Bi^{iii}	126.04 (16)	Li3^{i}—Bi—Bi^{vi}	136.094 (5)
Li1^{xiii}—Li3—Bi^{iii}	53.96 (16)	Li3^{iii}—Bi—Bi^{vi}	91.563 (7)
Li5^{xxxiv}—Li3—Bi^{iii}	123.701 (11)	Li3^{ii}—Bi—Bi^{vi}	136.094 (5)
In^{xxxiv}—Li3—Bi^{iii}	123.701 (11)	Li4—Bi—Bi^{xxv}	35.264 (5)
In—Li3—Bi^{iii}	56.299 (11)	Li1—Bi—Bi^{xxv}	93.3 (3)
Bi^{xxxv}—Li3—Bi^{iii}	180.0	Li1^{xv}—Bi—Bi^{xxv}	148.5 (4)
Li1^{xxxi}—Li3—Bi^{xxxvi}	125.1 (4)	Li1^{xvi}—Bi—Bi^{xxv}	93.3 (3)
Li1^{xiv}—Li3—Bi^{xxxvi}	54.9 (4)	Li1^{x}—Bi—Bi^{xxv}	39.0 (3)
Li1^{xxxii}—Li3—Bi^{xxxvi}	53.96 (16)	Li1^{xxxix}—Bi—Bi^{xxv}	93.3 (3)
Li1^{ii}—Li3—Bi^{xxxvi}	126.04 (16)	Li1^{viii}—Bi—Bi^{xxv}	93.3 (3)
Li1^{xxxiii}—Li3—Bi^{xxxvi}	53.96 (16)	In—Bi—Bi^{xxv}	144.736 (5)
Li1^{xiii}—Li3—Bi^{xxxvi}	126.04 (16)	Li2^{xxvii}—Bi—Bi^{xxv}	46.161 (11)
Li5^{xxxiv}—Li3—Bi^{xxxvi}	56.299 (8)	Li2^{vi}—Bi—Bi^{xxv}	46.161 (10)
In^{xxxiv}—Li3—Bi^{xxxvi}	56.299 (8)	Li2^{xxv}—Bi—Bi^{xxv}	91.625 (8)
In—Li3—Bi^{xxxvi}	123.701 (8)	Li3^{i}—Bi—Bi^{xxv}	91.563 (7)
Bi^{xxxv}—Li3—Bi^{xxxvi}	92.189 (10)	Li3^{iii}—Bi—Bi^{xxv}	136.094 (10)
Bi^{iii}—Li3—Bi^{xxxvi}	87.811 (10)	Li3^{ii}—Bi—Bi^{xxv}	136.094 (10)
Li1^{xxxi}—Li3—Bi^{i}	54.9 (4)	Bi^{vi}—Bi—Bi^{xxv}	59.999 (5)
Li1^{xiv}—Li3—Bi^{i}	125.1 (4)	Li4—Bi—Bi^{xxvii}	35.264 (5)
Li1^{xxxii}—Li3—Bi^{i}	126.04 (16)	Li1—Bi—Bi^{xxvii}	93.3 (3)
Li1^{ii}—Li3—Bi^{i}	53.96 (16)	Li1^{xv}—Bi—Bi^{xxvii}	93.3 (3)
Li1^{xxxiii}—Li3—Bi^{i}	126.04 (16)	Li1^{xvi}—Bi—Bi^{xxvii}	148.5 (4)
Li1^{xiii}—Li3—Bi^{i}	53.96 (16)	Li1^{x}—Bi—Bi^{xxvii}	93.3 (3)
Li5^{xxxiv}—Li3—Bi^{i}	123.701 (8)	Li1^{xxxix}—Bi—Bi^{xxvii}	93.3 (3)
In^{xxxiv}—Li3—Bi^{i}	123.701 (8)	Li1^{viii}—Bi—Bi^{xxvii}	39.0 (3)
In—Li3—Bi^{i}	56.299 (8)	In—Bi—Bi^{xxvii}	144.736 (5)

Bi^{xxxv}—Li3—Bi^{i}	87.811 (10)
Bi^{iii}—Li3—Bi^{i}	92.189 (10)
Bi^{xxxvi}—Li3—Bi^{i}	180.000 (10)
Li1^{xxxi}—Li3—Bi^{xxxii}	53.96 (16)
Li1^{xiv}—Li3—Bi^{xxxii}	126.04 (16)
Li1^{xxxii}—Li3—Bi^{xxxii}	53.96 (16)
Li1^{ii}—Li3—Bi^{xxxii}	126.04 (16)
Li1^{xxxiii}—Li3—Bi^{xxxii}	125.1 (4)
Li1^{xiii}—Li3—Bi^{xxxii}	54.9 (4)
Li5^{xxxiv}—Li3—Bi^{xxxii}	56.299 (9)
In^{xxxiv}—Li3—Bi^{xxxii}	56.299 (9)
In—Li3—Bi^{xxxii}	123.701 (8)
Bi^{xxxv}—Li3—Bi^{xxxii}	92.189 (10)
Bi^{iii}—Li3—Bi^{xxxii}	87.811 (10)
Bi^{xxxvi}—Li3—Bi^{xxxii}	92.189 (10)
Bi^{i}—Li3—Bi^{xxxii}	87.811 (10)
Li1^{xxxi}—Li3—Bi^{ii}	126.04 (16)
Li1^{xiv}—Li3—Bi^{ii}	53.96 (16)
Li1^{xxxii}—Li3—Bi^{ii}	126.04 (16)
Li1^{ii}—Li3—Bi^{ii}	53.96 (16)
Li1^{xxxiii}—Li3—Bi^{ii}	54.9 (4)
Li1^{xiii}—Li3—Bi^{ii}	125.1 (4)
Li5^{xxxiv}—Li3—Bi^{ii}	123.701 (8)
In^{xxxiv}—Li3—Bi^{ii}	123.701 (8)
In—Li3—Bi^{ii}	56.299 (9)
Bi^{xxxv}—Li3—Bi^{ii}	87.811 (10)
Bi^{iii}—Li3—Bi^{ii}	92.189 (10)
Bi^{xxxvi}—Li3—Bi^{ii}	87.811 (10)
Bi^{i}—Li3—Bi^{ii}	92.189 (10)
Bi^{xxxii}—Li3—Bi^{ii}	180.00 (2)
Li1^{xxxi}—Li3—Li3^{iii}	91.5 (3)
Li1^{xiv}—Li3—Li3^{iii}	88.5 (3)
Li1^{xxxii}—Li3—Li3^{iii}	146.4 (4)
Li1^{ii}—Li3—Li3^{iii}	33.6 (4)
Li1^{xxxiii}—Li3—Li3^{iii}	91.5 (3)
Li1^{xiii}—Li3—Li3^{iii}	88.5 (3)
Li5^{xxxiv}—Li3—Li3^{iii}	144.736 (8)
In^{xxxiv}—Li3—Li3^{iii}	144.736 (8)
In—Li3—Li3^{iii}	35.264 (8)
Bi^{xxxv}—Li3—Li3^{iii}	88.436 (7)
Bi^{iii}—Li3—Li3^{iii}	91.564 (7)
Bi^{xxxvi}—Li3—Li3^{iii}	133.884 (5)
Bi^{i}—Li3—Li3^{iii}	46.116 (5)
Bi^{xxxii}—Li3—Li3^{iii}	133.884 (5)
Li2^{xxvii}—Bi—Bi^{xxvii}	91.625 (8)
Li2^{vi}—Bi—Bi^{xxvii}	46.161 (10)
Li2^{xxv}—Bi—Bi^{xxvii}	46.161 (11)
Li3^{i}—Bi—Bi^{xxvii}	136.094 (10)
Li3^{iii}—Bi—Bi^{xxvii}	136.094 (10)
Li3^{ii}—Bi—Bi^{xxvii}	91.563 (7)
Bi^{vi}—Bi—Bi^{xxvii}	59.999 (5)
Bi^{xxv}—Bi—Bi^{xxvii}	59.999 (11)
Li4—Bi—Bi^{xl}	90.920 (4)
Li1—Bi—Bi^{xl}	90.832 (9)
Li1^{xv}—Bi—Bi^{xl}	35.7 (2)
Li1^{xvi}—Bi—Bi^{xl}	141.1 (2)
Li1^{x}—Bi—Bi^{xl}	148.06 (14)
Li1^{xxxix}—Bi—Bi^{xl}	88.996 (9)
Li1^{viii}—Bi—Bi^{xl}	35.11 (14)
In—Bi—Bi^{xl}	89.080 (4)
Li2^{xxvii}—Bi—Bi^{xl}	136.068 (5)
Li2^{vi}—Bi—Bi^{xl}	91.593 (8)
Li2^{xxv}—Bi—Bi^{xl}	43.839 (6)
Li3^{i}—Bi—Bi^{xl}	133.821 (6)
Li3^{iii}—Bi—Bi^{xl}	88.407 (8)
Li3^{ii}—Bi—Bi^{xl}	46.095 (5)
Bi^{vi}—Bi—Bi^{xl}	90.0
Bi^{xxv}—Bi—Bi^{xl}	121.296 (7)
Bi^{xxvii}—Bi—Bi^{xl}	61.306 (9)
Li4—Bi—Bi^{iv}	90.920 (16)
Li1—Bi—Bi^{iv}	35.7 (2)
Li1^{xv}—Bi—Bi^{iv}	90.832 (18)
Li1^{xvi}—Bi—Bi^{iv}	141.1 (2)
Li1^{x}—Bi—Bi^{iv}	88.996 (16)
Li1^{xxxix}—Bi—Bi^{iv}	148.06 (14)
Li1^{viii}—Bi—Bi^{iv}	35.11 (14)
In—Bi—Bi^{iv}	89.080 (16)
Li2^{xxvii}—Bi—Bi^{iv}	136.068 (10)
Li2^{vi}—Bi—Bi^{iv}	43.839 (10)
Li2^{xxv}—Bi—Bi^{iv}	91.593 (8)
Li3^{i}—Bi—Bi^{iv}	88.407 (8)
Li3^{iii}—Bi—Bi^{iv}	133.821 (11)
Li3^{ii}—Bi—Bi^{iv}	46.095 (11)
Bi^{vi}—Bi—Bi^{iv}	121.296 (8)
Bi^{xxv}—Bi—Bi^{iv}	89.999 (19)
Bi^{xxvii}—Bi—Bi^{iv}	61.306 (12)
Bi^{xl}—Bi—Bi^{iv}	62.595 (13)

Symmetry codes: (i) −*x*+1/4, *y*, −*z*+1/4; (ii) −*x*+1/4, −*y*+1/4, *z*; (iii) *x*, −*y*+1/4, −*z*+1/4; (iv) *x*+1/4, −*y*+1/2, *z*−1/4; (v) *x*+1/4, *y*−1/4, −*z*+1/2; (vi) *x*, −*y*+3/4, −*z*+3/4; (vii) *x*, *y*−1/2, *z*−1/2; (viii) *y*+1/4, −*z*+1/2, *x*−1/4; (ix) −*y*+1/2, −*z*, −*x*+1/2; (x) −*z*+1/2, *x*−1/4, *y*+1/4; (xi) −*z*+1/2, −*x*+1/2, −*y*; (xii) −*x*+1, −*y*+1/2, −*z*+1/2; (xiii) −*y*+1/4, *z*, −*x*+1/4; (xiv) *z*, −*x*+1/4, −*y*+1/4; (xv) *z*, *x*, *y*; (xvi) *y*, *z*, *x*; (xvii) −*x*+1, −*y*+1, −*z*+1; (xviii) −*y*+1/2, −*z*+1/2, −*x*+1; (xix) *x*, *y*+1/2, *z*+1/2; (xx) *y*+1/2, *z*+1/2, *x*; (xxi) −*z*+1/2, −*x*+1, −*y*+1/2; (xxii) *z*+1/2, *x*, *y*+1/2; (xxiii) −*x*+1, *y*+1/4, *z*+1/4; (xxiv) *x*+1/4, −*y*+1, *z*+1/4; (xxv) −*x*+3/4, *y*, −*z*+3/4; (xxvi) *x*+1/4, *y*+1/4, −*z*+1; (xxvii) −*x*+3/4, −*y*+3/4, *z*; (xxviii) *x*, −*y*+5/4, −*z*+5/4; (xxix) −*x*+5/4, *y*, −*z*+5/4; (xxx) −*x*+5/4, −*y*+5/4, *z*; (xxxi) −*z*, *x*−1/4, *y*−1/4; (xxxii) *x*−1/4, *y*−1/4, −*z*; (xxxiii) *y*−1/4, −*z*, *x*−1/4; (xxxiv) −*x*, −*y*, −*z*; (xxxv) −*x*, *y*−1/4, *z*−1/4; (xxxvi) *x*−1/4, −*y*, *z*−1/4; (xxxvii) *x*, −*y*−1/4, −*z*−1/4; (xxxviii) −*x*−1/4, *y*, −*z*−1/4; (xxxix) *x*−1/4, *y*+1/4, −*z*+1/2; (xl) −*x*+1/2, *y*+1/4, *z*−1/4.