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INTERMETALLIC COMPOUNDS  
BETWEEN LITHIUM AND LEAD  
V. BRILLOUIN POLYHEDRA  
OF THE VARIOUS PHASES

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UCRL-5801  
Chemistry-General  
TID-4500, UC-4  
15th Edition

UNIVERSITY OF CALIFORNIA  
Lawrence Radiation Laboratory  
Livermore, California

Contract No. W-7405-eng-48

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Printed for the U. S. Atomic Energy Commission

1950  
U.S. GOVERNMENT PRINTING OFFICE  
16-50811-1

THE  
OFFICE OF TECHNICAL SERVICES  
U. S. DEPARTMENT OF COMMERCE

WASHINGTON, D. C.

Printed in USA. Price 50 cents. Available from the  
Office of Technical Services  
U. S. Department of Commerce  
Washington 25, D.C.

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ABSTRACT

A determination of the Brillouin polyhedra for intermetallic compounds allows an estimation, prediction or explanation of some electromagnetic and structural properties. Brillouin polyhedra for the intermetallic compounds between lithium and lead are presented and discussed.

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\*This work was performed under the auspices of the U. S. Atomic Energy Commission.

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INTRODUCTION

Structures of the five intermetallic compounds between lithium and lead;  $\text{LiPb}$ ,<sup>1,2</sup>  $\text{Li}_3\text{Pb}$ ,<sup>3</sup>  $\text{Li}_8\text{Pb}_3$ ,<sup>4</sup>  $\text{Li}_7\text{Pb}_2$ ,<sup>3</sup> and  $\text{Li}_{22}\text{Pb}_5$ ,<sup>5</sup> have been determined by x-ray diffraction. Since the atomic scattering factor for x-rays (and electrons) of lead is quite large while that of lithium is small, structure assignments are made on the basis of lead lattice positions determined by diffraction and of lithium positions determined by stoichiometric and steric considerations.

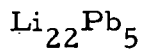
Once the structure of a phase is known, Brillouin polyhedra for that structure may be determined.<sup>6</sup> A systematic method for calculating volumes of Brillouin polyhedra for cubic, hexagonal, tetragonal, and orthorhombic systems has been presented.<sup>7</sup>

If  $\underline{n}$  is the number of nearly free electrons per unit cell of a structure, only those Brillouin polyhedra which contain about  $\underline{n}$  states per unit cell will be of interest in our approximation. Because the choice of valences of atoms in a structure determines the value of  $\underline{n}$ , that choice determines which polyhedra are thought to be significant. For example, Mott and Jones,<sup>6</sup> using valences of one for copper and two for zinc, find that the proper Brillouin

- 
- (1) H. Nowotny, Z. Metallkunde, 33, 388 (1941).  
 (2) A. Zalkin and W. J. Ramsey, J. Phys. Chem., 61, 1413 (1957).  
 (3) A. Zalkin and W. J. Ramsey, ibid., 60, 234 (1956).  
 (4) A. Zalkin, D. H. Tempelton, and W. J. Ramsey, ibid., 1275 (1956).  
 (5) A. Zalkin and W. J. Ramsey, ibid., 62, 689 (1958).  
 (6) Cf. N. F. Mott and H. Jones, The Theory of the Properties of Metals and Alloys, pp. 152-174, Dover Publs., N. Y., N. Y., 1958.  
 (7) D. P. Shoemaker and T. C. Huang, Acta Cryst., 7, 249 (1954).

polyhedron for  $\gamma$  brass ( $\text{Cu}_5\text{Zn}_8$  with 84 electrons per unit cell) is bounded by the forms  $\{330\}$  and  $\{411\}$  and contains just 90 electrons per unit cell. In sharp contrast for the same alloy, Shoemaker and Huang,<sup>7</sup> implying valences of about 5.5 for copper and 4.5 for zinc (i.e., about 254 electrons per unit cell), have calculated the volume of the polyhedron bounded by  $\{600\}$  and  $\{422\}$  to be 255.6 electrons per cell. Such a contrast in description should be experimentally resolvable.<sup>8</sup>

Insofar as a determination of the Brillouin polyhedra for intermetallic compounds makes possible an explanation of some properties and a prediction of other properties of the compounds, such a determination is of value. Proposed polyhedra for the lithium-lead intermetallic compounds together with a discussion are presented below.



$\text{Li}_{22}\text{Pb}_5$  has a complex face-centered cubic structure; space group, F23;  $a_0 = 20.08\text{\AA}$ ;  $Z = 16$ .<sup>5</sup> The lead atom positions in the cell are:<sup>9</sup>

$$\begin{aligned} 16e \text{ at } \underline{x}_1 &= -0.0859 \pm 0.0003 \\ 16e \text{ at } \underline{x}_1' &= \underline{x}_1 - \frac{1}{4} = -0.3359 \\ 24f \text{ at } \underline{x}_2 &= 0.3211 \pm 0.0003 \\ 24g \text{ at } \underline{x}_2' &= \underline{x}_2 - \frac{1}{4} = 0.0711 \end{aligned}$$

A valence of four for lead and one for lithium leads to a value of 672 for the number of electrons per unit cell. Four is taken to be the valence of lead because bond-order, bond-length considerations<sup>10</sup> give almost exactly four for the valence of lead in the other three most lithium rich compounds,  $\text{Li}_7\text{Pb}_2$ ,  $\text{Li}_3\text{Pb}$ , and  $\text{Li}_8\text{Pb}_3$ . Also it is reasonable to expect that lead would exhibit its maximum covalence, four, in the most lithium-rich compound. Lithium atom positions within the unit cell cannot be estimated with sufficient accuracy to allow meaningful calculations of bond orders.

(8) Cf. B. Lax, Rev. Mod. Phys. 30, 122 (1958).

(9) Terminology from "International Tables for X-Ray Crystallography" Kynoch Press, Birmingham, England, 1952.

(10) Cf. L. Pauling, The Electronic Structure of Metals and Alloys in "The Theory of Alloy Phases" pp. 220-242, Amer. Soc. for Metals, 1956.



With 672 electrons per unit cell, planes for which  $h^2 + k^2 + \ell^2$  is approximately 75 will be of interest. Structure factors are given by,

$$S_{hkl} = 8 \left\{ 1 + e^{2\pi i \left( \frac{-h+k+\ell}{4} \right)} \right\} \left\{ 2(\cos 2\pi h x_1 \cos 2\pi k x_1 \cos 2\pi \ell x_1 - i \sin 2\pi h x_1 \sin 2\pi k x_1 \sin 2\pi \ell x_1) + \cos 2\pi h x_2 + \cos 2\pi k x_2 + \cos 2\pi \ell x_2 \right\} . *$$

$S_{hkl}$  will have values other than zero only for  $h$ ,  $k$ , and  $\ell$  all even, or all odd. The following structure factors are computed:

$$\begin{array}{l} \{hkl\}: \{800\} \quad \{733\} \quad \{660\} \quad \{822\} \quad \{555\} \quad \{751\} \quad \{840\} \\ |S_{hkl}|: 5.3 \quad 26.2 \quad 76.8 \quad 37.7 \quad 43.6 \quad 3.0 \quad 4.8 \end{array}$$

In Table I are shown the volumes of polyhedra bounded by various combinations of these sets of planes, and the various forms are shown in Fig. 1.

Table I

<u>Bounding Planes</u>	<u>Volume (states per cell)</u>
{660}, {822}	720
{660}, {822}, {555}	696
{660}, {822}, {555}, {751}	690.7
{733}, {660}, {555}, {822}	643.1

$\text{Li}_3\text{Bi}$  is known to be a semiconductor<sup>11</sup> (see also, below, the discussion of  $\text{Li}_3\text{Pb}$ ). An attempt was made at this laboratory to observe the nuclear magnetic resonance of  $\text{Li}^7$  in  $\text{Li}_3\text{Bi}$  and the various Li-Pb intermetallic compounds.<sup>12</sup> Resonances were observed in  $\text{Li}_3\text{Bi}$ ,  $\text{Li}_{22}\text{Pb}_5$ ,  $\text{Li}_7\text{Pb}_2$ ,  $\text{Li}_3\text{Pb}$ , and  $\text{Li}_8\text{Pb}_3$ , and not in  $\text{LiPb}$ . It is suspected that the high electrical conductivity of  $\text{LiPb}$  made that observation difficult. The resonance lines were quite narrow for  $\text{Li}_3\text{Bi}$  and  $\text{Li}_{22}\text{Pb}_5$  while they were broad for  $\text{Li}_7\text{Pb}_2$ ,  $\text{Li}_3\text{Pb}$ , and  $\text{Li}_8\text{Pb}_3$ . In this case, a narrow resonance line strongly suggests semi-conducting properties.

\* This equation is incorrectly given in reference 5.

(11)E. Mosser and W. B. Pearson, Phys. Rev., 101, 492 (1956).

(12)Dr. B. E. Holder, this laboratory, personal communication.

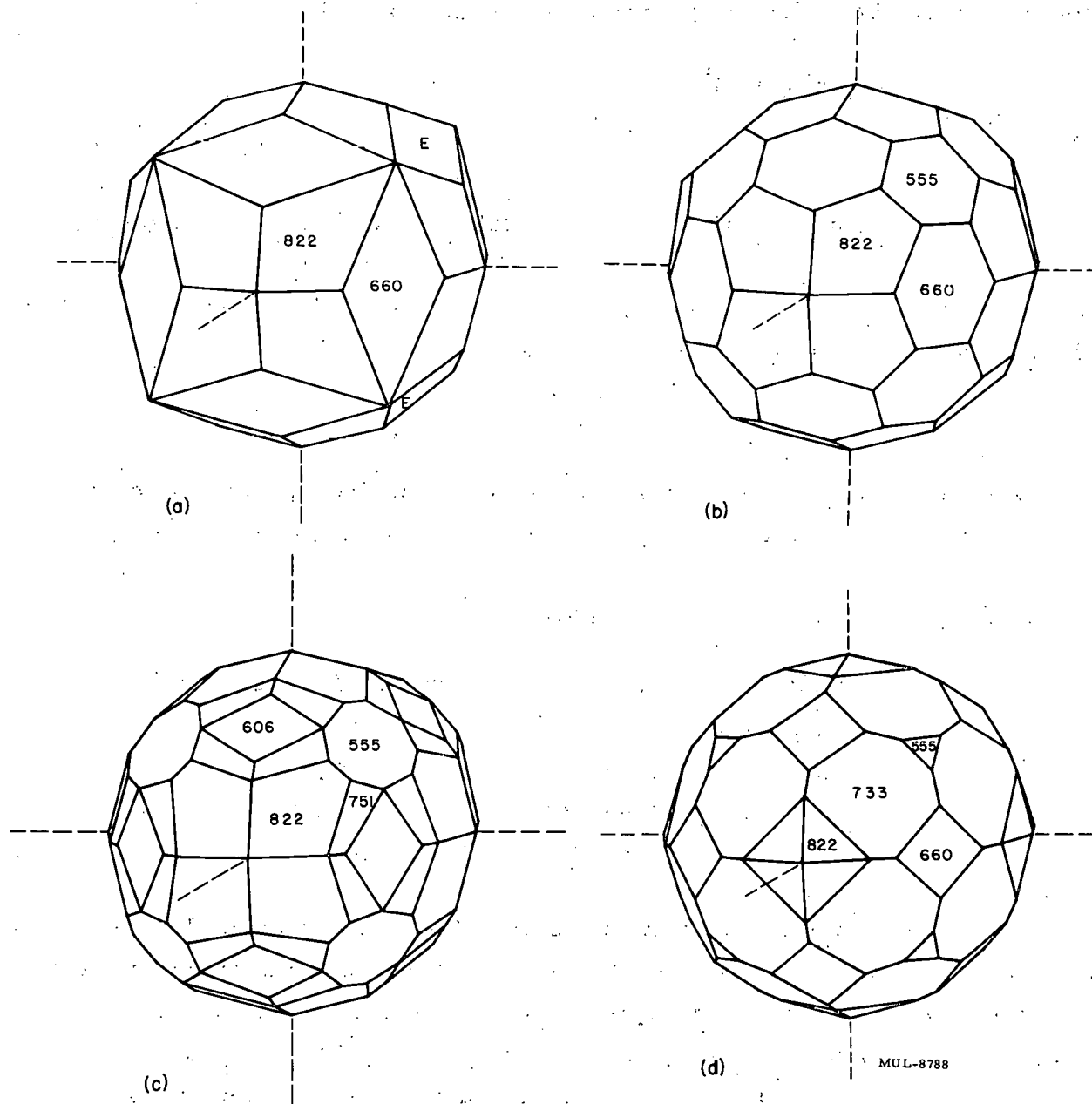
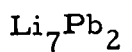


Fig. 1. Brillouin polyhedra of interest for  $\text{Li}_{22}\text{Pb}_5$ . (a) Bounded by  $\{822\}$ ,  $\{660\}$ \*; (b) by  $\{822\}$ ,  $\{660\}$ ,  $\{555\}$ ; (c) by  $\{822\}$ ,  $\{660\}$ ,  $\{555\}$ ,  $\{751\}$ ; (d) by  $\{822\}$ ,  $\{660\}$ ,  $\{555\}$ ,  $\{733\}$ .

\*This zone is exactly geometrically similar to the proposed first zone for  $\gamma$ -brass which is bounded by  $\{330\}$  and  $\{411\}$ . However, every picture of this zone with which we are familiar (Cf. Mott and Jones,<sup>6</sup> Fig. 71) is incorrectly drawn in that planes marked E in the figure are improperly foreshortened.

If  $\text{Li}_{22}\text{Pb}_5$  is indeed a semiconductor, we choose for the first Brillouin zone that one bounded by  $\{733\}$ ,  $\{822\}$ ,  $\{660\}$  and  $\{555\}$  (Fig. 1d). This zone is bounded by planes with large structure factors, and contains approximately 643 states per cell. The average composition of this phase should then be  $\text{Li}_{4.08}\text{Pb}$  to just fill this zone with electrons. In order to fill any of the somewhat larger zones of Fig. 1, either the interstitial addition of lithium to the lattice or the substitution of lead atoms for lithium atoms in the lattice would be necessary. Such filling would be quite costly energetically.



$\text{Li}_7\text{Pb}_2$  has a hexagonal structure,<sup>3</sup> space group  $D_3^2 - P321$ ,  $Z = 1$ ,  $a = 4.751\text{\AA}$ ,  $c = 8.589\text{\AA}$ , and  $c/a = 1.808$ . The proposed positions are:<sup>9</sup>

- 2 Pb in 2(d)  $1/3, 2/3, z, 2/3, 1/3, \bar{z}, z = +1/4$
- 4 Li(I) in 2(d)  $z = -1/12$  and  $z = -5/12$
- 2 Li(II) in 2(c)  $00z, 00\bar{z}, z = 1/3$
- 1 Li(III) in 1(a)  $000$

Structure factors for this phase are given by,

$$S_{hkl} = e^{2\pi i \left( \frac{h+2k}{3} + \frac{l}{4} \right)} + e^{2\pi i \left( \frac{2h+k}{3} - \frac{l}{4} \right)},$$

which gives rise to the following values:

$$\begin{array}{l} \{hkl\}: \{101\} \{102\} \{003\} \{110\} \{103\} \{111\} \{004\} \{112\} \\ |S_{hkl}|: 1.732 \quad 1 \quad 0 \quad 2 \quad 1.93 \quad 0 \quad 2 \quad 2 \end{array}$$

We choose the polyhedron bounded by  $\{110\}$ ,  $\{103\}$  and  $\{004\}$  which is shown in Fig. 2. A valence of one for lithium and four for lead gives 45 electrons per unit cell. The Brillouin zone contains 49.5 electrons per cell, while the inscribed sphere contains 39.4 electrons or 79.5 percent of the volume.

A choice of four for the valence of lead was made on the basis of bond-order, bond-length considerations<sup>10</sup> which led to a sum of four of the orders of bonds to near neighboring atoms. This theory was not applicable in the case of the lithium atoms because of the excessively low orders of the lithium-lithium bonds. A valence of one for lithium is however an obvious choice.

An equation relating the number of states per unit cell,  $N$ , which this polyhedron will contain to  $b(= \underline{a}/\underline{c})$  has been derived:

$$N = 36 \left( -\frac{5}{81b^2} + \frac{5}{3} - \frac{3}{8} b^2 + \frac{9}{32} b^4 \right), \quad 0.475 \leq b \leq 0.667. \quad (1)$$

At  $b = 0.475$ ,  $\{004\}$  begins to intersect  $\{110\}$ , while at  $b = 0.667$ ,  $\{112\}$  begins to truncate the polyhedron. A plot of equation (1) is shown in Fig. 3. Care must be taken in applying equation (1) to structures similar to  $\text{Li}_7\text{Pb}_2$ , e.g.,  $\text{Na}_3\text{As}$ , in that the more scarce atoms must be the predominant scatterers.

Since for this compound the zone is well over half full, and is bounded by planes of relatively large structure factors, the compound should prove to be a moderately poor, hole-type conductor.

### $\text{Li}_3\text{Pb}$

$\text{Li}_3\text{Pb}$  is face-centered cubic, space group  $O_h^5 - \text{Fm}3\text{m}$ ,  $Z = 4$ ,  $\underline{a} = 6.687\text{\AA}$ .<sup>3</sup> The positions suggested are:<sup>9</sup>

- 4 Pb in 4(a) 0, 0, 0; plus face-centering
- 4 Li(I) in 4(b) 1/2, 1/2, 1/2; plus face-centering
- 8 Li(II) in 8(c) 1/4, 1/4, 1/4; 3/4, 3/4, 3/4; plus face-centering

The structure factors,  $S_{hkl}$ , are equal to just four if  $\underline{h}$ ,  $\underline{k}$  and  $\underline{l}$  are all even or all odd and are equal to zero otherwise.

A valence of four for lead is taken on the basis of bond-order, bond-length considerations,<sup>10</sup> which give a value of almost exactly four for the sum of the orders of the bonds between lead atoms and near neighbors. A valence of one is taken for lithium, and the bond-order, bond-length theory is inapplicable because of the excessively low order of the bonds between lithium atoms. Thus there are 28 electrons per unit cell.

For this compound, a first Brillouin zone bounded by  $\{220\}$  and  $\{311\}$  is proper. This zone together with that bounded by  $\{220\}$  only are shown in Figs. 4a and 4b, respectively. Their volumes are exactly  $31\frac{2}{3}$  and 32 states, respectively, per unit cell. Truncation of the zone by  $\{311\}$  reduces its volume by only about one percent. The inscribed sphere contains 74.7% of the volume or about 23.6 states per cell. On the basis of the above considerations, it is predicted that  $\text{Li}_3\text{Pb}$  would be a relatively poor, hole-type conductor.

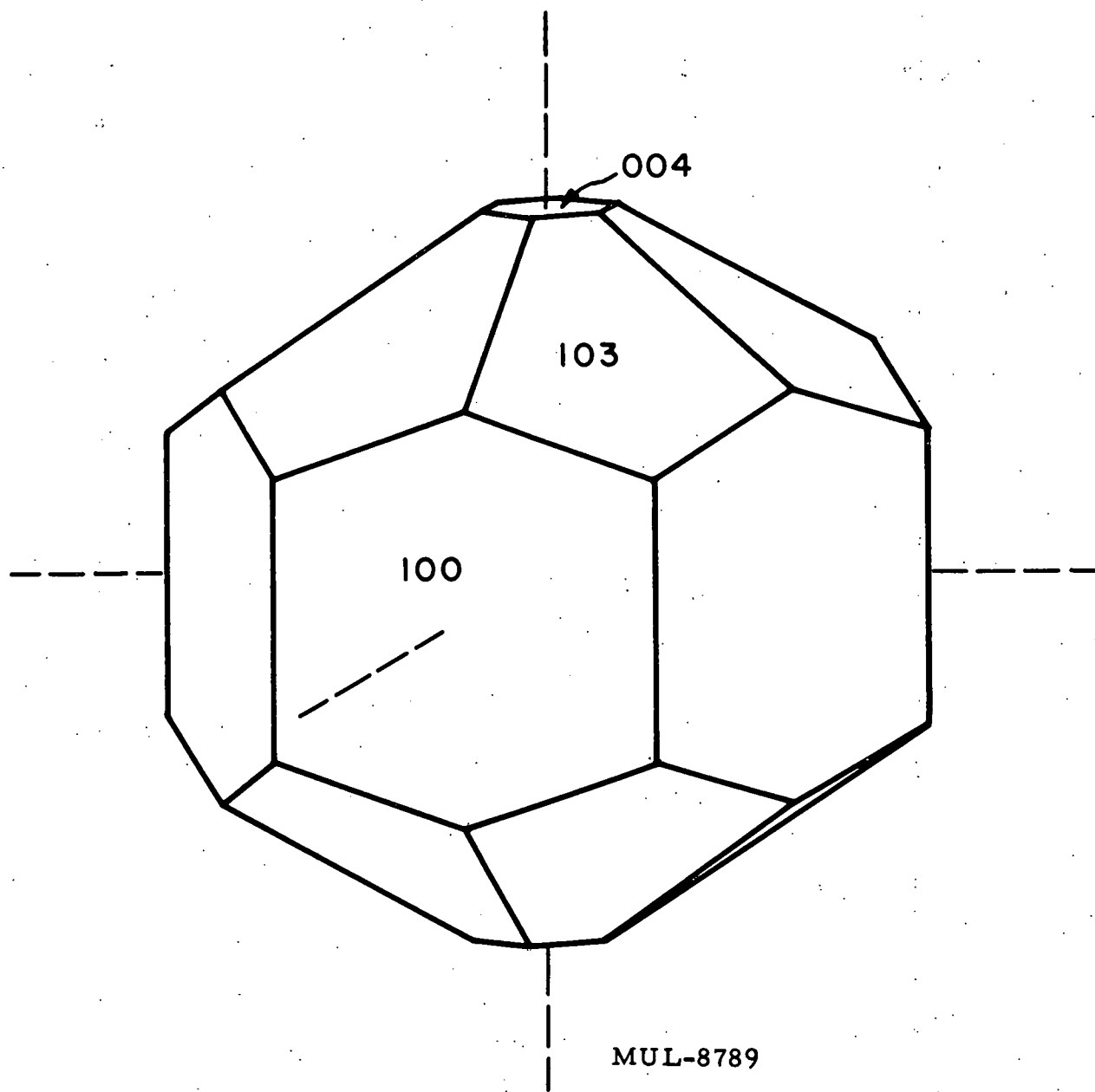
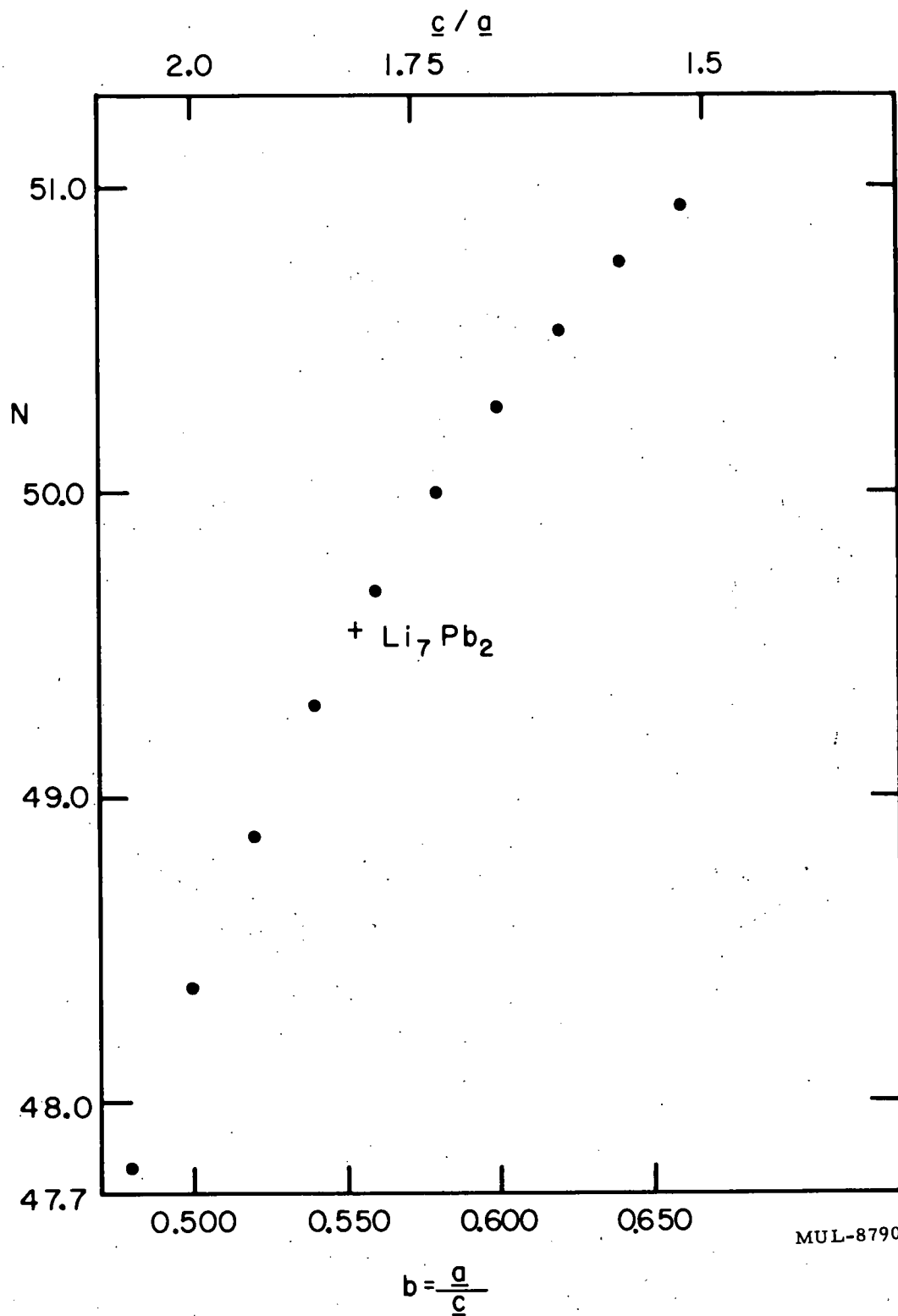


Fig. 2. The first Brillouin zone for  $\text{Li}_7\text{Pb}_2$ .



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Fig. 3. N, the number of states per cell in  $\text{Li}_7\text{Pb}_2$  like structures, vs  $b = \frac{a}{c}$ .

$\text{Li}_3\text{Bi}$  is isostructural and very nearly isometric to  $\text{Li}_3\text{Pb}$ .<sup>13</sup> With a valence of five for bismuth and one for lithium, there would be 32 electrons per unit cell for this compound, and it would be predicted to be a semiconductor on the basis of a full Brillouin zone bounded by {220}. The compound has been demonstrated to be a semiconductor.<sup>11</sup> However, since the planes {311} have the same large structure factors as the planes {220} they must represent as large an energy discontinuity. Thus the {220} planes would be overrun where they are closest to the origin before the {311} planes were overrun. Since  $\text{Li}_3\text{Bi}$  is a semiconductor, it would be predicted, on the basis of the free electron approximation, that this phase has the composition  $\text{Li}_{35}\text{Bi}_{12}$  with  $31\frac{2}{3}$  electrons per unit cell on the average. A choice between the free electron approximation and the concept of a semiconducting bond<sup>14</sup> for this phase, which makes the composition  $\text{Li}_3\text{Bi}$  necessary, could be made on the basis of a very careful determination of the stoichiometry of the phase.

$\text{Li}_8\text{Pb}_3$

$\text{Li}_8\text{Pb}_3$  is monoclinic, space group C2/m,  $a = 8.240\text{\AA}$ ,  $b = 4.757\text{\AA}$ ,  $c = 11.03\text{\AA}$ ,  $\beta = 104^\circ 25'$ , and  $Z = 2$ .<sup>3</sup> The suggested positions are:<sup>9</sup>

2 Pb(I) in 2(a): (0, 0, 0) + (c).

4 Pb(II) in 4(i):  $\pm (x, 0, z) + (c)$ ;  $x = 5/11$ ,  $z = 4/11$

4 Li(I) in 4(i):  $x = 4/11$ ,  $z = 1/11$

4 Li(II) in 4(i):  $x = 3/11$ ,  $z = 9/11$

4 Li(III) in 4(i):  $x = 2/11$ ,  $z = 6/11$

4 Li(IV) in 4(i):  $x = 1/11$ ,  $z = 3/11$

Structure factors,  $S_{hkl}$ , are given by

$$S_{hkl} = \{1 + 2 \cos 2\pi(hx + lz)\} \left(1 + e^{2\pi i \frac{h+k}{2}}\right).$$

And so,  $S_{hkl}$  has values other than zero only for  $h+k = 2n$ ,  $n = 0, 1, 2, \dots$

We give below the values of  $S_{hkl}$  for some values of  $h, k$ , and  $l$ :

$hkl$ :	202, $11\bar{3}$ ,	004	$20\bar{4}$ , 113	203, 020, $11\bar{4}$ , $31\bar{1}$	021, $31\bar{2}$
$S_{hkl}$ :	0.644	1.84	1.84	6	0.644
$hkl$ :	022, 311, $31\bar{3}$	005	$20\bar{5}$ , 114		
$S_{hkl}$ :	1.44	3.66	5.36		

(13) G. Brauer and E. Zintl, Z. Physik. Chem., **37B**, 323 (1937).

(14) E. Mosser and W. B. Pearson, J. Chem. Phys. **26**, 893 (1957).

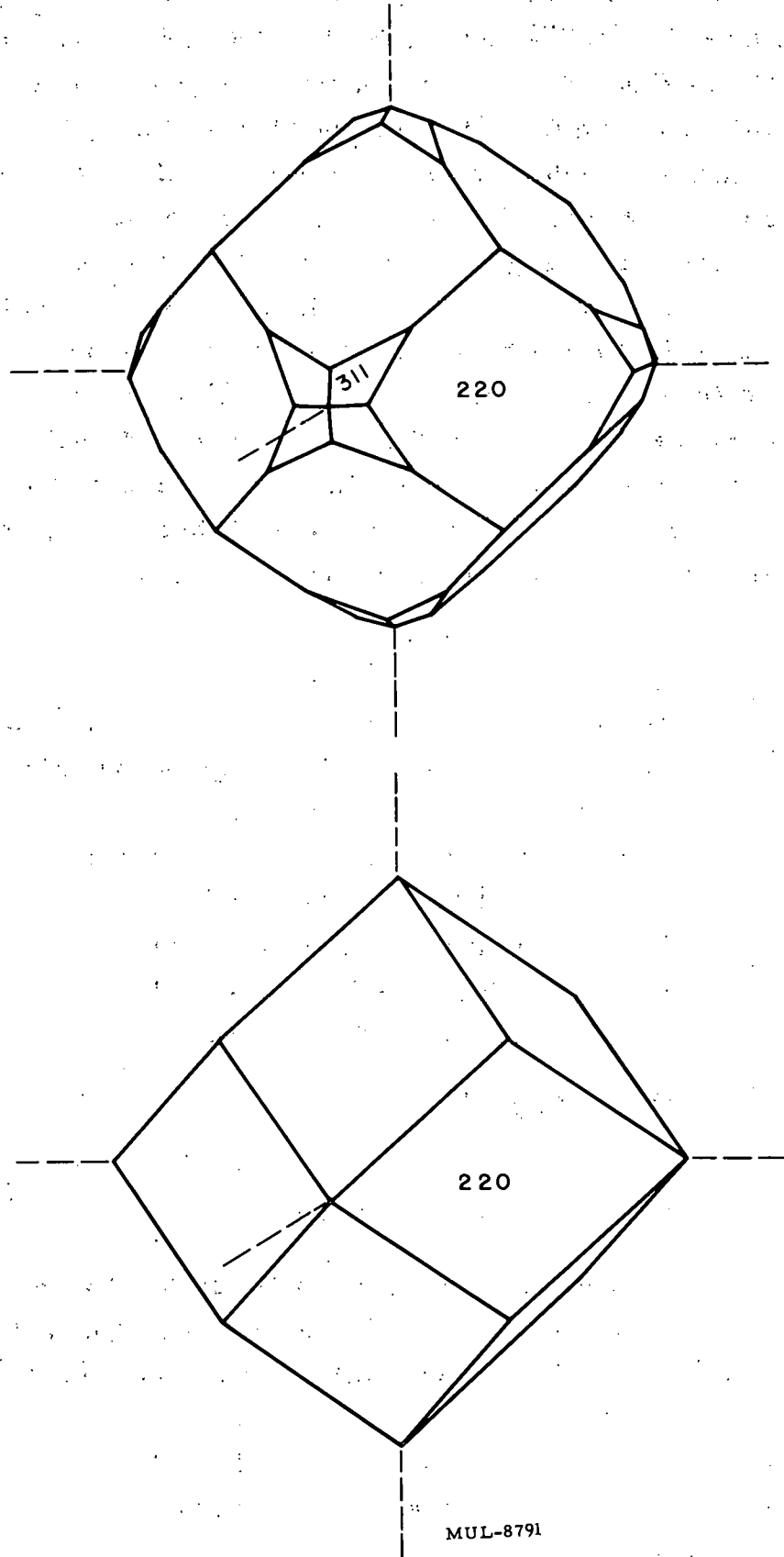


Fig.4. (a) The first Brillouin zone for  $\text{Li}_3\text{Pb}$ ; (b) A zone bounded by {220} only.



The selection of a valence of four for lead is based on bond-order, bond-length considerations<sup>10</sup> which give very nearly four for the sum of the orders of the bonds between any lead atom and its near neighbors (see below). A valence of one is taken for lithium, and the bond-order, bond-length theory is inapplicable. Thus for  $\text{Li}_8\text{Pb}_3$  there are 40 electrons per cell.

To accommodate 40 electrons per cell, a Brillouin zone bounded by  $\{203\}$ ,  $\{020\}$ ,  $\{11\bar{4}\}$ , and  $\{31\bar{1}\}$  is chosen. This zone contains 43.8 states per cell, and is shown in Fig. 5. It will be noted that this zone is identical, except for an isotropic scaling factor, to the zone bounded by  $\{110\}$  in the cubic system. The inscribed sphere contains 74 percent of the total volume of the zone, or 32.4 states per cell.

With 40 electrons in a zone capable of containing 43.8 electrons it could be reasonable to assert that the zone is 91.4 percent filled. However, in this structure there are two kinds of lead atoms, and in each unit cell there are two pairs of lead atoms and two single lead atoms. The distance between the lead atoms of a pair is  $2.91\text{\AA}$  which is almost exactly the lead-lead single covalent bond distance ( $2.86\text{\AA}$ <sup>10</sup>) for tetravalent lead. It is suggested therefore that these two single bonds per cell form a narrow band of their own, which band does not contribute to the conduction band. There are then 36 conduction electrons per cell, and the zone is 82.2 percent full. The compound will still be a hole-type conductor, but a better conductor than would be expected on the basis of a fully free electron approximation.

### LiPb

Stoichiometric LiPb has the CsCl, B2, structure above  $214^\circ\text{C}$ , at which temperature  $a_0 = 3.563\text{\AA}$ . Below this temperature the lattice continuously distorts rhombohedrally, and at room temperature the rhombohedral angle is  $89^\circ 30'$ .<sup>2</sup> At lower temperatures, the rhombohedral angle does not decrease much more. The homogeneity range for the phase is from 50 to approximately 53 atoms percent lithium.<sup>15</sup> As LiPb is saturated with lithium, the cell constant,  $a_0$ , decreases, at room temperature, from  $3.54_2$  to  $3.53_2\text{\AA}$ ; while the room temperature rhombohedral angle increases to very nearly  $90^\circ$ ; and the temperature of the transition, as measured by electrical resistivity, decreases from  $215^\circ\text{C}$  to  $185^\circ\text{C}$ .

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(15) G. Grube and H. Klaiber, Z. Electrochem., 40, 745 (1934); these authors determined the complete phase diagram for the Li-Pb system.

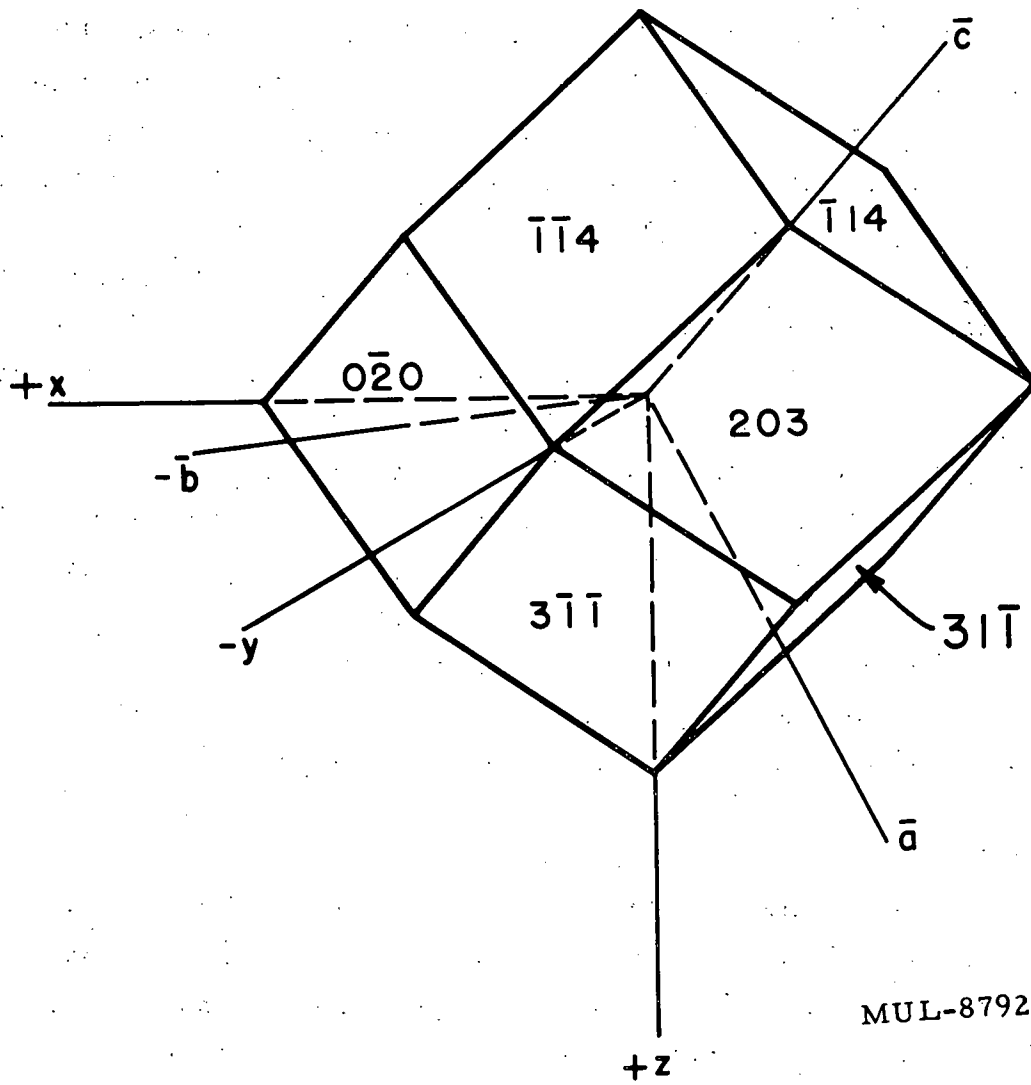


Fig.5. The first Brillouin zone for  $\text{Li}_8\text{Pb}_3$ . A set of orthogonal axes and the reciprocal lattice directions are shown.

Since the volume of the unit cell decreases with increasing relative lithium content, either the lithium atoms replace lead atoms in the lattice, or vacant lead atom sites are produced in the lattice. Either case leads to a calculation of fewer electrons per unit cell in the lithium-rich compound than in the stoichiometric compound.

For reasons to be described below, it is proposed that the lead atoms have a character that is partially that of  $\text{Pb}^{\text{II}}$  and partially that of  $\text{Pb}^{\text{III}+}$ , while the lithium atoms are characterized as partially  $\text{Li}^{\text{I}}$  and partially  $\text{Li}^{\text{II}-}$ . (Here the roman numerals indicate the valences for covalent bonding.) Following Pauling,<sup>16</sup> charge transfer is to be expected in order to restore the electrical neutrality of the atoms of the lattice. The electronegativity difference between lithium and lead is about 0.65,<sup>17</sup> and so bonds between lithium and lead will be about 10% ionic.<sup>18</sup> If  $\underline{c}$  is the fraction of charge transferred from the lead atoms to the lithium atoms, then  $\underline{c} + 1$  is the number of lithium, lead bonds that will be formed and,  $0.10 (\underline{c} + 1)$  is the fraction of charge transferred from the lithium to lead atoms because of the partial ionic character of the bonds. The condition for electroneutrality is, then

$$\underline{c} - 0.10 (\underline{c} + 1) = 0 .$$

Therefore the fraction of charge transferred is 0.11. For this model then, the average valence of the lead is 2.11 while that of the lithium is 1.11, and there are 3.22 electrons per unit cell.

A first Brillouin zone bounded by  $\{110\}$  planes contains four electrons per unit cell, while the inscribed sphere contains 3.08 electrons per unit cell. This zone is appropriate for  $\text{LiPb}$  and is exactly similar to that shown in Fig. 4b. On the basis of zone theory, it is predicted that  $\text{LiPb}$  should be a good "hole"-type conductor.

No explanation can be given for the existence of the rhombohedral phase of the compound. It would certainly appear that the rhombohedral distortion is due to some property of the state of the lead atoms in the lattice because

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(16) L. Pauling, Proceedings of the National Academy of Science, 39, 551 (1953).

(17) W. Gordy and W. J. O. Thomas, J. Chem. Phys., 24, 439 (1956).

(18) L. Pauling, p. 69, The Nature of the Chemical Bond, Cornell University Press, New York, 1948.

the distortion becomes weaker as the fraction of lead decreases. Thus a Jahn-Teller effect conceivably could be responsible for the distortion.<sup>19</sup>

### CONCLUSION

Although the zone theory is, at best, only qualitatively applicable to intermetallic compounds, it does provide a basis upon which to predict some of the properties of those compounds. As applied above to compounds between lithium and lead, the theory has led to the suggestion of further experiments which could provide a better understanding of these compounds in particular and of intermetallic compounds in general.

### ACKNOWLEDGMENTS

We wish to thank Drs. A. Zalkin and D. E. Sands for helpful discussions of structures and structure factors.

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(19) D. E. Abell, this laboratory, personal communication.

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