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Further Considerations on the Symmetry Properties of the Normal Vibrations of a Crystal*

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This paper supplements the preceding paper by Maradudin and Vosko on the same subject. Extensions and additions include discussions of (1) the group of the bond, (2) tabulations of the time-reversal invariance criterion, (3) the labeling of experimental dispersion curves, (4) compatibility relations, (5) accidental degeneracies, (6) the use of computers for extracting symmetry information, and (7) application to magnetic normal modes. The chief results of the preceding paper are summarized. Group theory is used to predict the connectivity of the phonon dispersion relations in CsCl and Mg. A collection of corrections to primary references useful in this field is included.

1. INTRODUCTION

This paper supplements the previous article [henceforth called (I)] and is the residue of an intended review article covering the same subject. I appreciated the opportunity to read (I) in its preprint form. It will probably be a classic in the field for its mathematical lucidity and the freshness of its viewpoint. In what follows I would like to extend some of the ideas discussed in (I) and add some new material. The extensions include an elaboration on what might be called the group of the bond, a few comments to be added to the very complete discussion of time-reversal invariance, and a discussion of how group theory is being used to label experimental and calculated phonon dispersion relations. The new material includes compatibility relations, rules for the crossing of dispersion curves, the use of computers along with group theory to extract symmetry information, and the eventual extension of the theory given in (I) to magnetic modes in solids. As further examples, we present the group theory for CsCl and Mg, and reference applications to other substances. It occurred to the author that it would be useful to workers in the field to have a summary of the main results of (I) without proofs or mathematical digressions. This is presented just before the examples. The article concludes with a tabulation of misprints and errors encountered by the author during his reading. Most of these are easily detected by the expert, but might be time-consuming for others.

2. NOTATION

Before taking up the main topics of this supplement, I would like to discuss the problem of notation. The rational content of mathematical theorems and physical laws is obviously independent of the symbols used in their statement. On the other hand, efficient communication among workers in the same field demands a standard notation for frequently used quantities. In some cases there is a rational basis for choosing a notation. In most cases there is not, and the notation devised by the person with a dominant intellect or personality usually prevails until a more dominant person appears. Where strong conflicts occur between schools of thought, committees are sometimes set up.

Perhaps the most outstanding example of such a cooperative effort is the *International Tables for X-Ray Crystallography*.[1] Although the major task of those three volumes is to summarize data and methods useful to crystallographers, it has also served to establish a universal notation for the point and space groups and to record various coordinate conventions adopted by the International Union of Crystallography. Another example of the usefulness of committee action is the paper "Standards on Piezoelectric Crystals, 1949," which was the work of the Standards Committee and the Piezoelectric Crystals Committee of the Institute of Radio Engineers.[2] This paper recommends standard Cartesian coordinate systems for all Bravais lattices, specifies standard plate orientation nomenclature, and recommends symbols and units for physical quantities. The use of such standards by all solid-state physicists seems highly desirable.

It appears to the author that the group theory of crystal lattices needs some standardization of notation. There is not even a universally accepted notation for the point group operations. Tables III, IV, and XIV, given later in this paper, illustrate some of the notations in current use. Three basic systems of notation emerge.

One system is based on a more or less arbitrary numbering of the operations, as is illustrated by Kovalev's[3] and Slater's[4] notation for the cubic groups. This is very useful for making concise multiplication tables. It is less useful in representation tables because it requires the reader either to memorize or constantly look up the geometric meaning of these symbols.

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* Work supported by the U.S. Atomic Energy Commission.

[1] K. Lonsdale, *International Tables for X-Ray Crystallography* (The Kynoch Press, Birmingham, England, 1952), 3 Vols.

[2] Standards 1949, Proc. Inst. Radio Engrs. **37,** 1378 (1949).

[3] O. V. Kovalev, *Irreducible Representations of the Space Groups* (Gordon and Breach Science Publishers, New York, 1965). [Translation by A. M. Gross. Originally published by Academy of Sciences USSR Press, Kiev, 1961)].

[4] J. C. Slater, *Quantum Theory of Molecules and Solids* (McGraw-Hill Book Co., Inc., New York, 1965), Vol. 2.

The second system is based on special symbols such as C for rotation, S for rotoreflections, and σ for reflections. Subscripts and superscripts are added to these symbols to indicate the order of the axis, i.e., twofold, threefold, etc., and to indicate the direction of rotation or reflection. There are two variants here. The notation for the axes of rotation are either tied to a provided diagram (as in Altmann and Cracknell[5]) or to a special coordinate system (as in McWeeny[6]). The use of a special diagram insures self-consistency and independence from future conventions. It has the disadvantage that one must continually refer to the author's diagram or memorize his system. The use of a special coordinate system appeals to the author since it involves less memory work. The choice of coordinate systems is essentially unique because of the two standards mentioned above.[1,2]

The third system of notation is exemplified by Slater's symbols for the operations of the hexagonal point group $6/mmm$ (in Table XIV, given later in this paper). Multiplication of operations is accomplished by adding subscripts and following simple rules for determining the rest of the symbol for the product operation. This obviates multiplication tables and is easily understood. If a similar system could be devised for the operations of the cube, this might have universal appeal.

The existence of so many notations frustrates easy comparison of tables, tends to divide people into different schools, and bespeaks the need for a standard reference.

The notational problem is also evident in the representations for the point groups and the space groups. Here there are two major competing notational systems. One is the outgrowth of atomic and molecular symmetry considerations in which the point groups are dominant. The other comes from band theory where the concept of the Brillouin zone (BZ) is central.

The first system, which appears to be due to Mulliken,[7] is characterized by symbols A, B for one-dimensional representations, E for two-dimensional representations, T for three-dimensional representations, etc. To these symbols are attached primes and subscripts whose meaning is given by a set of rules. (See, for example, Altmann[8] or McWeeny.[9]) The rules allow the reader to gain a great deal of information about the representation by merely examining the symbol. Although this system was devised expressly for point groups, it has application to space groups. In solid-state physics one is seldom interested in space groups per se, but more often in the factor group of the space groups which are isomorphic to the point groups. Also, as we have seen in (I), one can use multiplier representations of the point groups (rather than than full representations of the space groups) for many applications. For these reasons this notation makes a great deal of sense. It has been adopted by Altmann and his coworkers.[5,10]

The second notation for the irreducible representations has coalesced about the work of Bouckaert, Smoluchowski, and Wigner[11] (BSW). In their work, symmetry lines and points in the (BZ) are labeled with arbitrary letters, most of which are Greek. Points on the x axis in reciprocal space, for instance, are labeled Δ. For each wave vector in and on the (BZ) there are one or more irreducible representations of the space group. The representations of most interest are those associated with wave vectors on symmetry lines and at symmetry points. The irreducible representations along these lines or at these points are specified by adding arbitrary numerical subscripts and (sometimes) primes to the letter for the symmetry element. For example, Δ_1, Δ_1', Δ_2, Δ_2', and Δ_5 are the representations of the group of the wave vector which lies along the x axis in the (BZ). Unfortunately, there is not just one such system of labels. Different authors have chosen different letters and different subscripts for the same representation.[12] Koster[13] recorded a consistent set of letters for the symmetry elements in all Bravais lattices, but for various reasons it has not met with universal acceptance.[14] The situation may be further aggravated in the future by the appearance of books such as Kovalev's which use a wholly new arbitrary listing of wave vectors and representations.

The choice of notation here is a difficult problem. The band theorists have lived with it for over thirty years. The lattice dynamicists have remained relatively aloof until recent years. It is, however, now becoming common to find branches of phonon dispersion relations labeled with the (BSW) names of the irreducible representations.[15–18] For better or worse, Pandora's box has been opened. Wherever possible in this paper, current notations will be compared. It seems best at

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[5] S. L. Altmann and A. P. Cracknell, Rev. Mod. Phys. **37**, 19 (1965).

[6] R. McWeeny, *Symmetry* (The Macmillan Company, New York, 1963).

[7] R. S. Mulliken, Phys. Rev. **43**, 279 (1933).

[8] S. L. Altmann, "Group Theory" in *Quantum Theory*, D. R. Bates, Ed. (Academic Press Inc., New York, 1962), Vol. II, p. 163.

[9] Reference 6, p. 95.

[10] S. L. Altmann and C. J. Bradley, Rev. Mod. Phys. **37**, 33 (1965).

[11] L. P. Bouckaert, R. Smoluchowski, and E. Wigner, Phys. Rev. **50**, 58 (1936).

[12] H. Jones, *Theory of Brillouin Zones and Electronic States in Crystals* (North-Holland Publishing Co., Amsterdam, 1960), pp. 87–88.

[13] G. F. Koster, "Space Groups and their Representations" in *Solid State Physics*, F. Seitz and D. Turnbull, Eds. (Academic Press Inc., New York, 1957), Vol. 5, p. 173.

[14] The bismuth-type crystals are a good example. Slater (see Ref. 4) and M. H. Cohen [Phys. Rev. **121**, 387 (1961)] have each chosen a labeling of the symmetry points different than Koster's.

[15] A. D. B. Woods, *Symposium on Inelastic Scattering of Neutrons by Condensed Systems* (Brookhaven National Laboratory, Upton, N. Y., 1967), BNL–940.

[16] G. Dolling and R. A. Cowley, Proc. Phys. Soc. (London) **88**, 463 (1966).

[17] W. Cochran, R. A. Cowley, G. Dolling, and M. M. Elcombe, Proc. Roy. Soc. (London) **A293**, 433 (1966).

[18] J. L. Warren, J. L. Yarnell, G. Dolling, and R. A. Cowley, Phys. Rev. **158**, 805 (1967).

the present time not to suggest a new notation for the representations or to express any strong prejudice for a particular choice.

3. EXTENSIONS

The group of the bond is defined as the set of all operations which leave the force constant matrix $\mathbf{\Phi}(l\kappa;\, l'\kappa')$ invariant. As mentioned in (I) under Eq. (2.10), the transformation properties of $\mathbf{\Phi}(l\kappa;\, l'\kappa')$ under elements in the group of the bond may be used to determine the number of independent force constants. Let

$$\mathcal{S}_m=\{\mathbf{S}\mid \mathbf{v}(S)+\mathbf{x}(m)\}. \tag{3.1}$$

Then the transformation properties of $\mathbf{\Phi}(l\kappa;\, l'\kappa')$ are given by the equation

$$\Phi_{\mu\nu}(LK;\, L'K')=\sum_{\alpha\beta} S_{\mu\alpha}S_{\nu\beta}\Phi_{\alpha\beta}(l\kappa;\, l'\kappa'), \tag{3.2}$$

where

$$\mathbf{x}(LK)=\mathcal{S}_m\mathbf{x}(l\kappa). \tag{3.3}$$

There are two additional relations which are used below:

$$\Phi_{\mu\nu}(l\kappa;\, l'\kappa')=\Phi_{\nu\mu}(l'\kappa';\, l\kappa), \tag{3.4}$$

$$\begin{aligned}\Phi_{\mu\nu}(l\kappa;\, l'\kappa')&=\Phi_{\mu\nu}(l-l'\kappa;\, 0\kappa'),\\ &=\Phi_{\mu\nu}(0\kappa;\, l'-l\kappa').\end{aligned} \tag{3.5}$$

In (I) the last four equations are labeled (2.10b), (2.4), (2.3), and (2.11b), respectively. The force constant matrix $\mathbf{\Phi}(l\kappa;\, l'\kappa')$ describes the bonding between the atom at $\mathbf{x}(l\kappa)$ and the atom at $\mathbf{x}(l'\kappa')$.

The group of the bond contains not only the space group operations $\mathcal{R}_m=\{\mathbf{R}\mid \mathbf{v}(R)+\mathbf{x}(m)\}$, such that

$$\mathcal{R}_m\mathbf{x}(l\kappa)=\mathbf{x}(l+m\kappa) \tag{3.6a}$$

and

$$\mathcal{R}_m\mathbf{x}(l'\kappa')=\mathbf{x}(l'+m\kappa'), \tag{3.6b}$$

but also operations which are analogous to the antiunitary operations discussed in connection with the dynamical matrix. If the space group contains an operation $\mathcal{S}_{m-}$ such that

$$\mathcal{S}_{m-}\mathbf{x}(l\kappa)=\mathbf{x}(-l+m\kappa') \tag{3.7}$$

and similarly for $\mathbf{x}(l'\kappa')$, then Eq. (3.2) becomes

$$\Phi_{\mu\nu}(l'-l\kappa';\, 0\kappa)=\sum_{\alpha\beta} S_{-\mu\alpha}S_{-\nu\beta}\Phi_{\alpha\beta}(l-l'\kappa;\, 0\kappa'), \tag{3.8a}$$

or, in vector notation,

$$\mathbf{\Phi}(l'-l\kappa';\, 0\kappa)=\mathbf{S}_{-}\mathbf{\Phi}(l-l'\kappa;\, 0\kappa')\mathbf{S}_{-}^{-1} \tag{3.8b}$$

or

$$\mathbf{\Phi}(l'\kappa';\, l\kappa)=\mathbf{S}_{-}\mathbf{\Phi}(l\kappa;\, l'\kappa')\mathbf{S}_{-}^{-1}. \tag{3.8c}$$

Let $\mathfrak{J}$ be a transposition operator

$$\mathfrak{J}\mathbf{\Phi}\mathfrak{J}=\mathbf{\Phi}^{\mathrm{T}}. \tag{3.9}$$

When this operator is applied to Eq. (3.8c) and use is made of Eq. (3.4), we get

$$\mathbf{\Phi}(l\kappa;\, l'\kappa')=\mathfrak{J}\mathbf{S}_{-}\mathbf{\Phi}(l\kappa;\, l'\kappa')\mathbf{S}_{-}^{-1}\mathfrak{J}. \tag{3.10}$$

The operator $\mathfrak{J}$ plays a role similar to K in the antiunitary operators of (I). The combined operator $\mathfrak{J}\mathcal{S}_{m-}$ leaves the bond indices ${}_{\alpha\beta}(l\kappa;\, l'\kappa')$ invariant and hence is in the group of the bond.

A classic example of the use of this operation came in the discussion of the interaction of an atom with its second neighbors for germanium by Herman.[19] The lattice of germanium is two interpenetrating fcc lattices. The second neighbors of an atom at the corner of the cube are located on face centers. It turns out that the group of the bond contains space group operations of the form $\{E\mid \mathbf{x}(m)\}$ and $\{\sigma^{\bar{1}10}\mid \mathbf{x}(m)\}$. E is the identity operation and $\sigma^{\bar{1}10}$ is a reflection plane whose normal is in the direction $[\bar{1}10]$. The atom at the corner of the cube has indices $(l\kappa)=(0001)$, and the second neighbor that we are using in this example has indices $(l'\kappa')=(0011)$.[20] In Herman's notation, these operations simplify $\mathbf{\Phi}(0001;\, 0011)$ to

$$\mathbf{\Phi}(0001;\, 0011)=-\begin{pmatrix}\mu & \nu & \delta\\ \nu & \mu & \delta\\ \gamma & \gamma & \lambda\end{pmatrix}. \tag{3.11}$$

Application of the operator $\mathfrak{J}\{C_2^{001}\mid \mathbf{x}(m)\}$ shows that $\gamma=-\delta$. C_2^{001} is a twofold rotation about the z axis and changes (0011) to $(00\bar{1}1)$. (Further examples of this kind are found in Sec. 6.)

The discussion of time reversal in (I) is very good. The comments that I wish to add are related to the criteria for extra degeneracies, Eq. (5.61) in (I):

$$\sum_{\mathbf{A}} \phi(\mathbf{k};\, \mathbf{A},\, \mathbf{A})\chi^{(s)}(\mathbf{k};\, \mathbf{A}^2)=h, \qquad \text{first type,} \tag{3.12a}$$

$$=-h, \qquad \text{second type,} \tag{3.12b}$$

$$=0, \qquad \text{third type,} \tag{3.12c}$$

where

$$\phi(\mathbf{k};\, \mathbf{A},\, \mathbf{A})=\exp\left[i(\mathbf{k}+\mathbf{A}^{-1}\mathbf{k})\cdot\mathbf{v}(\mathbf{A})\right] \tag{3.13}$$

by Eq. (3.47) in (I). The **A**'s are operations in $G_0(\mathbf{k},\, -\mathbf{k})$ which are not in $G_0(\mathbf{k})$. In the practical application of this criteria it has been pointed out that $\phi(\mathbf{k};\, \mathbf{A},\, \mathbf{A})=1$ if the space group of the crystal is symmorphic or if $\mathbf{k}$ is in the interior of the (BZ) for crystals with nonsymmorphic space groups. In these two cases the irreducible multiplier representations are just the ordinary irreducible representations of the point group $G_0(\mathbf{k})$. Koster, Dimmock, Wheeler, and Satz[21] list the behavior of these representations under time reversal. In their tables of irreducible representations they include the letter a, b, or c, corresponding to the three

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[19] F. Herman, Phys. Chem. Solids **8**, 405 (1959).

[20] $l'=(001)$ gives the position vector $\mathbf{x}(l')=(a/2,\, a/2,\, 0)$ in Cartesian coordinates; a is the cubic lattice constant.

[21] G. F. Koster, J. O. Dimmock, R. G. Wheeler, and H. Statz, *Properties of the Thirty-Two Point Groups* (The M.I.T. Press, Cambridge, Mass., 1963).

cases above for each representation. They do not explain how this letter was arrived at, but Dimmock and Wheeler[22] derived a criteria for magnetic groups. The ordering of cases agrees with Wigner's 1932 choice,[23] which is consistent with Herring's criteria.[24] The authors of (I) have used Wigner's new terminology.[25] This means that b in Koster *et al.* is the third type and c is the second type. Koster *et al.* say that Case c does not occur for point groups without spin.[26] Upon looking through the tables, one finds that only for point groups 4, $\bar{4}$, $4/m$, 3, $\bar{3}$, 6, $\bar{6}$, $6/m$, 23, and $m3$ do some of the ordinary (no spin) representations correspond to Case b. Thus, for 22 of the 32 point groups we need not worry at all about time reversal. Of the point groups listed above, roughly half of their representations belong to Case b. Of course for **k** vectors on the surface of the (BZ) of nonsymmorphic crystals one must go back to the general criteria.

It was shown in (I) that each branch of the phonon dispersion relation belongs to a definite irreducible representation of the group of the wave vector. It is intuitively obvious that names of the irreducible representations would make good labels for experimental dispersion curves. When people began measuring phonon relations by means of neutron inelastic scattering some ten years ago, there was no need to use group theory to label the curves obtained. Measurements were made in elemental cubic substances along directions of very high symmetry so that the modes could be classified as pure transverse-acoustic (TA), longitudinal-acoustic (LA), transverse-optic (TO), or longitudinal-optic (LO).[27] This labeling scheme began to break down when measurements were made along directions of lower symmetry.[28] By the time measurements had been made on more complicated substances such as UO_2, Mg, and white tin, the use of group theory labels was fully established.[29–32] The names of the representations came from band theory and are almost exclusively taken from (BSW)[11] or Koster.[13] Perhaps one of the first papers to use this labeling was a theoretical paper by Johnson and Loudon,[33] which analyzed the critical points of the phonon spectra of diamond, Si, and Ge. No explanation of the notation was given in that paper.

Thus, while the authors of (I) base their labeling and calculation on the relatively recent tables of Kovalev, most of the experimental literature during the past four years is based on other sources. One reason for this could be that Kovalev's tables are the best complete set. It is also important that Kovalev bases his work on multiplier representations. Until very recently, most of the band theory calculations have been based on the representations of the factor group of the wave vector.[13] Another complete set of representations based on multiplier representations of the point groups has recently been published by Hurley.[34] It relies heavily on point group representations tabulated by McWeeny.[6] Because of its extreme compaction, it is not as convenient to use as Kovalev's work. Excellent though incomplete tables can be found in Slater.[35] Twenty of the most common lattice structures are treated fully. One must take care, however, to note Slater's unorthodox conventions.[36] These have been discussed by Altmann and Bradley[37] and by Hurley.[38] Hurley has pointed out that Slater's treatment of the cubic groups is not consistent with his treatment of the noncubic groups. The articles by Altmann and Cracknell[5] and by Altmann and Bradley[10] also contain extensive tables of irreducible representations.

Even without the use of irreducible representations and projection operators to find eigenvectors, a great deal of information useful for labeling curves can be obtained from compatibility relations, rules for crossing, and computer calculations. These are discussed in the next section.

4. ADDITIONS

Compatibility conditions are useful in establishing the connectivity of branches of the dispersion relation. The problem of connectivity arises when two symmetry lines in **k** space meet at a symmetry point.[39] An example of this can be seen in Fig. 1 for the diamond lattice. Starting at Γ, one can reach X by going along the line Δ or by going along the line Σ to K, which is identical with the point U, and then on along S.[40] One

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[22] J. O. Dimmock and R. G. Wheeler, J. Phys. Chem. Solids **23**, 729 (1962).

[23] E. Wigner, Nachr. Akad. Wiss. Goettingen, Math.—Kl. Physik, p. 546 (1932). [Translated in *Group Theory and Solid State Physics: I*, P. H. Meijer, Ed. (Gordon and Breach Science Publishers, New York, 1964)].

[24] C. Herring, Phys. Rev. **52**, 361 (1937); [See alternatively, Knox and Gold, *Symmetry in the Solid State* (W. A. Benjamin, Inc., New York, 1964), p. 235].

[25] E. P. Wigner, *Group Theory* (Academic Press Inc., New York, 1959), p. 343.

[26] Reference 21, p. 12.

[27] B. N. Brockhouse and P. K. Iyengar, Phys. Rev. **111**, 747 (1958).

[28] G. Dolling, *Inelastic Scattering of Neutrons* (International Atomic Energy Agency, Vienna, 1963), Vol. 2, p. 37.

[29] D. Long-Price, *Inelastic Scattering of Neutrons* (International Atomic Energy Agency, Vienna, 1965), Vol. 1, p. 109.

[30] P. K. Iyengar, G. Venkataraman, P. R. Vijayaraghavan, and A. P. Roy, *ibid.* p. 153.

[31] A. D. B. Woods, G. Dolling, and R. A. Cowley, *ibid.*, p. 373.

[32] W. Cochran, R. A. Cowley, G. Dolling, and M. M. Elcombe, Proc. Roy. Soc. (London) **A293**, 433 (1966). G. Dolling kindly pointed out to me that the labeling at L and M (or X) in Fig. 1 is in error. From top to bottom the labels should read L_1, L_2', L_3, L'_3, and X_4', X_5', X_4', X_5'.

[33] F. A. Johnson and R. Loudon, Proc. Roy. Soc. (London) **A281**, 274 (1964).

[34] A. C. Hurley, Phil. Trans. Roy. Soc. London, Ser. A. **A260**, 1 (1966).

[35] See Ref. 4, Appendix 3.

[36] J. C. Slater, Rev. Mod. Phys. **37**, 68 (1965).

[37] Reference 10; see note added in proof, p. 45.

[38] Reference 34, p. 26.

[39] The question of connectivity also arises when two symmetry planes intersect in a symmetry line. This case is of less interest however.

[40] The dispersion relation in the Σ direction is actually periodic in an interval twice the length of the interval from $\Gamma \rightarrow K$, $U \rightarrow X$. This can be seen by using an extended zone scheme in **k** space in which each reciprocal lattice point is enclosed in a Brillouin zone of the type shown in Fig. 1.

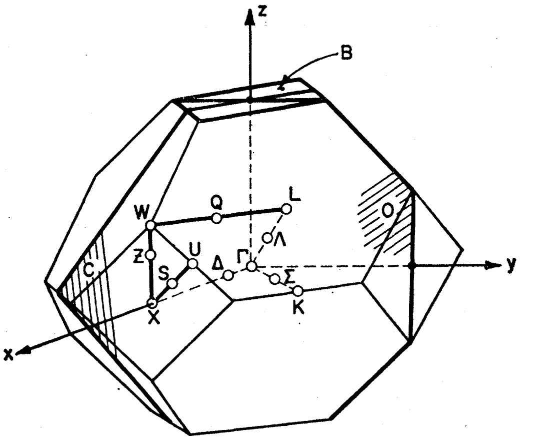

FIG. 1. Brillouin zone for face-centered cubic lattice. *C*, *O*, and *B* are symmetry planes.

of the better definitions of compatibility relations, their construction, and their use is to be found in Tinkham's discussion of band theory.[41] The basic idea is as follows. The point group of the wave vector along symmetry lines, like Δ and Σ, are subgroups of the point group of the wave vector at terminal symmetry points, like Γ and X. An irreducible representation of the point group of the wave vector at a terminal symmetry point must, perforce, provide a representation of its subgroups. In order to make a precise definition of compatibility, it is best to define our terms in advance.

Let $\tau^{(t)}=\{\boldsymbol{\tau}^{(t)}(\mathrm{R}),\ \mathrm{R}\in G\}$ be an irreducible representation of the group G, e.g., the point group of the wave vector at a terminal symmetry point. Let $\tau'^{(t)}=\{\boldsymbol{\tau}^{(t)}(\mathrm{R}),\ \mathrm{R}\in G'\}$ be the representation provided by $\tau^{(t)}$ for the subgroup G', e.g., the point group of the wave vector along a symmetry line. Let $\sigma^{(s)}=\{\boldsymbol{\delta}^{(s)}(\mathrm{R}),\ \mathrm{R}\in G'\}$, $s=1, 2, \cdots, n$ be the irreducible representations of G'. The representation $\tau'^{(t)}$ can be decomposed into the direct sum

$$\tau'^{(t)}=\sum_{s=1}^{n} c_s(t)\sigma^{(s)}, \tag{4.1}$$

where $c_s(t)$ is the number of times the irreducible representation $\sigma^{(s)}$ occurs in $\tau'^{(t)}$. The irreducible representation $\sigma^{(s)}$ is said to be compatible with the representation $\tau^{(t)}$ if $\sigma^{(s)}$ is in the decomposition of $\tau'^{(t)}$, i.e., if $c_s(t)\neq 0$. We say that a given branch of the dispersion relation along a symmetry line is compatible with a value of the dispersion relation at a symmetry point provided that the corresponding irreducible representations to which they belong are compatible. One can easily establish these compatibility relations by using the known irreducible multiplier representations and the decomposition formula for c_s [Eq. (4.36) from (I)]. For many of the common crystal structures these are listed in Appendix 3 of Slater.[4] It naturally follows that if branches measured or calculated along different symmetry lines are going to connect at a common symmetry point, they must be compatible with this symmetry point.

As an example of how these relations are used, let us establish the general shape and connectivity of the dispersion relations along the Σ direction in diamond assuming that the dispersion relations along Δ have been measured. In particular, let us assume that the solid curves and their labels in Fig. 2 are known. By constructing the multiplier representation $\{\mathbf{T}(\mathbf{k}_4;\ \mathrm{R})\}$ for $\mathbf{k}$ along Σ [see Eqs. (6.7) in (I)] and using the decomposition formula for c_s, the number of times the irreducible representation s is in $\mathbf{T}(\mathbf{k}_4;\ \mathrm{R})$, we find that

$$\{\mathbf{T}(\mathbf{k}_4;\ \mathrm{R})\}=2\tau^{(1)}(\mathbf{k}_4;\ \mathrm{R})\oplus\tau^{(2)}(\mathbf{k}_4;\ \mathrm{R})\oplus\tau^{(3)}(\mathbf{k}_4;\ \mathrm{R})\oplus 2\tau^{(4)}(\mathbf{k}_4;\ \mathrm{R}) \tag{4.2a}$$

in Kovalev's notation or

$$\{\mathbf{T}(\Sigma;\ \mathrm{R})\}=2\Sigma_1(\mathrm{R})\oplus\Sigma_2(\mathrm{R})\oplus\Sigma_4(\mathrm{R})\oplus 2\Sigma_3(\mathrm{R}) \tag{4.2b}$$

in the notation of (BSW). The compatibility relations for points Γ and X are in Tables I and II. The fact that Σ_4 starts from Γ_{15}, which is the origin of the acoustic modes, and ends on X_3 tells us that the lower Δ_5 branch ends in X_3. Table II tells us that X_1 is the endpoint of the longitudinal branches Δ_1 and Δ_2'. Thus, the labeling at X or $\mathbf{k}_{10}$ is unique. The dashed curves on Fig. 2 are drawn in by compatibility and by assuming that the crossing of branches belonging to the same representation is unlikely. The ordering of the branches coming out of symmetry points is not unique. This can be seen by comparing the experimental curves for diamond[18] in Fig. 3 with those for silicon[28] in Fig. 4. The order of the representations X_1 and X_4 are different

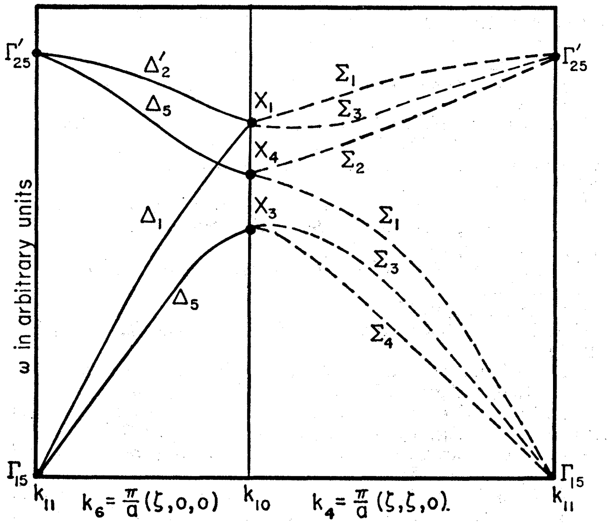

FIG. 2. Predicted connectivity of dispersion curves in the Σ direction of diamond assuming that the curves are known at Γ and along Δ. The figure is illustrative and not drawn to scale.

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[41] M. Tinkham, *Group Theory and Quantum Mechanics* (McGraw-Hill Book Co., Inc., New York, 1964), p. 286.

TABLE I. Compatibility relations for diamond at Γ or $\mathbf{k}_{11}$.[a]

Γ_{15}	Γ_{25}'
$\Delta_1 \oplus \Delta_5$	$\Delta_2' \oplus \Delta_5$
$\Sigma_1 \oplus \Sigma_3 \oplus \Sigma_4$	$\Sigma_1 \oplus \Sigma_2 \oplus \Sigma_3$

[a] Taken from Ref. 4, Table A3–31, p. 383.

in the two substances because of dynamical effects which cannot be predicted from group theory. This example shows us the power and limitations of compatibility relations. Under favorable circumstances labels can be assigned without calculating eigenvectors. These relations always serve as a useful crosscheck.

The second use of group theory mentioned at the beginning of this paper concerned the crossing of branches. The use here is combined with topological arguments and hence is less direct. Any crossing or contact of branches not predicted by group theory considerations is called an accidental degeneracy. Accidental degeneracies may be further subdivided into three types: (1) possible, (2) unlikely, and (3) vanishingly improbable.[42] The first type of degeneracy occurs between branches belonging to different representations. There is no known prohibition against their crossing. The other two types occur for branches belonging to the same representation. It should be recalled that for a general point in the Brillouin zone the group of the wave vector has only one irreducible representation. Therefore all branches of the dispersion relation in off-symmetry directions belong to the same representation.

von Neumann and Wigner[43] have shown that with three or more variable parameters in the system it is not impossible for two eigenvalues of a Hermitian matrix to become degenerate for some value of the parameters. The three components of the wave vector $\mathbf{k}$ in the dynamical matrix $\mathbf{D}(\mathbf{k})$ serve as variable parameters for our system. Herring[44] has examined the problem of accidental degeneracy for band theory. It is almost intuitively obvious that the arguments he made for the solutions of the Schrodinger equation can be carried over to the equations of motion in lattice dynamics. Herring defined an accidental degeneracy to be vanishingly improbable if it ceases to exist after some infinitesimal change is made in the form of the interaction which does not alter the symmetry of the interaction. In band theory the interaction is the self-consistent potential for the one electron problem. In lattice dynamics the interaction might be considered to be the set of Born–von Karman force constants.

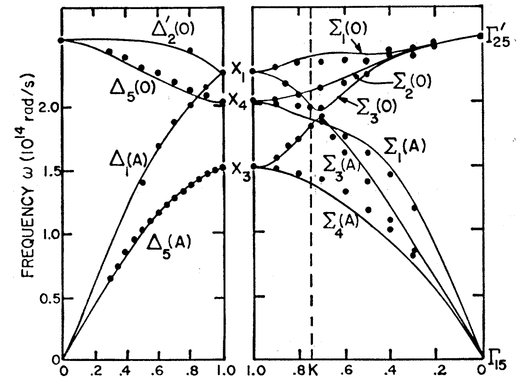

FIG. 3. Measured and calculated dispersion curves for diamond in two directions of high symmetry.

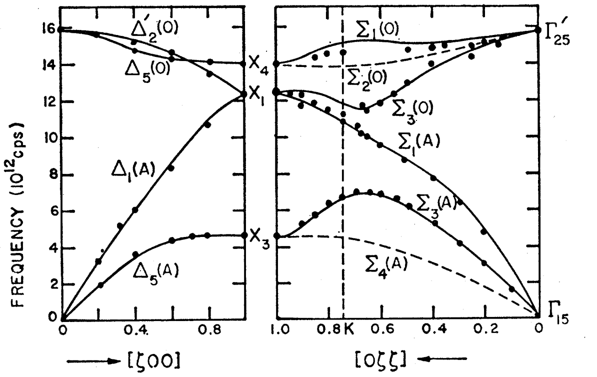

FIG. 4. Measured and calculated dispersion curves for silicon. Dotted branches have not been reported in the literature, but must have this connectivity by compatibility.

Most of the contacts or crossings of branches belonging to the same representation are of the vanishingly improbable type. Herring lists a set of what might be called *unlikely* accidental degeneracies. This list is summarized below.

For crystals with no center of inversion, contacts between branches belonging to the same representation may occur at isolated points which may lie in symmetry planes or in planes perpendicular to twofold axes, provided that time reversal does not cause these branches to have additional degeneracies. Points of contact must occur in multiples of four in the Brillouin zone.

For crystals with an inversion center, contacts between branches belonging to the same representation may occur at all points $\mathbf{k}$ of an endless curve, or a number of such curves in $\mathbf{k}$ space. It is vanishingly

TABLE II. Compatibility relations for diamond at X or $\mathbf{k}_{10}$.[a]

X_1	X_3	X_4
$\Delta_1 \oplus \Delta_2'$	Δ_5	Δ_5
$\Sigma_1 \oplus \Sigma_3$	$\Sigma_3 \oplus \Sigma_4$	$\Sigma_1 \oplus \Sigma_2$

[a] Taken from Ref. 4, Table A3–31, p. 383.

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[42] J. Callaway, *Energy Band Theory* (Academic Press Inc., New York, 1964), pp. 36, 37.

[43] J. von Neumann and E. Wigner, Physik. Z. **30**, 467 (1929) [Translated in R. S. Knox and A. Gold, *Symmetry in the Solid State* (W. A. Benjamin, Inc., New York, 1964), p. 167].

[44] C. Herring, Phys. Rev. **52**, 365 (1937). [See also Knox and Gold, Ref. 43, p. 240.]

improbable for such curves to lie in planes of symmetry in the Brillouin zone; however, a contact curve may pass through a symmetry axis at a point where necessary degeneracy or contact of inequivalent branches occurs. Herring also gives a discussion of the type of endless contact curves which can exist and a limited amount of information on the number of times a certain type may occur.

Because the situation is not clear-cut, one cannot categorically say that branches belonging to the same representation cannot cross. Each suspected case of crossing for equivalent branches must be investigated to see if it falls into the vanishingly improbable type or the unlikely type.

From the above discussion one can see that there are limitations on the usefulness of compatibility relations and crossing rules. Ultimately the assignment of branches to irreducible representations depends on the transformation properties of the eigenvectors. Projection operators are often inadequate to give eigenvectors. When a given representation occurs more than once in the multiplier representation $\{\mathbf{T}(\mathbf{k};\,\mathbf{R})\}$, then the projection operator method only gives a linear combination of eigenvectors.

One practical way of associating eigenvectors with eigenvalues is to do a computer calculation for the lattice dynamics of the crystal under investigation. This gives numerical values for eigenvalues and eigenvectors. The transformation properties of these eigenvectors can be checked by application of the matrices $\mathbf{T}(\mathbf{k};\,\mathbf{R})$. Even very crude models will work because the real symmetry-dependent properties are model-independent. One does have to be careful about possible accidental degeneracies introduced by a model. This method of assigning labels can be the by-product of doing a least-squares fit of a theoretical model to experimental data and therefore is very convenient for the experimenter.

Recently A. W. Luehrmann reported on a computer code that produces a complete set of irreducible representations for any point group. This suggests that it will soon be possible to do group theory analyses on a computer for complicated symmorphic crystals containing many atoms per unit cell. Programs for the irreducible representations of nonsymmorphic space groups are reportedly in progress.[45]

When a crystal has a magnetically ordered phase, there are magnetic normal modes. These are called spin waves or magnons. The symmetry group for the crystal is then one of the magnetic space groups. Application of group theory to magnetic modes has already been made by Brinkman.[46] The analysis is less fruitful because there are fewer symmetry operations in the magnetic groups. There are also complications arising in many cases from a lack of knowledge of the underlying spin arrangement, i.e., an uncertainty in the magnetic space group.

In some cases where the magnetic group is known there are other puzzlements. The experimental spin-wave dispersion curves show a symmetry higher than that of the magnetic space group according to Brinkman. He has used this knowledge as a basis for introducing what he calls spin–space type groups. These groups reflect the symmetry of the dominant interactions (Heisenberg exchange, crystal field contributions, etc.). By working out the symmetry of these interactions and comparing them with the observed symmetry of spin wave dispersion relation, something can be learned about the strength of less symmetric interactions. This, in turn, could be useful in determining the magnetic space group itself if it were unknown. Some magnetic modes are optically active.[47] Group theory will again be useful in establishing selection rules. Excellent magnon dispersion relations are beginning to be reported.[48] As the substances reported become more complicated, group theory labels will undoubtedly appear. In UO_2 the vibrational and magnetic modes interact strongly.[49] A proper treatment of substances like this will have to come from a unified approach in which the magnetic space group is the proper group for both the phonons and magnons.

5. PROCEDURE

This section outlines the procedure used in working out and presenting the group theoretical results given in the next section. The notation with minor exceptions is that used in (I). Formula numbers followed by asterisks refer to (I). This is done in order to make it easy to refer to the original discussion.

Each example in the next section begins with a discussion of the Cartesian coordinate system used to describe the direct and reciprocal lattice. This system conforms with the recommendation of the Piezoelectric Standards, 1949.[2] There are several properties of the dynamical matrix $\mathbf{D}(\mathbf{k})$ which are independent of the particular choice of $\mathbf{k}$. Some of these are listed below.

A. $\mathbf{D}(\mathbf{k})$ is Hermitian,

$$D_{\beta\alpha}(\kappa'\kappa\mid\mathbf{k})=D_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k})^{*}. \qquad (2.22)^{*}$$

B. $\mathbf{D}(\mathbf{k})$ is periodic in the reciprocal lattice,

$$D_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k}+\mathbf{K}(h))=D_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k}), \qquad (2.19)^{*}$$

where

$$\mathbf{K}(h)=\sum_{j=1}^{3}h_j\mathbf{b}_j, \qquad (5.1)$$

$$\mathbf{a}_i\cdot\mathbf{b}_j=2\pi\delta_{ij}, \qquad (5.2)$$

and

$$\mathbf{x}(l)=\sum_{i=1}^{3}l_i\mathbf{a}_i. \qquad (5.3)$$

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[45] A. W. Luehrmann, Bull. Am. Phys. Soc. **12**, 341 (1967).

[46] W. Brinkman, J. Appl. Phys. **38,** 939 (1967).

[47] A. J. Sievers, III and M. Tinkham, Phys. Rev. **129**, 1566 (1963).

[48] H. B. Moller and J. C. Gylden Houmann, Phys. Rev. Letters **16**, 737 (1966).

[49] G. Dolling and R. A. Cowley, Phys. Rev. Letters **16**, 683 (1966).

This definition of the reciprocal lattice differs in a minor way from that given in Eq. (2.18) in (I).

C. If the point group of the space group contains the inversion operation, there are the following simplifications that can be made under special circumstances.

(1) If every atom is at an inversion center, $\mathbf{D}(\mathbf{k})$ can be converted into a real symmetric matrix $\mathbf{C}(\mathbf{k})$ which has the same eigenvalues as $\mathbf{D}(\mathbf{k})$ and real eigenvectors $\mathbf{w}(\mathbf{k}j)$. The transformation is

$$C_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k}) = \exp\{-i\mathbf{k}\cdot[\mathbf{x}(\kappa)-\mathbf{x}(\kappa')]\}D_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k}), \tag{3.27*}$$

$$w_\alpha(\kappa \mid \mathbf{k}j) = \exp[-i\mathbf{k}\cdot\mathbf{x}(\kappa)]u_\alpha(\kappa \mid \mathbf{k}j). \tag{3.29*}$$

Note that j stands for the triplet of quantities $sa\lambda$. The number s is a label for the representation according to which $\mathbf{w}(\mathbf{k}j)$ transforms. The quantity a runs from 1 to c_s where c_s is the number of times that the irreducible representation $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R}\}$ occurs in the representation $\{\mathbf{T}(\mathbf{k},\mathbf{R})\}$. λ runs from 1 to f_s where f_s is the dimension of the irreducible representation $\{\boldsymbol{\tau}^{(s)}(\mathbf{k};\mathbf{R})\}$. The real form $\mathbf{C}(\mathbf{k})$ is very convenient for use on a computer. If, on the other hand, one wishes to keep the Hermitian form $\mathbf{D}(\mathbf{k})$, there are still the simplifications

$$D_{\alpha\beta}(\kappa\kappa \mid \mathbf{k})^* = D_{\alpha\beta}(\kappa\kappa \mid \mathbf{k}) \tag{5.4}$$

and

$$D_{\beta\alpha}(\kappa'\kappa \mid \mathbf{k}) = \exp\{2i\mathbf{k}\cdot[\mathbf{x}(\kappa)-\mathbf{x}(\kappa')]\}D_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k}). \tag{5.5}$$

(2) When only some of the atoms are located at centers of inversion, then Eqs. (5.4) and (5.5) apply to the corresponding values of κ and κ'.

(3) If two atoms of the same species occur in the lattice and are interchanged by the inversion operation, then

$$D_{\alpha\beta}(\mathcal{I}_m[\kappa], \mathcal{I}_m[\kappa] \mid \mathbf{k}) = D_{\beta\alpha}(\kappa\kappa \mid \mathbf{k}), \tag{3.30*}$$

where

$$\mathcal{I}_m = \{\mathbf{i} \mid \mathbf{v}(i) + \mathbf{x}(m)\} \tag{5.6}$$

and $\mathcal{I}_m[\kappa]$ is defined in such a way that the operation $\mathcal{I}_m$ interchanges sublattice κ with sublattice $\mathcal{I}_m[\kappa]$. Thus

$$\mathcal{I}_m[\mathcal{I}_m[\kappa]] = \kappa. \tag{5.7}$$

We also have

$$D_{\alpha\beta}(\mathcal{I}_m[\kappa]\kappa \mid \mathbf{k}) = D_{\alpha\beta}(\kappa\mathcal{I}_m[\kappa] \mid \mathbf{k})^*, \tag{3.31a*}$$

$$= D_{\beta\alpha}(\mathcal{I}_m[\kappa]\kappa \mid \mathbf{k}). \tag{3.31b*}$$

(4) If none of the above three conditions hold, there is still the general relation

$$D_{\alpha\beta}(\mathcal{I}_m[\kappa]\mathcal{I}_m[\kappa'] \mid \mathbf{k}) = \exp[i\Upsilon(\kappa\kappa' \mid \mathbf{k}; \mathcal{I}_m)]D_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k})^*, \tag{3.26*}$$

where

$$\Upsilon(\kappa\kappa' \mid \mathbf{k}; \mathcal{I}_m) = -\mathbf{k}\cdot[\mathbf{x}(\mathcal{I}_m[\kappa]) + \mathbf{x}(\kappa) - \mathbf{x}(\mathcal{I}_m[\kappa']) - \mathbf{x}(\kappa')]. \tag{5.8}$$

Returning now to the general properties of $\mathbf{D}(\mathbf{k})$ which hold for all $\mathbf{k}$ we have the following.

D. Even for general $\mathbf{k}$ not all the matrix elements are unrelated to one another in functional form. As an example,

$$D_{21}(\kappa\kappa' \mid k_1, k_2, k_3) = D_{12}(\kappa\kappa' \mid k_2, k_1, k_3)$$

in cubic lattices. k_1, k_2, and k_3 are the Cartesian components of $\mathbf{k}$. The relation between the functional forms of the matrix elements is found by applying the formula

$$D_{\alpha\beta}(\mathcal{S}_m[\kappa]\mathcal{S}_m[\kappa'] \mid \mathbf{Sk}) = \exp[i\Upsilon(\kappa\kappa' \mid \mathbf{k}; \mathcal{S}_m)] \sum_{\mu\nu} S_{\alpha\mu}S_{\beta\nu}D_{\mu\nu}(\kappa\kappa' \mid \mathbf{k}), \tag{3.4*}$$

where

$$\Upsilon(\kappa\kappa' \mid \mathbf{k}; \mathcal{S}_m) = \mathbf{Sk}\cdot[\mathbf{x}(\mathcal{S}_m[\kappa]) - \mathbf{Sx}(\kappa) - \mathbf{x}(\mathcal{S}_m[\kappa']) + \mathbf{Sx}(\kappa')]. \tag{5.9}$$

The definition of $\mathcal{S}_m[\kappa]$ is an obvious generalization of $\mathcal{I}_m[\kappa]$ given above. $\mathcal{S}_m[\kappa]$ is the same as $F_0(\kappa; \mathbf{S})$, Eq. (2.35b) of (I).

E. The form of the force constant matrices $\boldsymbol{\Phi}(l\kappa; l'\kappa')$ which enters into the definition of $\mathbf{D}(\mathbf{k})$ can be determined by using the group of the bond discussed in the previous section. Most current models of lattice dynamics treat interactions of nearest and next nearest neighbors using Born–von Karman force constants $\Phi_{\alpha\beta}(l\kappa; l'\kappa')$ as adjustable parameters. When longer range forces are necessary, these are treated in another fashion. As an aid in constructing models of this sort, in the next section we record the form of the force constant matrices for first and second neighbors. The general relations used to obtain the simplified forms of the force constant matrices are

$$\Phi_{\alpha\beta}(\mathcal{S}_m[l\kappa]; \mathcal{S}_m[l'\kappa']) = \sum_{\mu\nu} S_{\alpha\mu}S_{\beta\nu}\Phi_{\mu\nu}(l\kappa; l'\kappa') \tag{2.10b*}$$

and

$$\Phi_{\beta\alpha}(l'\kappa'; l\kappa) = \Phi_{\alpha\beta}(l\kappa; l'\kappa'). \tag{2.3*}$$

The discussion of general properties of $\mathbf{D}(\mathbf{k})$ is followed by a table listing the essential properties of typical symmetry planes, lines, and points in the Brillouin zone. For each of the symmetry points and lines in the table, starting with the most symmetric, we give the representation $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$:

$$T_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k}; \mathbf{R}) = \delta(\kappa, \mathcal{R}_m[\kappa']) \exp[i\theta(\kappa' \mid \mathbf{k}; \mathcal{R}_m)]R_{\alpha\beta}, \tag{3.17b*}$$

where

$$\theta(\kappa' \mid \mathbf{k}; \mathcal{R}_m) = \mathbf{k}\cdot[\mathbf{x}(\mathcal{R}_m[\kappa']) - \mathbf{Rx}(\kappa')]. \tag{5.10}$$

This representation has two significant uses. The first is based on the fact that all matrices in the representation commute with $\mathbf{D}(\mathbf{k})$. This gives an invariance condition

$$\mathbf{D}(\mathbf{k}) = \mathbf{T}(\mathbf{k};\mathbf{R})^{-1}\mathbf{D}(\mathbf{k})\mathbf{T}(\mathbf{k};\mathbf{R}), \tag{3.23*}$$

which simplifies to

$$D_{\alpha\beta}(\mathcal{R}_m[\kappa]\mathcal{R}_m[\kappa'] \mid \mathbf{k}) = \exp[i\Upsilon(\kappa\kappa' \mid \mathbf{k}; \mathcal{R}_m)] \sum_{\mu\nu} R_{\alpha\mu}R_{\beta\nu}D_{\mu\nu}(\kappa\kappa' \mid \mathbf{k}), \quad (5.11)$$

where

$$\Upsilon(\kappa\kappa' \mid \mathbf{k}; \mathcal{R}_m) = \theta(\kappa \mid \mathbf{k}; \mathcal{R}_m) - \theta(\kappa' \mid \mathbf{k}; \mathcal{R}_m). \quad (5.12)$$

As in (I), $\mathbf{R} \in G_0(\mathbf{k})$ and $\mathcal{R}_m \in G_{\mathbf{k}}$. The invariance condition is used to simplify the form of $\mathbf{D}(\mathbf{k})$. The second use of $\{\mathbf{T}(\mathbf{k}; \mathbf{R})\}$ is in the construction of symmetry-adapted eigenvectors $\mathbf{E}(\mathbf{k}; s\lambda)$. These are then used as trial solutions in the eigenvalue equation. In the process of obtaining $\mathbf{E}(\mathbf{k}; s\lambda)$, one can get much useful intermediate information.

In the next section, before giving the simplified form of $\mathbf{D}(\mathbf{k})$, we use the decomposition formula

$$c_s = h^{-1} \sum_{\mathbf{R}} \chi(\mathbf{k}; \mathbf{R})\chi^{(s)}(\mathbf{k}; \mathbf{R})^* \quad (4.36)^*$$

to find how many times the irreducible multiplier representation $\{\boldsymbol{\tau}^{(s)}(\mathbf{k}; \mathbf{R})\}$ is contained in $\{\mathbf{T}(\mathbf{k}; \mathbf{R})\}$. The order of the point group of the wave vector is h. $\chi(\mathbf{k}; \mathbf{R})$ and $\chi^{(s)}(\mathbf{k}; \mathbf{R})$ are the characters of the matrices $\mathbf{T}(\mathbf{k}; \mathbf{R})$ and $\boldsymbol{\tau}^{(s)}(\mathbf{k}; \mathbf{R})$, respectively.

At this point one is in a position to test for additional degeneracies due to time reversal. The test criteria can be written down for three special cases: (1) $\mathbf{k}$ in the Brillouin zone; (2) $\mathbf{k} = \frac{1}{2}\mathbf{K}(h)$; and (3) $\mathbf{k}$ on the surface of the Brillouin zone, but not equal to $\frac{1}{2}\mathbf{K}(h)$.[50] For points inside the Brillouin zone

$$d_s(\mathbf{k}) = h^{-1} \sum_{\mathbf{A}} \chi^{(s)}(\mathbf{k}; \mathbf{A}^2) = 1, \quad \text{first type}, \quad (5.13a)$$

$$= -1, \quad \text{second type}, \quad (5.13b)$$

$$= 0, \quad \text{third type}. \quad (5.13c)$$

$d_s(\mathbf{k}) = 1$ means that there is no additional degeneracy. When $d_s(\mathbf{k}) = -1$, there is an additional degeneracy $\omega_{sa}(\mathbf{k}) = \omega_{sa'}(\mathbf{k})$ for some a'. This is an indirect proof that the representation s must occur an even number of times in $\{\mathbf{T}(\mathbf{k}; \mathbf{R})\}$ if $d_s(\mathbf{k}) = -1$. Finally, for $d_s(\mathbf{k}) = 0$, then $\omega_{sa}(\mathbf{k}) = \omega_{s'a'}(\mathbf{k})$ for some $s' \neq s$ and some a'. This implies that there are an even number of representations of dimension f_s contained in $\{\mathbf{T}(\mathbf{k}; \mathbf{R})\}$. According to Koster *et al.*,[26] the second type does not occur within the Brillouin zone. The summation is over all elements $\mathbf{A}$ such that $\mathbf{A}\mathbf{k} = -\mathbf{k}$. [If no such elements $\mathcal{A}_m = \{\mathbf{A} \mid \mathbf{v}(A) + \mathbf{x}(m)\}$ exist in the space group, then time reversal can produce no degeneracies.] The above criteria for points within the zone has been checked by Koster *et al.* and may be looked up rather than worked out.

When $\mathbf{k} = \frac{1}{2}\mathbf{K}(h)$,

$$d_s(\tfrac{1}{2}\mathbf{K}(h)) = h^{-1} \sum_{\mathbf{R}} \times \exp\{-i\tfrac{1}{2}[\mathbf{K}(h) + \mathbf{R}^{-1}\mathbf{K}(h)]\cdot\mathbf{v}(R)\}\chi^{(s)}(\tfrac{1}{2}\mathbf{K}; \mathbf{R}^2), \quad (5.63)^*$$

where the sum is over $\mathbf{R} \in G_0(\mathbf{k})$, the point group of the wave vector. For symmorphic groups, $\mathbf{v}(R) = \mathbf{0}$, and the exponential is one.

For a general point on the surface of the zone,

$$d_s(\mathbf{k}) = h^{-1} \sum_{\mathbf{A}} \exp\{-i[\mathbf{k} + \mathbf{A}^{-1}\mathbf{k}]\cdot\mathbf{v}(A)\}\chi^{(s)}(\mathbf{k}; \mathbf{A}^2). \quad (5.61)^* \text{ and } (3.47)^*$$

Only under special conditions does the above test tell us a' when $d_s(\mathbf{k}) = -1$ or $s'a'$ when $d_s(\mathbf{k}) = 0$. This information is still implicit in $\mathbf{D}(\mathbf{k})$ and may be obtained in the process of finding eigenvectors and eigenvalues.

After obtaining the above information about the representation $\{\mathbf{T}(\mathbf{k}; \mathbf{R})\}$ from character tables, one can proceed to construct the symmetry-adapted eigenvectors $\mathbf{E}(\mathbf{k}; s\lambda)$ whose transformation properties are defined by the equation

$$\mathbf{T}(\mathbf{k}; \mathbf{R})\mathbf{E}(\mathbf{k}; s\lambda) = \sum_{\lambda'} \tau_{\lambda'\lambda}{}^{(s)}(\mathbf{k}; \mathbf{R})\mathbf{E}(\mathbf{k}; s\lambda'). \quad (4.44)^*$$

$\mathbf{E}(\mathbf{k}; s\lambda)$ is obtained by use of projection operators $\mathbf{P}_{\lambda\lambda'}{}^{(s)}(\mathbf{k})$:

$$\mathbf{E}(\mathbf{k}, s\lambda) = \mathbf{P}_{\lambda\lambda'}{}^{(s)}(\mathbf{k})\psi, \quad (4.38)^*$$

where ψ is an arbitrary $3r$-dimensional column matrix and

$$\mathbf{P}_{\lambda\lambda'}{}^{(s)}(\mathbf{k}) = (f_s/h) \sum_{R} \tau_{\lambda\lambda'}{}^{(s)}(\mathbf{k}; \mathbf{R})^*\mathbf{T}(\mathbf{k}; \mathbf{R}). \quad (4.37)^*$$

A good treatment of projection operators may be found in McWeeny.[51] In the next section, the $\mathbf{E}(\mathbf{k}; s\lambda)$'s are indicated for each $\mathbf{k}$ treated. When $c_s \leq 2$, these vectors will be substituted into the eigenvalue equation

$$\mathbf{D}(\mathbf{k})\mathbf{E}(\mathbf{k}; s\lambda) = \omega_{sa}{}^2(\mathbf{k})\mathbf{E}(\mathbf{k}; s\lambda), \quad (5.14)$$

and the eigenvectors $\mathbf{e}(\mathbf{k}\ sa\lambda)$ will be written out explicitly. For $c_s > 2$, only the determinant condition for branches belonging to s are recorded.

6. EXAMPLES

Using the procedure outlined in Sec. 5, we treat the lattices exemplified by CsCl and Mg. Not all the details are given here. Sec. 6 of (I) illustrated the essential intermediate steps. Further details on these and other materials such as Al, NaCl, diamond, Na, GaAs, white tin, and As are given in a forthcoming report.[52] The

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[50] One should not confuse h in $\mathbf{K}(h)$, which stands for a triplet of integers, with h which means the order of the point group of the wave vector.

[51] See Ref. 6, Sections 5.7 and 5.8, pp. 126–33.

[52] J. L. Warren, Los Alamos Scientific Laboratory Report (in preparation).

application of group theory to the lattice dynamics of more complicated substances (such as $LaCl_3$[53] and wurtzite[54]) appears in the literature.

CsCl Structure

The space group of CsCl is *Pm3m*.[55] The lattice is simple cubic with two atoms per unit cell. There exists no element which solidifies in a simple cubic lattice, and therefore CsCl is the simplest crystal lattice with this space group. This space group is symmorphic, which means that $\mathbf{v}(S)=0$ for all $\mathcal{S}_m$. The edges of the unit cell provide axes for a natural Cartesian coordinate system. Let $\mathbf{1}_1$, $\mathbf{1}_2$, and $\mathbf{1}_3$ be unit vectors directed parallel to the cube edges. The position vector for atoms in the lattice is

$$\mathbf{x}(l\kappa)=a_0\sum_{i=1}^{3}[l_i+\tfrac{1}{2}(\kappa-1)]\mathbf{1}_i, \qquad \kappa=1,2 \tag{6.1}$$

where a_0 is the lattice constant and the l_i's are integers. The point group of the space group is *m3m* which contains 48 operations. These operations can be divided into ten classes in the group-theoretic sense. The first class contains only the identity operation **1**. The second class contains three twofold rotations. Axes of rotation shall be considered to have direction. The direction of an axis is defined as being from a point called the origin to another point on the axis. The right-hand rule is used to define the positive sense of rotation (see Fig. 5). The twofold axes in the second class are parallel to the unit vectors $\mathbf{1}_i$. They are denoted by $\mathbf{2}[100]$, $\mathbf{2}[010]$, and $\mathbf{2}[001]$.[56] The third class contains eight threefold axes. The axes of rotation are directed along the body diagonals of the unit cell and are denoted $\mathbf{3}[111]$, $\mathbf{3}[1\bar{1}\bar{1}]$, $\mathbf{3}[\bar{1}1\bar{1}]$, $\mathbf{3}[\bar{1}\bar{1}1]$, $\mathbf{3}[\bar{1}\bar{1}\bar{1}]$, $\mathbf{3}[\bar{1}11]$, $\mathbf{3}[1\bar{1}1]$, and $\mathbf{3}[11\bar{1}]$. The above 12 elements constitute the tetrahedral group 23. The fourth and fifth classes of *m3m* are obtained from 23 by multiplication of each element in 23 by $\mathbf{4}[100]$. Multiplication here means the operation "followed by." Thus, $\mathbf{3}[111]$ "followed by" $\mathbf{4}[100]$ is equivalent to $\mathbf{2}[101]$:

$$\mathbf{4}[100]\,\mathbf{3}[111]=\mathbf{2}[101]. \tag{6.2}$$

The fourth class consists of six fourfold rotations: $\mathbf{4}[100]$, $\mathbf{4}[010]$, $\mathbf{4}[001]$, $\mathbf{4}[\bar{1}00]$, $\mathbf{4}[0\bar{1}0]$, and $\mathbf{4}[00\bar{1}]$. The six elements in the fifth class are twofold rotations about the face diagonals of the unit cell: $\mathbf{2}[011]$, $\mathbf{2}[101]$, $\mathbf{2}[110]$, $\mathbf{2}[01\bar{1}]$, $\mathbf{2}[\bar{1}01]$, and $\mathbf{2}[1\bar{1}0]$.

The collection of all elements in the first five classes is the octahedral point group 432. In set theoretical notation

$$432=23\cup\mathbf{4}[100]23. \tag{6.3}$$

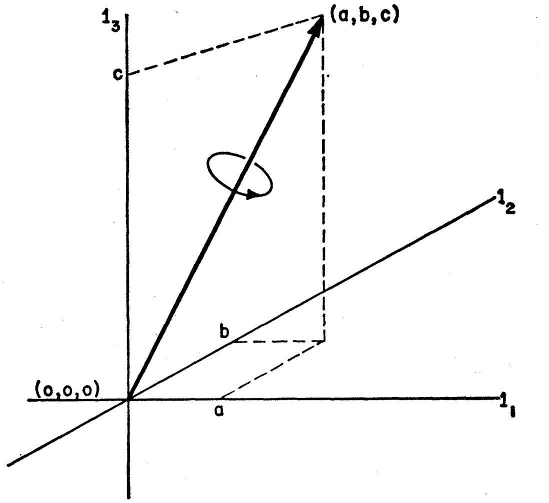

FIG. 5. Direction of rotation axis. Right-hand rule specifies the the sense of a positive rotation.

The next five classes of *m3m* can be obtained from the first five by multiplying each element in 432 by the inversion operation $\bar{\mathbf{1}}$. Class six consists of just the inversion operation. Class seven contains three reflection planes. Geometrically it is easily seen that a twofold rotation $\mathbf{2}[100]$ followed by an inversion is equivalent to a reflection through a mirror plane whose normal is in the [100] direction. The elements of the seventh class are $\bar{\mathbf{2}}[100]$, $\bar{\mathbf{2}}[010]$, and $\bar{\mathbf{2}}[001]$. Class eight is $\bar{\mathbf{1}}$ times class 3. For example,

$$\bar{\mathbf{1}}\mathbf{3}[111]=\bar{\mathbf{3}}[111]. \tag{6.4}$$

Threefold rotations followed by inversions are equivalent to sixfold rotations in the opposite sense followed by a reflection through a plane perpendicular to the rotation axis. (The symbol for a rotoreflection S_n has more or less been dropped by crystallographers.) The remaining two classes are obvious. Tables III and IV contain a comparison of this notation with that found in tables of irreducible representations. Tables III and IV also contain a symbol from the International Tables which shows the effect of the operations $\mathbf{n}[abc]$ or $\bar{\mathbf{n}}[abc]$ on a general point in the crystal. For example,

$$\mathbf{3}[111]xyz=yzx. \tag{6.5a}$$

A three-dimensional matrix which does the same thing is given below:

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix}=\begin{pmatrix} y \\ z \\ x \end{pmatrix}. \tag{6.5b}$$

This matrix can be used to represent $\mathbf{3}[111]$. The set of such matrices, one for each operation in *m3m*, forms

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[53] H. H. Caspers, J. Murphy, and R. A. Buchanan, *Lattice Dynamics*, R. F. Wallis, Ed. (Pergamon Press, Inc., London, 1965), p. 109.

[54] M. A. Nusimovici and J. L. Birman, Phys. Rev. **156**, 925 (1967). See references in this article for previous work on wurtzite.

[55] This is also called O_h. See Ref. 1, Vol. I, p. 330.

[56] This is an adaptation of notation in Vol. 1, p. 23 of Ref. 1. The general symbol is $n[abc]$. The integer n stands for a rotation of $2\pi/\bar{n}$; $\bar{n}$ is a rotoinversion, i.e., a rotation of $2\pi/n$ followed by an inversion through the origin. The symbol $[abc]$ specifies the direction of the rotation or rotoinversion axis. See Fig. 5.

TABLE III. Comparison of common notations for point group operations for the group 432; irreducible representation T_{1u} and its character are included.

W[a]	McW[b]	A&C[c]	HI[d]	HII[d]	S[e]	K[f]	Int[g]	$(T_{1u})_{1i}$	$(T_{1u})_{2i}$	$(T_{1u})_{3i}$	$\chi(T_{1u})$
1	E	E	e	a_1	R_1	h_1	xyz	100	010	001	3
$2[100]$	C_2^x	C_{2x}	C_2^x	a_2	R_2	h_2	$x\bar{y}\bar{z}$	100	$0\bar{1}0$	$00\bar{1}$	−1
$2[010]$	C_2^y	C_{2y}	C_2^y	a_3	R_3	h_3	$\bar{x}y\bar{z}$	$\bar{1}00$	010	$00\bar{1}$	−1
$2[001]$	C_2^z	C_{2z}	C_2^z	a_4	R_4	h_4	$\bar{x}\bar{y}z$	$\bar{1}00$	$0\bar{1}0$	001	−1
$3[111]$	C_3^{xyz}	C_{31}^+	$C_3^{(4)}$	a_5	R_5	h_9	zxy	001	100	010	0
$3[1\bar{1}\bar{1}]$	$C_3^{x\bar{y}\bar{z}}$	C_{33}^+	$C_3^{(3)}$	a_6	R_6	h_{12}	$\bar{z}\bar{x}y$	$00\bar{1}$	$\bar{1}00$	010	0
$3[\bar{1}1\bar{1}]$	$C_3^{\bar{x}y\bar{z}}$	C_{34}^+	$C_3^{(2)}$	a_7	R_7	h_{10}	$z\bar{x}\bar{y}$	001	$\bar{1}00$	$0\bar{1}0$	0
$3[\bar{1}\bar{1}1]$	$C_3^{\bar{x}\bar{y}z}$	C_{32}^+	$C_3^{(1)}$	a_8	R_8	h_{11}	$\bar{z}x\bar{y}$	$00\bar{1}$	100	$0\bar{1}0$	0
$3[\bar{1}\bar{1}\bar{1}]$	$\bar{C}_3^{xyz}$	C_{31}^-	$C_3^{(8)}$	a_9	R_9	h_5	yzx	010	001	100	0
$3[\bar{1}11]$	$\bar{C}_3^{x\bar{y}\bar{z}}$	C_{33}^-	$C_3^{(7)}$	a_{10}	R_{10}	h_7	$\bar{y}z\bar{x}$	$0\bar{1}0$	001	$\bar{1}00$	0
$3[1\bar{1}1]$	$\bar{C}_3^{\bar{x}y\bar{z}}$	C_{34}^-	$C_3^{(5)}$	a_{11}	R_{11}	h_8	$\bar{y}\bar{z}x$	$0\bar{1}0$	$00\bar{1}$	100	0
$3[11\bar{1}]$	$\bar{C}_3^{\bar{x}\bar{y}z}$	C_{32}^-	$C_3^{(6)}$	a_{12}	R_{12}	h_6	$y\bar{z}\bar{x}$	010	$00\bar{1}$	$\bar{1}00$	0
$4[100]$	C_4^x	C_{4x}^+	C_4^x	a_{14}	R_{14}'	h_{19}	$x\bar{z}y$	100	$00\bar{1}$	010	1
$4[010]$	C_4^y	C_{4y}^+	C_4^y	a_{16}	R_{16}'	h_{24}	$zy\bar{x}$	001	010	100	1
$4[001]$	C_4^z	C_{4z}^+	C_4^z	a_{18}	R_{18}'	h_{14}	$\bar{y}xz$	$0\bar{1}0$	100	001	1
$4[\bar{1}00]$	$\bar{C}_4^x$	C_{4x}^-	C_4^{-x}	a_{13}	R_{13}'	h_{20}	$xz\bar{y}$	100	001	$0\bar{1}0$	1
$4[0\bar{1}0]$	$\bar{C}_4^y$	C_{4y}^-	C_4^{-y}	a_{15}	R_{15}'	h_{22}	$\bar{z}yx$	$00\bar{1}$	010	100	1
$4[00\bar{1}]$	$\bar{C}_4^z$	C_{4z}^-	C_4^{-z}	a_{17}	R_{17}'	h_{15}	$y\bar{x}z$	010	$\bar{1}00$	001	1
$2[011]$	C_2^{yz}	C_{2d}	C_2^b	a_{20}	R_{20}'	h_{18}	$\bar{x}zy$	$\bar{1}00$	001	010	−1
$2[101]$	C_2^{xz}	C_{2c}	C_2^d	a_{22}	R_{22}'	h_{23}	$z\bar{y}x$	001	$0\bar{1}0$	100	−1
$2[110]$	C_2^{xy}	C_{2a}	C_2^f	a_{24}	R_{24}'	h_{16}	$yx\bar{z}$	010	100	$00\bar{1}$	−1
$2[01\bar{1}]$	$C_2^{y\bar{z}}$	C_{2f}	C_2^a	a_{19}	R_{19}'	h_{17}	$\bar{x}\bar{z}\bar{y}$	$\bar{1}00$	$00\bar{1}$	$0\bar{1}0$	−1
$2[\bar{1}01]$	$C_2^{z\bar{x}}$	C_{2e}	C_2^c	a_{21}	R_{21}'	h_{21}	$\bar{z}\bar{y}\bar{x}$	$00\bar{1}$	$0\bar{1}0$	$\bar{1}00$	−1
$2[1\bar{1}0]$	$C_2^{x\bar{y}}$	C_{2b}	C_2^e	a_{23}	R_{23}'	h_{13}	$\bar{y}\bar{x}\bar{z}$	$0\bar{1}0$	$\bar{1}00$	$00\bar{1}$	−1

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[a] Warren, the author, has introduced his own notation to avoid confusion with other authors. He does not feel strongly that this notation is any better than the rest.

[b] McWeeny, see Ref. 6, p. 74. McWeeny uses another notation for elements of the various subgroups of $m3m$.

[c] Altmann and Cracknell, see Ref. 5, p. 26.

[d] Hurley, see Ref. 34, p. 7. Hurley has no geometrical notation HI for $\bar{1}$ 432.

[e] Slater, see Ref. 4, p. 28. Note that the convention $R_i\psi(x, y, z) = \psi(R_i^{-1}(x, y, z))$ is assumed.

[f] Kovalev, see Ref. 3, pp. 6, 7.

[g] *International Tables for X-Ray Crystallography*, see Ref. 1, Vol. 1, p. 330.

Table IV. Comparison of common notations for point group operations for the coset $\bar{1}$ 432; irreducible representation T_{1u} and its character are included.

W[a]	McW[b]	A&C[c]	HII[d]	S[e]	K[f]	Int[g]	$(T_{1u})_{1i}$	$(T_{1u})_{2i}$	$(T_{1u})_{3i}$	$\chi(T_{1u})$
1	i	i	a_1'	R_1'	h_{25}	$\bar{x}\bar{y}\bar{z}$	$\bar{1}00$	$0\bar{1}0$	$00\bar{1}$	-3
$\bar{2}[100]$	σ^x	σ_x	a_2'	R_2'	h_{26}	$\bar{x}yz$	$\bar{1}00$	010	001	1
$\bar{2}[010]$	σ^y	σ_y	a_3'	R_3'	h_{27}	$x\bar{y}z$	100	$0\bar{1}0$	001	1
$\bar{2}[001]$	σ^z	σ_z	a_4'	R_4'	h_{28}	$xy\bar{z}$	100	010	$00\bar{1}$	1
$\bar{3}[111]$	$\bar{S}_6^{xyz}$	S_{61}^-	a_5'	R_5'	h_{33}	$\bar{z}\bar{x}\bar{y}$	$00\bar{1}$	$\bar{1}00$	$0\bar{1}0$	0
$\bar{3}[1\bar{1}\bar{1}]$	$\bar{S}_6^{x\bar{y}\bar{z}}$	S_{63}^-	a_6'	R_6'	h_{36}	$zx\bar{y}$	001	100	$0\bar{1}0$	0
$\bar{3}[\bar{1}1\bar{1}]$	$\bar{S}_6^{\bar{x}y\bar{z}}$	S_{64}^-	a_7'	R_7'	h_{34}	$\bar{z}xy$	$00\bar{1}$	100	010	0
$\bar{3}[\bar{1}\bar{1}1]$	$S_6^{\bar{x}\bar{y}z}$	S_{62}^-	a_8'	R_8'	h_{35}	$z\bar{x}y$	001	$\bar{1}00$	010	0
$\bar{3}[\bar{1}\bar{1}\bar{1}]$	S_6^{xyz}	S_{61}^+	a_9'	R_9'	h_{29}	$\bar{y}\bar{z}\bar{x}$	$0\bar{1}0$	$00\bar{1}$	$\bar{1}00$	0
$\bar{3}[\bar{1}11]$	$S_6^{x\bar{y}\bar{z}}$	S_{63}^+	a_{10}'	R_{10}'	h_{31}	$y\bar{z}x$	010	$00\bar{1}$	100	0
$\bar{3}[1\bar{1}1]$	$S_6^{\bar{x}y\bar{z}}$	S_{64}^+	a_{11}'	R_{11}'	h_{32}	$yz\bar{x}$	010	001	$\bar{1}00$	0
$\bar{3}[11\bar{1}]$	$S_6^{\bar{x}\bar{y}z}$	S_{62}^+	a_{12}'	R_{12}'	h_{30}	$\bar{y}zx$	$0\bar{1}0$	001	100	0
$\bar{4}[100]$	$\bar{S}_4^x$	S_{4x}^-	a_{14}'	R_{14}	h_{43}	$\bar{x}z\bar{y}$	$\bar{1}00$	001	$0\bar{1}0$	-1
$\bar{4}[010]$	$\bar{S}_4^y$	S_{4y}^-	a_{16}'	R_{16}	h_{48}	$\bar{z}\bar{y}x$	$00\bar{1}$	$0\bar{1}0$	100	-1
$\bar{4}[001]$	$\bar{S}_4^z$	S_{4z}^-	a_{18}'	R_{18}	h_{38}	$y\bar{x}\bar{z}$	010	$\bar{1}00$	$00\bar{1}$	-1
$\bar{4}[\bar{1}00]$	S_4^x	S_{4x}^+	a_{13}'	R_{13}	h_{44}	$\bar{x}\bar{z}y$	$\bar{1}00$	$00\bar{1}$	010	-1
$\bar{4}[0\bar{1}0]$	S_4^y	S_{4y}^+	a_{15}'	R_{15}	h_{46}	$z\bar{y}\bar{x}$	001	$0\bar{1}0$	$\bar{1}00$	-1
$\bar{4}[00\bar{1}]$	S_4^z	S_{4z}^+	a_{17}'	R_{17}	h_{39}	$\bar{y}x\bar{z}$	$0\bar{1}0$	100	$00\bar{1}$	-1
$\bar{2}[011]$	σ^{yz}	σ_{dd}	a_{20}'	R_{20}	h_{42}	$x\bar{z}\bar{y}$	100	$00\bar{1}$	$0\bar{1}0$	1
$\bar{2}[101]$	σ^{zx}	σ_{dc}	a_{22}'	R_{22}	h_{47}	$\bar{z}y\bar{x}$	$00\bar{1}$	010	$\bar{1}00$	1
$\bar{2}[110]$	σ^{xy}	σ_{da}	a_{24}'	R_{24}	h_{40}	$\bar{y}\bar{x}z$	$0\bar{1}0$	$\bar{1}00$	001	1
$\bar{2}[01\bar{1}]$	$\sigma^{y\bar{z}}$	σ_{df}	a_{19}'	R_{19}	h_{41}	xzy	100	001	010	1
$\bar{2}[\bar{1}01]$	$\sigma^{z\bar{x}}$	σ_{de}	a_{21}'	R_{21}	h_{45}	zyx	001	010	100	1
$\bar{2}[1\bar{1}0]$	$\sigma^{x\bar{y}}$	σ_{db}	a_{23}'	R_{23}	h_{37}	yxz	010	100	001	1

[a–g] See corresponding footnotes for Table III.

a representation of the group. It so happends that this representation is irreducible and is known as T_{1u} or as Γ_{15} in the notation of (BSW). (Strictly speaking, Γ_{15} is the name of a particular representation of a space group whose point group is $m3m$.) Since T_{1u} is used extensively in constructing the representation $\{\mathbf{T}(\mathbf{k};\,\mathbf{R})\}$ for all wave vectors $\mathbf{k}$ and all crystal structures whose point group is a subgroup of $m3m$, it is written out by rows. The character of the representation is also given.

Properties Independent of k

Each atom is at a center of inversion and hence $\mathbf{D}(\mathbf{k})$ can be made real. Although the real matrix $\mathbf{C}(\mathbf{k})$ is no longer periodic in reciprocal space, $\omega^2(\mathbf{k})$ still has this property. When converted to real form, Eq. (3.23)* becomes

$$\sum_{\mu\nu} S_{\alpha\mu}S_{\beta\nu}C_{\mu\nu}(\kappa\kappa' \mid \mathbf{k}) = C_{\alpha\beta}(\mathcal{S}_m[\kappa]\mathcal{S}_m[\kappa'] \mid \mathbf{Sk}). \qquad (6.6)$$

Since the two atoms in the unit cell are different, they cannot be transformed into one another by any operation of the space group. This means that $\mathcal{S}_m[\kappa]=\kappa$ for all $\mathcal{S}_m$. With $\mathbf{S}=\mathbf{3}[111]$ and

$$\mathbf{3}[111]\begin{pmatrix} k_1 \\ k_2 \\ k_3 \end{pmatrix} = \begin{pmatrix} k_3 \\ k_1 \\ k_2 \end{pmatrix}, \qquad (6.7)$$

Eq. (6.6) gives the following relations:

$$C_{22}(\kappa\kappa' \mid k_1, k_2, k_3) = C_{33}(\kappa\kappa' \mid k_3, k_1, k_2);$$

$$C_{33}(\kappa\kappa' \mid k_1, k_2, k_3) = C_{11}(\kappa\kappa' \mid k_3, k_1, k_2);$$

$$C_{23}(\kappa\kappa' \mid k_1, k_2, k_3) = C_{31}(\kappa\kappa' \mid k_3, k_1, k_2);$$

$$C_{31}(\kappa\kappa' \mid k_1, k_2, k_3) = C_{12}(\kappa\kappa' \mid k_3, k_1, k_2);$$

$$C_{13}(\kappa\kappa' \mid k_1, k_2, k_3) = C_{21}(\kappa\kappa' \mid k_3, k_1, k_2);$$

$$C_{32}(\kappa\kappa' \mid k_1, k_2, k_3) = C_{13}(\kappa\kappa' \mid k_3, k_1, k_2).$$

By using Eq. (6.6) with $\mathbf{S}=\mathbf{2}[1\bar{1}0]$, one additional independent relation can be found:

$$C_{21}(\kappa\kappa' \mid k_1, k_2, k_3) = C_{12}(\kappa\kappa' \mid k_2, k_1, k_3).$$

TABLE V. Force constant matrices for the eight nearest neighbors to $(l\kappa)=(0001)$ in CsCl lattice; $\mathbf{\Phi}(n)=\mathbf{S}_n\mathbf{\Phi}(1)\mathbf{S}_n^{-1}$, $n=1, 2, \cdots, 8$.

n	l_1'	l_2'	l_3'	κ'	S_n	$-\Phi_{1\nu}$	$-\Phi_{2\nu}$	$-\Phi_{3\nu}$
1	0	0	0	2	$\mathbf{1}$	$\alpha\beta\beta$	$\beta\alpha\beta$	$\beta\beta\alpha$
2	$\bar{1}$	0	0	2	$4[001]$	$\alpha\bar{\beta}\bar{\beta}$	$\bar{\beta}\alpha\beta$	$\bar{\beta}\beta\alpha$
3	$\bar{1}$	$\bar{1}$	0	2	$2[001]$	$\alpha\beta\bar{\beta}$	$\beta\alpha\bar{\beta}$	$\bar{\beta}\bar{\beta}\alpha$
4	0	$\bar{1}$	0	2	$4[00\bar{1}]$	$\alpha\bar{\beta}\beta$	$\bar{\beta}\alpha\bar{\beta}$	$\bar{\beta}\beta\alpha$
5	$\bar{1}$	$\bar{1}$	$\bar{1}$	2	$\bar{\mathbf{1}}$	$\alpha\beta\beta$	$\beta\alpha\beta$	$\beta\beta\alpha$
6	0	$\bar{1}$	$\bar{1}$	2	$\bar{4}[00\bar{1}]$	$\alpha\bar{\beta}\bar{\beta}$	$\bar{\beta}\alpha\beta$	$\bar{\beta}\beta\alpha$
7	0	0	$\bar{1}$	2	$\bar{2}[001]$	$\alpha\beta\bar{\beta}$	$\beta\alpha\bar{\beta}$	$\bar{\beta}\bar{\beta}\alpha$
8	1	0	$\bar{1}$	2	$\bar{4}[001]$	$\alpha\bar{\beta}\beta$	$\bar{\beta}\alpha\bar{\beta}$	$\beta\bar{\beta}\alpha$

The other operations give no new information. The above relations are sufficient to show that there are only two independent functional forms. These can be taken to be $C_{11}(\kappa\kappa'\mid\mathbf{k})$ and $C_{12}(\kappa\kappa'\mid\mathbf{k})$. For given values of κ and κ' the other seven components can be obtained from $C_{11}(\kappa\kappa'\mid\mathbf{k})$ and $C_{12}(\kappa\kappa'\mid\mathbf{k})$ by cyclic permutations and interchanges of the Cartesian components of $\mathbf{k}$. These relations are summarized below.

$$C_{22}(\kappa\kappa'\mid\mathbf{k})=C_{11}(\kappa\kappa'\mid k_2, k_3, k_1); \tag{6.8a}$$

$$C_{33}(\kappa\kappa'\mid\mathbf{k})=C_{11}(\kappa\kappa'\mid k_3, k_1, k_2); \tag{6.8b}$$

$$C_{13}(\kappa\kappa'\mid\mathbf{k})=C_{12}(\kappa\kappa'\mid k_1, k_3, k_2); \tag{6.8c}$$

$$C_{21}(\kappa\kappa'\mid\mathbf{k})=C_{12}(\kappa\kappa'\mid k_2, k_1, k_3); \tag{6.8d}$$

$$C_{23}(\kappa\kappa'\mid\mathbf{k})=C_{12}(\kappa\kappa'\mid k_2, k_3, k_1); \tag{6.8e}$$

$$C_{31}(\kappa\kappa'\mid\mathbf{k})=C_{12}(\kappa\kappa'\mid k_3, k_1, k_2); \tag{6.8f}$$

$$C_{32}(\kappa\kappa'\mid\mathbf{k})=C_{12}(\kappa\kappa'\mid k_3, k_2, k_1). \tag{6.8g}$$

Since $\mathbf{C}(\mathbf{k})$ is symmetric, we have the additional relations

$$C_{11}(21\mid\mathbf{k})=C_{11}(12\mid\mathbf{k}), \tag{6.9a}$$

$$C_{12}(21\mid\mathbf{k})=C_{12}(12\mid\mathbf{k}). \tag{6.9b}$$

It therefore follows that there are only six independent functional forms in $\mathbf{C}(\mathbf{k})$.

As a further aid to construction of a model, the first and second neighbor force-constant matrices will be derived. The atom $(l\kappa)=(0001)$ has eight nearest neighbors. It is assumed that the force-constant matrix for the interaction of this atom with the atom $(l'\kappa')=(0002)$ is of the form[57]

$$\mathbf{\Phi}(0001;0002)=-\begin{pmatrix}\alpha & \beta & \gamma\\ \zeta & \epsilon & \delta\\ \eta & \theta & \iota\end{pmatrix}. \tag{6.10}$$

The group of the bond for this interaction is one of the symmorphic space groups whose point group is $3m$. Because the transformation properties of $\mathbf{\Phi}(l\kappa;\, l'\kappa')$ are independent of the translational part of the operations in the space group, we need consider only the operations of the point group $3m$ in order to determine the symmetry of $\mathbf{\Phi}(l\kappa;\, l'\kappa')$. For this bond

$$3m=\{\mathbf{1}, \mathbf{3}[111], \mathbf{3}[\bar{1}\bar{1}\bar{1}], \bar{\mathbf{2}}[01\bar{1}], \bar{\mathbf{2}}[\bar{1}01], \bar{\mathbf{2}}[1\bar{1}0]\}. \tag{6.11}$$

Equation (2.10b)* and the representation T_{1u} from Tables III and IV impose the following conditions on the matrix elements. With $\mathbf{S}=\mathbf{3}[111]$,

$$\epsilon=\iota=\alpha, \quad \eta=\delta=\beta, \quad \theta=\zeta=\gamma. \tag{6.12a}$$

Letting $\mathbf{S}=\bar{\mathbf{2}}[1\bar{1}0]$ in (2.10b)* gives the additional relations

$$\epsilon=\alpha, \quad \zeta=\beta, \quad \delta=\gamma, \quad \eta=\theta. \tag{6.12b}$$

No further information is obtained by applying the other operations of the point group. When these results are put together, the matrix becomes

$$\mathbf{\Phi}(0001;0002)=-\begin{pmatrix}\alpha & \beta & \beta\\ \beta & \alpha & \beta\\ \beta & \beta & \alpha\end{pmatrix}. \tag{6.13}$$

The seven other force-constant matrices associated with the other nearest neighbors are obtained by applying rotations to the matrix in Eq. (6.13). All of this information is summarized in Table V. The force constant matrices $\mathbf{\Phi}(0002;\, l'1)$ are obtained by the relation

$$\Phi_{\alpha\beta}(0002;\, l'1)=\Phi_{\beta\alpha}(0001;\, -l'2), \tag{6.14}$$

which follows from Eq. (2.3)* and the fact that $\mathbf{\Phi}(l\kappa;\, l'\kappa')$ depends only on the difference between l and l'.

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[57] The minus sign is introduced here because $\mathbf{\phi}(l\kappa;\, l'\kappa')\cdot\mathbf{u}(l'\kappa')$ is minus the force on the atom $(l\kappa)$ due to the displacement $\mathbf{u}(l'\kappa')$.

There are six second neighbors. Take the prototype bond matrix to be

$$\mathbf{\Phi}(0001;\,1001)=-\begin{pmatrix}\lambda & \mu & \nu\\ \sigma & \rho & \xi\\ \tau & \upsilon & \varphi\end{pmatrix}. \tag{6.15}$$

The point group of the bond contains $4mm$ plus the coset of reversal operators $\mathfrak{I}\mathbf{1}\ 4mm$. It will be recalled that the operator $\mathfrak{I}$ transposes the matrix $\mathbf{\Phi}(l\kappa;\,l'\kappa')$. In this case the operator $\mathbf{S}=\mathbf{4}[100]$ tells us that

$$\mu=\nu=\sigma=\tau=\xi=\upsilon=0,\qquad \varphi=\rho.$$

All of the other operations add nothing to our knowledge. Therefore

$$\mathbf{\Phi}(0001;\,1001)=-\begin{pmatrix}\lambda & 0 & 0\\ 0 & \rho & 0\\ 0 & 0 & \rho\end{pmatrix}. \tag{6.16}$$

The information on the other five neighbors is contained in Table VI. This completes the discussion of those properties of $\mathbf{D}(\mathbf{k})$ which are independent of $\mathbf{k}$.

Symmetry of Brillouin Zone

The reciprocal lattice for this crystal lattice is also simple cubic:

$$\mathbf{K}(h)=\left(\frac{2\pi}{a_0}\right)\sum_{i=1}^{3}h_i\mathbf{l}_i. \tag{6.17}$$

The Brillouin zone is shown in Fig. 6.[58] Typical planes, lines, and points of symmetry are shown. Most figures of this sort do not show planes of symmetry since band structure calculations are not usually carried out over whole planes. One should note, however, that any line in a symmetry plane has the symmetry of the plane. Table VII lists the symmetry elements in the nomenclature of (BSW) and Kovalev for the typical elements shown in Fig. 6. Other information given in the table is the point group $G_0(\mathbf{k})$, the principal axis of the point group, the order of the group h, the wave vectors related to $\mathbf{k}$ by a reciprocal lattice vector, the wave vectors in the star of $\mathbf{k}$, i.e., those obtained from $\mathbf{k}$ by applying operation in $G_0(\mathbf{k})$, and the number of wave vectors related to $\mathbf{k}$ at which the phonon energy is the same by symmetry. A quick examination of the $G_0(\mathbf{k})$'s in this table reveals that time inversion caused no additional degeneracies. [See the discussion under Eq. (3.13).]

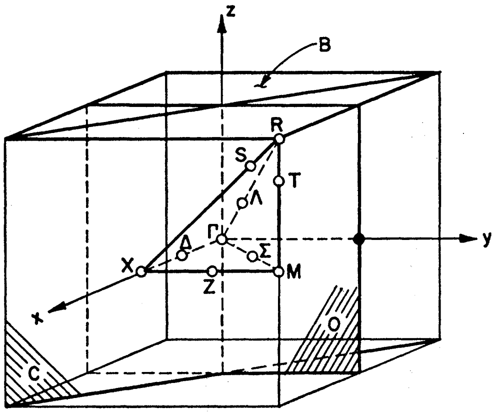

Fig. 6. Brillouin zone for simple cubic lattice. Symmetry planes are labeled *C*, *O*, and *B*.

Table VI. Force constant matrices for the six second-nearest neighbors to $(l\kappa)$ = (0001) in CsCl lattice: $\mathbf{\Phi}(n)=\mathbf{S}_n\mathbf{\Phi}(9)\mathbf{S}_n^{-1}$, $n=9, 10, \cdots, 14$.

n	l_1'	l_2'	l_3'	κ'	S_n	$-\Phi_{1\nu}$	$-\Phi_{2\nu}$	$-\Phi_{3\nu}$
9	1	0	0	1	$\mathbf{1}$	$\lambda 00$	$0\rho 0$	00ρ
10	0	1	0	1	$\mathbf{4}[001]$	$\rho 00$	$0\lambda 0$	00ρ
11	0	0	1	1	$\mathbf{4}[0\bar{1}0]$	$\rho 00$	$0\rho 0$	00λ
12	$\bar{1}$	0	0	1	$\mathbf{2}[001]$	$\lambda 00$	$0\rho 0$	00ρ
13	0	$\bar{1}$	0	1	$\mathbf{4}[00\bar{1}]$	$\rho 00$	$0\lambda 0$	00ρ
14	0	0	$\bar{1}$	1	$\mathbf{4}[0\bar{1}0]$	$\rho 00$	$0\rho 0$	00λ

Symmetry at Γ, $\mathbf{k}_{12}=(0, 0, 0)$

Consider the form of the multiplier representation $\{\mathbf{T}(\mathbf{k};\,\mathbf{R})\}$. Since $\mathcal{R}_m[\kappa']=\kappa'$ and $\mathbf{k}_{12}=\mathbf{0}$, Eq. (3.17b)* reduces to

$$T_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k}_{12};\,\mathbf{R})=\delta(\kappa,\,\kappa')R_{\alpha\beta}. \tag{6.18}$$

The matrix elements $R_{\alpha\beta}$ are given in Tables III and IV under the heading $(T_{1u})_{\alpha\beta}$. The character of $\mathbf{T}(\mathbf{k}_{12};\,\mathbf{R})$ is just twice the character $\chi^{(T_{1u})}$ given in the last column of these tables.

The real symmetric matrix $\mathbf{C}(\mathbf{k})$ has the following transformation properties [as can be verified by making the transformation Eq. (3.27)* on Eq. (5.11)]:

$$C_{\alpha\beta}(\kappa,\,\kappa'\mid\mathbf{k})=\exp\{i[\mathbf{k}-\mathbf{Rk}]\cdot[\mathbf{x}(\kappa)-\mathbf{x}(\kappa')]\}\times\sum_{\mu\nu}R_{\alpha\mu}R_{\beta\nu}C_{\mu\nu}(\kappa\kappa'\mid\mathbf{k}). \tag{6.19}$$

The exponential is nonzero only for $\kappa\neq\kappa'$ and $\mathbf{k}$'s on the surface of the (BZ). This relation holds for all $\mathbf{k}$ in the Brillouin Zone. Application of Eq. (6.19) shows that there are only three independent nonzero matrix elements:

$$A=C_{11}(11\mid\mathbf{k}_{12}),$$

$$B=C_{11}(22\mid\mathbf{k}_{12}), \tag{6.20a}$$

and

$$C=C_{11}(12\mid\mathbf{k}_{12}). \tag{6.20b}$$

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[58] This figure appears in many places. Seldom are two such figures exactly the same. The fact that (BSW) in 1936 used a left-handed system in their figure has probably helped to produce variations.

TABLE VII. Symmetries for the Brillouin zone of a simple cubic attice.

Typical $a_0\mathbf{k}/\pi$	BSW name[a]	Kovalev number	$G_0(\mathbf{k})$	Principal axis	h	Equivalent points	n[b]	Star of **k**	m[b]	N[b]
$(0, \zeta_1, \zeta_2)$	0[a]	1	m	[100]	2	$(0, \zeta_1, \zeta_2)$	1	$(0, \pm\zeta_1, \pm\zeta_2)$, $(\pm\zeta_1, 0, \pm\zeta_2)$, $(\pm\zeta_1, \pm\zeta_2, 0)$ $(0, \pm\zeta_2, \pm\zeta_1)$, $(\pm\zeta_2, 0, \pm\zeta_1)$, $(\pm\zeta_2, \pm\zeta_1, 0)$	24	24
$(\zeta_1, \zeta_2, 1)$	B[a]	2	m	[001]	2	$(\zeta_1, \zeta_2, \pm 1)$	2	$(\pm\zeta_1, \pm\zeta_2, 1)$, $(\pm\zeta_1, 1, \pm\zeta_2)$, $(1, \pm\zeta_1, \pm\zeta_2)$ $(\pm\zeta_2, \pm\zeta_1, 1)$, $(\pm\zeta_2, 1, \pm\zeta_1)$, $(1, \pm\zeta_2, \pm\zeta_1)$	24	48
$(-\zeta_1, \zeta_1, \zeta_2)$	C[a]	3	m	[110]	2	$(-\zeta_1, \zeta_1, \zeta_2)$	1	$(\pm\zeta_1, \pm\zeta_1, \pm\zeta_2)$, $(\pm\zeta_1, \pm\zeta_2, \pm\zeta_1)$ $(\pm\zeta_2, \pm\zeta_1, \pm\zeta_1)$,	24	24
$(\zeta, \zeta, 0)$	Σ	4	$mm2$	[110]	4	$(\zeta, \zeta, 0)$	1	$(\pm\zeta, \pm\zeta, 0)$, $(\pm\zeta, 0, \pm\zeta)$, $(0, \pm\zeta, \pm\zeta)$	12	12
$(1, \zeta, \zeta)$	S	5	$mm2$	[011]	4	$(\pm 1, \zeta, \zeta)$	2	$(1, \pm\zeta, \pm\zeta)$, $(\pm\zeta, 1, \pm\zeta)$, $(\pm\zeta, \pm\zeta, 1)$	12	24
$(1, \zeta, 0)$	Z	6	$mm2$	[010]	4	$(\pm 1, \zeta, 0)$	2	$(1, \pm\zeta, 0)$, $(\pm\zeta, 1, 0)$, $(\pm\zeta, 0, 1)$ $(0, \pm\zeta, 1)$, $(1, 0, \pm\zeta)$, $(0, 1, \pm\zeta)$	12	24
(ζ, ζ, ζ)	Λ	9	$3m$	[111]	6	(ζ, ζ, ζ)	1	$(\pm\zeta, \pm\zeta, \pm\zeta)$	8	8
$(1, 1, \zeta)$	T	7	$4mm$	[001]	8	$(\pm 1, \pm 1, \zeta)$	4	$(1, 1, \pm\zeta)$, $(1, \pm\zeta, 1)$, $(\pm\zeta, 1, 1)$	6	24
$(\zeta, 0, 0)$	Δ	8	$4mm$	[100]	8	$(\zeta, 0, 0)$	1	$(\pm\zeta, 0, 0)$, $(0, \pm\zeta, 0)$, $(0, 0, \pm\zeta)$	6	6
$(1, 0, 0)$	X	10	$4/mmm$	[100]	16	$(\pm 1, 0, 0)$	2	$(1, 0, 0)$, $(0, 1, 0)$, $(0, 0, 1)$	3	3
$(1, 1, 0)$	M	11	$4/mmm$	[001]	16	$(\pm 1, \pm 1, 0)$	4	$(1, 1, 0)$, $(1, 0, 1)$, $(0, 1, 1)$	3	12
$(1, 1, 1)$	R	13	$m3m$	[111]	48	$(\pm 1, \pm 1, \pm 1)$	8	$(1, 1, 1)$	1	8
$(0, 0, 0)$	Γ	12	$m3m$	[000]	48	$(0, 0, 0)$	1	$(0, 0, 0)$	1	1

[a] The names of the symmetry planes are not due to BSW, but appear in Altmann and Cracknell. See Ref. 5, p. 20, Fig. 1.

[b] n is the number of equivalent points, m is the number of points in the star, and N is the number of places in the zone which have the same energy by symmetry alone. One should have $hm=48$ and $nm=N$.

The final form of $\mathbf{C}(\mathbf{k}_{12})$ is

$$\mathbf{C}(\mathbf{k}_{12}) = \begin{pmatrix} A & & & C & & \\ & A & & & C & \\ & & A & & & C \\ C & & & B & & \\ & C & & & B & \\ & & C & & & B \end{pmatrix}. \tag{6.21}$$

The irreducible representations may be found in Slater[4] (Table A3-20, p. 375), or in Altmann and Cracknell[5] (Tables II and III), or in Kovalev[3] [T205, p. 92 (see Table XXVI, given later in this paper, for correction to T205)], or McWeeny[6] (Table 4.22, p. 105). None of these tables are perfectly convenient to use. All of them give only a portion of the representations and require the reader to complete the table by some given rule. A comparison of the names of the ten irreducible representation is given in Table VIII. The correspondences were made by matching characters. It is sometimes difficult to compare representations directly because they may differ by a unitary transformation.

Either by inspection or by using Eq. (4.36)* for c_s, one finds that $\{\mathbf{T}(\mathbf{k}_{12};\, \mathbf{R})\}$ may be reduced to the direct sum of two identical three-dimensional representations:

$$\{\mathbf{T}(\mathbf{k}_{12};\, \mathbf{R})\} = 2\Gamma_{15} = 2T_{1u} = 2\tau^{(10)}. \tag{6.22}$$

This suggests that there are three degenerate acoustic modes and three degenerate optic modes. The frequency of the optical mode in ionic solids very close to $\mathbf{k}=\mathbf{0}$ can be measured by optical absorption and Raman scattering. These measurements show a large splitting between the longitudinal and transverse modes. At first sight this appears to be in contradiction to the degeneracy required by group theory at $\mathbf{k}=\mathbf{0}$. There are three good recent discussions of this problem in the literature.[59–61] All parties agree that there must be a degeneracy at $\mathbf{k}=\mathbf{0}$ for the optical modes. They are not in total agreement on the source of the apparent difficulty. Rosenstock has questioned the validity of using cyclic boundary conditions for calculations involving long-range Coulomb forces. Barron advances arguments showing that cyclic boundary conditions are not essential. He feels that Coulomb retardation effects alone are adequate to understand the apparent discontinuity. Maradudin and Weiss, on the other hand, have demonstrated that the conditionally convergent Coulomb summations depend on how one takes the limit

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[59] H. B. Rosenstock, Phys. Rev. **121,** 416 (1961).

[60] A. A. Maradudin and G. H. Weiss, Phys. Rev. **123,** 1968 (1961).

[61] T. H. K. Barron, Phys. Rev. **123,** 1995 (1961).

TABLE VIII. Comparison of names for the irreducible representation of $m3m$ at Γ.

A and C, McW[a]	A_{1g}	A_{2g}	E_g	T_{1g}	T_{2g}	A_{1u}	A_{2u}	E_u	T_{1u}	T_{2u}
BSW[b]	Γ_1	Γ_2	Γ_{12}	Γ_{15}'	Γ_{25}'	Γ_1'	Γ_2'	Γ_{12}'	Γ_{15}	Γ_{25}
K[c]	τ^1	τ^2	τ^3	τ^5	τ^4	τ^6	τ^7	τ^8	τ^{10}	τ^9

[a] Altmann and Cracknell (see Ref. 5) and McWeeny (see Ref. 6, p. 105) use the same notation.

This association with BSW is given in Altmann and Cracknell.

[c] Kovalev (see Ref. 3, T205, p. 92).

as **k** approaches zero. For a finite size crystal one obtains the degeneracy; for crystals which become infinite before **k** goes to zero, there are two distinct optical frequencies. They suggest that it might be possible to see the longitudinal and transverse branches become degenerate by making measurements on very small crystals or powders. No experimental information exists on this point. It is fairly easy to understand why there is a difference in energy between the longitudinal and transverse modes for **k** not equal to zero. Consider the equation

$$\nabla\cdot\mathbf{E}(\mathbf{x})=-\rho(\mathbf{x}) \tag{6.23a}$$

for the electric field. $\rho(\mathbf{x})$ is the macroscopic charge density. It is zero in the interior of the solid when no disturbance is present. Let us Fourier-transform this equation:

$$\mathbf{k}\cdot\mathbf{E}(\mathbf{k})=-\rho(\mathbf{k}). \tag{6.23b}$$

For definiteness, let the solid be finite in size and let

$$\rho(\mathbf{k})=\frac{1}{2\pi}\int\rho(\mathbf{x})\exp(-i\mathbf{k}\cdot\mathbf{x})\,d\mathbf{x}, \tag{6.24}$$

where the integral goes over all space. $\rho(\mathbf{k})=0$ for the static solid. A transverse mode does not change the charge density within the bulk of the solid. There may be charge induced at the surface, but the electric field contributed by this will depend on the size and shape of the crystal. What field there is will be nearly perpendicular to **k**, which is consistent with $\rho(\mathbf{k})$ in Eq. (6.23b) being small. This macroscopic field will contribute in a negligible fashion to the restoring forces in the solid. For the longitudinal modes, however, $\rho(\mathbf{x})$ is not zero throughout the bulk of the solid, and hence $\rho(\mathbf{k})$ is larger. This will give a larger restoring field from Eq. (6.23b). The energy of the longitudinal mode will therefore be higher. For $\mathbf{k}=0$, however, there is a discontinuity. Equation (6.24) must give zero if there is charge neutrality, and Eq. (6.23b) places no restriction on $\mathbf{E}(\mathbf{k})$. The field that does exist is due to surface charge density and is the same for longitudinal and transverse modes, since there is no physical way of telling them apart for $\mathbf{k}=\mathbf{0}$. The energy of the displacement is degenerate for isotropic solids. The above argument is qualitative and should not be taken too seriously. This discussion also has to be modified in the case of anistropic solids. As an example of what can occur, the reader is referred to an article by Nusimovici and Birman[54] which predicted the "displacement of both the Γ_1 and Γ_5 modes when observed for $k\parallel x$ compared to $k\parallel z$" in the wurtzite structure. Γ_1 is transverse-optic and Γ_5 is longitudinal-optic.

Let us return now to the problem of finding the eigenvalues and eigenvectors for $\mathbf{C}(\mathbf{k}_{12})$. At first sight the construction of a symmetry-adapted eigenvector by the projection-operator method might seem a little onerous since it involves the addition of 48 six-by-six matrices. A close examination of the irreducible representation shows that many of the matrix elements $(\tau_{\lambda\lambda}{}^{(10)}(\mathbf{k}_{12},\mathbf{R})$ entering into the projection operator are zero. Only 16 matrices have to be added. Furthermore, $\mathbf{T}(\mathbf{k}_{12};\mathbf{R})$ has two equal three-by-three nonzero blocks, and hence it is only necessary to do the addition for one block to infer the form of the whole six-by-six matrix. The projection operator for $\lambda=\lambda'=1$ is

$$P_{11}{}^{(10)}(\mathbf{k}_{12})=\begin{pmatrix}1&&&&&\\&0&&&&\\&&0&&&\\&&&1&&\\&&&&0&\\&&&&&0\end{pmatrix}. \tag{6.25}$$

The symmetry-adapted eigenvector is

$$\mathbf{E}(\mathbf{k}_{12};10\;1)=\begin{pmatrix}\psi_1\\0\\0\\\psi_4\\0\\0\end{pmatrix}. \tag{6.26}$$

When this is substituted into the eigenvalue equation, one obtains a set of two simultaneous homogeneous linear equations:

$$(A-\omega^2)\psi_1+C\psi_2=0; \tag{6.27a}$$

$$C\psi_1+(B-\omega^2)\psi_2=0. \tag{6.27b}$$

TABLE IX. Decomposition of the representation $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ for all symmetry elements in the Brillouin zone of CsCl lattice.

$\mathbf{k}$	(BSW)	McWeeny	Kovalev
O, k_1	$4O_1\oplus 2O_2$	$4A'\oplus 2A''$	$4\tau^{(1)}\oplus 2\tau^{(2)}$
B, k_2	$3B_1\oplus 3B_2$	$3A'\oplus 3A''$	$3\tau^{(1)}\oplus 3\tau^{(2)}$
C, k_3	$4C_1\oplus 2C_2$	$4A'\oplus 2A''$	$4\tau^{(1)}\oplus 2\tau^{(2)}$
Σ, k_4	$2(\Sigma_1\oplus\Sigma_3\oplus\Sigma_4)$	$2(A_1\oplus B_2\oplus B_1)$	$2(\tau^{(1)}\oplus\tau^{(4)}\oplus\tau^{(3)})$
S, k_5	$2S_1\oplus S_2\oplus 2S_3\oplus S_4$	$2A_1\oplus A_2\oplus 2B_1\oplus B_2$	$2\tau^{(1)}\oplus\tau^{(2)}\oplus 2\tau^{(3)}\oplus\tau^{(4)}$
Z, k_6	$2Z_1\oplus Z_2\oplus 2Z_3\oplus Z_4$	$2A_1\oplus A_2\oplus 2B_1\oplus B_2$	$2\tau^{(1)}\oplus\tau^{(2)}\oplus 2\tau^{(3)}\oplus\tau^{(4)}$
Λ, k_9	$2\Lambda_1\oplus 2\Lambda_3$	$2A_1\oplus 2E$	$2\tau^{(1)}\oplus 2\tau^{(3)}$
T, k_7	$T_1\oplus T_2'\oplus 2T_5$	$A_1\oplus B_2\oplus 2E$	$\tau^{(1)}\oplus\tau^{(4)}\oplus 2\tau^{(5)}$
Δ, k_8	$2\Delta_1\oplus 2\Delta_5$	$2A_1\oplus 2E$	$2\tau^{(1)}\oplus 2\tau^{(5)}$
X, k_{10}	$X_1\oplus X_5\oplus X_4'\oplus X_5'$	$A_{1g}\oplus E_g\oplus A_{2u}\oplus E_u$	$\tau^{(1)}\oplus\tau^{(9)}\oplus\tau^{(4)}\oplus\tau^{(10)}$
M, k_{11}	$M_2'\oplus M_4'\oplus 2M_5'$	$B_{1u}\oplus A_{2u}\oplus 2E_u$	$\tau^{(8)}\oplus\tau^{(4)}\oplus 2\tau^{(10)}$
R, k_{13}	$\Gamma_{15}\oplus\Gamma_{25}'$	$T_{1u}\oplus T_{2g}$	$\tau^{(10)}\oplus\tau^{(4)}$
Γ, k_{12}	$2\Gamma_{15}$	$2T_{1u}$	$2\tau^{(10)}$

This set is supplemented by a normalization condition:

$$\psi_1^2+\psi_2^2=1. \tag{6.28}$$

ψ_1 and ψ_2 are real quantities. The eigenvalues are

$$\omega_{101}^2(\mathbf{k}_{12})=\tfrac{1}{2}[A+B]-\{\tfrac{1}{4}[A+B]^2-AB+C^2\}^{1/2}, \tag{6.29a}$$

$$\omega_{102}^2(\mathbf{k}_{12})=\tfrac{1}{2}[A+B]+\{\tfrac{1}{4}[A+B]^2-AB+C^2\}^{1/2}. \tag{6.29b}$$

The eigenvectors corresponding to these are

$$\mathbf{e}(\mathbf{k}_{12}\ 10i1)=\begin{pmatrix} -C/N(i) \\ 0 \\ 0 \\ (A-\omega_{10i}^2(\mathbf{k}_{12}))/N(i) \\ 0 \\ 0 \end{pmatrix}, \tag{6.30a}$$

where $i=1$, 2 and

$$N(i)=\{C^2+(A-\omega_{10i}^2(\mathbf{k}_{12}))^2\}^{1/2}. \tag{6.30b}$$

By examining the limit as $\mathbf{k}$ approaches zero in $\mathbf{C}(\mathbf{k})$, one can show that $C^2=AB$. This is done in Appendix A. This means that $\omega_{101}^2(\mathbf{k}_{12})=0$. Now that one knows the general form of the symmetry-adapted trial eigenvector for $\lambda=1$, it is not too hard to guess $\mathbf{E}(\mathbf{k}_{12};102)$ and $\mathbf{E}(\mathbf{k}_{12};103)$:

$$\mathbf{E}(\mathbf{k}_{12};102)=\begin{pmatrix} 0 \\ \psi_2 \\ 0 \\ 0 \\ \psi_5 \\ 0 \end{pmatrix} \tag{6.31}$$

and

$$\mathbf{E}(\mathbf{k}_{12};103)=\begin{pmatrix} 0 \\ 0 \\ \psi_3 \\ 0 \\ 0 \\ \psi_6 \end{pmatrix}. \tag{6.32}$$

It is easily seen that

$$\psi_2=\psi_3=-C/N(i), \tag{6.33}$$

$$\psi_5=\psi_6=(A-\omega_{10i}^2(\mathbf{k}_{12}))/N(i). \tag{6.34}$$

In Appendix A it is also shown that the solution $i=1$ has the atoms moving in phase. The above results may be summarized by giving the unitary transformation matrix which will diagonalize $\mathbf{C}(\mathbf{k}_{12})$:

$$\mathbf{U}^{-1}\mathbf{C}\mathbf{U}=\mathbf{\Omega}, \tag{6.35}$$

$$\mathbf{U}^{-1}=\begin{pmatrix} -C/N(1) & 0 & 0 & -C/N(2) & 0 & 0 \\ 0 & -C/N(1) & 0 & 0 & -C/N(2) & 0 \\ 0 & 0 & -C/N(1) & 0 & 0 & -C/N(2) \\ A/N(1) & 0 & 0 & -B/N(2) & 0 & 0 \\ 0 & A/N(1) & 0 & 0 & -B/N(2) & 0 \\ 0 & 0 & A/N(1) & 0 & 0 & -B/N(2) \end{pmatrix}. \tag{6.36}$$

The columns of this matrix are the eigenvectors, i.e.,

$$\mathbf{U}^{-1}=(\mathbf{e}(\mathbf{k}_{12}1011),\mathbf{e}(\mathbf{k}_{12}1012),\mathbf{e}(\mathbf{k}_{12}1013),\mathbf{e}(\mathbf{k}_{12}1021),\times\mathbf{e}(\mathbf{k}_{12}1022),\mathbf{e}(\mathbf{k}_{12}1023)). \quad (6.37)$$

The diagonal matrix $\mathbf{\Omega}$ is

$$\mathbf{\Omega}=\begin{pmatrix}0&&&&&\\&0&&&&\\&&0&&&\\&&&A+B&&\\&&&&A+B&\\&&&&&A+B\end{pmatrix}. \quad (6.38)$$

Symmetry at R, $\mathbf{k}_{13}=(\pi/a_0)(1, 1, 1)$

Let us begin with the construction of $\{\mathbf{T}(\mathbf{k}_{13};\mathbf{R})\}$.

$$T_{\alpha\beta}(\kappa\kappa'\mid\mathbf{k}_{13};\mathbf{R})=\delta(\kappa,\kappa')\exp[i\theta(\kappa\mid\mathbf{k}_{13};\mathcal{R}_m)]R_{\alpha\beta}, \quad (6.39a)$$

where

$$\theta(\kappa\mid\mathbf{k}_{13};\mathcal{R}_m)=\mathbf{k}_{13}\cdot[\mathbf{x}(\kappa)-\mathbf{R}\mathbf{x}(\kappa)]. \quad (6.39b)$$

Since $\mathbf{x}(1)=\mathbf{0}$, it follows that $\theta(1\mid\mathbf{k};\mathcal{R}_m)=0$ for all $\mathbf{k}$ and $\mathcal{R}_m$. It turns out that $\bar{\theta}=\exp[i\theta(2\mid\mathbf{k};\mathcal{R}_m)]$ is ±1 for all $\mathbf{k}$ that we shall consider below. Thus

$$\mathbf{T}(\mathbf{k};\mathbf{R})=\begin{pmatrix}\mathbf{R}&\mathbf{0}\\\mathbf{0}&\bar{\theta}\mathbf{R}\end{pmatrix}. \quad (6.40)$$

Whether $\bar{\theta}$ is one or minus one depends on the particular $\mathbf{k}$ and on the element $\mathbf{R}$. For instance, when $\mathbf{k}=\mathbf{k}_{13}$, then

$$\begin{aligned}\bar{\theta}&=+1, \qquad \mathbf{R}\in\bar{4}3m\\&=-1, \qquad \mathbf{R}\in\bar{\mathbf{1}}\,\bar{4}3m.\end{aligned} \quad (6.41)$$

$\bar{4}3m$ is a subgroup of $m3m$; $\bar{\mathbf{1}}\,\bar{4}3m$ is the set of elements obtained by multiplying each element in $\bar{4}3m$ by the inversion **1**. The character can likewise be expressed in terms of $\bar{\theta}$:

$$\chi(\mathbf{k};\mathbf{R})=(1+\bar{\theta})\chi^{(T_{1u})}(\mathbf{R}). \quad (6.42)$$

In order to save space, only $\bar{\theta}$ will be given for the other symmetry points, lines, and planes. Equations (6.40) and (6.42) shall be understood. For convenience of reference the decomposition of $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ into its irreducible parts for all symmetry points, lines, and planes is given in Table IX.

There remains the problem of listing the eigenvectors and eigenvalues in terms of the matrix elements of $\mathbf{C}(\mathbf{k})$. This can be done most efficiently by giving the form of $\mathbf{C}(\mathbf{k})$ after the invariance relations (6.19) have been applied for all operations in the group of the wave vector. This will serve to identify the nonzero elements of $\mathbf{C}(\mathbf{k})$. Thus, for $\mathbf{k}=\mathbf{k}_{13}$,

$$\mathbf{C}(\mathbf{k}_{13})=\begin{pmatrix}A&&&&&\\&A&&&&\\&&A&&&\\&&&B&&\\&&&&B&\\&&&&&B\end{pmatrix}. \quad (6.43)$$

It is obvious that

$$A=C_{11}(11\mid\mathbf{k}_{13}) \quad (6.44a)$$

and

$$B=C_{11}(22\mid\mathbf{k}_{13}). \quad (6.44b)$$

Next we give the matrix $\mathbf{U}^{-1}$ whose columns are the eigenvectors. For $\mathbf{k}_{13}$ this is just the six by six unit matrix because $\mathbf{C}(\mathbf{k}_{13})$ is already diagonal. Finally, the eigenvalues are given:

$$\omega_{10}^2(\mathbf{k}_{13})=A; \quad (6.45a)$$

$$\omega_4^2(\mathbf{k}_{13})=B. \quad (6.45b)$$

The labels on the eigenvalues are those due to Kovalev. One can easily convert to (BSW) labels by using the correspondences in Table IX.

Symmetry at M, $\mathbf{k}_{11}=(\pi/a_0)(1, 1, 0)$

$$\begin{aligned}\bar{\theta}&=+1, \qquad \mathbf{R}\in mmm\\&=-1, \qquad \mathbf{R}\in\mathbf{4}[100]\,mmm.\end{aligned} \quad (6.46)$$

$$mmm=\{\mathbf{1},\mathbf{2}[001],\mathbf{2}[110],\mathbf{2}[1\bar{1}0],\bar{\mathbf{1}},\bar{\mathbf{2}}[001],\times\bar{\mathbf{2}}[110],\bar{\mathbf{2}}[1\bar{1}0]\}. \quad (6.47)$$

$$\mathbf{C}(\mathbf{k}_{11})=\begin{pmatrix}A&&&&C&\\&A&&C&&\\&&D&&&\\&C&&B&&\\C&&&&B&\\&&&&&E\end{pmatrix}. \quad (6.48)$$

$$\mathbf{U}^{-1}=\begin{pmatrix}0&0&0&u_1&0&u_2\\0&0&u_1&0&u_2&0\\0&1&0&0&0&0\\0&0&v_1&0&v_2&0\\0&0&0&v_1&0&v_2\\1&0&0&0&0&0\end{pmatrix}. \quad (6.49)$$

Let $\alpha_{11}=A$, $\alpha_{22}=B$, and $\alpha_{12}=C$, then

$$u_i=-\alpha_{12}/N_i, \tag{6.50a}$$

$$v_i=[\alpha_{11}-\omega_{10i}^2(\mathbf{k}_{11})]/N_i, \tag{6.50b}$$

$$N_i=\{\alpha_{12}^2+[\alpha_{11}-\omega_{10i}(\mathbf{k}_{11})]^2\}^{1/2}, \tag{6.50c}$$

$$\omega_{10i}^2(\mathbf{k}_{11})=\tfrac{1}{2}[\alpha_{11}+\alpha_{22}] +(2i-3)\{\tfrac{1}{4}[\alpha_{11}+\alpha_{22}]^2-\alpha_{11}\alpha_{22}+\alpha_{12}^2\}^{1/2}. \tag{6.50d}$$

This form of solution occurs so often in what follows that we refer to this set of equations and give the particular form of α_{11}, α_{22}, and α_{12} for each case. The other eigenvalues are

$$\omega_8^2(\mathbf{k}_{11})=E, \tag{6.51}$$

$$\omega_4^2(\mathbf{k}_{11})=D. \tag{6.52}$$

In these modes one of the sublattices is standing still.

Symmetry at X, $\mathbf{k}_{10}=(\pi/a_0)(1,0,0)$

$$\begin{aligned}\bar{\theta}&=+1, & R&\in 4mm\\ &=-1, & R&\in \bar{1}\,4mm,\end{aligned} \tag{6.53}$$

$$4mm=\{1, 2[100], 4[100], 4[\bar{1}00], \bar{2}[010], \times\bar{2}[001], \bar{2}[011], \bar{2}[01\bar{1}]\}. \tag{6.54}$$

$$\mathbf{C}(\mathbf{k}_{10})=\begin{pmatrix} A&&&&&\\ &B&&&&\\ &&B&&&\\ &&&C&&\\ &&&&D&\\ &&&&&D \end{pmatrix}. \tag{6.55}$$

$$\mathbf{U}^{-1}=\begin{pmatrix} 0&0&0&1&0&0\\ 0&0&0&0&1&0\\ 0&0&0&0&0&1\\ 1&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&1&0&0&0 \end{pmatrix}. \tag{6.56}$$

The eigenvectors are listed in the same order as the representations in Table IX:

$$\omega_1^2(\mathbf{k}_{10})=C; \tag{6.57}$$

$$\omega_9^2(\mathbf{k}_{10})=D; \tag{6.58}$$

$$\omega_4^2(\mathbf{k}_{10})=A; \tag{6.59}$$

$$\omega_{10}^2(\mathbf{k}_{10})=B. \tag{6.60}$$

Symmetry on Δ, $\mathbf{k}_8=(\pi/a_0)(\zeta,0,0)$

$$\bar{\theta}=1,\ R\in 4mm. \tag{6.61}$$

$$\mathbf{C}(\mathbf{k}_8)=\begin{pmatrix} A&&&C&&\\ &D&&&F&\\ &&D&&&F\\ C&&&B&&\\ &F&&&E&\\ &&F&&&E \end{pmatrix}. \tag{6.62}$$

$$\mathbf{U}^{-1}=\begin{pmatrix} u_1&u_2&0&0&0&0\\ 0&0&u_1'&0&u_2'&0\\ 0&0&0&u_1'&0&u_2'\\ v_1&v_2&0&0&0&0\\ 0&0&v_1'&0&v_2'&0\\ 0&0&0&v_1'&0&v_2' \end{pmatrix}. \tag{6.63}$$

Let

$$\alpha_{11}=A,\quad \alpha_{22}=B,\quad\text{and}\quad \alpha_{12}=C \tag{6.64}$$

to get the solutions for u_i, v_i, and $\omega_{1i}^2(\mathbf{k}_8)$ from (6.50).

Symmetry on T, $\mathbf{k}_7=(\pi/a_0)(1,1,\zeta)$

$$\begin{aligned}\bar{\theta}&=+1, & R&\in mm2\\ &=-1, & R&\in 4[001]\,mm2\end{aligned} \tag{6.66}$$

$$mm2=\{1, 2[001], \bar{2}[011], \bar{2}[01\bar{1}]\}. \tag{6.67}$$

$$\mathbf{C}(\mathbf{k}_7)=\begin{pmatrix} A&&&&C&\\ &A&&C&&\\ &&D&&&\\ &C&&B&&\\ C&&&&B&\\ &&&&&E \end{pmatrix}. \tag{6.68}$$

$$\mathbf{U}^{-1}=\begin{pmatrix} 0&0&0&u_1&0&u_2\\ 0&0&u_1&0&u_2&0\\ 1&0&0&0&0&0\\ 0&0&v_1&0&v_2&0\\ 0&0&0&v_1&0&v_2\\ 0&1&0&0&0&0 \end{pmatrix}. \tag{6.69}$$

$$\omega_1^2(\mathbf{k}_7)=D; \tag{6.70}$$

$$\omega_4^2(\mathbf{k}_7)=E. \tag{6.71}$$

Let

$$\alpha_{11}=A, \qquad \alpha_{22}=B, \quad \text{and} \quad \alpha_{12}=C \tag{6.72}$$

to get the solutions for u_i, v_i, and $\omega_{5i}^2(\mathbf{k}_7)$ from (6.50).

Symmetry on Λ, $\mathbf{k}_9=(\pi/a_0)(\zeta, \zeta, \zeta)$

$$\bar{\theta}=1, \qquad \mathbf{R}\in 3m, \tag{6.73}$$

$$3m=\{\mathbf{1}, \mathbf{3}[111], \mathbf{3}[\bar{1}\bar{1}\bar{1}], \bar{\mathbf{2}}[01\bar{1}], \mathbf{2}[\bar{1}01], \bar{\mathbf{2}}[1\bar{1}0]\}. \tag{6.74}$$

$$\mathbf{C}(\mathbf{k}_9)=\begin{pmatrix} A & C & C & E & F & F \\ C & A & C & F & E & F \\ C & C & A & F & F & E \\ E & F & F & B & D & D \\ F & E & F & D & B & D \\ F & F & E & D & D & B \end{pmatrix}. \tag{6.75}$$

$$\mathbf{U}^{-1}=\begin{pmatrix} u_1/\sqrt{3} & u_2/\sqrt{3} & 2u_1'/(6)^{1/2} & 0 & 2u_2'/(6)^{1/2} & 0 \\ u_1/\sqrt{3} & u_2/\sqrt{3} & -u_1'/(6)^{1/2} & u_1'/\sqrt{2} & -u_2'/(6)^{1/2} & u_2'/\sqrt{2} \\ u_1/\sqrt{3} & u_2/\sqrt{3} & -u_1'/(6)^{1/2} & -u_1'/\sqrt{2} & -u_2'/(6)^{1/2} & -u_2'/\sqrt{2} \\ v_1/\sqrt{3} & v_2/\sqrt{3} & 2v_1'/(6)^{1/2} & 0 & 2v_2'/(6)^{1/2} & 0 \\ v_1/\sqrt{3} & v_2/\sqrt{3} & -v_1'/(6)^{1/2} & v_1'/\sqrt{2} & -v_2'/(6)^{1/2} & v_2'/\sqrt{2} \\ v_1/\sqrt{3} & v_2/\sqrt{3} & -v_1'/(6)^{1/2} & -v_1'/\sqrt{2} & -v_2'/(6)^{1/2} & -v_2'/\sqrt{2} \end{pmatrix}. \tag{6.76}$$

Let

$$\alpha_{11}=A+2C, \qquad \alpha_{22}=B+2D, \quad \text{and} \quad \alpha_{12}=E+2F \tag{6.77}$$

to get the solutions for u_i, v_i, and $\omega_{1i}^2(\mathbf{k}_9)$ from 6.50.
Let

$$\alpha_{11}=A-C, \qquad \alpha_{22}=B-D, \quad \text{and} \quad \alpha_{12}=E-F \tag{6.78}$$

to get the solutions for u_i', v_i', and $\omega_{3i}^2(\mathbf{k}_9)$ from (6.50).

Symmetry on Z, $\mathbf{k}_6=(\pi/a_0)(1, \zeta, 0)$

$$\begin{aligned} \bar{\theta}&=+1, \qquad \mathbf{R}\in\{\mathbf{1}, \mathbf{2}[001]\}, \\ &=-1, \qquad \mathbf{R}\in\{\mathbf{2}[100], \mathbf{2}[010]\}, \end{aligned} \tag{6.79}$$

$$\mathbf{C}(\mathbf{k}_6)=\begin{pmatrix} A & & & & H & \\ & B & & G & & \\ & & C & & & \\ & G & & D & & \\ H & & & & E & \\ & & & & & F \end{pmatrix}. \tag{6.80}$$

TABLE X. Compatibility relations at Γ for representations of CsCl.

	Δ	Λ	Σ
Γ_{15}	$\Delta_1\oplus\Delta_5$	$\Lambda_1\oplus\Lambda_3$	$\Sigma_1\oplus\Sigma_3\oplus\Sigma_4$

$$\mathbf{U}^{-1}=\begin{pmatrix} u_1 & u_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & u_1' & u_2' & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & v_1' & v_2' & 0 \\ v_1 & v_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}. \tag{6.81}$$

Let

$$\alpha_{11}=A, \qquad \alpha_{22}=E, \quad \text{and} \quad \alpha_{12}=H \tag{6.82}$$

to get the solutions for u_i, v_i, and $\omega_{1i}^2(\mathbf{k}_6)$ from (6.50).

$$\omega_2^2(\mathbf{k}_6)=F. \tag{6.83}$$

Let

$$\alpha_{11}=B; \qquad \alpha_{22}=D, \quad \text{and} \quad \alpha_{12}=G \tag{6.84}$$

to get the solutions for u_i', v_i', and $\omega_3^2(\mathbf{k}_6)$ from (6.50).

$$\omega_4^2(\mathbf{k}_6)=C. \tag{6.85}$$

Symmetry on S, $\mathbf{k}_5=(\pi/a_0)(1, \zeta, \zeta)$

$$\begin{aligned} \bar{\theta}&=+1, \qquad \mathbf{R}\in\{\mathbf{1}, \bar{\mathbf{2}}[01\bar{1}]\} \\ &=-1, \qquad \mathbf{R}\in\{\mathbf{2}[011], \bar{\mathbf{2}}[100]\}. \end{aligned} \tag{6.86}$$

$$\mathbf{C}(\mathbf{k}_5)=\begin{pmatrix} A & & & & H & H \\ & B & C & G & & \\ & C & B & G & & \\ & G & G & D & & \\ H & & & & E & F \\ H & & & & F & E \end{pmatrix}. \tag{6.87}$$

$$\mathbf{U}^{-1}=\begin{pmatrix} 0 & 0 & 0 & u_1' & u_2' & 0 \\ u_1/\sqrt{2} & u_2/\sqrt{2} & 0 & 0 & 0 & 1/\sqrt{2} \\ u_1/\sqrt{2} & u_2/\sqrt{2} & 0 & 0 & 0 & -1/\sqrt{2} \\ v_1 & v_2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} & v_1'/\sqrt{2} & v_2'/\sqrt{2} & 0 \\ 0 & 0 & -1/\sqrt{2} & v_1'/\sqrt{2} & v_2'/\sqrt{2} & 0 \end{pmatrix}. \tag{6.88}$$

Let

$$\alpha_{11}=B+C, \qquad \alpha_{22}=D, \quad \text{and} \quad \alpha_{12}=\sqrt{2}G \tag{6.89}$$

to get the solutions for u_i, v_i, and $\omega_{1i}^2(\mathbf{k}_5)$ from (6.50).

$$\omega_2^2(\mathbf{k}_5)=E-F. \tag{6.90}$$

Let

$$\alpha_{11}=A, \qquad \alpha_{22}=E+F, \quad \text{and} \quad \alpha_{12}=\sqrt{2}H \tag{6.91}$$

to get the solutions for u_i', v_i', and $\omega_{3i}^2(\mathbf{k}_5)$ from (6.50).

$$\omega_4^2(\mathbf{k}_5)=B-C. \tag{6.92}$$

Symmetry on $\sum$, $\mathbf{k}_4=(\pi/a_0)(\zeta,\zeta,0)$

$$\bar{\theta}=1, \qquad \mathbf{R}\in mm2. \tag{6.93}$$

$$mm2=\{\bar{1}, 2[110], \bar{2}[001], \bar{2}[\bar{1}10]\}. \tag{6.94}$$

$$\mathbf{C}(\mathbf{k}_4)=\begin{pmatrix} A & C & & G & I & \\ C & A & & I & G & \\ & & B & & & H \\ G & I & & D & F & \\ I & G & & F & D & \\ & & H & & & E \end{pmatrix}. \tag{6.95}$$

$$\mathbf{U}^{-1}=\begin{pmatrix} u_1/\sqrt{2} & u_2/\sqrt{2} & 0 & 0 & u_1''/\sqrt{2} & u_2''/\sqrt{2} \\ u_1/\sqrt{2} & u_2/\sqrt{2} & 0 & 0 & -u_1''/\sqrt{2} & -u_2''/\sqrt{2} \\ 0 & 0 & u_1' & u_2' & 0 & 0 \\ v_1/\sqrt{2} & v_2/\sqrt{2} & 0 & 0 & v_1''/\sqrt{2} & v_2''/\sqrt{2} \\ v_1/\sqrt{2} & v_2/\sqrt{2} & 0 & 0 & -v_1''/\sqrt{2} & -v_2''/\sqrt{2} \\ 0 & 0 & v_1' & v_2' & 0 & 0 \end{pmatrix}. \tag{6.96}$$

Let

$$\alpha_{11}=A+C, \qquad \alpha_{22}=D+F, \quad \text{and} \quad \alpha_{12}=G+I \tag{6.97}$$

to get the solutions u_i, v_i, and $\omega_{1i}^2(\mathbf{k}_4)$ from (6.50). Let

$$\alpha_{11}=B, \qquad \alpha_{22}=E, \quad \text{and} \quad \alpha_{12}=H \tag{6.98}$$

to get the solutions u_i', v_i', and $\omega_{3i}^2(\mathbf{k}_4)$ from (6.50). Let

$$\alpha_{11}=A-C, \qquad \alpha_{22}=D-F, \quad \text{and} \quad \alpha_{12}=G-I \tag{6.99}$$

to get the solutions u_i'', v_i'', and $\omega_{4i}^2(\mathbf{k}_4)$ from (6.50).

Symmetry on Plane C, $\mathbf{k}_3=\pi(-\zeta_1,\zeta_1,\zeta_2)/a_0$

$$\bar{\theta}=1, \qquad \mathbf{R}\in\{1, \bar{2}[110]\}. \tag{6.100}$$

$$\mathbf{C}(\mathbf{k}_3)=\begin{pmatrix} A & C & D & I & K & L \\ C & A & -D & K & I & -L \\ D & -D & B & L & -L & J \\ I & K & L & E & G & H \\ K & I & -L & G & E & -H \\ L & -L & J & H & -H & F \end{pmatrix}. \tag{6.101}$$

The decomposition of $\{\mathbf{T}(\mathbf{k};\,\mathbf{R})\}$ in Table IX shows that it is not practical to write the eigenvectors in terms of the matrix elements of $\mathbf{C}\,(\mathbf{k})$. $\tau^{(1)}$ occurs four times, and hence the components of the eigenvectors transforming as $\tau^{(1)}$ are solutions of a quartic equation. We give the symmetrized trial solutions which decompose the equations of motion into two independent sets of different symmetry:

$$\mathbf{E}(\mathbf{k}_3;\,11)=\begin{pmatrix}\psi_1/\sqrt{2}\\ -\psi_1/\sqrt{2}\\ \psi_3\\ \psi_4/\sqrt{2}\\ -\psi_4/\sqrt{2}\\ \psi_6\end{pmatrix},\qquad(6.102\text{a})$$

$$\mathbf{E}(\mathbf{k}_3;\,21)=\begin{pmatrix}\psi_1'/\sqrt{2}\\ \psi_1'/\sqrt{2}\\ 0\\ \psi_4'/\sqrt{2}\\ \psi_4'/\sqrt{2}\\ 0\end{pmatrix}.\qquad(6.102\text{b})$$

This latter vector would lead to a solution which could be written out as above. The modes are perpendicular to the plane C and correspond to a TA and TO.

Symmetry on Plane B, $\mathbf{k}_2=\pi(\zeta_1,\,\zeta_2,\,1)/a_0$

$$\begin{aligned}\bar{\theta}&=+1, & \mathbf{R}&=1,\\ &=-1, & \mathbf{R}&=\bar{2}[001].\end{aligned}\qquad(6.103)$$

$$\mathbf{C}(\mathbf{k}_2)=\begin{pmatrix}A & D & & & & L\\ D & B & & & & M\\ & & C & I & K & \\ & & I & E & H & \\ & & K & H & F & \\ L & M & & & & G\end{pmatrix}.\qquad(6.104)$$

TABLE XI. Compatibility relations at R for representations of CsCl.

	Λ	S	T
R_{15}	$\Lambda_1\oplus\Lambda_3$	$S_1\oplus S_3\oplus S_4$	$T_1\oplus T_5$
R_{25}'	$\Lambda_1\oplus\Lambda_3$	$S_1\oplus S_2\oplus S_3$	$T_2'\oplus T_5$

The symmetrized trial solutions are

$$\mathbf{E}(\mathbf{k}_2;\,11)=\begin{pmatrix}\psi_1\\ \psi_2\\ 0\\ 0\\ 0\\ \psi_6\end{pmatrix},\qquad(6.105\text{a})$$

$$\mathbf{E}(\mathbf{k}_2;\,21)=\begin{pmatrix}0\\ 0\\ \psi_3\\ \psi_4\\ \psi_5\\ 0\end{pmatrix}.\qquad(6.105\text{b})$$

This gives two sets of three simultaneous linear equations.

Symmetry on Plane O, $\mathbf{k}_1=(0,\,\zeta_1,\,\zeta_2)$

$$\bar{\theta}=1,\qquad \mathbf{R}\in\{1,\,\bar{2}[100]\}.\qquad(6.106)$$

$$\mathbf{C}(\mathbf{k}_1)=\begin{pmatrix}A & & & I & & \\ & B & D & & J & L\\ & D & C & & M & K\\ I & & & E & & \\ & J & M & & F & H\\ & L & K & & H & G\end{pmatrix}.\qquad(6.107)$$

The symmetrized trial solutions are

$$\mathbf{E}(\mathbf{k}_1;\,11)=\begin{pmatrix}0\\ \psi_2\\ \psi_3\\ \psi_4\\ \psi_5\\ 0\end{pmatrix},\qquad(6.108\text{a})$$

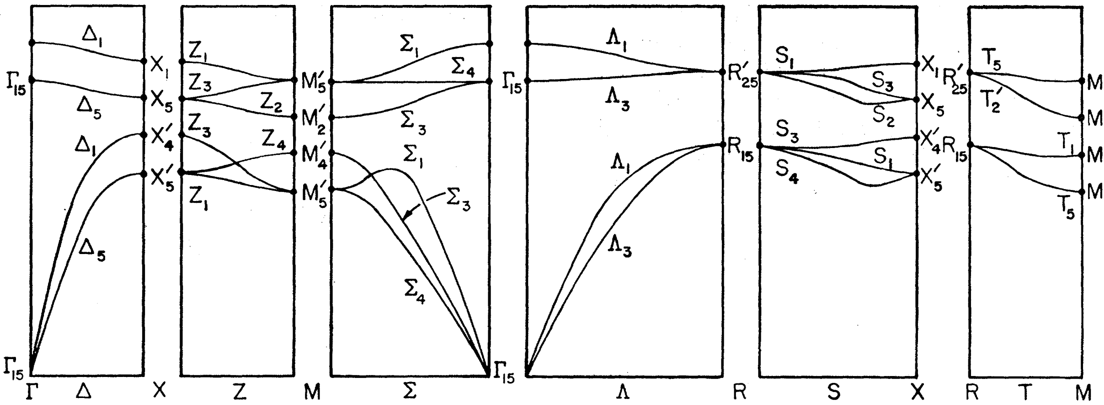

FIG. 7. Possible arrangement of dispersion curves for CsCl obtained by group theory. No physical data have been used.

$$\mathbf{E}(\mathbf{k}_1;21)=\begin{pmatrix}\psi_1\\0\\0\\0\\0\\\psi_6\end{pmatrix}. \qquad (6.108\text{b})$$

Predictions

No experimental dispersion relations for CsCl-type substances have been reported in the literature. It is not possible to predict dispersion relations uniquely from the above information. Nevertheless, it is an interesting exercise to use the group-theoretical results above, Tables X, XI, XII, and XIII listing the compatibility, and a little intuition to sketch the expected connectivity. This has been done in Fig. 7. In ordering the branches at symmetry points it was assumed that $C_{\alpha\beta}(11\mid\mathbf{k})<C_{\alpha\beta}(22\mid\mathbf{k})$. This corresponds to placing the Cs atom at the origin. A knowledge of the eigenvectors was used in choosing the ordering.

Mg Structure

A fairly good group-theoretical analysis of the lattice dynamics of magnesium already is in the literature.[30] The methods used differ slightly from those expounded in (I). The results of the two analyses differ occasionally.

The space group of Mg is D_{6h}^4 or $P6_3/mmc$.[62] The lattice is hexagonal close-packed. There are two atoms in a unit cell. Just as in the case of simple cubic, there are no elements forming a hexagonal lattice with only one atom per unit cell. The hcp lattice is nonsymmorphic.

TABLE XII. Compatibility relations at M for representations of CsCl.

	Σ	Z	T
M_2'	Σ_3	Z_2	T_2'
M_4'	Σ_3	Z_4	T_1
M_5'	$\Sigma_1\oplus\Sigma_4$	$Z_1\oplus Z_3$	T_5

The origin of the coordinate system preferred by the International Tables differs from the one most commonly used by physicists. The origin is placed at a point with symmetry ($\bar{3}m1$), i.e., at an inversion center on a threefold axis which lies in a mirror plane. The sites occupied by Mg atoms do not have this symmetry. It is usual to take the origin at an atomic site. Slater, however, has chosen a coordinate system whose origin is consistent with the International Tables. The atomic basis is located within the unit cell. We follow Slater. The position vector is

$$\mathbf{x}(l\kappa)=[l_1+\tfrac{1}{3}\kappa]\mathbf{a}_1+[l_2+\tfrac{1}{3}(3-\kappa)]\mathbf{a}_2+(l_3+\tfrac{1}{4}(2\kappa-1)]\mathbf{a}_3. \qquad (6.109)$$

The primitive translation vectors $\mathbf{a}_i$ are the usual ones. $\mathbf{a}_3$ is along the sixfold or so-called c axis. $\mathbf{a}_1$ and $\mathbf{a}_2$ are perpendicular to $\mathbf{a}_3$ and are 120° apart. Each axis is perpendicular to a mirror plane in the hcp lattice. According to (6.109), the two atoms in the atomic basis are located at $(\frac{1}{3},\frac{2}{3},\frac{1}{4})_\mathrm{H}$ and $(\frac{2}{3},\frac{1}{3},\frac{3}{4})_\mathrm{H}$ in this system.[63] Figure 8 illustrates the arrangement of atoms. The origin of coordinates is located in a plane $\frac{1}{4}\mid\mathbf{a}_3\mid$ down from the plane of solid dots. The open circles are on a plane $\frac{1}{2}\mid\mathbf{a}_3\mid$ up from the plane of solid dots.

In addition to this hexagonal coordinate system, it is useful to have a Cartesian coordinate system because

TABLE XIII. Compatibility relations at X for representations of CsCl.

	Δ	Z	S
X_1	Δ_1	Z_1	S_1
X_5	Δ_5	$Z_2\oplus Z_3$	$S_2\oplus S_3$
X_4'	Δ_1	Z_3	S_3
X_5'	Δ_5	$Z_1\oplus Z_4$	$S_1\oplus S_4$

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[62] Some of the properties of this group are found in Ref. 1, p. 304.

[63] A subscript H on the brackets indicates that the hexagonal basis was used.

TABLE XIV. Comparison of common notations for point group operations in D_{6h}; reducible representation R and its character are included.

W[a]	McW[b]	A&B[c]	HI[d]	HII[d]	S[e]	K[f]	Int[g]	R_{1i}	R_{2i}	R_{3i}	$\chi(R)$	I[h]
1	E	E	e	b_1	X_0	h_1	x, y, z	$1, 0, 0$	$0, 1, 0$	$0, 0, 1$	3	
2[001]	C_2	C_2	$C_2{}^z$	b_2	X_3	h_4	$\bar{x}, \bar{y}, z$	$\bar{1}, 0, 0$	$0, \bar{1}, 0$	$0, 0, 1$	−1	*
3[001]	C_3	$C_3{}^+$	$C_3{}^z$	b_3	X_{-2}	h_3	$\bar{y}, x-y, z$	$\frac{\bar{1}}{2}, \frac{\bar{1}}{2}\sqrt{3}, 0$	$\frac{1}{2}\sqrt{3}, \frac{\bar{1}}{2}, 0$	$0, 0, 1$	0	
3[001]	$\bar{C}_3$	$C_3{}^-$	$C_3{}^{-z}$	b_4	X_2	h_5	$y-x, \bar{x}, z$	$\frac{\bar{1}}{2}, \frac{1}{2}\sqrt{3}, 0$	$\frac{\bar{1}}{2}\sqrt{3}, \frac{1}{2}, 0$	$0, 0, 1$	0	
6[001]	C_6	$C_6{}^+$	$C_6{}^z$	b_5	X_{-1}	h_2	$x-y, x, z$	$\frac{1}{2}, \frac{\bar{1}}{2}\sqrt{3}, 0$	$\frac{1}{2}\sqrt{3}, \frac{1}{2}, 0$	$0, 0, 1$	2	*
6[00$\bar{1}$]	$\bar{C}_6$	$C_6{}^-$	$C_6{}^{-z}$	b_6	X_1	h_6	$y, y-x, z$	$\frac{1}{2}, \frac{1}{2}\sqrt{3}, 0$	$\frac{\bar{1}}{2}\sqrt{3}, \frac{1}{2}, 0$	$0, 0, 1$	2	*
2[100]	$C_2{}^{(1)}$	$C_{21}{}''$	$C_2{}^{(6)}$	b_{12}	$Y_{-1}{}'$	h_9	$x-y, \bar{y}, \bar{z}$	$1, 0, 0$	$0, \bar{1}, 0$	$0, 0, \bar{1}$	−1	*
2[110]	$C_2{}^{(2)}$	$C_{23}{}''$	$C_2{}^{(5)}$	b_{11}	$Y_1{}'$	h_{11}	$y, x, \bar{z}$	$\frac{\bar{1}}{2}, \frac{1}{2}\sqrt{3}, 0$	$\frac{1}{2}\sqrt{3}, \frac{1}{2}, 0$	$0, 0, \bar{1}$	−1	*
2[010]	$C_2{}^{(3)}$	$C_{22}{}''$	$C_2{}^{(4)}$	b_{10}	$Y_3{}'$	h_7	$\bar{x}, y-x, \bar{z}$	$\frac{\bar{1}}{2}, \frac{1}{2}\sqrt{3}, 0$	$\frac{\bar{1}}{2}\sqrt{3}, \frac{1}{2}, 0$	$0, 0, \bar{1}$	−1	*
2[210]	$C_2{}^{(12)}$	$C_{22}{}'$	$C_2{}^{(1)}$	b_7	$Y_0{}'$	h_{10}	$x, x-y, z$	$\frac{1}{2}, \frac{1}{2}\sqrt{3}, 0$	$\frac{1}{2}\sqrt{3}, \frac{\bar{1}}{2}, 0$	$0, 0, \bar{1}$	−1	
2[120]	$C_2{}^{(23)}$	$C_{21}{}'$	$C_2{}^{(2)}$	b_8	$Y_2{}'$	h_{12}	$y-x, y, \bar{z}$	$\bar{1}, 0, 0$	$0, 1, 0$	$0, 0, \bar{1}$	−1	
2[$\bar{1}$20]	$C_2{}^{(34)}$	$C_{23}{}'$	$C_2{}^{(3)}$	b_9	$Y_{-2}{}'$	h_8	$\bar{y}, \bar{x}, \bar{z}$	$\frac{1}{2}, \frac{\bar{1}}{2}\sqrt{3}, 0$	$\frac{\bar{1}}{2}\sqrt{3}, \frac{\bar{1}}{2}, 0$	$0, 0, \bar{1}$	−1	
1	i	i		$b_1{}'$	$X_3{}'$	h_{13}	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}, 0, 0$	$0, \bar{1}, 0$	$0, 0, \bar{1}$	−3	*
$\bar{\mathbf{2}}$[001]	σ_h	σ_h		$b_2{}'$	$X_0{}'$	h_{16}	$x, y, \bar{z}$	$1, 0, 0$	$0, 1, 0$	$0, 0, \bar{1}$	1	
$\bar{\mathbf{3}}$[001]	$\bar{S}_6$	$S_6{}^-$		$b_3{}'$	$X_1{}'$	h_{15}	$y, y-x, \bar{z}$	$\frac{1}{2}, \frac{1}{2}\sqrt{3}, 0$	$\frac{\bar{1}}{2}\sqrt{3}, \frac{1}{2}, 0$	$0, 0, \bar{1}$	0	*
3[00$\bar{1}$]	S_6	$S_6{}^+$		$b_4{}'$	$X_{-1}{}'$	h_{17}	$x-y, x, \bar{z}$	$\frac{1}{2}, \frac{\bar{1}}{2}\sqrt{3}, 0$	$\frac{1}{2}\sqrt{3}, \frac{1}{2}, 0$	$0, 0, \bar{1}$	0	*
$\bar{\mathbf{6}}$[001]	$\bar{S}_3$	$S_3{}^-$		$b_5{}'$	$X_2{}'$	h_{14}	$y-x, \bar{x}, \bar{z}$	$\frac{\bar{1}}{2}, \frac{1}{2}\sqrt{3}, 0$	$\frac{\bar{1}}{2}\sqrt{3}, \frac{1}{2}, 0$	$0, 0, \bar{1}$	−2	
$\bar{\mathbf{6}}$[00$\bar{1}$]	S_3	$S_3{}^+$		$b_6{}'$	$X_{-2}{}'$	h_{18}	$\bar{y}, x-y, \bar{z}$	$\frac{1}{2}, \frac{\bar{1}}{2}\sqrt{3}, 0$	$\frac{1}{2}\sqrt{3}, \frac{\bar{1}}{2}, 0$	$0, 0, \bar{1}$	−2	
$\bar{\mathbf{2}}$[100]	$\sigma^{(23)}$	σ_{v1}		$b_{12}{}'$	Y_2	h_{21}	$y-x, y, z$	$\bar{1}, 0, 0$	$0, 1, 0$	$0, 0, 1$	1	
$\bar{\mathbf{2}}$[110]	$\sigma^{(34)}$	σ_{v3}		$b_{11}{}'$	Y_{-2}	h_{23}	$\bar{y}, \bar{x}, z$	$\frac{1}{2}, \frac{\bar{1}}{2}\sqrt{3}, 0$	$\frac{\bar{1}}{2}\sqrt{3}, \frac{\bar{1}}{2}, 0$	$0, 0, 1$	1	
$\bar{\mathbf{2}}$[010]	$\sigma^{(12)}$	σ_{v2}		$b_{10}{}'$	Y_0	h_{19}	$x, x-y, z$	$\frac{1}{2}, \frac{1}{2}\sqrt{3}, 0$	$\frac{1}{2}\sqrt{3}, \frac{\bar{1}}{2}, 0$	$0, 0, 1$	1	
$\bar{\mathbf{2}}$[210]	$\sigma^{(3)}$	σ_{d2}		$b_7{}'$	Y_3	h_{22}	$\bar{x}, y-x, z$	$\frac{\bar{1}}{2}, \frac{\bar{1}}{2}\sqrt{3}, 0$	$\frac{1}{2}\sqrt{3}, \frac{1}{2}, 0$	$0, 0, 1$	1	*
2[120]	$\sigma^{(1)}$	σ_{d1}		$b_8{}'$	Y_{-1}	h_{24}	$x-y, \bar{y}, z$	$1, 0, 0$	$0, \bar{1}, 0$	$0, 0, 1$	1	*
$\bar{\mathbf{2}}$[$\bar{1}$20]	$\sigma^{(2)}$	σ_{d3}		$b_9{}'$	Y_1	h_{20}	y, x, z	$\frac{\bar{1}}{2}, \frac{1}{2}\sqrt{3}, 0$	$\frac{1}{2}\sqrt{3}, \frac{1}{2}, 0$	$0, 0, 1$	1	*

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[a] Warren, notation explained in the text.

[b] McWeeny, see Ref. 6, p. 69.

[c] Altmann and Bradley, see Ref. 10, p. 34, Fig. 1. The reciprocal lattice vectors in this figure are in error.

[d] Hurley, see Ref. 15, p. 8. No geometrical notation HI is given for the last twelve operations.

[e] Slater, see Ref. 4, p. 36–7. The correspondence in this table has been chosen so that Slater's representation tables can be used directly without making allowance for his special convention $\mathbf{R}\psi(\mathbf{r})=\psi(\mathbf{Rr})$.

[f] Kovalev, see Ref. 3, p. 8.

[g] International Tables, see Ref. 1, Vol. 1, p. 304.

[h] The symbol I stands for interchange. Those operations with an asterisk in this column interchange sublattices.

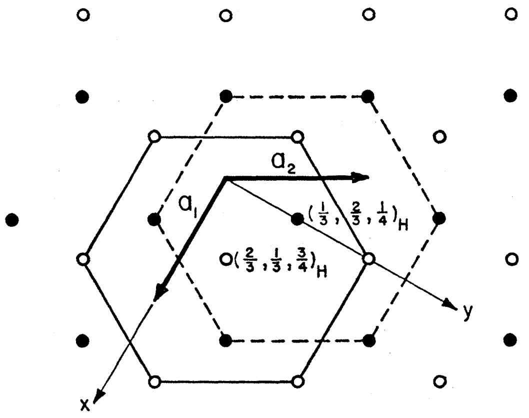

FIG. 8. Direct lattice for hexagonal close-packed crystal. Two layers perpendicular to the sixfold axis $\mathbf{a}_3$ are shown. The origin of coordinates is on a plane $\frac{1}{4}\,|\,\mathbf{a}_3\,|$ below the plane of the solid dots.[63]

the dynamical matrix is implicitly assumed to be expressed in Cartesian coordinates. Our choice is

$$\mathbf{l}_1=\mathbf{a}_1/a_{\mathrm{H}}, \qquad (6.110\mathrm{a})$$

$$\mathbf{l}_3=\mathbf{a}_3/c_{\mathrm{H}}, \qquad (6.110\mathrm{b})$$

$$\mathbf{l}_2=[\mathbf{a}_1+2\mathbf{a}_2]/(\sqrt{3}\,a_{\mathrm{H}}), \qquad (6.110\mathrm{c})$$

where $a_{\mathrm{H}}=|\,\mathbf{a}_1\,|$ and $c_{\mathrm{H}}=|\,\mathbf{a}_3\,|$. This Cartesian system conforms with the Standards, 1949. (Slater chooses a system in which the $\mathbf{l}_2$ axis coincides in direction with $\mathbf{a}_2$.) The position vector in this Cartesian system is

$$\mathbf{x}(l\kappa)=\tfrac{1}{2}a_{\mathrm{H}}[2l_1-l_2+(\kappa-1)]\mathbf{l}_1+\tfrac{1}{2}\sqrt{3}\,a_{\mathrm{H}}[l_2+1-\tfrac{1}{3}\kappa)\mathbf{l}_2 +c_{\mathrm{H}}[l_3+\tfrac{1}{2}(\kappa-\tfrac{1}{2})]\mathbf{l}_3. \qquad (6.111)$$

The point group operations are divided into twelve classes. These classes are indicated in Table XIV by slight separations. The direction part of the operation symbol $n[abc]$ is expressed in the hexagonal system since this gives integer components. Thus

$2[100]$—180° rotation about the $\mathbf{a}_1$ axis;

$2[210]$—180° rotation about line 30° from $\mathbf{a}_1$ axis;

$2[110]$—180° rotation about line 60° from $\mathbf{a}_1$ axis;

$2[120]$—180° rotation about line 90° from $\mathbf{a}_1$ axis;

$2[010]$—180° rotation about the $\mathbf{a}_2$ axis;

$2[\bar{1}20]$—180° rotation about line 150° from $\mathbf{a}_1$ axis.

This notation is perhaps geometrically less transparent than desirable, but at least it is consistent with the idea behind the notation for the cubic system.

Properties Independent of k

Inversion is an element of the group and it interchanges sublattices. By (3.32) in (I),

$$\mathbf{D}(\mathbf{k})=\begin{pmatrix}\mathbf{D}(11\,|\,\mathbf{k}) & \mathbf{D}(12\,|\,\mathbf{k})\\ \mathbf{D}(12\,|\,\mathbf{k})^* & \mathbf{D}(11\,|\,\mathbf{k})^*\end{pmatrix}, \qquad (6.112)$$

where $\mathbf{D}(11\,|\,\mathbf{k})$ is Hermitian and $\mathbf{D}(12\,|\,\mathbf{k})$ is symmetric. The functional relationships between matrix elements are not so useful for hexagonal crystals. The operations lead to linear combinations. For example, if we let $\mathbf{S}=6[001]$ in (3.4)*, then

$$D_{11}(11\,|\,\tfrac{1}{2}(k_1-\sqrt{3}\,k_2),\,\tfrac{1}{2}(\sqrt{3}\,k_1+k_2),\,k_3)=\tfrac{1}{4}[D_{11}(11\,|\,\mathbf{k}) -\sqrt{3}\,D_{21}(11\,|\,\mathbf{k})-\sqrt{3}\,D_{12}(11\,|\,\mathbf{k})+3D_{22}(11\,|\,\mathbf{k})].$$

This and other relations like it may be useful under special circumstances, but do not allow one to save time in setting up the dynamical matrix.

The force constant matrices have been written out in full for first through fourth neighbors by Iyengar *et al.*[64]

Symmetry of Brillouin Zone

The reciprocal lattice is also hexagonal:

$$\mathbf{K}(h)=(2\pi/a_{\mathrm{H}})h_1\mathbf{l}_1+(2\pi/\sqrt{3}\,a_{\mathrm{H}})(h_1+2h_2)\mathbf{l}_2 +(2\pi/c_{\mathrm{H}})h_3\mathbf{l}_3. \qquad (6.113)$$

Typical symmetry planes, lines, and points in the (BZ) are shown in Fig. 9. The notation for lines and points is due to Herring.[65] That for planes has been introduced for completeness. Table XV contains a list of these symmetry elements. This is the analog of Table VII. The meaning of the column headings was explained there. The coordinates of the equivalent points are in a reciprocal hexagonal coordinate system. The basis vectors for this system $\mathbf{b}_j$ are defined by the relation

$$\mathbf{a}_i\cdot\mathbf{b}_j=2\pi\,\delta_{ij}. \qquad (6.114)$$

The vector $\mathbf{b}_2$ makes a 60° angle with $\mathbf{b}_1$. The expression for the wave vector is

$$\mathbf{k}=\tfrac{1}{2}\sum_{j=1}^{3}\eta_j\mathbf{b}_j. \qquad (6.115)$$

This choice was made so that $\eta_j=1$ is true at certain

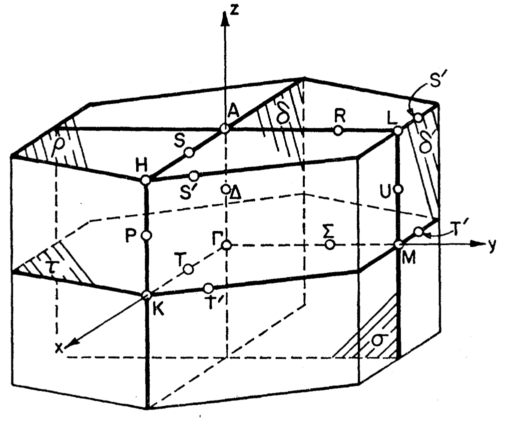

FIG. 9. Brillouin zone for hexagonal lattice. Symmetry planes are labeled δ, δ', σ, ρ, and τ.

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[64] P. K. Iyengar, G. Venkataraman, P. R. Vijayaraghavan, and A. P. Roy. *Lattice Dynamics*, R. F. Wallis, Ed. (Pergamon Press, Ltd., London, 1965) p. 223.

[65] C. Herring, J. Franklin Inst. **233**, 525 (1942). [Alternatively, see Knox and Gold, p. 257 cited in Ref. 43].

TABLE XV. Planes, lines, and points of symmetry in the Brillouin zone of a hexagonal close-packed lattice.

$\sqrt{3}a_{\mathrm{H}}\mathbf{k}/\pi$[a]	H[b]	K#[c]	$G_0(\mathbf{k})$	Axis[d]	h[e]	Equivalent points[f] (2k)	n[e]	m[e]	N[e]
$(\zeta_1, \zeta_2, 0)$	τ	1	m	[001]	2	$(\eta_1, \eta_2, 0)_{\mathrm{RH}}$	1	12	12
(ζ_1, ζ_2, ξ)	ρ	2	m	[001]	2	$(\eta_1, \eta_2, \pm 1)_{\mathrm{RH}}$	2	12	24
$(0, 2\eta_1, \xi\eta_2)$	σ	3	m	[100]	2	$(0, \eta_1, \eta_2)_{\mathrm{RH}}$	1	12	12
$(2\sqrt{3}\eta_1, 0, \xi\eta_2)$	δ	4	m	[120]	2	$(2\eta_1, -\eta_1, \eta_2)_{\mathrm{RH}}$	1	12	12
$(\zeta_1, 2, \zeta_2)$	δ'		m	[120]	2	$(2\eta_1-2, 2-\eta_1, \eta_2)_{\mathrm{RH}}$, $(2\eta_1-2, -\eta_1, \eta_2)_{\mathrm{RH}}$	2	12	24
$(0, 2\eta, 0)$	Σ	5	$mm2$	[120]	4	$(0, \eta, 0)_{\mathrm{RH}}$	1	6	4
$(2\sqrt{3}\eta, 0, 0)$	T	6	$mm2$	[100]	4	$(2\eta, -\eta, 0)_{\mathrm{RH}}$	1	6	6
$(\sqrt{3}(2\eta-2), 2, 0)$	T'		$mm2$	[100]	4	$(2\eta-2, 2-\eta, 0)_{\mathrm{RH}}$, $(2\eta-2, -\eta, 0)_{\mathrm{RH}}$	2	6	12
$(0, 2\eta, \xi)$	R	7	$mm2$	[120]	4	$(0, \eta, \pm 1)_{\mathrm{RH}}$	2	6	12
$(2\sqrt{3}\eta, 0, \xi)$	S	8	$mm2$	[100]	4	$(2\eta, -\eta, \pm 1)_{\mathrm{RH}}$	2	6	12
$(\sqrt{3}(2\eta-2), 2, \xi)$	S'		$mm2$	[100]	4	$(2\eta-2, 2-\eta, \pm 1)_{\mathrm{RH}}$, $(2\eta-2, -\eta, \pm 1)_{\mathrm{RH}}$	4	6	24
$(0, 2, \xi\eta)$	U	9	$mm2$	[001]	4	$(0, \pm 1, \eta)_{\mathrm{RH}}$	2	6	12
$(4/\sqrt{3}, 0, \xi\eta)$	P	10	$3m$	[001]	6	$(\frac{4}{3}, -\frac{2}{3}, \eta)_{\mathrm{RH}}$, $(-\frac{2}{3}, \frac{4}{3}, \eta)_{\mathrm{RH}}$, $(-\frac{2}{3}, -\frac{2}{3}, \eta)_{\mathrm{RH}}$	3	4	12
$(0, 2, 0)$	M	12	mmm	[120]	8	$(0, \pm 1, 0)_{\mathrm{RH}}$	2	3	6
$(0, 2, \xi)$	L	14	mmm	[120]	8	$(0, \pm 1, \pm 1)_{\mathrm{RH}}$	4	3	12
$(0, 0, \xi\eta)$	Δ	11	$6mm$	[001]	12	$(0, 0, \eta)_{\mathrm{RH}}$	1	2	2
$(4/\sqrt{3}, 0, 0)$	K	13	$\bar{6}m2$	[001]	12	$(\frac{4}{3}, -\frac{2}{3}, 0)_{\mathrm{RH}}$, $(-\frac{2}{3}, \frac{4}{3}, 0)_{\mathrm{RH}}$, $(-\frac{2}{3}, -\frac{2}{3}, 0)_{\mathrm{RH}}$	3	2	6
$(4/\sqrt{3}, 0, \xi)$	H	15	$\bar{6}m2$	[001]	12	$(\frac{4}{3}, -\frac{2}{3}, \pm 1)_{\mathrm{RH}}$, $(-\frac{2}{3}, \frac{4}{3}, \pm 1)_{\mathrm{RH}}$, $(-\frac{2}{3}, -\frac{2}{3}, \pm 1)_{\mathrm{RH}}$	6	2	12
$(0, 0, \xi)$	A	17	$6/mmm$	[001]	24	$(0, 0, \pm 1)_{\mathrm{RH}}$	2	1	2
$(0, 0, 0)$	Γ	16	$6/mmm$	[001]	24	$(0, 0, 0)_{\mathrm{RH}}$	1	1	1

[a] Cartesian components of **k** are used here. $\xi = \sqrt{3}\ a_H/c_H$. ζ_1 and ζ_2 can be found by using Eq. (6.116).

[b] H stands for Herring. The labels for the planes are new.

[c] K # means Kovalev number.

[d] Direction of the principal axes of the point group $G_0(\mathbf{k})$ in the hexagonal basis.

[e] The quantities h, n, m, and N have the same meaning as in Table VIII except that $hm = 24$.

[f] The equivalent points are given in a reciprocal hexagonal basis (RH).

zone boundary points. The Cartesian coordinates of **k** found in column one of Table XV are related to the η_j's by the matrix equation

$$\begin{pmatrix} k_1 \\ k_2 \\ k_3 \end{pmatrix} = \frac{\pi}{\sqrt{3}\ a_{\mathrm{H}}} \begin{pmatrix} \sqrt{3} & 0 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & \xi \end{pmatrix} \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{pmatrix}, \tag{6.116}$$

where $\xi = \sqrt{3}\ a_{\mathrm{H}}/c_{\mathrm{H}}$. The reciprocal hexagonal coordinates are useful in forming scaler products with position vectors expressed as in (6.109). The star of **k** was omitted from the table to save space.

The tables of Koster *et al.*[21] show that there are no additional degeneracies due to time reversal in the interior of the zone. By applying (5.61) it is found that there are additional degeneracies at general points on the upper surface of the (BZ) ρ and along the line R lying in this surface.[66]

Symmetry at Γ, $\mathbf{k}_{16}$

As in the previous example we begin by constructing the representation $\{\mathbf{T}(\mathbf{k};\ \mathbf{R})\}$. The formula is

$$T_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k};\ \mathbf{R}) = \delta(\kappa,\ \mathcal{R}_m[\kappa'])\ \exp\left[i\theta(\kappa' \mid \mathbf{k};\ \mathcal{R}_m)\right] R_{\alpha\beta}, \tag{6.117a}$$

where

$$\theta(\kappa' \mid k;\ \mathcal{R}_m) = \mathbf{k}\cdot\left[\mathbf{x}(\mathcal{R}_m[\kappa']) - \mathbf{R}\mathbf{x}(\kappa')\right]. \tag{6.117b}$$

Since $\mathbf{k} = \mathbf{0}$, the exponential factor is unity here. Nevertheless, it is useful to discuss the factor $[\mathbf{x}(\mathcal{R}_m[\kappa']) - \mathbf{R}\mathbf{x}(\kappa')]$ now because it is needed at all of the other symmetry points. The point group is $6/mmm$. It contains 24 elements. The space group is nonsymmorphic and therefore some of the elements have nonprimitive translations which must be used when finding the $\mathcal{R}_m[\kappa']$'s. A study of the space group operations shows that half of the operations interchange sublattices. These are marked in Table XIV with an asterisk in the last column. Furthermore, it is found by working with (6.117b) that for $\mathcal{R}_m$ which do not interchange sublattices

$$\mathbf{T}(\mathbf{k};\ \mathbf{R}) = \begin{pmatrix} \bar{\theta}\mathbf{R} & 0 \\ 0 & \bar{\theta}^*\mathbf{R} \end{pmatrix}, \tag{6.118a}$$

$\mathbf{T}(\mathbf{k};\ \mathbf{R})$ for operations which do interchange sublattices have the form

$$\mathbf{T}(\mathbf{k};\ \mathbf{R}) = \begin{pmatrix} 0 & \bar{\theta}^*\mathbf{R} \\ \bar{\theta}\mathbf{R} & 0 \end{pmatrix}, \tag{6.118b}$$

where

$$\bar{\theta} = \exp\left[i\theta(1 \mid \mathbf{k};\ \mathcal{R}_m)\right] \tag{6.118c}$$

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[66] A. A. Maradudin has pointed out to me that Sullivan has also found time-reversal degeneracies in wurtzite. See Ref. 54 for further information on this.

TABLE XVI. The factor $\bar{\theta}$ used in the calculation of $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$; column headings are Herring's labels for the symmetry elements in the (BZ).

$\mathcal{R}_0$[a]		$(L)_H$[b]	A	H[c]	K	Δ[d]	L	M	P
$\{1\mid 0\}$		000	1	1	1	1	1	1	1
$\{2[001]\mid \mathbf{v}\}$	*	$11\frac{1}{2}$	i			d	$-i$	-1	
$\{3[001]\mid 0\}$		110	1	ω^2	ω^2	1			ω^2
$\{3[00\bar{1}]\mid 0\}$		010	1	ω^{-2}	ω^{-2}	1			ω^{-2}
$\{6[001]\mid \mathbf{v}\}$	*	$10\frac{1}{2}$	i			d			
$\{6[00\bar{1}]\mid \mathbf{v}\}$	*	$00\frac{1}{2}$	i			d			
$\{2[100]\mid 0\}$	*	111	-1	ω^{-1}	ω^2		1	-1	
$\{2[110]\mid 0\}$	*	001	-1	-1	1				
$\{2[010]\mid 0\}$	*	101	-1	ω	ω^{-2}				
$\{2[210]\mid \mathbf{v}\}$		$01\frac{1}{2}$	i						
$\{2[120]\mid \mathbf{v}\}$		$00\frac{1}{2}$	i				i	1	
$\{2[\bar{1}20]\mid \mathbf{v}\}$		$11\frac{1}{2}$	i						
$\{\bar{1}\mid 0\}$	*	111	-1				1	-1	
$\{\bar{2}[001]\mid \mathbf{v}\}$		$00\frac{1}{2}$	i	i	1		i	1	
$\{\bar{3}[001]\mid 0\}$	*	001	-1						
$\{\bar{3}[00\bar{1}]\mid 0\}$	*	101	-1						
$\{\bar{6}[001]\mid \mathbf{v}\}$		$01\frac{1}{2}$	i	$i\omega^{-2}$	ω^{-2}				
$\{\bar{6}[00\bar{1}]\mid \mathbf{v}\}$		$11\frac{1}{2}$	i	$i\omega^2$	ω^2				
$\{\bar{2}[100]\mid 0\}$		000	1			1	1	1	
$\{\bar{2}[110]\mid 0\}$		110	1			1			
$\{\bar{2}[010]\mid 0\}$		010	1			1			
$\{\bar{2}[210]\mid \mathbf{v}\}$	*	$10\frac{1}{2}$	i	$i\omega^{-2}$	ω^{-2}	d			$\omega^{-2}d$
$\{\bar{2}[120]\mid \mathbf{v}\}$	*	$11\frac{1}{2}$	i	$i\omega^2$	ω^2	d	$-i$	-1	$\omega^2 d$
$\{\bar{2}[\bar{1}20]\mid \mathbf{v}\}$	*	$00\frac{1}{2}$	i	i	1	d			d

[a] Space-group operators $\mathcal{R}_m$ for $m=0$, $\mathbf{v}=\frac{1}{2}a_3$. The asterisk indicates that this operation interchanges sublattices.

[b] The symbol $(L)_H$ means $[\mathbf{x}\mathcal{R}_0[1]-\mathbf{R}\mathbf{x}(1)]$ expressed in the hexagonal basis.

[c] $\omega=\exp[2\pi\ i/6]$.

[d] $d=\exp[\pi\ \eta\ i/2]$, where η is the appropriate coordinate of $\mathbf{k}$ in the reciprocal hexagonal basis.

and the **R**'s are the three by three matrices in Table XIV. Thus, once $\bar{\theta}$ is known, it is easy to write out $\{\mathbf{T}(\mathbf{k},\mathbf{R})\}$. In Table XVI, XVII, and XVIII $\bar{\theta}$ is evaluated for the operations $\mathcal{R}_0$, i.e., $m=0$, and the symmetry elements in the (BZ). Γ is omitted because obviously $\bar{\theta}=1$ for all $\mathcal{R}_0$'s.

The character of this representation is given by the relation

$$\begin{aligned} \chi^{(T)}(\mathbf{R}) &= 0, && \text{for } \mathbf{R} \text{ with } *, \\ &= (\bar{\theta}+\bar{\theta}^*)\chi(\mathbf{R}), && \text{for } \mathbf{R} \text{ without } *. \end{aligned} \tag{6.119}$$

$\chi(\mathbf{R})$ is found in Table XIV.

With the above information we are in a position to decompose $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ into its irreducible parts. One could proceed as above to apply the formula for c_s at each point of symmetry. There is, however, a short cut which makes use of the compatibility relations. If one calculates c_s at points Γ, A, H, L, M, and K, then one can obtain the decomposition on the lines joining these points by examining the compatibility. (See Tables XIX–XXIII.) The results are in Table XXIV. Since compatibility conditions have not been written down between lines and planes, c_s has been worked out for these cases.

The quantity $\bar{\theta}$ is also needed to calculate the transformation properties of $\mathbf{D}(\mathbf{k})$. Thus

$$D_{\alpha\beta}(\mathcal{R}_m[\kappa]\mathcal{R}_m[\kappa'] \mid \mathbf{k}) = \bar{\Upsilon} \sum_{\mu\nu} R_{\alpha\mu}R_{\beta\nu}D_{\mu\nu}(\kappa\kappa' \mid \mathbf{k}), \tag{6.120a}$$

where

$$\begin{aligned} \bar{\Upsilon} &= 1 && \kappa=\kappa' \\ &= \bar{\theta}^2 && \kappa=1,\ \kappa'=2 \\ &= (\bar{\theta}^*)^2 && \kappa=2,\ \kappa'=1. \end{aligned} \tag{6.120b}$$

This follows from Eqs. (5.11) and (5.12) by using the

TABLE XVII. The factor $\bar{\theta}$ used in the calculation of $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$. (See Tables XV and XVI for the meaning of the column headings and other symbols.)

$\mathcal{R}_0$		U	S'	S	R	T'	T	Σ
$\{1\mid 0\}$		1	1	1	1	1	1	1
$\{2[001]\mid \mathbf{v}\}$	*	$-d$						
$\{2[100]\mid 0\}$	*		$-d^2$	$-d^2$		d^2	d^2	
$\{2[010]\mid 0\}$	*							
$\{2[120]\mid \mathbf{v}\}$					i			1
$\{\bar{2}[001]\mid \mathbf{v}\}$			i	i	i	1	1	1
$\{\bar{2}[100]\mid 0\}$		1			1			1
$\{\bar{2}[210]\mid \mathbf{v}\}$	*							
$\{\bar{2}[120]\mid \mathbf{v}\}$	*	$-d$	$-d^2$	$-d^2$		d^2	d^2	
$\{\bar{2}[\bar{1}20]\mid \mathbf{v}\}$	*							

fact that $\theta(2\mid\mathbf{k}\cdot\mathcal{R}_m)=\theta(1\mid\mathbf{k};\mathcal{R}_m)^*$ for this example. At Γ, $\bar{\Upsilon}=1$ for all κ, κ' and $\mathcal{R}_m$.

With this information one can find the independent matrix elements in $\mathbf{D}(\mathbf{k})$. Consider first operations which do not interchange sublattice. For example, let $\mathcal{R}_0=\{3[001]\mid\mathbf{0}\}$. The application of (6.120) gives a set of linear equations which ultimately tells us that

$$D_{22}(\kappa\kappa'\mid\mathbf{k}_{16})=D_{11}(\kappa\kappa'\mid\mathbf{k}_{16}), \tag{6.121a}$$

$$D_{21}(\kappa\kappa'\mid\mathbf{k}_{16})=D_{12}(\kappa\kappa'\mid\mathbf{k}_{16}), \tag{6.121b}$$

$$D_{13}=D_{23}=D_{31}=D_{32}=0. \tag{6.121c}$$

Setting $\mathcal{R}_0=\{2[120]\mid\mathbf{v}\}$ results in

$$D_{12}(\kappa\kappa'\mid\mathbf{k}_{16})=0. \tag{6.121d}$$

The other operations introduce no other relations. Therefore

$$\mathbf{D}(\mathbf{k}_{16})=\begin{pmatrix} A & & & C & & \\ & A & & & C & \\ & & B & & & D \\ C & & & A & & \\ & C & & & A & \\ & & D & & & B \end{pmatrix}. \tag{6.121e}$$

The eigenvectors are found by using projection operators. The matrix $\mathbf{U}^{-1}$ whose columns are the eigenvectors is

$$\mathbf{U}^{-1}=\begin{pmatrix} 0 & 0 & 0 & 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 0 & 1/\sqrt{2} & 0 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 0 & -1/\sqrt{2} & 0 & 1/\sqrt{2} & 0 \\ -1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{6.122}$$

The order of the vectors is the same as the representations in Table XXIV. The eigenvalues are[67]

$$\omega_{3+}{}^2(\mathbf{k}_{16})=B-D, \tag{6.123a}$$

$$\omega_{2-}{}^2(\mathbf{k}_{16})=B+D. \tag{6.123b}$$

These are longitudinal-optic and -acoustic modes, respectively. At $\mathbf{k}_{16}$, $D=-B$. This follows from Appendix A, Eq. (A.9). The transverse modes are given by

$$\omega_{5+}{}^2(\mathbf{k}_{16})=A-C, \tag{6.123c}$$

$$\omega_{6-}{}^2(\mathbf{k}_{16})=A+C. \tag{6.123d}$$

Once again $C=-A$ and ω_{5+} is the optic mode. This is in disagreement with the assignment made by Iyengar *et al.*,[30] in their Fig. 5. The reduced matrices in their Table III agree with our Eqs. (6.123). It is helpful to note that at Γ, acoustic modes are odd under inversion, while optic modes are even.

In succeeding subsections we list the final form of $\mathbf{D}(\mathbf{k})$, the eigenvector matrix $\mathbf{U}^{-1}$, and the eigenvalues. This is done until one representation appears more than twice in $\{\mathbf{T}(\mathbf{k};\ \mathbf{R})\}$. When this occurs then the symmetrized trial eigenvector $\mathbf{E}(\mathbf{k};\ s\lambda)$ is indicated in place of $\mathbf{U}^{-1}$.

TABLE XVIII. The factor $\bar{\theta}$ used in the calculation of $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$. (This is a continuation of Tables XVI and XVII.) $d_i=\exp[\pi\eta_i i/2]$.

$\mathcal{R}_0$		δ'	δ	σ	ρ	τ
$\{1\mid 0\}$		1	1	1	1	1
$\{\bar{2}[001]\mid \mathbf{v}\}$					-1	1
$\{\bar{2}[100]\mid 0\}$				1		
$\{\bar{2}[120]\mid \mathbf{v}\}$	*	$d_1{}^2d_2$	$d_1{}^2d_2$			

---

[67] The s on $\omega_{sa}(\mathbf{k})$ is Herring's label. These labels were used here in place of Kovalev's just to be democratic.

Symmetry at A, $\mathbf{k}_{17}$

$$\mathbf{D}(\mathbf{k})=\begin{pmatrix} A &&&&& \\ & A &&&& \\ && B &&& \\ &&& A && \\ &&&& A & \\ &&&&& B \end{pmatrix}. \tag{6.124}$$

$$\mathbf{U}^{-1}=\begin{pmatrix} 0 & 0 & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & \frac{1}{2}i & -\frac{1}{2}i & \frac{1}{2}i & -\frac{1}{2}i \\ 1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2}i & -\frac{1}{2}i & -\frac{1}{2}i & \frac{1}{2}i \\ 0 & 0 & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ i/\sqrt{2} & -i/\sqrt{2} & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{6.125}$$

$$\omega_1^2(\mathbf{k}_{17})=B, \tag{6.126a}$$

$$\omega_3^2(\mathbf{k}_{17})=A. \tag{6.126b}$$

Symmetry at H, $\mathbf{k}_{15}$

If one uses Slater's matrix element Table A3–10 to decompose $\{\mathbf{T}(\mathbf{k}, \mathbf{R})\}$, the numbers in this table must be multiplied by $\exp[-i\mathbf{k}\cdot\mathbf{v}(R)]$ to get the multiplier representations of Kovalev. Kovalev may be used directly.

$$\mathbf{D}(\mathbf{k}_{15})=\begin{pmatrix} A & C &&&& D \\ -C & A &&&& -iD \\ && B & D & -iD & \\ && D^* & A & C & \\ && iD^* & C & A & \\ D^* & iD^* &&&& B \end{pmatrix}, \tag{6.127a}$$

where

$$D^*=\exp(2\pi i/6)\ D=\omega D. \tag{6.127b}$$

$$\mathbf{U}^{-1}=\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & u_1/\sqrt{2} & 0 & u_2/\sqrt{2} & 0 \\ \frac{1}{2}i & \frac{1}{2}i & -iu_1/\sqrt{2} & 0 & -iu_2/\sqrt{2} & 0 \\ 0 & 0 & 0 & v_1^* & 0 & v_2^* \\ \frac{1}{2}\omega^{-1} & -\frac{1}{2}\omega^{-1} & 0 & u_1^*/\sqrt{2} & 0 & u_2^*/\sqrt{2} \\ -\frac{1}{2}\omega^{-1} & \frac{1}{2}i\omega^{-1} & 0 & iu_1^*/\sqrt{2} & 0 & iu_2^*/\sqrt{2} \\ 0 & 0 & v_1 & 0 & v_2 & 0 \end{pmatrix}, \tag{6.128a}$$

where

$$\alpha_{11}=A-iC, \qquad \alpha_{22}=B, \quad \text{and} \quad \alpha_{12}=\sqrt{2}\,D, \tag{6.128b}$$

$$u_i=-\alpha_{12}/N_i, \tag{6.128c}$$

$$v_i=[\alpha_{11}-\omega_{3i}^2(\mathbf{k}_{15})]/N_i, \tag{6.128d}$$

$$N_i=\{|\alpha_{12}|^2+[\alpha_{11}-\omega_{3i}^2(\mathbf{k}_{15})]^2\}^{1/2}, \tag{6.128e}$$

$$\omega_{3i}^2(\mathbf{k}_{15})=\tfrac{1}{2}[\alpha_{11}+\alpha_{22}]+(2i-3)\{\tfrac{1}{4}[\alpha_{11}+\alpha_{22}]^2-\alpha_{11}\alpha_{22}+|\alpha_{12}|^2\}^{1/2}. \tag{6.128f}$$

The $s=1$ mode is given by

$$\omega_1^2(\mathbf{k}_{15})=A+iC. \tag{6.129}$$

Symmetry at K, $\mathbf{k}_{13}$

$$\mathbf{D}(\mathbf{k}_{13})=\begin{pmatrix} A & C && D & iD & \\ -C & A && iD & -D & \\ && B &&& \\ D^* & -iD^* && A & -C & \\ -iD^* & -D^* && C & A & \\ &&&&& B \end{pmatrix}, \tag{6.130a}$$

Table XIX. Compatibility relations at Γ for hcp lattice.

Γ_2^-	Γ_3^+	Γ_5^+	Γ_6^-
Δ_1	Δ_2	Δ_5	Δ_6
Σ_3	Σ_3	$\Sigma_1\oplus\Sigma_4$	$\Sigma_1\oplus\Sigma_4$
T_3	T_2	$T_1\oplus T_4$	$T_1\oplus T_4$

where

$$D^*=\exp\left(-2\pi i/3\right)\, D=\omega^{-2}D. \tag{6.130b}$$

$$\mathbf{U}^{-1}=\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 1/\sqrt{2} & 0 & 0 \\ \frac{1}{2}i & \frac{1}{2}i & 0 & -i/\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ \frac{1}{2}\omega^2 & -\frac{1}{2}\omega^2 & 1/\sqrt{2} & 0 & 0 & 0 \\ -\frac{1}{2}i\omega^2 & \frac{1}{2}i\omega^2 & i/\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{6.131}$$

$$\omega_1^2(\mathbf{k}_{13})=A+iC+2\omega^2D, \tag{6.132a}$$

$$\omega_3^2(\mathbf{k}_{13})=A+iC-2\omega^2D, \tag{6.132b}$$

$$\omega_5^2(\mathbf{k}_{13})=A-iC, \tag{6.132c}$$

$$\omega_6^2(\mathbf{k}_{13})=B. \tag{6.132d}$$

There may be a nontrivial difference between these results and those appearing in Table III of Iyengar.[30] Note that they have the representation K_2 in place of our K_3.

Symmetry at Δ, $\mathbf{k}_{11}$

$$\mathbf{D}(\mathbf{k}_{11})=\begin{pmatrix} A & & & C & & \\ & A & & & C & \\ & & B & & & D \\ C^* & & & A & & \\ & C^* & & & A & \\ & & D^* & & & B \end{pmatrix}, \tag{6.133a}$$

Table XX. Compatibility relations at A for hcp lattice.

A_1	A_3
$\Delta_1\oplus\Delta_2$	$\Delta_5\oplus\Delta_6$
$R_1\oplus R_3$	$R_1\oplus R_2\oplus R_3\oplus R_4$
S	S

Table XXI. Compatibility relations at H and L for hcp lattice.

H_1	H_3	L_1	L_2
S	S	S	S
$P_1\oplus P_2$	P_3	$U_1\oplus U_2$	$U_3\oplus U_4$
		$R_1\oplus R_3$	$R_2\oplus R_4$

where

$$C^*=\exp\left(i\pi\eta\right)\, C=d^2C, \tag{6.133b}$$

$$D^*=\exp\left(i\pi\eta\right)\, D=d^2D. \tag{6.133c}$$

$$\mathbf{U}^{-1}=\begin{pmatrix} 0 & 0 & 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 1/\sqrt{2} & 0 & 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -d/\sqrt{2} & d/\sqrt{2} & 0 \\ 0 & 0 & -d/\sqrt{2} & 0 & 0 & d/\sqrt{2} \\ d/\sqrt{2} & -d/\sqrt{2} & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{6.134}$$

$$\omega_1^2(\mathbf{k}_{11})=B+dD, \tag{6.135a}$$

$$\omega_2^2(\mathbf{k}_{11})=B-dD, \tag{6.135b}$$

$$\omega_5^2(\mathbf{k}_{11})=A-dC, \tag{6.135c}$$

$$\omega_6^2(\mathbf{k}_{11})=A+dC. \tag{6.135d}$$

Symmetry at L, $\mathbf{k}_{14}$

$$\mathbf{D}(\mathbf{k}_{14})=\begin{pmatrix} A & & & & & \\ & B & & & & D \\ & & C & & D & \\ & & & A & & \\ & & D & & B & \\ & D & & & & C \end{pmatrix}. \tag{6.136}$$

Table XXII. Compatibility relations at M for hcp lattice.

M_1^+	M_2^-	M_3^+	M_3^-	M_4^+	M_4^-
T_1	T_4	T_2	T_1	T_4	T_3
Σ_1	Σ_1	Σ_3	Σ_4	Σ_4	Σ_3
U_1	U_2	U_2	U_3	U_4	U_1

$$\mathbf{U}^{-1}=\begin{pmatrix} 0 & 0 & 0 & 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ u_1/\sqrt{2} & u_1^*/\sqrt{2} & u_2/\sqrt{2} & u_2^*/\sqrt{2} & 0 & 0 \\ v_1/\sqrt{3} & v_1/\sqrt{2} & v_2/\sqrt{2} & v_2/\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -i/\sqrt{2} & i/\sqrt{2} \\ -u_1/\sqrt{2} & -u_1^*/\sqrt{2} & -u_2/\sqrt{2} & -u_2^*/\sqrt{2} & 0 & 0 \\ iv_1/\sqrt{2} & -iv_1/\sqrt{2} & iv_2/\sqrt{2} & -iv_2/\sqrt{2} & 0 & 0 \end{pmatrix}, \tag{6.137a}$$

where u_i, v_i, and $\omega_{1i}^2(\mathbf{k}_{14})$ are found by setting

$$\alpha_{11}=B, \qquad \alpha_{22}=C, \quad \text{and} \quad \alpha_{12}=iD \tag{6.137b}$$

in Eqs. (6.128). It is easily seen that

$$\omega_2^2(\mathbf{k}_{14})=A. \tag{6.138}$$

Symmetry at M, $\mathbf{k}_{12}$

$$\mathbf{D}(\mathbf{k}_{12})=\begin{pmatrix} A & & & D & & \\ & B & & & E & \\ & & C & & & F \\ D & & & A & & \\ & E & & & B & \\ & & F & & & C \end{pmatrix}. \tag{6.139}$$

$$\mathbf{U}^{-1}=\begin{pmatrix} 0 & 0 & 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 1/\sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} & 0 & 0 & 1/\sqrt{2} \\ 0 & 0 & 0 & -1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 1/\sqrt{2} & 0 & 0 & -1/\sqrt{2} \end{pmatrix}. \tag{6.140}$$

$$\omega_{1+}^2(\mathbf{k}_{14})=B+E\ (\text{LA}), \tag{6.141a}$$

$$\omega_{2-}^2(\mathbf{k}_{14})=B-E\ (\text{LO}), \tag{6.141b}$$

$$\omega_{3+}^2(\mathbf{k}_{14})=C+F\ (\text{TO}\perp), \tag{6.141c}$$

$$\omega_{3-}^2(\mathbf{k}_{14})=A-D\ (\text{TO}\,||), \tag{6.141d}$$

$$\omega_{4+}^2(\mathbf{k}_{14})=A+D\ (\text{TA}\,||), \tag{6.141e}$$

$$\omega_{4-}^2(\mathbf{k}_{14})=C-F\ (\text{TA}\perp). \tag{6.141f}$$

These results are not in agreement with Iyengar *et al.*[30] The disagreement is either a sign error [interchange plus for minus in (6.141)] or a difficulty in assigning labels to solutions. The descriptive labels given in (6.141) are those given by Iyengar *et al.* They must be based on experiment or a model calculation. Without this knowledge one would normally expect ω_{3+} to be acoustic and ω_{4-} to be optic because the $\kappa=1$, $\kappa'=2$ elements of $\mathbf{D}(\mathbf{k})$ are negative for positive force constants. There is no rule, however, that this must always be true.

Symmetry along P, $\mathbf{k}_{10}$

$$\mathbf{D}(\mathbf{k}_{10})=\begin{pmatrix} A & C & & D & iD & E \\ -C & A & & iD & -D & -iE \\ & & B & E & -iE & \\ D^* & -iD^* & E^* & A & -C & \\ -D^* & -D^* & iE^* & C & A & \\ E & iE^* & & & & B \end{pmatrix}, \tag{6.142a}$$

where

$$D^*=\omega^{-2}d^{-2}D, \quad \text{and} \quad E^*=\omega^{-2}d^{-2}E. \tag{6.142b}$$

Table XXIII. Compatibility relations at K for hcp lattice.

K_1	K_3	K_5	K_6
T_1	T_4	$T_1\oplus T_4$	$T_2\oplus T_3$
P_1	P_2	P_3	P_3

TABLE XXIV. Decomposition of $\{\mathbf{T}(\mathbf{k};\mathbf{R})\}$ for all symmetry elements in the (BZ) of a hexagonal close-packed lattice.

	Herring	Altmann and Bradley[a]	Kovalev
τ	$4\tau_1\oplus2\tau_2$		$4\tau^{(1)}\oplus2\tau^{(2)}$
ρ	$3\rho_1\oplus3\rho_2$		$3\tau^{(1)}\oplus3\tau^{(2)}$
σ	$4\sigma_1\oplus2\sigma_2$		$4\tau^{(1)}\oplus2\tau^{(2)}$
δ	$3\delta_1\oplus3\delta_2$		$3\tau^{(1)}\oplus3\tau^{(2)}$
δ'	$3\delta_1'\oplus3\delta_2'$		$3\tau^{(1)}\oplus3\tau^{(2)}$
Σ	$2(\Sigma_1\oplus\Sigma_3\oplus\Sigma_4)$	$2(\mathcal{A}'\oplus\mathcal{B}''\oplus\mathcal{B}')$	$2(\tau^{(1)}\oplus\tau^{(4)}\oplus\tau^{(3)})$
T, T'	$2T_1\oplus T_2\oplus T_3\oplus2T_4$	$2\mathcal{A}'\oplus\mathcal{A}''\oplus\mathcal{B}''\oplus2\mathcal{B}'$	$2\tau^{(1)}\oplus\tau^{(2)}\oplus\tau^{(4)}\oplus2\tau^{(3)}$
R	$2R_1\oplus R_2\oplus2R_3\oplus R_4$	$2\mathcal{A}'\oplus\mathcal{A}''\oplus2\mathcal{B}''\oplus\mathcal{B}'$	$2\tau^{(1)}\oplus\tau^{(2)}\oplus2\tau^{(4)}\oplus\tau^{(3)}$
S, S'	$3S_1$	$3\mathcal{E}(1)$	$3\tau^{(1)}$
U	$2U_1\oplus2U_2\oplus U_3\oplus U_4$	$2\mathcal{A}_p\oplus2\mathcal{A}_m\oplus\mathcal{B}_m\oplus\mathcal{B}_p$	$2\tau^{(1)}\oplus2\tau^{(3)}\oplus\tau^{(4)}\oplus\tau^{(2)}$
P	$P_1\oplus P_2\oplus2P_3$	$A_p\oplus A_m\oplus2E$	$\tau^{(1)}\oplus\tau^{(2)}\oplus2\tau^{(3)}$
M	$M_1^+\oplus M_2^-\oplus M_3^+\oplus M_3^-\oplus M_4^+$	$\mathcal{A}_+'\oplus\mathcal{A}_-'\oplus\mathcal{B}_+''\oplus\mathcal{B}_-'\oplus\mathcal{B}_+'$	$\tau^{(1)}\oplus\tau^{(8)}\oplus\tau^{(5)}\oplus\tau^{(6)}\oplus\tau^{(3)}\oplus\tau^{(4)}$
L	$2L_1\oplus L_2$	$2\mathcal{E}_1\oplus\mathcal{E}_2$	$2\tau^{(1)}\oplus\tau^{(2)}$
Δ	$\Delta_1\oplus\Delta_2\oplus\Delta_5\oplus\Delta_6$	$A_{1p}\oplus A_{1m}\oplus E_p\oplus E_m$	$\tau^{(1)}\oplus\tau^{(3)}\oplus\tau^{(6)}\oplus\tau^{(5)}$
K	$K_1\oplus K_3\oplus K_5\oplus K_6$	$A_1'\oplus A_2'\oplus E'\oplus E''$	$\tau^{(1)}\oplus\tau^{(3)}\oplus\tau^{(5)}\oplus\tau^{(6)}$
H	$H_1\oplus2H_3$	$A^{(2)}\oplus2E^*$	$\tau^{(1)}\oplus\tau^{(3)}$
A	$A_1\oplus A_3$	$A^{(2)}\oplus E^{(4)}$	$\tau^{(1)}\oplus\tau^{(3)}$
Γ	$\Gamma_2^-\oplus\Gamma_3^+\oplus\Gamma_5^+\oplus\Gamma_6^-$	$A_{2-}''\oplus A_{2+}''\oplus E_+'\oplus E_-'$	$\tau^{(4)}\oplus\tau^{(5)}\oplus\tau^{(11)}\oplus\tau^{(10)}$

[a] See Ref. 10, p. 38, for an explanation of the symbols used in this column.

$$\mathbf{U}^{-1}=\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & u_1/\sqrt{2} & 0 & u_2/\sqrt{2} & 0 \\ \frac{1}{2}i & \frac{1}{2}i & -iu_1/\sqrt{2} & 0 & -iu_2/\sqrt{2} & 0 \\ 0 & 0 & 0 & v_1 & 0 & v_2 \\ \frac{1}{2}d\omega^2 & -d\omega^2 & 0 & u_1^*/\sqrt{2} & 0 & u_2^*/\sqrt{2} \\ -\frac{1}{2}id\omega^2 & id\omega^2 & 0 & iu_1^*/\sqrt{2} & 0 & iu_2^*/\sqrt{2} \\ 0 & 0 & v_1 & 0 & v_2 & 0 \end{pmatrix}, \tag{6.143a}$$

where

$$\omega^2=\exp(2\pi i/3), \qquad d=\exp(i\pi\eta/2) \tag{6.143b}$$

and the solutions u_i, v_i, and $\omega_{3i}(\mathbf{k}_{10})$ are found from (6.128) by setting

$$\alpha_{11}=A-iC, \qquad \alpha_{22}=B, \quad \text{and} \quad \alpha_{12}=\sqrt{2}E, \tag{6.143c}$$

$$\omega_1^2(\mathbf{k}_{10})=A+iC+2\omega^2\,dD. \tag{6.144}$$

Symmetry along U, $\mathbf{k}_9$

$$\mathbf{D}(\mathbf{k}_9)=\begin{pmatrix} A & & & E & & \\ & B & D & & F & H \\ & -D & C & & H & G \\ E^* & & & A & & \\ & F^* & H^* & & B & -D \\ & H^* & G^* & & D & C \end{pmatrix}, \tag{6.145a}$$

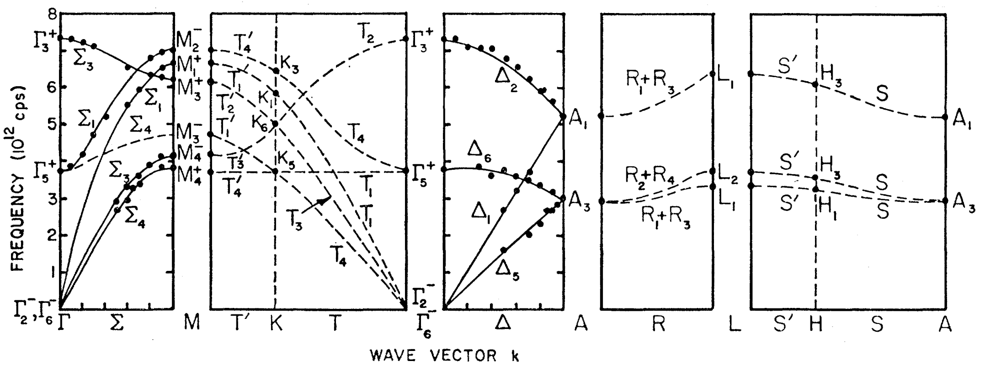

FIG. 10. Possible arrangement of dispersion curves for Mg obtained by group theory and the data of Iyengar *et al.*[30] for the Δ and Σ directions. Dashed curves are predictions.

where

$$E^*=d^2E,\qquad F^*=d^2F,$$

$$G^*=d^2G,\quad\text{and}\quad H^*=-d^2H. \tag{6.145b}$$

$$\mathbf{U}^{-1}=\begin{pmatrix} 0 & 0 & 0 & 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ u_1/\sqrt{2} & u_2/\sqrt{2} & u_1'/\sqrt{2} & u_2'/\sqrt{2} & 0 & 0 \\ v_1/\sqrt{2} & v_2/\sqrt{2} & v_1'/\sqrt{2} & v_2'/\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -d/\sqrt{2} & d/\sqrt{2} \\ du_1/\sqrt{2} & du_2/\sqrt{2} & -du_1'/\sqrt{2} & -du_2'/\sqrt{2} & 0 & 0 \\ -dv_1/\sqrt{2} & -dv_2/\sqrt{2} & dv_1'/\sqrt{2} & dv_2'/\sqrt{2} & 0 & 0 \end{pmatrix}, \tag{6.146a}$$

where d is $\exp[\pi i\eta/2]$ as before and u_i, v_i, $\omega_{1i}^2(\mathbf{k}_9)$ are determined from (6.128) by setting

$$\alpha_{11}=B+dF,\qquad \alpha_{22}=C-d^{-1}G^*,\quad\text{and}\quad \alpha_{12}=D-dH. \tag{6.146b}$$

The u_i', and v_i', and $\omega_{2i}^2(\mathbf{k}_9)$ are determined by setting

$$\alpha_{11}=B-dF,\qquad \alpha_{22}=C+dG,\quad\text{and}\quad \alpha_{12}=D+dH. \tag{6.146c}$$

For the pure modes we find

$$\omega_3^2(\mathbf{k}_9)=A-dE, \tag{6.147a}$$

$$\omega_4^2(\mathbf{k}_9)=A+dE. \tag{6.147b}$$

Symmetry along S, S', $\mathbf{k}_8$

$$\mathbf{D}(\mathbf{k}_8)=\begin{pmatrix} A & D & & & & E \\ -D & B & & & & F \\ & & C & E & F & \\ & & E^* & A & -D & \\ & & F^* & D & B & \\ E^* & F^* & & & & C \end{pmatrix}, \tag{6.148a}$$

where

$$E^*=-d^4E,\quad\text{and}\quad F^*=-d^4F. \tag{6.148b}$$

Since there is only one irreducible representation along S which is two dimensional and occurs three times, the eigenvectors will not be written down. The form of $\mathbf{D}(\mathbf{k}_8)$ suggests a trial solution which is simpler than that obtained by projection operators.

The line S' is essentially continuous with S as seen in an extended zone scheme. Instead of letting η go from 0 to $\frac{2}{3}$, we can let it go from 0 to 1.

Symmetry along R, $\mathbf{k}_7$

$$\mathbf{D}(\mathbf{k}_7)=\begin{pmatrix} A & & & & & \\ & B & & & & \\ & & C & & & \\ & & & A & & \\ & & & & B & \\ & & & & & C \end{pmatrix}. \tag{6.149}$$

$$\mathbf{U}^{-1}=\begin{pmatrix}0&0&1&0&0&0\\0&0&0&1&0&0\\1&0&0&0&0&0\\0&0&0&0&0&1\\0&1&0&0&0&0\\0&0&0&0&1&0\end{pmatrix}. \qquad (6.150)$$

$$\omega_{11}^2(\mathbf{k}_7)=C=\omega_{32}^2(\mathbf{k}_7), \qquad (6.151a)$$

$$\omega_{12}(\mathbf{k}_7)=B=\omega_{31}^2(\mathbf{k}_7), \qquad (6.151b)$$

$$\omega_2(\mathbf{k}_7)=A=\omega_4(\mathbf{k}_7). \qquad (6.151c)$$

The degeneracy seen here is predicted by time-reversal invariance.

Symmetry along T, T', $\mathbf{k}_6$

$$\mathbf{D}(\mathbf{k}_6)=\begin{pmatrix}A&D&&E&H&\\-D&B&&H&F&\\&&C&&&G\\E^*&H^*&&A&-D&\\H^*&F^*&&D&B&\\&&G^*&&&C\end{pmatrix}, \qquad (6.152a)$$

where

$$E^*=d^4E, \qquad F^*=d^4F,$$

$$G^*=d^4G, \quad \text{and} \quad H^*=-d^4F. \qquad (6.152b)$$

The eigenvector matrix is

$$\mathbf{U}^{-1}=\begin{pmatrix}u_1/\sqrt{2}&u_2/\sqrt{2}&0&0&u_1'/\sqrt{2}&u_2'/\sqrt{2}\\v_1/\sqrt{2}&v_2/\sqrt{2}&0&0&v_1'/\sqrt{2}&v_2'/\sqrt{2}\\0&0&1/\sqrt{2}&1/\sqrt{2}&0&0\\d^2u_1/\sqrt{2}&d^2u_2/\sqrt{2}&0&0&-d^2u_1'/\sqrt{2}&-d^2u_2'/\sqrt{2}\\-dv_1/\sqrt{2}&-d^2v_2/\sqrt{2}&0&0&d^2v_1'/\sqrt{2}&d^2v_2'/\sqrt{2}\\0&0&-d^2/\sqrt{2}&d^2/\sqrt{2}&0&0\end{pmatrix}, \qquad (6.153a)$$

where $d=\exp[i\pi\eta/2]$ and the solutions u_i, v_i, and $\omega_{1i}^2(\mathbf{k}_6)$ are found by substituting

$$\alpha_{11}=A+d^2E, \qquad \alpha_{22}=B-d^2F, \quad \text{and} \quad \alpha_{12}=D-d^2H \qquad (6.153b)$$

into (6.128). The solutions for u_i', v_i', and $\omega_{4i}^2(\mathbf{k}_6)$ are found by substituting

$$\alpha_{11}=A-d^2E, \qquad \alpha_{22}=B+d^2F, \quad \text{and} \quad \alpha_{12}=D+d^2H \qquad (6.153c)$$

into (6.128). The other two eigenvalues are

$$\omega_2^2(\mathbf{k}_6)=C-d^2G,$$

$$\omega_3^2(\mathbf{k}_6)=C+d^2G. \qquad (6.154)$$

The above results do not appear to be in agreement with those of Iyengar *et al.* The factor d^2 is missing from $\omega_2^2(\mathbf{k}_6)$ and $\omega_3^2(\mathbf{k}_6)$. There are also terms missing from the $s=1$ and 4 solutions also.

T′ is a continuation of T in the sense that S′ is a continuation of S.

Symmetry along Σ, $\mathbf{k}_5$

$$\mathbf{D}(\mathbf{k}_5)=\begin{pmatrix}A&&&D&&\\&B&&&E&\\&&C&&&F\\D^*&&&A&&\\&E^*&&&B&\\&&F^*&&&C\end{pmatrix}. \qquad (6.155)$$

$$\mathbf{U}^{-1}=\begin{pmatrix}0&0&0&0&u_1''&u_2''\\u_1&u_2&0&0&0&0\\0&0&u_1'&u_2'&0&0\\0&0&0&0&v_1''&v_2''\\v_1&v_2&0&0&0&0\\0&0&v_1'&v_2'&0&0\end{pmatrix}, \qquad (6.156a)$$

where

$$\alpha_{11}=\alpha_{22}=B, \quad \text{and} \quad \alpha_{12}=E \qquad (6.156b)$$

for u_i, v_i, and $\omega_{1i}^2(\mathbf{k}_5)$. If we set

$$\alpha_{11}=\alpha_{22}=C, \quad \text{and} \quad \alpha_{12}=F, \qquad (6.156c)$$

then we get u_i', v_i', and $\omega_{3i}^2(\mathbf{k}_5)$. With the relations

$$\alpha_{11}=\alpha_{22}=A, \quad \text{and} \quad \alpha_{12}=D, \qquad (6.156d)$$

one finds u_i'', v_i'', and $\omega_{4i}^2(\mathbf{k}_5)$.

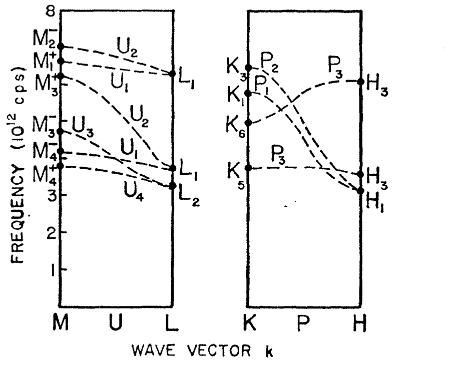

Fig. 11. Continuation of Fig. 10 for the symmetry directions P and U.

Symmetry on δ, δ', $\mathbf{k}_4$

The plane δ contains the lines T and S. The plane δ' is an extension of δ in the same sense that T′ and S′ are extensions of T and S. The two irreducible representation in the plane are each contained three times in $\{\mathbf{T}(\mathbf{k}_4, \mathbf{R})\}$ and hence the eigenvectors will not be given.

$$\mathbf{D}(\mathbf{k}_4)=\begin{pmatrix} A & D & E & G & J & K \\ -D & B & F & J & H & L \\ E^* & -F & C & K & L & I \\ d_1^2d_2G & -d_1^2d_2J & d_1^2d_2K & A & -D & E^* \\ -d_1^2d_2J & d_1^2d_2H & d_1^2d_2L & D & B & -F \\ d_1^2d_2K & -d_1^2d_2L & d_1^2d_2I & E & F & C \end{pmatrix}, \tag{6.157}$$

where

$$d_i=\exp[\pi i\eta_i/2].$$

This can be broken into two three-by-three matrices by symmetry.

Symmetry on σ, $\mathbf{k}_3$

This is the plane containing Σ and R.

$$\mathbf{D}(\mathbf{k}_3)=\begin{pmatrix} A & & & E & & \\ & B & D & & F & H \\ & D^* & C & & H & G \\ E^* & & & A & & \\ & F^* & H^* & & B & D^* \\ & H^* & G^* & & D & C \end{pmatrix}. \tag{6.158}$$

The form of $\mathbf{D}(\mathbf{k}_3)$ shows that vibrations with polarization perpendicular to the plane are pure. Their frequencies are

$$\omega_{2i}^2(\mathbf{k}_3)=A+(2i-3)\,|\,E\,|. \tag{6.159}$$

The frequencies belonging to $s=1$ are found from a quartic equation. The trial solutions are obvious.

Symmetry on ρ, $\mathbf{k}_2$

Time reversal predicts a degeneracy between the two representations. Each is one-dimensional and occurs three times. We find that

$$\mathbf{D}(\mathbf{k}_2)=\begin{pmatrix} A & D & & & & E \\ D^* & B & & & & F \\ & & C & E & F & \\ & & E^* & A & D^* & \\ & & F^* & D & B & \\ E^* & F^* & & & & C \end{pmatrix}. \tag{6.160}$$

Once again, the trial solutions are obvious from the block structure of $\mathbf{D}(\mathbf{k}_2)$.

Table XXV. Corrections to R. McWeeny, *Symmetry* (The Macmillan Co., New York, 1963).

Location	Correction
p. 61 last line	$(S_n\neq i\bar{C}_n$. There is no simple rule.)[a]
p. 62 Fig. 3.5	"Axis for $C_2^{(k+1)}$ [also defines plane for $\sigma^{(k+1)}$]"[b]
p. 74 Table 3.12	"$T\mid E\mid C_2^xC_2^yC_2^z\mid C_3^{xyz}\ldots$"
p. 99 Table 4.12	"$iC_6=i\bar{S}_6S_6\sigma_h\bar{S}_3S_3$"
p. 99 Table 4.13	"$iD_6=i\bar{S}_6S_6\sigma_h\bar{S}_3S_3\cdots$"
p. 102 Table 4.18	This table is wrong. There are 4 classes and only 3 representations listed. See Slater, Ref. 4, Table A3–35, p. 392 for a correct table.
p. 104 Table 4.21	Because the table for T is wrong, one cannot use it to generate the table for T_h.

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[a] M. J. Buerger, *Elementary Crystallography* (John Wiley & Sons, Inc., New York, 1956), p. 30.

[b] The plane σ^k is *not* defined by the direction of its normal. This is not an error, but a case where one convention is used for operations in the cubic groups and another convention for other point groups. It is not unique to McWeeny.

TABLE XXVI. Corrections to O. V. Kovalev, ***Irreducible Representations of the Space Groups*** (Gordon and Breach Science Publishers, New York, 1965).

Location	Correction
p. 6 line beginning $h_{13}=$	"$h_{13}=(\bar{y}, \bar{x}, \bar{z})\cdots$"
p. 7 line beginning $h_{47}=$	"$h_{47}=(\bar{z}, \bar{y}, \bar{x})\cdots$"
p. 8 line beginning $h_5=$	"$h_5=(y-x, \bar{x}, z)\cdots$"
p. 8 line beginning $h_8=$	"$\cdots$—rotation about $(\bar{1}10)$."
p. 8 line beginning $h_{12}=$	"$h_{12}=(y-x, y, \bar{z})\cdots$"
p. 8 line beginning $h_{14}=$	$h_{14}=(y-x, \bar{x}, \bar{z})\cdots$"
p. 8 line beginning $h_{18}=$	"$h_{18}=(\bar{y}, x-y, \bar{z})\cdots$"
p. 8 line beginning $h_{20}=$	"$\cdots$—reflection in the plane $(\bar{1}10)$."
p. 9 line beginning $\Gamma_0{}^b=$	$\Gamma_0{}^b$—base-centered$\cdots$"
p. 23 sixth line	This formula does not appear to be right. Could it be $\psi_{\mathbf{k}\mu}(g^{-1}\mathbf{r})=\tau_{\mu'\mu}(g)\psi_{\mathbf{k}\mu'}(\mathbf{r})$?
p. 24 14th line	$T(g)$ is really not defined by the formula below except by implication that it is the coefficient of $\psi_{k_s\mu}'(\mathbf{r})$.
p. 30 3rd line	"$\cdots$have unequal"
p. 92 5th line under $T205$	"erator $\tau(h_k)$ corresponds to the element h_k and the operator $-\tau(h_{k+24})$ corresponds to the element h_{k+24}," This may be a translation difficulty. The sentence is so garbled that this may not be the correct interpretation.
p. 111 Table T70	The matrix under elements h_{20}, h_{22}, h_{24} should be $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

Symmetry on τ, $\mathbf{k}_1$

$$\mathbf{D}(\mathbf{k}_1)=\begin{pmatrix} A & D & & E & H & \\ D^* & B & & H & F & \\ & & C & & & G \\ E^* & H^* & & A & D & \\ H^* & F^* & & D^* & B & \\ & & G^* & & & C \end{pmatrix}. \qquad (6.161)$$

Modes with polarization perpendicular to the plane are pure:

$$x_{2i}{}^2(\mathbf{k}_1)=C+(2i-3)\,|G|. \qquad (6.162)$$

The four frequencies $x_{1i}{}^2(\mathbf{k}_1)$ are found from a quartic.

Predictions

Phonon dispersion curves have been measured in Mg along Δ and Σ.[30] It is again of interest to use the above group theory along with the data to predict the connectivity of the dispersion relation in other symmetry directions. The predictions are shown in Fig. 10 and 11. These predictions cannot be very unique for S, U, and P. The most interesting results are along T. These are predicated on the experimental assignments at M.

Dispersion curves have been measured for Be[68] and Zn.[69] The above theory can be taken over for these substances. It has often been said and should be emphasized again that group theory is useful in separating symmetry from dynamics. It is not a substitute for detailed calculations.

7. CORRECTIONS

It is next to impossible to make a book or journal article without some misprints and trivial errors. The errata section of journals serves as a vehicle for making corrections to these references. It is more difficult to

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[68] R. E. Schmunk, R. M. Brugger, P. D. Randolph, and K. A. Strong, Phys. Rev. **128**, 562 (1962).

[69] G. Borgonovi, G. Caglioti, and J. J. Antal, Phys. Rev. **132**, 683 (1963).

TABLE XXVII. Corrections to G. F. Koster, "Space Groups and their Representations" in *Solid State Physics*, F. Seitz and D. Turnbull, Eds. (Academic Press Inc., New York, 1957), Vol. 5, p. 173.[a]

Location	Correction
p. 179 4th line below Eq. (2–3)	"spond in turn to screw axes and glide planes···"
p. 179 6th line below Eq. (2–3)	"···Moreover the translational part···"
p. 181 8th line	"We now list the 32 point groups and *the character tables of* their irreducible representations."
p. 184 Table IX	The order of the labels in column one should be W_1, W_2, W_3, W_4.
p. 185 Table XIII	The order of the labels in column two should be W_1, W_2, W_1', W_2', W_3.
p. 186 Table XIV	The order of the labels in column one should be M_1, M_4, M_3, M_2, M_5, M_1', M_4', M_3', M_2', M_5'.
p. 188 Table XIX	The order of the labels in column one should be L_1, L_2, L_3, L_2', L_1', L_3'.
p. 197 8th line	"···subgroup C_4···"
p. 197 last line	"equal angles *of 60°* with one another···"
p. 214 Eq. (2–7), lower line	"$\mathbf{R}_n\cdot\alpha^{-1}\mathbf{k}_j=2\pi\times$(integer)"
p. 216 2nd line	"···appear as often as exp $(i\mathbf{k}_1\cdot\mathbf{R}_n)$···"
p. 218 2nd line after Eq. (2–23)	"group *of* k_1, ···"
p. 222 3rd line	"tions form *a basis for* an irreducible representation···"
p. 224 2nd line above Eq. (3–4)	"tion (3–2) remains unchanged···" Eq. (2–29) is nonexistent. (3–2) seems to me to be what is meant.
p. 224 5th line below Eq. (3–4)	"···by use of (3–1)." Again (2–38) is nonexistent and (3–1) seems appropriate.
p. 227 bottom of page	A description of the symmetry point N seems to be missing. It is the center of the rhombic face and has symmetry D_{2h}. The principal twofold axis is on the line $k_x=k_y$ and $k_z=0$.
p. 230 2nd line of reference 23	"···R. J. Elliot, Phys. Rev. **96**, 280 (1954)."
p. 233 Table XXXIII	Koster does not seem to agree with Elliot, whom he quotes as reference. Slater (Ref. 4 in the present paper) Table A3–28 agrees with neither Koster nor Elliot.
p. 233 6th line of Table XXXIV	The two operations $\{C_2' \mid \tau\}$ are lumped together as if they had the same character. They correspond to the operations R_{19}' and R_{20}' in Slater Table A3–25. There they are given different characters. They are also given different characters in Döring and Zehler.[b] These operations are also confused in Herring.[c]
p. 234 2nd line	"···vectors $t_1=sj$, ···" [Cf. p. 210, Eq. (4–13).]

[a] See also Ref. 21, p. 1 for some further errors.

[b] W. Doring and V. Zehler, Ann. Physik **13**, 214 (1953), Table 7.

[c] See Ref. 65, Table X.

make corrections to books before a new printing or edition.

A review article is an appropriate place to make corrections to books and articles used as references to the subject. It is hoped that the authors mentioned in this section will not take offense. These minor corrections are intended to make life easier for the beginner and should not detract from the stature of the published work.

Tables XXV to XXVIII contain a list of corrections to errors found by the author during his reading and use of tables. No claim can be made for completeness.

Notes added in proof. The phonon dispersion curves for TlBr, which has the CsCl structure, have recently

TABLE XXVIII. Corrections to J. C. Slater, *Quantum Theory of Molecules and Solids* (McGraw-Hill Book Co., Inc., New York, 1965), Vol. II.

Location	Correction
p. 350, 16th line from bottom	Eq. (A3–2) seems inappropriate; I couldn't find suitable replacement.
p. 360, Table A3–9	This table does not agree with Kovalev's Table T41 on p. 104. It was not possible to get a correct projection operator using this table.
p. 367, 2nd line from bottom	"L_1 L_2 L_1 L_2"
p. 380, Table A3–26	Change $(L_4)_{ij}$ to $(L_3')_{ij}$ in column one

appeared in print. [See E. R. Cowley and A. Okazaki, Proc. Roy. Soc. (London) **A300**, 45 (1967)]. Measurements were made along the symmetry lines Δ, **S**, Σ, **T**, and Λ. The connectivity is the same as the predictions illustrated on Fig. 7. The ordering at the symmetry point **M** is different. The lower $\mathbf{M}_5'$ and $\mathbf{M}_4'$ points are interchanged. Similarly, there is an interchange at **X** of the $\mathbf{X}_5$ and $\mathbf{X}_4'$ points. In comparing the predictions with the data one must note further that Cowley and Okazaki's representation labels $\mathbf{S}_3$ and $\mathbf{S}_4$ are what we have called $\mathbf{S}_4$ and $\mathbf{S}_3$, respectively.

A private communication with G. Venkataraman has disclosed that the labeling given above for Mg at Γ and **K** is correct. We have not been able to resolve our differences at **M** and **T** or for eigenfrequencies at **K**. Any resolution of this problem will be published in Ref. 52.

ACKNOWLEDGMENTS

I would like to acknowledge helpful discussions with John L. Yarnell, J. Larry Verble, Darryl Smith, Gerald Dolling, and Roger Cowley.

APPENDIX A

This appendix demonstrates the explicit form of ω^2 and the eigenvectors at Γ, $\mathbf{k}_{12}=\mathbf{0}$ for CsCl lattice. The equations of motion are

$$M_\kappa \ddot{u}_\alpha(l\kappa) = -\sum_{l'\kappa'\beta} \Phi_{\alpha\beta}(l\kappa;\, l'\kappa')u_\beta(l'\kappa'). \tag{A1}$$

This is Eq. (2.12) in (I). In order to put this into a form more closely related to Hooke's law we will define

$$K_{\alpha\beta}(l\kappa;\, l'\kappa') = -\Phi_{\alpha\beta}(l\kappa;\, l'\kappa'). \tag{A2}$$

Furthermore,

$$K_{\alpha\beta}(l\kappa;\, l\kappa) = -{\sum_{l'\kappa'}}' K_{\alpha\beta}(l\kappa;\, l'\kappa'), \tag{A3}$$

where the prime on the summation means that the term $(l'\kappa')=(l\kappa)$ is omitted. Equation (A1) becomes

$$M_\kappa \ddot{u}_\alpha(l\kappa) = -{\sum_{l'\kappa'\beta}}' K_{\alpha\beta}(l\kappa;\, l'\kappa')[u_\beta(l\kappa)-u_\beta(l'\kappa')]. \tag{A4}$$

In this form it is readily seen that if the atom $(l\kappa)$ is displaced while all others are held fixed, then there will be a restoring force provided that the tensor force constants $\mathbf{K}(l\kappa;\, l'\kappa')$ are positive. Actually, in this case it is only required that

$${\sum_{l'\kappa'}}' \mathbf{K}(l\kappa;\, l'\kappa') > 0. \tag{A5}$$

When one carries out the usual analysis to arrive at the dynamical matrix, the result is

$$D_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k}) = -(M_\kappa M_{\kappa'})^{-1/2} \sum_{l'} K_{\alpha\beta}(l\kappa;\, l'\kappa') \times \exp\{i\mathbf{k}\cdot[\mathbf{x}(l')-\mathbf{x}(l)]\}. \tag{A6}$$

This must be written out for two cases: (1) $\kappa=\kappa'$; and (2) $\kappa\neq\kappa'$.

$$D_{\alpha\beta}(\kappa\kappa \mid \mathbf{k}) = M_\kappa^{-1}\Big({\sum_{\kappa'}}' \sum_{l'} K_{\alpha\beta}(l\kappa;\, l'\kappa') + {\sum_{l'}}'' K_{\alpha\beta}(l\kappa;\, l'\kappa)[1-\exp\{i\mathbf{k}\cdot[\mathbf{x}(l')-\mathbf{x}(l)]\}]\Big). \tag{A7}$$

The prime on the first sum means $\kappa'\neq\kappa$; the double prime on the second summations means $l'\neq l$. When $\kappa\neq\kappa'$ the formula is the same as Eq. (A6). The equations for $\mathbf{C}(\mathbf{k})$ obtained from the above by using Eq. (3.27)* are

$$C_{\alpha\beta}(\kappa\kappa \mid \mathbf{k}) = \exp\{i\mathbf{k}\cdot[\mathbf{x}(\kappa')-\mathbf{x}(\kappa)]\}D_{\alpha\beta}(\kappa\kappa \mid \mathbf{k}), \tag{A8a}$$

$$C_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k}) = -(M_\kappa M_{\kappa'})^{-1/2} \sum_{l'} K_{\alpha\beta}(l\kappa;\, l'\kappa') \times \exp\{i\mathbf{k}\cdot[\mathbf{x}(l'\kappa')-\mathbf{x}(l\kappa)]\}. \tag{A8b}$$

At Γ these expressions reduce to

$$C_{\alpha\beta}(\kappa\kappa \mid \mathbf{k}_{12}) = M_\kappa^{-1} {\sum_{\kappa'}}' \sum_{l'} K_{\alpha\beta}(l\kappa;\, l'\kappa'), \tag{A9a}$$

$$C_{\alpha\beta}(\kappa\kappa' \mid \mathbf{k}_{12}) = -(M_\kappa M_{\kappa'})^{-1/2} \sum_{l'} K_{\alpha\beta}(l\kappa;\, l'\kappa'). \tag{A9b}$$

It will be recalled that

$$\mathrm{A} = C_{11}(11 \mid \mathbf{k}_{12}) = M_1^{-1} \sum_{l'} K_{11}(l1;\, l'2), \tag{A10a}$$

$$\mathrm{B} = C_{11}(22 \mid \mathbf{k}_{12}) = M_2^{-1} \sum_{l'} K_{11}(l2;\, l'1), \tag{A10b}$$

$$\mathrm{C} = C_{11}(12 \mid \mathbf{k}_{12}) = -(M_1M_2)^{1/2} \sum_{l'} K_{11}(l1;\, l'2). \tag{A10c}$$

Since

$$K_{11}(l2;\, l'1) = K_{11}(l'1;\, l2) = K_{11}(0\,1;\, l-l'2) \tag{A11}$$

and since the summation over l' is independent of l and is symmetric in l', A, B, and C may be expressed in terms of the one sum

$$K_0=\sum_{l'} K_{11}(l1\cdot l'2). \tag{A12}$$

Thus

$$\mathrm{A}=K_0/M_1, \tag{A13a}$$

$$\mathrm{B}=K_0/M_2, \tag{A 3b}$$

$$\mathrm{C}=-K_0/(M_1M_2)^{1/2}. \tag{A13c}$$

From this is easily seen that

$$-\mathrm{AB}+\mathrm{C}^2=0. \tag{A14}$$

The eigenvectors $\mathbf{e}(\mathbf{k}_{12}\ 10i1)$ are

$$\mathbf{e}(\mathbf{k}_{12}\ 1011)=\begin{pmatrix} K_0(M_1)^{1/2}/[\,|K_0|\,(M_1+M_2)^{1/2}] \\ 0 \\ 0 \\ K_0(M_2)^{1/2}/[\,|K_0|\,(M_1+M_2)^{1/2}] \\ 0 \\ 0 \end{pmatrix} \tag{A15a}$$

and

$$\mathbf{e}(\mathbf{k}_{12}\ 1021)=\begin{pmatrix} K_0(M_2)^{1/2}/[\,|K_0|\,(M_1+M_2)^{1/2}] \\ 0 \\ 0 \\ -K_0(M_1)^{1/2}/[\,|K_0|\,(M_1+M_2)^{1/2}] \\ 0 \\ 0 \end{pmatrix}. \tag{A15b}$$

Clearly the first mode is acoustic and the second is optic. At first sight it might appear strange that the acoustic mode does not have equal amplitudes for the two atoms in the unit cell. It must be remembered that the true amplitude is

$$u_\alpha(l\kappa\,|\,\mathbf{k}sa\lambda)=(M_\kappa)^{-1/2}u(\mathbf{k})e_\alpha(\kappa\,|\,\mathbf{k}sa\lambda)\times\exp\{i\mathbf{k}\cdot\mathbf{x}(l\kappa)-\omega_{sa}(\mathbf{k})t\}, \tag{A16}$$

where $u(\mathbf{k})$ is an arbitrary amplitude factor. The factor $(M_\kappa)^{-1/2}$ cancels out the corresponding factor in Eq. (A15a).