Space Group Selection Rules: Diamond and Zinc Blende

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General methods for the reduction of direct products of space-group irreducible representations are discussed, based on the use of the full irreducible representations of the space group. The reduction proceeds in two stages: First, wave vector selection rules are obtained when the direct product of two stars is decomposed into a direct sum of stars; finally, the species of irreducible representations occurring for each star in the sum is found. The latter stage is accomplished by using the "reduction group," or by "direct inspection," depending on convenience. These methods can be applied to the reduction of the ordinary Kronecker products, and the symmetrized Kronecker powers, of the full space group irreducible representations of any space group.

The methods are applied here to the diamond and zinc-blende space groups. For both, the explicit reduction is given of all direct products: $\Gamma^{(m)}\otimes{}^\star X^{(m')}$, $\Gamma^{(m)}\otimes{}^\star L^{(m')}$, $\Gamma^{(m)}\otimes{}^\star\Lambda^{(m')}$, $\Gamma^{(m)}\otimes{}^\star\Delta^{(m')}$, ${}^\star X^{(m)}\otimes{}^\star X^{(m')}$, ${}^\star L^{(m)}\otimes{}^\star L^{(m')}$, ${}^\star L^{(m)}\otimes{}^\star X^{(m')}$, ${}^\star W^{(m)}\otimes{}^\star W^{(m')}$, ${}^\star\Sigma^{(m)}\otimes{}^\star\Sigma^{(m')}$, ${}^\star\Lambda^{(m)}\otimes{}^\star\Lambda^{(m')}$, ${}^\star\Delta^{(m)}\otimes{}^\star\Delta^{(m')}$, and ${}^\star\Delta^{(m)}\otimes{}^\star\Lambda^{(m')}$. The reduction is given of symmetrized Kronecker squares and cubes of $\Gamma^{(m)}$, ${}^\star X^{(m)}$, ${}^\star L^{(m)}$, ${}^\star\Lambda^{(m)}$, ${}^\star\Delta^{(m)}$, ${}^\star W^{(m)}$, ${}^\star\Sigma^{(m)}$ and ${}^\star Z^{(m)}$. Only single group (no spin-orbit or time-reversal effects) rules are given, although the same method will yield rules for the double groups. A later paper will discuss applications of these rules.

1. INTRODUCTION

IN this paper we shall obtain and discuss selection rules for processes which can occur in diamond and zinc-blende structures. The processes involved may be electronic, vibrational, or a mixture of the two, as well as caused by perturbations of one or another sort. Of the external perturbations which one normally considers, light is of primary importance. Among the specific types of processes in these structures to which the selection rules can be applied are optical absorption due to excitation of combination or overtone lattice vibrations, direct and indirect exciton creation, intervalley and intravalley scattering transitions, and band-band processes. These applications will be discussed in a later paper. Of perhaps equal interest to the selection rules which we have derived is the method of derivation. We utilize rigorous and general methods which are based explicitly on the character table for full space group irreducible representations.[1,2]

Neglecting accidental degeneracy the symmetry of a crystal as epitomized by its space group determines the nature, number, and type of eigenfunctions which may arise. For example, each solution of the electronic[3] and vibrational[4] crystal Schrödinger equation must belong to an irreducible function space of the crystal space group. The behavior of these eigenfunctions under transformation by crystal symmetry operation is fully determined by the space group irreducible representations. To determine selection rules for processes in crystals we assume that the initial and final states involved in the process are eigenstates of the appropriate Hamiltonian, with their necessary degeneracy specified by crystal symmetry. A given process is allowed if the direct product of the irreducible representations of the factors (initial and final state functions, and the perturbation) contains the trivial or identity representation of the space group. The reduction of the direct product of two irreducible representations of the space group into a direct sum of space group irreducible representations is thus the central problem at hand.

Consider a finite group, consisting of g elements R, with r classes, and character systems $\chi^{(j)}(R)$, $j=1, \cdots, r$ for the unitary irreducible representations $\Gamma^{(j)}$. We can reduce the direct product $\Gamma^{(j)}\otimes\Gamma^{(j')}$, as usual[5]:

$$\chi^{(j)}(R)\chi^{(j')}(R)=\sum_{j''=1}^{r}(jj'|j'')\chi^{(j'')}(R),\qquad R=1,\cdots g. \quad (1.1)$$

The coefficient $(jj'|j'')$ also can be found from

$$(jj'|j'')=\frac{1}{g}\sum_{R=1}^{g}\chi^{(j)}(R)\chi^{(j')}(R)\chi^{(j'')}(R)^*,\qquad j''=1,\cdots r. \quad (1.2)$$

In (1.1) the sum is over all r irreducible representations, in (1.2) the sum is over all group elements. Let the l_j functions

$$\psi_\mu{}^{(j)}(r),\quad \mu=1,\cdots l_j \quad (1.3)$$

transform under the symmetry operations of the group as partners in the irreducible representation $\Gamma^{(j)}$, and let the $l_{j'}$ functions $\psi'_{\mu'}{}^{(j')}(\mathbf{r})$ transform as partners in the irreducible representation $\Gamma^{(j')}$. Then, in general, the $(l_j\times l_{j'})$ functions

$$\theta_{\mu\mu'}{}^{(j,j')}(r)\equiv(\psi_\mu{}^{(j)}(r)\cdot\psi'_{\mu'}{}^{(j')}(r)),\qquad \mu=1,\cdots l_j;\quad \mu'=1,\cdots l_{j'}, \quad (1.4)$$

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[1] F. Seitz, Ann. Math. **37**, 17 (1936).

[2] J. S. Lomont, *Applications of Finite Groups* (Academic Press Inc., New York, 1959), Chap. 5. G. F. Koster, *Solid State Physics 5*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1957).

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

[4] E. Wigner, Nachr. Akad. Wiss. Göttingen, Math.-physik Kl. **2**, 133 (1930).

[5] A. Speiser, *Die Theorie der Gruppen* (Dover Publications, Inc., New York, 1945), p. 170.

generate the direct product representation $\Gamma^{(j)}\otimes\Gamma^{(j')}$, whose character system is given in (1.1). If $j'=j$, but the sets $\psi_\mu^{(j)}$ and $\psi'_{\mu'}{}^{(j)}$ are distinct, then (1.4) will in general generate the ordinary Kronecker square of $\Gamma^{(j)}$.

Now consider the $\frac{1}{2}l_j(l_j+1)$ functions

$$\varphi_{\mu\mu'}{}^{(j)}(r)=(\psi_\mu{}^{(j)}(r)\cdot\psi_{\mu'}{}^{(j)}(r)),\quad \mu\leqslant\mu'=1,\cdots l_j, \tag{1.5}$$

formed by taking all distinct pairs from the same set $\psi_\mu{}^{(j)}$. The basis (1.5) generates the symmetrized Kronecker square[6] representation of $\Gamma^{(j)}$, which is denoted $[\Gamma^{(j)}]_{(2)}$. The characters in this, generally reducible, representation can be obtained from

$$[\chi^{(j)}(R)]_{(2)}=\tfrac{1}{2}\{[\chi^{(j)}(R)]^2+\chi(R^2)\}. \tag{1.6}$$

The reduction of this representation can be carried out in analogy to (1.1)

$$[\chi^{(j)}(R)]_{(2)}=\textstyle\sum_{j'}([j]_{(2)}|j')\chi^{(j')}(R). \tag{1.7}$$

Finally, the $\frac{1}{6}l_j(l_j+1)(l_j+2)$ functions

$$\omega_{\mu\mu'\mu''}{}^{(j)}(r)=(\psi_\mu{}^{(j)}(r)\cdot\psi_{\mu'}{}^{(j)}(r)\cdot\psi_{\mu''}{}^{(j)}(r)),\quad \mu\leqslant\mu'\leqslant\mu''=1,\cdots l_j, \tag{1.8}$$

generate the symmetrized Kronecker cube of $\Gamma^{(j)}$ denoted $[\Gamma^{(j)}]_{(3)}$. The characters in this representation are obtained from

$$[\chi^{(j)}(R)]_{(3)}=\tfrac{1}{6}\{[\chi^{(j)}(R)]^3+3\chi^{(j)}(R)\chi^{(j)}(R^2)+2\chi^{(j)}(R^3)\}. \tag{1.9}$$

This can also be reduced in analogy to (1.1):

$$[\chi^{(j)}(R)]_{(3)}=\textstyle\sum_{j'}([j]_{(3)}|j')\chi^{(j')}(R). \tag{1.10}$$

This general theory can be applied to any finite group, and in particular to the space groups; for the determination of selection rules for physical processes.

Recently Elliott and Loudon,[7] and Lax and Hopfield[8] have obtained selection rules for special processes in crystals with the diamond structure. The former authors recognized that the "unallowed" irreducible representations of the factor group $\mathcal{G}(\mathbf{k})/\mathcal{T}(\mathbf{k})$ correspond to representations with wave vectors $2\mathbf{k}$, $3\mathbf{k}$, $\cdots$ and may be used to discuss processes involving transitions between these related families. They also utilized the irreducible representations of a new group which was the intersection of several subgroups of the full space group. By reducing the irreducible representation of the subgroups with respect to those of the intersection group, they were able to obtain selection rules for more general processes. The latter authors utilized a variant of the method of finding an intersection group, but no new group or group representations, appeared beyond what is in the literature. Both approaches utilize only part of the space group theory, or symmetry, which is available. Hence, they only obtain part of the selection rules governing processes in solids. Further, these methods do not seem applicable to the problem of constructing, and reducing symmetrized Kronecker powers of space group irreducible representations which are central to the discussion of lattice vibration (infrared and Raman) processes, and of configurational instability, in solids.

We therefore re-examined this problem, starting from first principles. Character tables for every space group element in each full space group irreducible representation can be obtained from the general theory.[1,2] For the representations in which we are generally interested, simplifications arise since these are homomorphic, not isomorphic to the space group. The most striking example is the representations with wave vector $\Gamma=(0,0,0)$. Using these character tables, we evaluate the character systems for the ordinary Kronecker product and for the symmetrized Kronecker power representations. These representations are reduced in two stages, as will be described below, to obtain the appropriate coupling coefficients. To our knowledge this is the first time the reduction of products of space group representations has been treated generally and completely. Thus the space groups can be put on an equal footing with the simpler point groups, or the more complicated rotation groups, from the point of view of obtaining selection rules.

Before proceeding with this program, we shall introduce some notations which we feel will be helpful. We shall then review the principles involved in constructing space group irreducible representations. The principles of the complete reduction of direct products will then be discussed. Finally specific selection rules for the diamond and zinc-blende space groups will be obtained using this general theory. In a later paper, the rules will be applied.

In this paper we consider only "single groups"; we neglect spin-orbit and time-reversal effects. Our methods can be applied to these cases, too.

2. NOTATION

$\mathcal{G}$, the space group, order $h\mathfrak{L}=g$;

$\mathcal{T}$, invariant subgroup of translations;

$\mathfrak{L}$, order of $\mathcal{T}$;

$\mathcal{G}/\mathcal{T}=\mathcal{P}$, factor group of the space group, order h;

$\mathcal{G}(\mathbf{k}_j)$, space group of $\mathbf{k}_j$, contains $\mathcal{T}$ and all rotational elements $\boldsymbol{\phi}$ such that $\boldsymbol{\phi}\cdot\mathbf{k}_j=\mathbf{k}_j+\mathbf{B}_h$, where $\mathbf{B}_h$ is a lattice vector in Fourier Space;

$\mathcal{T}(\mathbf{k}_j)$, translation group of $\mathbf{k}_j$, contains all translations $\mathbf{R}_L$, such that $\mathbf{k}_j\cdot\mathbf{R}_L=2\pi p$, where p is an integer;

$\mathbf{k}_j{}^{(m)}(\{\boldsymbol{\phi}|\boldsymbol{\tau}+\mathbf{R}_L\})$, character of the crystal symmetry operation $\{\boldsymbol{\phi}|\boldsymbol{\tau}+\mathbf{R}_L\}$ in the mth irreducible representation (dimension l_m) of $\mathcal{G}(\mathbf{k}_j)/\mathcal{T}(\mathbf{k}_j)$;

$\star\mathbf{k}_j=\{\mathbf{k}_j,\mathbf{k}_{j_2},\mathbf{k}_{j_3},\cdots\mathbf{k}_{j_s}\}$, star of $\mathbf{k}_j$, contains s distinct wave vectors;

[6] F. D. Murnaghan, *The Theory of Group Representations* (Johns Hopkins Press, Baltimore, 1938), p. 73 ff.; L. Tisza, Z. Physik **82**, 48 (1933).

[7] R. J. Elliott and R. Loudon, J. Phys. Chem. Solids **15**, 146 (1960).

[8] M. Lax and J. J. Hopfield, Phys. Rev. **124**, 115 (1961).

$^{\star}\mathbf{k}_j^{(m)}(\{\phi|\mathbf{R}_L+\boldsymbol{\tau}\})$, character of the operation $\{\phi|\mathbf{R}_L+\boldsymbol{\tau}\}$ in the full space group irreducible representation, based on the mth irreducible representation of each of the $\mathcal{G}(\mathbf{k}_j)/\mathcal{T}(\mathbf{k}_j)$, one for each $\mathbf{k}_j$ in $^{\star}\mathbf{k}_j$. This irreducible representation is of dimension $(s\cdot l_m)$;

$\mathcal{K}_j^{(m)}$, kernel of $^{\star}\mathbf{k}_j^{(m)}$: the collection of all elements in $\mathcal{T}$ such that each such element has a matrix in $^{\star}\mathbf{k}_j^{(m)}$ identical to that representing $\{\boldsymbol{\varepsilon}|0\}$;

$^{\star}\mathbf{k}_j^{(m)}/\mathcal{K}_j^{(m)}$, factor group of the matrix group $^{\star}\mathbf{k}_j^{(m)}$, with respect to $\mathcal{K}_j^{(m)}$;

$\mathcal{R}$, the reduction group, which is the largest of three factor groups;

$(\mathbf{k}_j\mathbf{k}_{j'}|\mathbf{k}_{j''})$, coupling coefficients for the reduction of the direct product of two stars: $^{\star}\mathbf{k}_j$ and $^{\star}\mathbf{k}_{j'}$;

$(\mathbf{k}_j^{(m)}\mathbf{k}_{j'}^{(m')}|\mathbf{k}_{j''}^{(m'')})$, coupling coefficients for the reduction of the direct product of two space group irreducible representations: $^{\star}\mathbf{k}_j^{(m)}$ and $^{\star}\mathbf{k}_{j'}^{(m')}$;

$[^{\star}\mathbf{k}_j^{(m)}]_{(2)}$, the symmetrized Kronecker square of the space group irreducible representation $^{\star}\mathbf{k}_j^{(m)}$;

$[^{\star}\mathbf{k}_j^{(m)}]_{(3)}$, the symmetrized Kronecker cube of $^{\star}\mathbf{k}_j^{(m)}$;

$([l_m\mathbf{k}_j]_{(2)}|\mathbf{k}_{j'})$, wave vector reduction coefficient for the reduction of $[^{\star}\mathbf{k}_j^{(m)}]_{(2)}$;

$([l_m\mathbf{k}_j]_{(3)}|\mathbf{k}_{j'})$, wave vector reduction coefficient for the reduction of $[^{\star}\mathbf{k}_j^{(m)}]_{(3)}$;

$([\mathbf{k}_j^{(m)}]_{(2)}|\mathbf{k}_{j'}^{(m')})$, complete reduction coefficient for $[^{\star}\mathbf{k}_j^{(m)}]_{(2)}$;

$([\mathbf{k}_j^{(m)}]_{(3)}|\mathbf{k}_{j'}^{(m')})$, complete reduction coefficient for $[^{\star}\mathbf{k}_j^{(m)}]_{(3)}$;

$\oplus$, direct sum of two representations;

$\otimes$, direct product of two representations;

$\times$, ordinary arithmetical product.

3. CHARACTERS OF SYMMETRY ELEMENTS

Our first task is to obtain the character of every element in the space group in a specified irreducible representation by applying the general theory.[1,2] We choose a wave vector $\mathbf{k}_j$, and find the space group $\mathcal{G}(\mathbf{k}_j)$; it is a subgroup of $\mathcal{G}$. The translational elements $\{\boldsymbol{\varepsilon}|\mathbf{R}_L\}$ which are in $\mathcal{T}(\mathbf{k}_j)$, are all represented by the same matrix as $\{\boldsymbol{\varepsilon}|0\}$, and form the kernel, or center of a representation of the group $\mathcal{G}(\mathbf{k}_j)$. The characters of the remaining elements in $\mathcal{G}(\mathbf{k}_j)$ can be found from the characters of the cosets in the irreducible representations of the factor group $\mathcal{G}(\mathbf{k}_j)/\mathcal{T}(\mathbf{k}_j)$, by selecting the allowable irreducible representations of this factor group, in a well-known manner. An allowable irreducible representation of $\mathcal{G}(\mathbf{k}_j)/\mathcal{T}(\mathbf{k}_j)$ will be called $\mathbf{k}_j^{(m)}$, and the character of $\{\phi_j|\boldsymbol{\tau}_j\}$ in such a representation is $\mathbf{k}_j^{(m)}(\{\phi_j|\boldsymbol{\tau}_j\})$.

Now consider an independent wave vector $\mathbf{k}_{j_2}$ in $^{\star}\mathbf{k}_j$, where

$$\mathbf{k}_{j_2}=\boldsymbol{\alpha}\cdot\mathbf{k}_j \tag{3.1}$$

and $\boldsymbol{\alpha}$ is the rotation which takes $\mathbf{k}_j$ into $\mathbf{k}_{j_2}$; $\{\boldsymbol{\alpha}|\boldsymbol{\tau}_\alpha\}$ is the corresponding space group element in $\mathcal{G}$. Now if $\{\phi_j|\boldsymbol{\tau}_j\}$ is an element in $\mathcal{G}(\mathbf{k}_j)$ so that

$$\phi_j\cdot\mathbf{k}_j=\mathbf{k}_j+\mathbf{B}_h, \tag{3.2}$$

then

$$\{\phi_{j_2}|\boldsymbol{\tau}_{j_2}\}\equiv\{\boldsymbol{\alpha}|\boldsymbol{\tau}_\alpha\}\{\phi_j|\boldsymbol{\tau}_j\}\{\boldsymbol{\alpha}|\boldsymbol{\tau}_\alpha\}^{-1} \tag{3.3}$$

is in $\mathcal{G}(\mathbf{k}_{j_2})$ and has the same character in $\mathcal{G}(\mathbf{k}_{j_2})$ as $\{\phi_j|\boldsymbol{\tau}_j\}$ in $\mathcal{G}(\mathbf{k}_j)$. Thus, each symmetry element in $\mathcal{G}(\mathbf{k}_{j_2})$ is conjugate to a symmetry element in $\mathcal{G}(\mathbf{k}_j)$ with respect to an element which takes $\mathbf{k}_j$ into $\mathbf{k}_{j_2}$. The subgroups $\mathcal{G}(\mathbf{k}_j)$ and $\mathcal{G}(\mathbf{k}_{j_2})$ of $\mathcal{G}$, are isomorphic and conjugate subgroups. Similarly, the factor groups $\mathcal{G}(\mathbf{k}_j)/\mathcal{T}(\mathbf{k}_j)$ and $\mathcal{G}(\mathbf{k}_{j_2})/\mathcal{T}(\mathbf{k}_{j_2})$ are isomorphic and their cosets conjugate. Continuing for the remaining space groups $\mathcal{G}(\mathbf{k}_{j_3})\cdots\mathcal{G}(\mathbf{k}_{j_s})$ for the other arms in $^{\star}\mathbf{k}_j$ we find these also are conjugate as are the factor groups $\mathcal{G}(\mathbf{k}_{j_3})/\mathcal{T}(\mathbf{k}_{j_3})\cdots\mathcal{G}(\mathbf{k}_{j_s})/\mathcal{T}(\mathbf{k}_{j_s})$. The matrices for conjugate cosets from these factor groups, in the corresponding irreducible representations $\mathbf{k}_j^{(m)}$, $\mathbf{k}_{j_2}^{(m)}$, $\cdots\mathbf{k}_{j_s}^{(m)}$, are identical.

A space group irreducible representation of $\mathcal{G}$ is obtained by combining corresponding allowable irreducible representations of the factor groups. The space group irreducible representation so formed is said to be induced[2] by the allowable irreducible representation $\mathbf{k}_j^{(m)}$ of $\mathcal{G}(\mathbf{k}_j)/\mathcal{T}(\mathbf{k}_j)$. We call this space group irreducible representation $^{\star}\mathbf{k}_j^{(m)}$ and the character of $\{\phi|\boldsymbol{\tau}\}$ in this representation is $^{\star}\mathbf{k}_j^{(m)}(\{\phi|\boldsymbol{\tau}\})$. If l_m is the dimension of the irreducible representation $\mathbf{k}_j^{(m)}$, and s the number of arms in $^{\star}\mathbf{k}_j$, then $(s\times l_m)$ is the dimension of $^{\star}\mathbf{k}_j^{(m)}$.

The character of $\{\phi|\boldsymbol{\tau}\}$ in the direct product of two space group irreducible representations is the ordinary product of the characters

$$^{\star}\mathbf{k}_j^{(m)}\otimes{}^{\star}\mathbf{k}_{j'}^{(m')}(\{\phi|\boldsymbol{\tau}\})={}^{\star}\mathbf{k}_j^{(m)}(\{\phi|\boldsymbol{\tau}\})\times{}^{\star}\mathbf{k}_{j'}^{(m')}(\{\phi|\boldsymbol{\tau}\}). \tag{3.4}$$

The problem of reducing the direct product representation (3.4) into a direct sum of irreducible space group representations,

$$^{\star}\mathbf{k}_j^{(m)}\otimes{}^{\star}\mathbf{k}_{j'}^{(m')}=\sum_{j''}\sum_{m''}(\mathbf{k}_j^{(m)}\mathbf{k}_{j'}^{(m')}|\mathbf{k}_{j''}^{(m'')})\times{}^{\star}\mathbf{k}_{j''}^{(m'')}, \tag{3.5}$$

is then one of determining the coefficients

$$(\mathbf{k}_j^{(m)}\mathbf{k}_{j'}^{(m')}|\mathbf{k}_{j''}^{(m'')}). \tag{3.6}$$

In (3.5) the sum on j'' is a sum on stars which may arise, that on m'' is a sum on allowable irreducible representations. The direct product representation (3.4) is of dimension $(ss')(l_m\cdot l_{m'})$.

The symmetrized Kronecker square of $^{\star}\mathbf{k}_j^{(m)}$ is of dimension $\frac{1}{2}(s\times l_m)(s\times l_m+1)$. The characters of space group elements in this representation can be found from (1.6) by using the multiplication law for space group elements[1]:

$$\{\phi|\mathbf{t}\}^2=\{\phi\cdot\phi|\phi\cdot\mathbf{t}+\mathbf{t}\}. \tag{3.7}$$

In analogy to (3.5) we have in this case

$$[^{\star}\mathbf{k}_j^{(m)}]_{(2)}=\sum_{j'}\sum_{m'}([\mathbf{k}_j^{(m)}]_{(2)}|\mathbf{k}_{j'}^{(m')})\,{}^{\star}\mathbf{k}_{j'}^{(m')}, \tag{3.8}$$

which also defines the reduction coefficients.

The symmetrized Kronecker cube of ${}^\star\mathbf{k}_j{}^{(m)}$ is of dimension $\frac{1}{6}(s\times l_m)(s\times l_m+1)(s\times l_m+2)$. Characters in this representation can be found from the space group multiplication law, (3.7) and (1.9). For this case we have

$$[{}^\star\mathbf{k}_j{}^{(m)}]_{(3)}=\sum_{j'}\sum_{m'}([\mathbf{k}_j{}^{(m)}]_{(3)}|\mathbf{k}_{j'}{}^{(m')})\,{}^\star\mathbf{k}_{j'}{}^{(m')}. \quad (3.9)$$

The determination of the reduction coefficients (3.6), (3.8), and (3.9) is carried out in two stages. In each case complete wave vector selection rules are obtained when the ordinary direct product of two stars, or symmetrized power of a star, is reduced into a direct sum of stars. This provides a necessary limitation on the work required to complete the reduction.

4. DIRECT PRODUCT OF TWO STARS

In a space group irreducible representation ${}^\star\mathbf{k}_j{}^{(m)}$ each translation, e.g., $\{\varepsilon|\mathbf{R}_L\}$ is represented by a diagonal matrix, with diagonal elements $\exp(i\mathbf{k}_j\cdot\mathbf{R}_L)$, $\exp(i\mathbf{k}_{j_2}\cdot\mathbf{R}_L)$, $\cdots$ $\exp(i\mathbf{k}_{j_s}\cdot\mathbf{R}_L)$. In general, the matrix is $(s\times l_m)$ dimensional, with each element repeated l_m times. In the direct product (3.5) each translation is represented by a diagonal $(s\cdot s')(l_m\cdot l_{m'})$ matrix, whose elements are of the form

$$\exp[i(\mathbf{k}_j+\mathbf{k}_{j'})\cdot\mathbf{R}_L];\quad \exp[i(\mathbf{k}_j+\mathbf{k}_{j'_2})\cdot\mathbf{R}_L];\quad\cdots;\quad \exp[i(\mathbf{k}_j+\mathbf{k}_{j'_{s'}})\cdot\mathbf{R}_L];\quad\cdots;\quad \exp[i(\mathbf{k}_{j_s}+\mathbf{k}_{j'_{s'}})\cdot\mathbf{R}_L], \quad (4.1)$$

with each element repeated $l_ml_{m'}$ times.

The first step in reducing (3.5) is to reduce these diagonal matrices. Consider the case where $l_m=l_{m'}=1$. The $s\cdot s'$ wave vectors in (4.1) are obtained by forming all pairs of wave vectors with one wave vector chosen from ${}^\star\mathbf{k}_j$, and the other from ${}^\star\mathbf{k}_{j'}$. In fully reduced form, this diagonal matrix will be a direct sum of diagonal matrices (which it is already) with each matrix bloc containing all the wave vectors in one star. Our task is then one of recognizing, and rearranging, the elements (4.1) into groups, each group containing all arms in one star.

We use the notation

$${}^\star\mathbf{k}_j\otimes{}^\star\mathbf{k}_{j'}=\sum_{j''}(\mathbf{k}_j\mathbf{k}_{j'}|\mathbf{k}_{j''})\,{}^\star\mathbf{k}_{j''}. \quad (4.2)$$

The coefficients $(\mathbf{k}_j\mathbf{k}_{j'}|\mathbf{k}_{j''})$ are integers since only complete stars arise on the right-hand side of (4.2). We also have

$$s\cdot s'=\sum_{\mathbf{k}_{j''}}(\mathbf{k}_j\mathbf{k}_{j'}|\mathbf{k}_{j''})s''. \quad (4.3)$$

Now

$${}^\star\mathbf{k}_{j'}\otimes{}^\star\mathbf{k}_j\equiv{}^\star\mathbf{k}_j\otimes{}^\star\mathbf{k}_{j'}, \quad (4.4)$$

so that

$$(\mathbf{k}_j\mathbf{k}_{j'}|\mathbf{k}_{j''})\equiv(\mathbf{k}_{j'}\mathbf{k}_j|\mathbf{k}_{j''}). \quad (4.5)$$

In other words, the coefficients $(\mathbf{k}_j\mathbf{k}_{j'}|\mathbf{k}_{j''})$ tell us the total dimensionality of all irreducible representations of the space group based on ${}^\star\mathbf{k}_{j''}$ which arise in the reduction of the direct product of irreducible representations ${}^\star\mathbf{k}_j{}^{(m)}$ and ${}^\star\mathbf{k}_{j'}{}^{(m')}$ if $l_m=l_{m'}=1$. In addition, these coefficients give us the complete wave vector selection rules for processes involving transitions between eigenstates of the crystal.

As a systematic procedure for determining the ${}^\star\mathbf{k}_{j''}$ and hence the $(\mathbf{k}_j\mathbf{k}_{j'}|\mathbf{k}_{j''})$, we construct a table with s rows and s' columns. We label the s rows with the arms of ${}^\star\mathbf{k}_j$

$$\mathbf{k}_j,\ \mathbf{k}_{j_2}=\boldsymbol{\alpha}_2\cdot\mathbf{k}_j,\ \cdots,\ \mathbf{k}_{j_s}=\boldsymbol{\alpha}_s\cdot\mathbf{k}_j, \quad (4.6)$$

and the s' columns with the arms of ${}^\star\mathbf{k}_{j'}$

$$\mathbf{k}_{j'},\ \mathbf{k}_{j_2'}=\boldsymbol{\beta}_2\cdot\mathbf{k}_j,\ \cdots,\ \mathbf{k}_{j_{s'}'}=\boldsymbol{\beta}_s\cdot\mathbf{k}_{j'}. \quad (4.7)$$

Now as the pqth element in the table (intersection of the pth row and qth column) we take

$$\boldsymbol{\alpha}_p\cdot(\mathbf{k}_j+\boldsymbol{\beta}_q\cdot\mathbf{k}_{j'})=\boldsymbol{\alpha}_p\cdot\mathbf{k}_j+\alpha_p\cdot\beta_q\cdot\mathbf{k}_{j'}, \quad (4.8)$$

which is a vector in ${}^\star(\mathbf{k}_j+\beta_q\mathbf{k}_{j'})$. Note that in a given row one of the terms is constant $\alpha_p\cdot\mathbf{k}_j$, but this is not so of the columns. However, every column in this table then contains only wave vectors in the star of the wave vector in the first row of the column, e.g., for the qth column in ${}^\star(\mathbf{k}_j+\beta_q\cdot\mathbf{k}_{j'})$. For particular pairs of wave vectors ${}^\star\mathbf{k}_j$ and ${}^\star\mathbf{k}_{j'}$ the star of their sum contains more than s arms. In this case we need to take together two or more entire columns to obtain all arms in the star. Conversely, it may be that the star of their sum consists of fewer than s arms, and in this case $(\mathbf{k}_j\mathbf{k}_{j'}|\mathbf{k}_j+\boldsymbol{\beta}_q\cdot\mathbf{k}_{j'})>1$. With a little practice one easily recognizes all such cases in any particular space group. Because of (4.5) we may equally work with a transposed array, with the s' arms of $\mathbf{k}_{j'}$ as row lables and the s arms of $\mathbf{k}_j$ as column heads. If l_m or $l_{m'}>1$, (4.2) will become

$$l_m\,{}^\star\mathbf{k}_j\otimes l_{m'}\,{}^\star\mathbf{k}_{j'}=\sum_{j''}(\mathbf{k}_j\mathbf{k}_{j'}|\mathbf{k}_{j''})^{(m,m')}\,{}^\star\mathbf{k}_{j''}, \quad (4.9)$$

where

$$(\mathbf{k}_j\mathbf{k}_{j'}|\mathbf{k}_{j''})^{(m,m')}=l_ml_{m'}(\mathbf{k}_j\mathbf{k}_{j'}|\mathbf{k}_{j''}), \quad (4.10)$$

and then

$$(s\cdot s')(l_m\cdot l_{m'})=\sum_{\mathbf{k}_{j''}}(\mathbf{k}_j\mathbf{k}_{j'}|\mathbf{k}_{j''})^{(m,m')}s''. \quad (4.11)$$

The $(\mathbf{k}_j\mathbf{k}_{j'}|\mathbf{k}_{j''})^{(m,m')}$ now give us dimensionality and wave vector selection rules for the ordinary Kronecker products but include multiplicity.

To obtain wave vector selection rules for the symmetrized Kronecker power representations we can use the results (4.2), but multiplicity must be included *ab initio*. By an application of (1.6) to this problem we find, for $l_m=1$, for the symmetrized square of a star,

$$\begin{aligned}[{}^\star\mathbf{k}_j]_{(2)}&=\tfrac{1}{2}\{{}^\star\mathbf{k}_j\otimes{}^\star\mathbf{k}_j\oplus{}^\star(2\mathbf{k}_j)\}\\&=\sum_{j'}([\mathbf{k}_j]_{(2)}|\mathbf{k}_{j'})\,{}^\star\mathbf{k}_{j'}.\end{aligned} \quad (4.12)$$

For $l_m>1$,

$$\begin{aligned}[l_m\,{}^\star\mathbf{k}_j]_{(2)}&=\tfrac{1}{2}\{l_m{}^2\,{}^\star\mathbf{k}_j\otimes{}^\star\mathbf{k}_j\oplus l_m\,{}^\star(2\mathbf{k}_j)\}\\&=\sum_{j'}([l_m\mathbf{k}_j]_{(2)}|\mathbf{k}_{j'})\,{}^\star\mathbf{k}_{j'}.\end{aligned} \quad (4.13)$$

For the symmetrized cube, in general,

$$\begin{aligned}[l_m\,{}^\star\mathbf{k}_j]_{(3)}&=\tfrac{1}{6}\{l_m{}^3\,{}^\star\mathbf{k}_j\otimes{}^\star\mathbf{k}_j\otimes{}^\star\mathbf{k}_j\\&\quad\oplus 3l_m{}^2\,{}^\star\mathbf{k}_j\otimes{}^\star(2\mathbf{k}_j)\oplus 2l_m\,{}^\star(3\mathbf{k}_j)\}\\&=\sum_{j'}([l_m\mathbf{k}_j]_{(3)}|\mathbf{k}_{j'})\,{}^\star\mathbf{k}_{j'}.\end{aligned} \quad (4.14)$$

Equations (4.10), (4.13), and (4.14) define the wave vector reduction coefficients, and hence the total dimensionality of representations based on a particular star which arise. In a case where $l_{m''}>1$, such as for representations $^{\star}X^{(m)}$ in diamond, a given representation in the reduction may "use up" several stars. As with (4.3) and (4.11), the total number of wave vectors which arise in taking a symmetrized product of stars must obey a conservation condition. In each case this is an obvious and useful check on the reductions.

5. COMPLETION OF THE REDUCTION

With the determination of coefficients (4.10), (4.13), and (4.14), a partial reduction of the Kronecker product (3.4), and the Kronecker powers (3.8) and (3.9), respectively, has been achieved. We now know which stars appear in the reduction, and we need to find the m'' which arise in $\mathbf{k}_{j''}^{(m'')}$. We base our final reduction of the Kronecker product on the use of Eqs. (1.1) and (1.2). Transcribing these equations into our space group notation

$$^{\star}\mathbf{k}_j^{(m)}(R)\cdot{}^{\star}\mathbf{k}_{j'}^{(m')}(R) = \sum_{j''}\sum_{m''}(\mathbf{k}_j^{(m)}\mathbf{k}_{j'}^{(m')}|\mathbf{k}_{j''}^{(m'')})\,^{\star}\mathbf{k}_{j''}^{(m'')}(R), \quad R=1,\cdots h\mathfrak{L}, \tag{5.1}$$

and

$$(\mathbf{k}_j^{(m)}\mathbf{k}_{j'}^{(m')}|\mathbf{k}_{j''}^{(m'')}) = (1/h\mathfrak{L})\sum_R {}^{\star}\mathbf{k}_j^{(m)}(R)\,^{\star}\mathbf{k}_{j'}^{(m')}(R) \times{}^{\star}\mathbf{k}_{j''}^{(m'')}(R)^*, \tag{5.2}$$

where R is a space-group element. In (5.1) the summations are over all stars and all allowable irreducible representations. In (5.2) the summation is over all space group elements. When we use (5.2) to determine coefficients, we call this the reduction group method. When we use (5.1), we call this the direct inspection method. Both methods will yield all coefficients without ambiguity. A third method, useful in special cases, is based on the construction of a basis which spans one star of those which arise in (4.10), (4.13), and (4.14). This basis will be a subset of the complete sets (1.4), (1.5), or (1.8); using it we can generate the required reducible character system which can then be reduced using the character tables of the appropriate space group irreducible representations having that star. For the symmetrized Kronecker square, Eqs. (5.1) and (5.2) will become

$$[^{\star}\mathbf{k}_j^{(m)}(R)]_{(2)} = \sum_{j'}\sum_{m'}([\mathbf{k}_j^{(m)}]_{(2)}|\mathbf{k}_{j'}^{(m')})\,^{\star}\mathbf{k}_{j'}^{(m')}(R)$$

and

$$([\mathbf{k}_j^{(m)}]_{(2)}|\mathbf{k}_{j'}^{(m')}) = (1/h\mathfrak{L})\sum_R [^{\star}\mathbf{k}_j^{(m)}(R)]_{(2)}\,^{\star}\mathbf{k}_{j'}^{(m')}(R)^*,$$

respectively. The equations for the cube are analogous. Reduction of the square and cube can also be completed using the three methods mentioned. We shall discuss the two general methods which we use, in terms of the ordinary products; application to the symmetrized powers follows *mutatis mutandis.*

We now describe the reduction group method of carrying out the evaluation (5.2). Consider the three matrix groups $^{\star}\mathbf{k}_j^{(m)}$, $^{\star}\mathbf{k}_{j'}^{(m')}$, $^{\star}\mathbf{k}_{j''}^{(m'')}$ involved in (5.2). For any star with $s<h$ these groups are homomorphic to the underlying space group $\mathcal{G}$. By construction, each of these is an irreducible representation of $\mathcal{G}$. Now collect together all the elements of $\mathcal{G}$ (actually of $\mathcal{T}$) which are represented in $^{\star}\mathbf{k}_j^{(m)}$ by the same matrix as $\{\boldsymbol{\varepsilon}|0\}$. These form the center of $^{\star}\mathbf{k}_j^{(m)}$ and we call this invariant matrix subgroup $\mathcal{K}_j^{(m)}$. We form the matrix factor group $^{\star}\mathbf{k}_j^{(m)}/\mathcal{K}_j^{(m)}$, which consists of a number of cosets and will have order (n_jh), where n_j is a small integer and h the order of $\mathcal{P}$. In a similar fashion we form the matrix factor groups for the other factors in the direct product to be reduced; these are $^{\star}\mathbf{k}_{j'}^{(m')}/\mathcal{K}_{j'}^{(m')}$, $^{\star}\mathbf{k}_{j''}^{(m'')}/\mathcal{K}_{j''}^{(m'')}$, of order $(n_{j'}h)$ and $(n_{j''}h)$, respectively. Call the largest of these three factor groups the matrix reduction group $\mathcal{R}$ whose order is, say, $(n_{j''}h)$ so $n_{j''}>n_{j'}$ or n_j. We next augment the matrix group $^{\star}\mathbf{k}_j^{(m)}/\mathcal{K}_j^{(m)}$ by including elements from the center $\mathcal{K}_j^{(m)}$ so as to construct a matrix group

$$^{\star}\mathbf{k}_j^{(m)}/\mathcal{K}_{j''}^{(m'')} = (^{\star}\mathbf{k}_j^{(m)}/\mathcal{K}_j^{(m)})\cdot(\mathcal{K}_j^{(m)}/\mathcal{K}_{j''}^{(m'')}). \tag{5.3}$$

This matrix group has $(n_{j''}h)$ elements and is isomorphic to $\mathcal{R}$. Likewise, we form

$$^{\star}\mathbf{k}_{j'}^{(m')}/\mathcal{K}_{j''}^{(m'')} = (^{\star}\mathbf{k}_{j'}^{(m')}/\mathcal{K}_{j'}^{(m')}) \times(\mathcal{K}_{j'}^{(m')}/\mathcal{K}_{j''}^{(m'')}), \tag{5.4}$$

also isomorphic to $\mathcal{R}$. Now the three matrix groups

$$^{\star}\mathbf{k}_{j''}^{(m'')}/\mathcal{K}_{j''}^{(m'')};\quad {}^{\star}\mathbf{k}_{j'}^{(m')}/\mathcal{K}_{j''}^{(m'')};\quad {}^{\star}\mathbf{k}_j^{(m)}/\mathcal{K}_{j''}^{(m'')}$$

are of equal order, and if R is a coset in $\mathcal{R}$, there is some matrix representing R in each group. This procedure defines the cosets R in the reduction group $\mathcal{R}$, and their characters in each of the space group irreducible representations under consideration.[9] The characters of these cosets, in the irreducible representations $^{\star}\mathbf{k}_j^{(m)}$, $^{\star}\mathbf{k}_{j'}^{(m')}$, $^{\star}\mathbf{k}_{j''}^{(m'')}$ satisfy the completeness relation

$$\sum_R|^{\star}\mathbf{k}_j^{(m)}(R)|^2=(n_{j''}h), \tag{5.5}$$

where the sum is over all R in $\mathcal{R}$. In (5.5) we can substitute $j\to j'$ and $m\to m'$; or $j\to j''$ and $m\to m''$ on the left side and the same constant occurs on the right. Also these characters satisfy orthogonality relations

$$\sum_R {}^{\star}\mathbf{k}_{j'}^{(m')}(R)\,^{\star}\mathbf{k}_j^{(m)}(R)^*=0, \quad j\neq j',\ m\neq m'', \tag{5.6}$$

where the sum is over all R in $\mathcal{R}$. We note that the reduction group $\mathcal{R}$ is defined for a particular combination of stars, and applies as well to any m, m', m'' which may appear in the direct products to be reduced. It must be clearly understood that (5.5) and (5.6) follow because the matrix groups $^{\star}\mathbf{k}_j^{(m)}$, $^{\star}\mathbf{k}_{j'}^{(m')}$, and

[9] If $n_{j'}$, $n_{j''}$ are not common multiples of n_j, this procedure can be easily generalized.

TABLE I. Geometry of the diamond structure.

Translational symmetry	
Cubic vector set	$\mathbf{a}_1=(1,0,0)a$
	$\mathbf{a}_2=(0,1,0)a$
	$\mathbf{a}_3=(0,0,1)a$
Primitive vector set	$\mathbf{t}_{xy}=(\frac{1}{2},\frac{1}{2},0)a=\mathbf{t}_1$
	$\mathbf{t}_{xz}=(\frac{1}{2},0,\frac{1}{2})a=\mathbf{t}_2$
	$\mathbf{t}_{yz}=(0,\frac{1}{2},\frac{1}{2})a=\mathbf{t}_3$
Basic vectors	$\boldsymbol{\tau}_1=(\frac{1}{4},\frac{1}{4},\frac{1}{4})a$
	$\boldsymbol{\tau}_2=(\frac{1}{4},-\frac{1}{4},-\frac{1}{4})a$
	$\boldsymbol{\tau}_3=(-\frac{1}{4},\frac{1}{4},-\frac{1}{4})a$
	$\boldsymbol{\tau}_4=(-\frac{1}{4},-\frac{1}{4},\frac{1}{4})a$
Fourier vector set	$\mathbf{B}_1=(2\pi,2\pi,-2\pi)(1/a)$
	$\mathbf{B}_2=(2\pi,-2\pi,2\pi)(1/a)$
	$\mathbf{B}_3=(-2\pi,2\pi,2\pi)(1/a)$
	$\mathbf{B}_j\cdot\mathbf{t}_i=2\pi\delta_{ij}$

Rotational Symmetry Operations

Type $\{\boldsymbol{\phi}\|0\}$		Type $\{\boldsymbol{\phi}\|\boldsymbol{\tau}_1\}$	
$\boldsymbol{\varepsilon}$	xyz	$\mathbf{i}$	$\bar{x}\bar{y}\bar{z}$
$\boldsymbol{\delta}_{2x}$	$x\bar{y}\bar{z}$	$\boldsymbol{\varrho}_x$	$\bar{x}yz$
$\boldsymbol{\delta}_{2y}$	$\bar{x}y\bar{z}$	$\boldsymbol{\varrho}_y$	$x\bar{y}z$
$\boldsymbol{\delta}_{2z}$	$\bar{x}\bar{y}z$	$\boldsymbol{\varrho}_z$	$xy\bar{z}$
$\boldsymbol{\sigma}_{4x}$	$\bar{x}z\bar{y}$	$\boldsymbol{\delta}_{4x}$	$x\bar{z}y$
$(\boldsymbol{\sigma}_{4x})^{-1}$	$\bar{x}\bar{z}y$	$(\boldsymbol{\delta}_{4x})^{-1}$	$xz\bar{y}$
$\boldsymbol{\sigma}_{4y}$	$\bar{z}\bar{y}x$	$\boldsymbol{\delta}_{4y}$	$zy\bar{x}$
$(\boldsymbol{\sigma}_{4y})^{-1}$	$z\bar{y}\bar{x}$	$(\boldsymbol{\delta}_{4y})^{-1}$	$\bar{z}yx$
$\boldsymbol{\sigma}_{4z}$	$y\bar{x}\bar{z}$	$\boldsymbol{\delta}_{4z}$	$\bar{y}xz$
$(\boldsymbol{\sigma}_{4z})^{-1}$	$\bar{y}x\bar{z}$	$(\boldsymbol{\delta}_{4z})^{-1}$	$y\bar{x}z$
$\boldsymbol{\varrho}_{xy}$	$\bar{y}\bar{x}z$	$\boldsymbol{\delta}_{2xy}$	$yx\bar{z}$
$\boldsymbol{\varrho}_{x\bar{y}}$	yxz	$\boldsymbol{\delta}_{2x\bar{y}}$	$\bar{y}\bar{x}\bar{z}$
$\boldsymbol{\varrho}_{xz}$	$\bar{z}y\bar{x}$	$\boldsymbol{\delta}_{2xz}$	$z\bar{y}x$
$\boldsymbol{\varrho}_{x\bar{z}}$	zyx	$\boldsymbol{\delta}_{2x\bar{z}}$	$\bar{z}\bar{y}\bar{x}$
$\boldsymbol{\varrho}_{yz}$	$x\bar{z}\bar{y}$	$\boldsymbol{\delta}_{2yz}$	$\bar{x}zy$
$\boldsymbol{\varrho}_{y\bar{z}}$	xzy	$\boldsymbol{\delta}_{2y\bar{z}}$	$\bar{x}\bar{z}\bar{y}$
$\boldsymbol{\delta}_{3xyz}$	zxy	$\boldsymbol{\sigma}_{6xyz}$	$\bar{z}\bar{x}\bar{y}$
$(\boldsymbol{\delta}_{3xyz})^{-1}$	yzx	$(\boldsymbol{\sigma}_{6xyz})^{-1}$	$\bar{y}\bar{z}\bar{x}$
$\boldsymbol{\delta}_{3\bar{x}\bar{y}z}$	$\bar{z}x\bar{y}$	$\boldsymbol{\sigma}_{6\bar{x}\bar{y}z}$	$z\bar{x}y$
$(\boldsymbol{\delta}_{3\bar{x}\bar{y}z})^{-1}$	$y\bar{z}\bar{x}$	$(\boldsymbol{\sigma}_{6\bar{x}\bar{y}z})^{-1}$	$\bar{y}zx$
$\boldsymbol{\delta}_{3\bar{x}y\bar{z}}$	$z\bar{x}\bar{y}$	$\boldsymbol{\sigma}_{6\bar{x}y\bar{z}}$	$\bar{z}xy$
$(\boldsymbol{\delta}_{3\bar{x}y\bar{z}})^{-1}$	$\bar{y}\bar{z}x$	$(\boldsymbol{\sigma}_{6\bar{x}y\bar{z}})^{-1}$	$yz\bar{x}$
$\boldsymbol{\delta}_{3x\bar{y}\bar{z}}$	$\bar{z}\bar{x}y$	$\boldsymbol{\sigma}_{6x\bar{y}\bar{z}}$	$zx\bar{y}$
$(\boldsymbol{\delta}_{3x\bar{y}\bar{z}})^{-1}$	$\bar{y}z\bar{x}$	$(\boldsymbol{\sigma}_{6x\bar{y}\bar{z}})^{-1}$	$y\bar{z}x$

${}^\star\mathbf{k}_{j''}{}^{(m'')}$ are irreducible representations of the full space group $\mathcal{G}$; they are representations, but not irreducible, of $\mathcal{R}$. Using the character tables for each element or coset R in the reduction group $\mathcal{R}$, in each of the irreducible representations we can complete the reduction of the direct product by determining the coefficients from

$$(\mathbf{k}_j{}^{(m)}\mathbf{k}_{j'}{}^{(m')}|\mathbf{k}_{j''}{}^{(m'')})=(1/n_{j''}h)\textstyle\sum_R {}^\star\mathbf{k}_j{}^{(m)}(R)\times{}^\star\mathbf{k}_{j'}{}^{(m')}(R)\,{}^\star\mathbf{k}_{j''}{}^{(m'')}(R)^*. \quad (5.7)$$

In (5.7) the summation is over the $(n_{j''}h)$ elements in $\mathcal{R}$, rather than over every element in the entire space group. Since the $n_{j''}$ are usually small integers, and many of the characters vanish, the sum (5.7) is not difficult to evaluate. In all cases where we can construct a reduction group ($n_{j''}<\mathcal{L}$), (5.7) is actually equivalent to carrying out the summation over all space group elements. Clearly, if the summation is taken over all elements R in $\mathcal{G}$, the value of the sum in (5.7) will be obtained $(\mathcal{L}/n_{j''})$ times, but the denominator should be [see (5.2)] $h\mathcal{L}=(n_{j''}h)(\mathcal{L}/n_{j''})$. Thus, the reduction group method is a rigorous device by which the sum (5.2) is made tractable.

In the direct inspection, or trial and error method, we use (5.1) to determine reduction coefficients. We have found this method most helpful in cases where one or more of the wave vectors in (5.1) depend on a parameter, i.e., is on a line or plane of symmetry. We use (5.1) as a set of linear inhomogeneous algebraic equations for the reduction coefficients. This procedure is slightly more difficult than the reduction group method since we must determine all coefficients essentially simultaneously. The number of such coefficients which must be considered, and hence the number of simultaneous equations to be solved, is fully determined by the wave vector selection rules. If ξ is the number of distinct stars which occur in the reduction (4.2) and r_ξ the total number of different species of irreducible representations at each star, then we need ξr_ξ linearly independent simultaneous equations (5.1) to find these coefficients. Some of these equations will express wave vector selection rules (4.2) or (4.6). The remaining equations are chosen for convenience. These equations can be solved by direct inspection since we know: (a) all reduction coefficients (5.1) are positive integers; (b) there is one and only one unique method of completely reducing a representation into irreducible components. One quickly finds that the wrong trial solution for a subset of the coefficients produces inconsistencies in the remainder.

TABLE II. Coordinates of zone points for diamond and zinc blende.[a]

Points	Coordinates	$s=$ multiplicity
Γ	$(0,0,0)(1/a)$	1
X	$(2\pi,0,0)(1/a)$	3
L	$(\pi,\pi,\pi)(1/a)$	4
W	$(2\pi,0,\pi)(1/a)$	6
Δ	$(\kappa,0,0)(1/a)$	6
Λ	$(\kappa,\kappa,\kappa)(1/a)$	8 (4)
Z	$(2\pi,0,\kappa)(1/a)$	12
Σ	$(\kappa,\kappa,0)(1/a)$	12
G	$(2\pi,\kappa,\kappa)(1/a)$	12
M	$(\kappa_1,\kappa_1,\kappa_2)(1/a)$	24 (12)
H	$(\kappa,\pi,2\pi-\kappa)(1/a)$	24
N	$(\kappa_1,\kappa_2,0)(1/a)$	24
P	$(\kappa_1,\kappa_2,2\pi)(1/a)$	24
k	$(\kappa_1,\kappa_2,\kappa_3)(1/a)$	48 (24)

[a] Multiplicity in zinc blende is given in parentheses.

TABLE III. Wave vector selection rules in diamond: coefficients $(\mathbf{k}_j\mathbf{k}_{j'}|\mathbf{k}_{j''})$.

$(\Gamma k_{j'}\|k_{j'})=1$	for all $k_{j'}$
$(XX\|\Gamma)=3$	
$(XX\|X)=2$	
$(XL\|L)=3$	
$(XW\|\Delta)=2;$	$\Delta_1=(\pi,0,0)(1/a)$
$(XW\|W)=1$	
$(XZ\|\Delta)=2;$	$\Delta_1=(\kappa,0,0)(1/a)$
$(XZ\|\Delta')=2;$	$\Delta_1'=(2\pi-\kappa,0,0)(1/a)$
$(XZ\|Z)=2;$	$Z_1=(2\pi,0,\kappa)(1/a)$
$(X\Sigma\|\Sigma')=1;$	$\Sigma_1'=(\kappa-2\pi,\kappa-2\pi,0)(1/a)$
$(X\Sigma\|N)=1;$	$N_1=(\kappa-2\pi,\kappa,0)(1/a)$
$(X\Delta\|\Delta')=1;$	$\Delta_1'=(\kappa-2\pi,0,0)(1/a)$
$(X\Delta\|Z)=1;$	$Z_1=(2\pi,0,\kappa)(1/a)$
$(X\Lambda\|M)=1;$	$M_1=(\kappa,\kappa,\kappa-2\pi)(1/a)$
$(LL\|\Gamma)=4$	
$(LL\|X)=4$	
$(LW\|\Sigma)=2;$	$\Sigma_1=(\pi,\pi,0)(1/a)$
$(LZ\|M)=2;$	$M_1=(\pi,\pi,\pi+\kappa)(1/a)$
$(L\Sigma\|M)=2;$	$M_1=(\kappa-\pi,\kappa-\pi,\pi)(1/a)$
$(L\Delta\|M)=1;$	$M_1=(\pi,\pi,\pi+\kappa)(1/a)$
$(L\Lambda\|\Lambda')=1;$	$\Lambda_1'=(\pi+\kappa,\pi+\kappa,\pi+\kappa)(1/a)$
$(L\Lambda\|M)=1;$	$M_1=(\pi+\kappa,\pi+\kappa,\kappa-\pi)(1/a)$
$(WW\|\Gamma)=6$	
$(WW\|X)=2$	
$(WW\|\Sigma)=2;$	$\Sigma_1=(\pi,\pi,0)(1/a)$
$(WZ\|\Delta)=4;$	$\Delta_1=(\pi+\kappa,0,0)(1/a)$
$(WZ\|N)=1;$	$N_1=(\pi,2\pi-\kappa,0)(1/a)$
$(WZ\|N')=1;$	$N_1'=(\pi,\kappa,0)(1/a)$
$(W\Sigma\|N)=1;$	$N_1=(2\pi+\kappa,\kappa-\pi,0)(1/a)$
$(W\Sigma\|P)=1;$	$P_1=(\kappa,\kappa+\pi,2\pi)(1/a)$
$(W\Sigma\|H)=1;$	$H_1=(\kappa,\pi,2\pi+\kappa)(1/a)$
$(W\Delta/Z)=1;$	$Z_1=(2\pi,0,\pi+\kappa)(1/a)$
$(W\Delta\|N)=1;$	$N_1=(2\pi+\kappa,\pi,0)(1/a)$
$(W\Lambda\|k)=1;$	$k_1=(2\pi+\kappa,\pi+\kappa,\kappa)(1/a)$
$(ZZ'\|\Delta)=2;$	$\Delta_1=(\kappa+\kappa',0,0)(1/a)$
$(ZZ'\|\Delta')=2;$	$\Delta_1'=(\kappa-\kappa',0,0)(1/a)$
$(ZZ'\|\Delta'')=2;$	$\Delta_1''=(\kappa+\kappa'-2\pi,0,0)(1/a)$
$(ZZ'\|\Delta''')=2;$	$\Delta_1'''=(\kappa-\kappa'-2\pi,0,0)(1/a)$
$(ZZ'\|N)=3;$	$N_1=(\kappa,\kappa',0)(1/a)$
$(ZZ'\|N')=1;$	$N_1'=(2\pi-\kappa,\kappa',0)(1/a)$
$(Z\Sigma/N)=1;$	$N_1=(2\pi+\kappa,\kappa+\kappa',0)(1/a)$
$(Z\Sigma\|N')=1;$	$N_1'=(2\pi+\kappa,\kappa-\kappa',0)(1/a)$
$(Z\Sigma\|P)=1;$	$P_1=(\kappa+\kappa',\kappa,2\pi)(1/a)$
$(Z\Sigma\|P')=1;$	$P_1'=(\kappa-\kappa',\kappa,2\pi)(1/a)$
$(Z\Sigma\|k)=1;$	$k_1=(2\pi+\kappa,\kappa,\kappa')(1/a)$
$(Z\Delta\|Z')=1;$	$Z_1'=(2\pi,0,\kappa+\kappa')(1/a)$
$(Z\Delta\|Z'')=1;$	$Z_1''=(2\pi,0,\kappa-\kappa')(1/a)$
$(Z\Delta\|N)=1;$	$N_1=(2\pi+\kappa',\kappa,0)(1/a)$
$(Z\Delta\|P)=1;$	$P_1=(\kappa,\kappa',2\pi)(1/a)$
$(Z\Lambda\|k)=1;$	$k_1=(2\pi+\kappa',\kappa',\kappa+\kappa')(1/a)$
$(Z\Lambda\|k')=1;$	$k_1'=(2\pi+\kappa',\kappa',\kappa-\kappa')(1/a)$
$(\Sigma\Sigma'\|\Sigma'')=1;$	$\Sigma_1''=(\kappa+\kappa',\kappa+\kappa',0)(1/a)$
$(\Sigma\Sigma'\|\Sigma''')=1;$	$\Sigma_1'''=(\kappa-\kappa',\kappa-\kappa',0)(1/a)$
$(\Sigma\Sigma'\|N)=1;$	$N_1=(\kappa-\kappa',\kappa+\kappa',0)(1/a)$
$(\Sigma\Sigma'\|k)=1;$	$k_1=(\kappa,\kappa',\kappa+\kappa')(1/a)$
$(\Sigma\Sigma'\|k')=1;$	$k_1'=(\kappa,\kappa',\kappa-\kappa')(1/a)$
$(\Sigma\Delta\|N)=1;$	$N_1=(\kappa,\kappa+\kappa',0)(1/a)$
$(\Sigma\Delta\|N')=1;$	$N_1'=(\kappa,\kappa-\kappa',0)(1/a)$
$(\Sigma\Delta\|M)=1;$	$M_1=(\kappa,\kappa,\kappa')(1/a)$
$(\Sigma\Lambda\|M)=1;$	$M_1=(\kappa+\kappa',\kappa+\kappa',\kappa')(1/a)$
$(\Sigma\Lambda\|M')=1;$	$M_1'=(\kappa-\kappa',\kappa-\kappa',\kappa')(1/a)$
$(\Sigma\Lambda\|k)=1;$	$k_1=(\kappa+\kappa',\kappa-\kappa',\kappa')(1/a)$
$(\Delta\Delta'\|\Delta'')=1;$	$\Delta_1''=(\kappa+\kappa',0,0)(1/a)$
$(\Delta\Delta'\|\Delta''')=1;$	$\Delta_1'''=(\kappa-\kappa',0,0)(1/a)$
$(\Delta\Delta'\|N)=1;$	$N_1=(\kappa,\kappa',0)(1/a)$
$(\Delta\Lambda\|M)=1;$	$M_1=(\kappa',\kappa',\kappa+\kappa')(1/a)$
$(\Delta\Lambda\|M')=1;$	$M_1'=(\kappa',\kappa',\kappa'-\kappa)(1/a)$
$(\Lambda\Lambda'\|\Lambda'')=1;$	$\Lambda_1''=(\kappa+\kappa',\kappa+\kappa',\kappa+\kappa')(1/a)$
$(\Lambda\Lambda'\|\Lambda''')=1;$	$\Lambda_1'''=(\kappa-\kappa',\kappa-\kappa',\kappa-\kappa')(1/a)$
$(\Lambda\Lambda'\|M)=1;$	$M_1=(\kappa+\kappa',\kappa+\kappa',\kappa-\kappa')(1/a)$
$(\Lambda\Lambda'\|M')=1;$	$M_1'=(\kappa-\kappa',\kappa-\kappa',\kappa+\kappa')(1/a)$

TABLE IV. Wave vector selection rules in diamond coefficients $([l_m\mathbf{k}_j]_{(2)}|\mathbf{k}_{j'})$.

$([\Gamma]_{(2)}\|\Gamma)=1$
$([2\Gamma]_{(2)}\|\Gamma)=3$
$([3\Gamma]_{(2)}\|\Gamma)=6$
$([L]_{(2)}\|\Gamma)=4;\quad (\|X)=2$ [a]
$([2L]_{(2)}\|\Gamma)=12;\quad (\|X)=8$ [a]
$([2X]_{(2)}\|\Gamma)=9;\quad (\|X)=4$ [a]
$([\Delta]_{(2)}\|\Gamma)=3;\quad (\|\Delta')=1;\quad (\|\Sigma)=1$
$([2\Delta]_{(2)}\|\Gamma)=12;\quad (\|\Delta')=3;\quad (\|\Sigma)=4$
$([\Lambda]_{(2)}\|\Gamma)=4;\quad (\|\Delta')=2;\quad (\|\Lambda')=1;\quad (\|\Sigma')=1$
$([2\Lambda]_{(2)}\|\Gamma)=16;\quad (\|\Delta')=8;\quad (\|\Lambda')=3;\quad (\|\Sigma')=4$
$([2W]_{(2)}\|\Gamma)=12;\quad (\|X)=6;\quad (\|\Sigma'')=4$ [b]
$([\Sigma'']_{(2)}\|\Gamma)=6;\quad (\|X)=8;\quad (\|\Sigma'')=4$ [b]
$([K]_{(2)}\|\Gamma)=6;\quad (\|K)=2;\quad (\|M)=1;\quad (\|\Delta)=2;\quad (\|\Sigma'')=1$ [b]
$([2Z]_{(2)}\|\Gamma)=24;\quad (\|\Delta')=6;\quad (\|\Delta'')=4;\quad (\|N)=4;\quad (\|X)=8;\quad (\|\Sigma)=4;\quad (\|\Sigma'')=4$
$([k]_{(2)}\|\Gamma)=24;\quad (\|k')=24$ [c]

[a] Since all $\star X^{(m)}$ have $l_m=2$, we must use up two stars whenever an $(|X)\neq 0$.
[b] $\Sigma_1''=(\pi,\pi,0)(1/a)$.
[c] $\mathbf{k}$ here is a general vector, whose symmetrized square contains only general vectors except for Γ.

6. APPLICATIONS TO DIAMOND STRUCTURE: O_h^7

In Table I, geometrical information regarding the diamond structure is given. Note the two types of fundamental rotational symmetry operations in this structure: those combined with fractionals, and those not. In Table II we give the coordinates of wave vectors

TABLE V. Wave vector selection rules in diamond coefficients $([l_m\mathbf{k}_j]_{(3)}|\mathbf{k}_{j'})$.

$([\Gamma]_{(3)}\|\Gamma)=1$
$([2\Gamma]_{(3)}\|\Gamma)=4$
$([3\Gamma]_{(3)}\|\Gamma)=10$
$([L]_{(3)}\|L)=5$
$([2L]_{(3)}\|L)=30$
$([2X]_{(3)}\|\Gamma)=8;\quad (\|X)=16$
$([2W]_{(3)}\|W)=26;\quad (\|\Delta)=24;\quad (\|L)=16$
$([K]_{(3)}\|\Gamma)=8;\quad (\|K)=8;\quad (\|N)=2;\quad (\|\Sigma)=2;\quad (\|\Sigma')=1;\quad (\|M)=4;\quad (\|H)=2;\quad (\|L)=2;\quad (\|\Delta)=4$

TABLE VI. Reduction coefficients for diamond.[a]

$(\Gamma^{(1+)}k_j^{(m)}|k_j^{(m)})=1$

$(\Gamma^{(2)}\Gamma^{(2)}|\Gamma^{(1)})=1$

$(\Gamma^{(2)}\Gamma^{(12)}|\Gamma^{(12)})=1$

$(\Gamma^{(2)}\Gamma^{(15)}|\Gamma^{(25)})=1$

$(\Gamma^{(2)}\Gamma^{(25)}|\Gamma^{(15)})=1$

$(\Gamma^{(12)}\Gamma^{(12)}|\Gamma^{(1)})=(|\Gamma^{(2)})=(|\Gamma^{(12)})=1$

$(\Gamma^{(12)}\Gamma^{(15)}|\Gamma^{(15)})=(|\Gamma^{(25)})=1$

$(\Gamma^{(12)}\Gamma^{(25)}|\Gamma^{(15)})=(|\Gamma^{(25)})=1$

$(\Gamma^{(15)}\Gamma^{(25)}|\Gamma^{(1)})=(|\Gamma^{(12)})=(|\Gamma^{(15)})=(|\Gamma^{(25)})=1$

$(\Gamma^{(15)}\Gamma^{(25)}|\Gamma^{(2)})=(|\Gamma^{(12)})=(|\Gamma^{(15)})=(|\Gamma^{(25)})=1$

$(\Gamma^{(25)}\Gamma^{(25)}|)=(\Gamma^{(15)}\Gamma^{(15)}|)$.

(For the above, the product of even $\times$ odd yields odd representations, etc.).

$(\Gamma^{(1-)}L^{(1+)}|L^{(1-)})=1$

$(\Gamma^{(1-)}L^{(1-)}|L^{(1+)})=1$

$(\Gamma^{(1-)}L^{(2+)}|L^{(2-)})=1$

$(\Gamma^{(1-)}L^{(2-)}|L^{(2+)})=1$

$(\Gamma^{(1-)}L^{(3+)}|L^{(3-)})=1$

$(\Gamma^{(1-)}L^{(3-)}|L^{(3+)})=1$

$(\Gamma^{(1-)}X^{(1)}|X^{(2)})=1$

$(\Gamma^{(1-)}X^{(2)}|X^{(1)})=1$

$(\Gamma^{(1-)}X^{(3)}|X^{(3)})=1$

$(\Gamma^{(1-)}X^{(4)}|X^{(4)})=1$

$(\Gamma^{(2+)}L^{(1+)}|)=(\Gamma^{(2-)}L^{(1-)}|)=(\Gamma^{(1-)}L^{(2-)}|)$

$(\Gamma^{(2+)}L^{(1-)}|)=(\Gamma^{(2-)}L^{(1+)}|)=(\Gamma^{(1-)}L^{(2+)}|)$

$(\Gamma^{(2+)}L^{(2+)}|)=(\Gamma^{(2-)}L^{(2-)}|)=(\Gamma^{(1-)}L^{(1-)}|)$

$(\Gamma^{(2+)}L^{(2-)}|)=(\Gamma^{(2-)}L^{(2+)}|)=(\Gamma^{(1-)}L^{(1+)}|)$

$(\Gamma^{(2+)}L^{(3+)}|)=(\Gamma^{(2-)}L^{(3-)}|)=(\Gamma^{(1-)}L^{(3-)}|)$

$(\Gamma^{(2+)}L^{(3-)}|)=(\Gamma^{(2-)}L^{(3+)}|)=(\Gamma^{(1-)}L^{(3+)}|)$

$(\Gamma^{(2+)}X^{(1)}|)=(\Gamma^{(2-)}X^{(2)}|)=(\Gamma^{(1-)}X^{(1)}|)$

$(\Gamma^{(2+)}X^{(2)}|)=(\Gamma^{(2-)}X^{(1)}|)=(\Gamma^{(1-)}X^{(2)}|)$

$(\Gamma^{(2+)}X^{(3)}|)=(\Gamma^{(2-)}X^{(3)}|)=(\Gamma^{(1-)}X^{(4)}|)$

$(\Gamma^{(2+)}X^{(4)}|)=(\Gamma^{(2-)}X^{(4)}|)=(\Gamma^{(1-)}X^{(3)}|)$

$(\Gamma^{(12+)}L^{(1+)}|L^{(3+)})=1$

$(\Gamma^{(12+)}L^{(1-)}|L^{(3-)})=1$

$(\Gamma^{(12+)}L^{(2+)}|L^{(3+)})=1$

$(\Gamma^{(12+)}L^{(2-)}|L^{(3-)})=1$

$(\Gamma^{(12+)}L^{(3+)}|L^{(1+)})=(|L^{(2+)})=(|L^{(3+)})=1$

$(\Gamma^{(12+)}L^{(3-)}|L^{(1-)})=(|L^{(2-)})=(|L^{(3-)})=1$

$(\Gamma^{(12+)}X^{(1)}|X^{(1)})=(|X^{(2)})=1$

$(\Gamma^{(12+)}X^{(2)}|X^{(1)})=(|X^{(2)})=1$

$(\Gamma^{(12+)}X^{(3)}|X^{(3)})=(|X^{(4)})=1$

$(\Gamma^{(12+)}X^{(4)}|X^{(3)})=(|X^{(4)})=1$

$(\Gamma^{(12-)}L^{(m\pm)}|)=(\Gamma^{(12+)}L^{(m\mp)}|)$

$(\Gamma^{(12-)}X^{(m)}|)=(\Gamma^{(12+)}X^{(m)}|)$

$(\Gamma^{(15+)}L^{(1+)}|L^{(2+)})=(|L^{(3+)})=1$

$(\Gamma^{(15+)}L^{(1-)}|L^{(2-)})=(|L^{(3-)})=1$

$(\Gamma^{(15+)}L^{(2+)}|L^{(1+)})=(|L^{(3+)})=1$

$(\Gamma^{(15+)}L^{(2-)}|L^{(1-)})=(|L^{(3-)})=1$

$(\Gamma^{(15+)}L^{(3+)}|L^{(1+)})=(|L^{(2+)})=1;\quad(|L^{(3+)})=2$

$(\Gamma^{(15+)}L^{(3-)}|L^{(1-)})=(|L^{(2-)})=1;\quad(|L^{(3-)})=2$

$(\Gamma^{(15+)}X^{(1)}|X^{(2)})=(|X^{(3)})=(|X^{(4)})=1$

$(\Gamma^{(15+)}X^{(2)}|X^{(1)})=(|X^{(3)})=(|X^{(4)})=1$

$(\Gamma^{(15+)}X^{(3)}|X^{(1)})=(|X^{(2)})=(|X^{(4)})=1$

$(\Gamma^{(15+)}X^{(4)}|X^{(1)})=(|X^{(2)})=(|X^{(3)})=1$

$(\Gamma^{(15-)}L^{(m\pm)}|)=(\Gamma^{(15+)}L^{(m\mp)}|)$

$(\Gamma^{(15-)}X^{(1)}|)=(\Gamma^{(15+)}X^{(2)}|)$

$(\Gamma^{(15-)}X^{(2)}|)=(\Gamma^{(15+)}X^{(1)}|)$

$(\Gamma^{(15-)}X^{(3)}|)=(\Gamma^{(15+)}X^{(3)}|)$

$(\Gamma^{(15-)}X^{(4)}|)=(\Gamma^{(15+)}X^{(4)}|)$

$(\Gamma^{(25+)}L^{(1+)}|L^{(1+)})=(|L^{(3+)})=1$

$(\Gamma^{(25+)}L^{(1-)}|L^{(1-)})=(|L^{(3-)})=1$

$(\Gamma^{(25+)}L^{(2+)}|L^{(2+)})=(|L^{(3+)})=1$

$(\Gamma^{(25+)}L^{(2-)}|L^{(2-)})=(|L^{(3-)})=1$

$(\Gamma^{(25+)}L^{(3+)}|L^{(1+)})=(|L^{(2+)})=1;\quad(|L^{(3+)})=2$

$(\Gamma^{(25+)}L^{(3-)}|L^{(1-)})=(|L^{(2-)})=1;\quad(|L^{(3-)})=2$

$(\Gamma^{(25+)}X^{(1)}|X^{(1)})=(|X^{(3)})=(|X^{(4)})=1$

$(\Gamma^{(25+)}X^{(2)}|X^{(2)})=(|X^{(3)})=(|X^{(4)})=1$

$(\Gamma^{(25+)}X^{(3)}|X^{(1)})=(|X^{(2)})=(|X^{(3)})=1$

$(\Gamma^{(25+)}X^{(4)}|X^{(1)})=(|X^{(2)})=(|X^{(4)})=1$

$(\Gamma^{(25-)}L^{(m\pm)}|)=(\Gamma^{(25+)}L^{(m\mp)}|)$

$(\Gamma^{(25-)}X^{(1)}|)=(\Gamma^{(25+)}X^{(2)}|)$

$(\Gamma^{(25-)}X^{(2)}|)=(\Gamma^{(25+)}X^{(1)}|)$

$(\Gamma^{(25-)}X^{(3)}|)=(\Gamma^{(25+)}X^{(3)}|)$

$(\Gamma^{(25-)}X^{(4)}|)=(\Gamma^{(25+)}X^{(4)}|)$

$(L^{(1+)}L^{(1+)}|\Gamma^{(1+)})=(|\Gamma^{(25+)})=(|X^{(1)})=(|X^{(3)})=1$

$(L^{(1+)}L^{(1-)}|\Gamma^{(1-)})=(|\Gamma^{(25-)})=(|X^{(2)})=(|X^{(3)})=1$

$(L^{(1+)}L^{(2+)}|\Gamma^{(2+)})=(|\Gamma^{(15+)})=(|X^{(2)})=(|X^{(4)})=1$

$(L^{(1+)}L^{(2-)}|\Gamma^{(2-)})=(|\Gamma^{(15-)})=(|X^{(1)})=(|X^{(4)})=1$

$(L^{(1+)}L^{(3+)}|\Gamma^{(12+)})=(|\Gamma^{(15+)})=(|\Gamma^{(25+)})=(|X^{(1)})$
$=(|X^{(2)})=(|X^{(3)})=(|X^{(4)})=1$

$(L^{(1+)}L^{(3-)}|\Gamma^{(12-)})=(|\Gamma^{(15-)})=(|\Gamma^{(25-)})=(|X^{(1)})$
$=(|X^{(2)})=(|X^{(3)})=(|X^{(4)})=1$

$(L^{(1+)}X^{(1)}|L^{(1+)})=(|L^{(2-)})=(|L^{(3+)})=(|L^{(3-)})=1$

$(L^{(1+)}X^{(2)}|L^{(1-)})=(|L^{(2+)})=(|L^{(3+)})=(|L^{(3-)})=1$

$(L^{(1+)}X^{(3)}|L^{(1+)})=(|L^{(1-)})=(|L^{(3+)})=(|L^{(3-)})=1$

$(L^{(1+)}X^{(4)}|L^{(2+)})=(|L^{(2-)})=(|L^{(3+)})=(|L^{(3-)})=1$

$(L^{(1-)}L^{(1-)}|)=(L^{(1+)}L^{(1+)}|)$

$(L^{(1-)}L^{(2+)}|)=(L^{(1+)}L^{(2-)}|)$

$(L^{(1-)}L^{(2-)}|)=(L^{(1+)}L^{(2+)}|)$

$(L^{(1-)}L^{(3+)}|)=(L^{(1+)}L^{(3-)}|)$

$(L^{(1-)}L^{(3-)}|)=(L^{(1+)}L^{(3+)}|)$

$(L^{(1-)}X^{(1)}|)=(L^{(1+)}X^{(2)}|)$

$(L^{(1-)}X^{(2)}|)=(L^{(1+)}X^{(1)}|)$

$(L^{(1-)}X^{(3)}|)=(L^{(1+)}X^{(3)}|)$

$(L^{(1-)}X^{(4)}|)=(L^{(1+)}X^{(4)}|)$

$(L^{(2+)}L^{(2+)}|)=(L^{(1+)}L^{(1+)}|)$

$(L^{(2+)}L^{(2-)}|)=(L^{(1+)}L^{(1-)}|)$

$(L^{(2+)}L^{(3+)}|)=(L^{(1+)}L^{(3+)}|)$

$(L^{(2+)}L^{(3-)}|)=(L^{(1+)}L^{(3-)}|)$

$(L^{(2+)}X^{(1)}|)=(L^{(1+)}X^{(2)}|)$

$(L^{(2+)}X^{(2)}|)=(L^{(1+)}X^{(1)}|)$

$(L^{(2+)}X^{(3)}|)=(L^{(1+)}X^{(4)}|)$

$(L^{(2+)}X^{(4)}|)=(L^{(1+)}X^{(3)}|)$

$(L^{(2-)}L^{(2-)}|)=(L^{(1+)}L^{(1+)}|)$

$(L^{(2-)}L^{(3+)}|)=(L^{(1+)}L^{(3-)}|)$

$(L^{(2-)}L^{(3-)}|)=(L^{(1+)}L^{(3+)}|)$

$(L^{(2-)}X^{(1)}|)=(L^{(1+)}X^{(1)}|)$

$(L^{(2-)}X^{(2)}|)=(L^{(1+)}X^{(2)}|)$

$(L^{(2-)}X^{(3)}|)=(L^{(1+)}X^{(4)}|)$

$(L^{(2-)}X^{(4)}|)=(L^{(1+)}X^{(3)}|)$

$(L^{(3+)}L^{(3+)}|\Gamma^{(1+)})=(|\Gamma^{(2+)})=(|\Gamma^{(12+)})=1;\quad(|\Gamma^{(15+)})$
$=(|\Gamma^{(25+)})=(|X^{(1)})=(|X^{(2)})=(|X^{(3)})$
$=(|X^{(4)})=2$

$(L^{(3+)}L^{(3-)}|\Gamma^{(1-)})=(|\Gamma^{(2-)})=(|\Gamma^{(12-)})=1;\quad(|\Gamma^{(15-)})$
$=(|\Gamma^{(25-)})=(|X^{(1)})=(|X^{(2)})=(|X^{(3)})$
$=(|X^{(4)})=2$

$(L^{(3+)}X^{(1)}|L^{(1+)})=(|L^{(1-)})=(|L^{(2+)})=(|L^{(2-)})=1;$
$(|L^{(3+)})=(|L^{(3-)})=2$

TABLE VI. (*continued*)

$$(L^{(3+)}X^{(2)}|\,)=(L^{(3+)}X^{(3)}|\,)=(L^{(3+)}X^{(4)}|\,)=(L^{(3+)}X^{(1)}|\,)$$
$$(L^{(3-)}L^{(3-)}|\,)=(L^{(3+)}L^{(3+)}|\,)$$
$$\begin{aligned}(L^{(3-)}X^{(1)}|\,)&=(L^{(3-)}X^{(2)}|\,)=(L^{(3-)}X^{(3)}|\,)=(L^{(3-)}X^{(4)}|\,)\\&=(L^{(3+)}X^{(1)}|\,)\end{aligned}$$

$$\begin{aligned}(X^{(1)}X^{(1)}|\Gamma^{(1+)})&=(|\Gamma^{(2-)})=(|\Gamma^{(12+)})=(|\Gamma^{(12-)})\\&=(|\Gamma^{(15-)})=(|\Gamma^{(25+)})=(|X^{(1)})\\&=(|X^{(2)})=(|X^{(3)})=(|X^{(4)})=1\end{aligned}$$
$$\begin{aligned}(X^{(1)}X^{(2)}|\Gamma^{(1-)})&=(|\Gamma^{(2+)})=(|\Gamma^{(12+)})=(|\Gamma^{(12-)})\\&=(|\Gamma^{(15+)})=(|\Gamma^{(25-)})=(|X^{(1)})\\&=(|X^{(2)})=(|X^{(3)})=(|X^{(4)})=1\end{aligned}$$
$$\begin{aligned}(X^{(1)}X^{(3)}|\Gamma^{(15+)})&=(|\Gamma^{(15-)})=(|\Gamma^{(25+)})=(|\Gamma^{(25-)})\\&=(|X^{(1)})=(|X^{(2)})=(|X^{(3)})=(|X^{(4)})=1\end{aligned}$$
$$(X^{(1)}X^{(4)}|\,)=(X^{(1)}X^{(3)}|\,)$$
$$(X^{(2)}X^{(2)}|\,)=(X^{(1)}X^{(1)}|\,)$$
$$(X^{(2)}X^{(3)}|\,)=(X^{(1)}X^{(3)}|\,)$$
$$(X^{(2)}X^{(4)}|\,)=(X^{(1)}X^{(3)}|\,)$$
$$\begin{aligned}(X^{(3)}X^{(3)}|\Gamma^{(1+)})&=(|\Gamma^{(1-)})=(|\Gamma^{(12+)})=(|\Gamma^{(12-)})\\&=(|\Gamma^{(25+)})=(|\Gamma^{(25-)})=(|X^{(1)})\\&=(|X^{(2)})=(|X^{(3)})=(|X^{(4)})=1\end{aligned}$$
$$\begin{aligned}(X^{(3)}X^{(4)}|\Gamma^{(2+)})&=(|\Gamma^{(2-)})=(|\Gamma^{(12+)})=(|\Gamma^{(12-)})\\&=(|\Gamma^{(15+)})=(|\Gamma^{(15-)})=(|X^{(1)})\\&=(|X^{(2)})=(|X^{(3)})=(|X^{(4)})=1\end{aligned}$$
$$(X^{(4)}X^{(4)}|\,)=(X^{(3)}X^{(3)}|\,)$$
$$(\Gamma^{(1-)}W^{(1)}|W^{(2)})=1$$
$$(\Gamma^{(1-)}W^{(2)}|W^{(1)})=1$$
$$(\Gamma^{(2+)}W^{(m)}|\,)=(\Gamma^{(1-)}W^{(m)}|\,)$$
$$(\Gamma^{(2-)}W^{(m)}|\,)=(\Gamma^{(1+)}W^{(m)}|\,)$$
$$(\Gamma^{(12+)}W^{(1)}|W^{(1)})=(|W^{(2)})=1$$
$$(\Gamma^{(12+)}W^{(2)}|\,)=(\Gamma^{(12+)}W^{(1)}|\,)$$
$$(\Gamma^{(12-)}W^{(m)}|\,)=(\Gamma^{(12+)}W^{(m)}|\,)$$
$$(\Gamma^{(15+)}W^{(1)}|W^{(2)})=1;\quad(|W^{(1)})=2$$
$$(\Gamma^{(15+)}W^{(2)}|W^{(1)})=1;\quad(|W^{(2)})=2$$

$$\begin{aligned}(\Gamma^{(15-)}W^{(1)}|\,)&=(\Gamma^{(15+)}W^{(2)}|\,)=(\Gamma^{(25+)}W^{(1)}|\,)\\&=(\Gamma^{(25-)}W^{(2)}|\,)\end{aligned}$$
$$\begin{aligned}(\Gamma^{(15-)}W^{(2)}|\,)&=(\Gamma^{(15+)}W^{(1)}|\,)=(\Gamma^{(25+)}W^{(2)}|\,)\\&=(\Gamma^{(25-)}W^{(1)}|\,)\end{aligned}$$

$$\begin{aligned}(W^{(1)}W^{(1)}|\Gamma^{(1+)})&=(|\Gamma^{(2-)})=(|\Gamma^{(12+)})=(|\Gamma^{(12-)})=(|\Gamma^{(15-)})\\&=(|\Gamma^{(25+)})=(|X^{(1)})=(|X^{(2)})=(|X^{(3)})\\&=(|X^{(4)})=1;\quad(|\Sigma^{(1)})=(|\Sigma^{(2)})=(|\Sigma^{(3)})\\&=(|\Sigma^{(4)}=(|\Gamma^{(15+)})=(|\Gamma^{(25-)})=2\end{aligned}$$
$$\begin{aligned}(W^{(1)}W^{(2)}|\Gamma^{(1-)})&=(|\Gamma^{(2+)})=(|\Gamma^{(12+)})=(|\Gamma^{(12-)}=(|\Gamma^{(15+)})\\&=(|\Gamma^{(25-)})=(|X^{(1)})=(|X^{(2)})=(|X^{(3)})\\&=(|X^{(4)})=1;\quad(|\Sigma^{(1)})=(|\Sigma^{(2)})=(|\Sigma^{(3)})\\&=(|\Sigma^{(4)})=(|\Gamma^{(15-)})=(|\Gamma^{(25+)})=2.\end{aligned}$$
$$(W^{(2)}W^{(2)}|\,)=(W^{(1)}W^{(1)}|\,).$$

$$\begin{aligned}(\Sigma^{(1)}\Sigma^{(1)}|\Sigma^{(1)})&=(|\Sigma^{(2)})=(|\Sigma^{(3)})=(|\Sigma^{(4)})=(|X^{(1)})\\&=(|X^{(4)})=2;\quad(|X^{(2)})=(|X^{(3)})=(|\Gamma^{(1+)})\\&=(|\Gamma^{(12+)})=(|\Gamma^{(15-)})=(|\Gamma^{(25+)})\\&=(|\Gamma^{(25-)})=1.\end{aligned}$$
$$\begin{aligned}(\Sigma^{(1)}\Sigma^{(2)}|\Sigma^{(1)})&=(|\Sigma^{(2)})=(|\Sigma^{(3)})=(|\Sigma^{(4)})=(|X^{(2)})\\&=(|X^{(4)})=2;\quad(|X^{(1)})=(|X^{(3)})=(|\Gamma^{(1-)})\\&=(|\Gamma^{(12-)})=(|\Gamma^{(15+)})=(|\Gamma^{(25+)})\\&=(|\Gamma^{(25-)})=1.\end{aligned}$$
$$\begin{aligned}(\Sigma^{(1)}\Sigma^{(3)}|\Sigma^{(1)})&=(|\Sigma^{(2)})=(|\Sigma^{(3)})=(|\Sigma^{(4)})=(|X^{(1)})\\&=(|X^{(3)})=2;\quad(|X^{(2)})=(|X^{(4)})=(|\Gamma^{(2-)})\\&=(|\Gamma^{(12-)})=(|\Gamma^{(15+)})=(|\Gamma^{(15-)})\\&=(|\Gamma^{(25+)})=1.\end{aligned}$$
$$\begin{aligned}(\Sigma^{(1)}\Sigma^{(4)}|\Sigma^{(1)})&=(|\Sigma^{(2)})=(|\Sigma^{(3)})=(|\Sigma^{(4)})\\&=(|X^{(2)})=(|X^{(3)})=2;\quad(|X^{(1)})=(|X^{(4)})\\&=(|\Gamma^{(2+)})=(|\Gamma^{(12+)})=(|\Gamma^{(15+)})=(|\Gamma^{(15-)}\\&=(|\Gamma^{(25-)})=1.\end{aligned}$$
$$(\Sigma^{(m)}\Sigma^{(m)}|\,)=(\Sigma^{(1)}\Sigma^{(1)}|\,)\quad m=2,3,4$$
$$(\Sigma^{(3)}\Sigma^{(4)}|\,)=(\Sigma^{(1)}\Sigma^{(2)}|\,)$$
$$(\Sigma^{(2)}\Sigma^{(4)}|\,)=(\Sigma^{(1)}\Sigma^{(3)}|\,)$$
$$(\Sigma^{(2)}\Sigma^{(3)}|\,)=(\Sigma^{(1)}\Sigma^{(4)}|\,)$$

[a] In the last 11 lines of this table, $\Sigma_1\equiv(\pi,\pi,0)(1/a)$: see note b of Table IV.

of high symmetry in the zone: one wave vector from a star is given. In Table III wave vector selection rules for 28 combinations are given; these are the ordinary Kronecker product of the stars so indicated. The coefficients listed are those defined by the equation (4.2); for representations with $l_m>1$ such as may occur at Γ, $\star L$, $\star\Lambda$, $\star\Delta$, and must occur at $\star X$, $\star W$, $\star Z$, we must use (4.10). When $\mathbf{k}_j$ and $\mathbf{k}_{j'}$ are on a line or plane (as distinct from a point) of symmetry we shall take the most general case, with different components. For example, in $(\Delta\Delta'|\mathbf{k}_{j''})$ we take Δ and Δ' to be two different wave vectors of the Δ symmetry. Special cases, with particular values of components, can then easily be constructed. In Table III for the coefficients we give the components of one of the arms of $\mathbf{k}_{j''}$; this defines the entire star, since the components of the other arms can easily be found by applying all rotations in O_h to the components given. Note, too, that for special values of components a given star may degenerate into stars of higher symmetry. For example, if $\kappa_1=\kappa_2$, $\star N\rightarrow 2\,\star\Sigma$; if $\kappa=0$, $\star\Sigma\rightarrow 12\Gamma$; etc. In Table IV we give wave vector selection rules for the reduction of the symmetrized Kronecker square, and in Table V for the symmetrized cube of certain representations.

The reduction group method was applied, *inter alia*, to reduce the ordinary Kronecker products of representations $\Gamma^{(m)}$, $\star X^{(m)}$, and $\star L^{(m)}$. From Table III, the relevant wave vector selection rules are

$$\star X\otimes\star X=3\Gamma\oplus 2\,\star X,\tag{6.1}$$

$$\star L\otimes\star L=4\Gamma\oplus 4\,\star X,\tag{6.2}$$

$$\star X\otimes\star L=3\,\star L.\tag{6.3}$$

When using (6.1)–(6.3) we must recall that all $l_m=2$ in $\star X^{(m)}$.

We find, for the four cosets in $\mathcal{T}/\mathcal{K}_X$

$$\mathcal{T}/\mathcal{K}_X=\mathcal{K}_X,\quad\{\boldsymbol{\varepsilon}|\mathbf{t}_{xy}\}\mathcal{K}_X,\quad\{\boldsymbol{\varepsilon}|\mathbf{t}_{xz}\}\mathcal{K}_X,\quad\{\boldsymbol{\varepsilon}|\mathbf{t}_{yz}\}\mathcal{K}_X.\tag{6.4}$$

There are eight cosets in $\mathcal{T}/\mathcal{K}_L$

$$\begin{aligned}\mathcal{T}/\mathcal{K}_L=\mathcal{K}_L,\quad&\{\boldsymbol{\varepsilon}|\mathbf{t}_{xy}\}\mathcal{K}_L,\quad\{\boldsymbol{\varepsilon}|\mathbf{t}_{xz}\}\mathcal{K}_L,\\&\{\boldsymbol{\varepsilon}|\mathbf{t}_{yz}\}\mathcal{K}_L,\quad\{\boldsymbol{\varepsilon}|\mathbf{Q}\}\mathcal{K}_L,\quad\{\boldsymbol{\varepsilon}|\mathbf{t}_{xy}+\mathbf{Q}\}\mathcal{K}_L,\\&\{\boldsymbol{\varepsilon}|\mathbf{t}_{xz}+\mathbf{Q}\}\mathcal{K}_L,\quad\{\boldsymbol{\varepsilon}|\mathbf{t}_{yz}+\mathbf{Q}\}\mathcal{K}_L,\end{aligned}\tag{6.5}$$

TABLE VII. Reduction coefficients for diamond.[a]

$(\Gamma^{(1+)}\Delta^{(m)}|\Delta^{(m)})=1$

$(\Gamma^{(1-)}\Delta^{(1)}|\Delta^{(4)})=1 \quad (\Gamma^{(2-)}\Delta^{(1)}|\Delta^{(3)})=1$

$(\Gamma^{(1-)}\Delta^{(2)}|\Delta^{(3)})=1 \quad (\Gamma^{(2-)}\Delta^{(2)}|\Delta^{(4)})=1$

$(\Gamma^{(1-)}\Delta^{(3)}|\Delta^{(2)})=1 \quad (\Gamma^{(2-)}\Delta^{(3)}|\Delta^{(1)})=1$

$(\Gamma^{(1-)}\Delta^{(4)}|\Delta^{(1)})=1 \quad (\Gamma^{(2-)}\Delta^{(4)}|\Delta^{(2)})=1$

$(\Gamma^{(1-)}\Delta^{(5)}|\Delta^{(5)})=1 \quad (\Gamma^{(2-)}\Delta^{(5)}|\Delta^{(5)})=1$

$(\Gamma^{(2+)}\Delta^{(1)}|\Delta^{(2)})=1 \quad (\Gamma^{(12+)}\Delta^{(1)}|\Delta^{(1)})=(|\Delta^{(2)})=1$

$(\Gamma^{(2+)}\Delta^{(2)}|\Delta^{(1)})=1 \quad (\Gamma^{(12+)}\Delta^{(2)}|\,)=(\Gamma^{(12+)}\Delta^{(1)}|\,)$

$(\Gamma^{(2+)}\Delta^{(3)}|\Delta^{(4)})=1 \quad (\Gamma^{(12+)}\Delta^{(3)}|\Delta^{(3)})=(|\Delta^{(4)})=1$

$(\Gamma^{(2+)}\Delta^{(4)}|\Delta^{(3)})=1 \quad (\Gamma^{(12+)}\Delta^{(4)}|\,)=(\Gamma^{(12+)}\Delta^{(3)}|\,)$

$(\Gamma^{(2+)}\Delta^{(5)}|\Delta^{(5)})=1 \quad (\Gamma^{(12+)}\Delta^{(5)}|\Delta^{(5)})=2$

$(\Gamma^{(12-)}\Delta^{(1)}|\,)=(\Gamma^{(12+)}\Delta^{(3)}|\,)=(\Gamma^{(12-)}\Delta^{(2)}|\,)$

$(\Gamma^{(12-)}\Delta^{(3)}|\,)=(\Gamma^{(12+)}\Delta^{(1)}|\,)=(\Gamma^{(12-)}\Delta^{(4)}|\,)$

$(\Gamma^{(12-)}\Delta^{(5)}|\,)=(\Gamma^{(12+)}\Delta^{(5)}|\,)$

$(\Gamma^{(15+)}\Delta^{(1)}|\Delta^{(4)})=(|\Delta^{(5)})=1$

$(\Gamma^{(15+)}\Delta^{(2)}|\Delta^{(3)})=(|\Delta^{(5)})=1$

$(\Gamma^{(15+)}\Delta^{(3)}|\Delta^{(2)})=(|\Delta^{(5)})=1$

$(\Gamma^{(15+)}\Delta^{(4)}|\Delta^{(1)})=(|\Delta^{(5)})=1$

$(\Gamma^{(15+)}\Delta^{(5)}|\Delta^{(1)})=(|\Delta^{(2)})=(|\Delta^{(3)})=(|\Delta^{(4)})=(|\Delta^{(5)})=1$

$(\Gamma^{(15-)}\Delta^{(1)}|\,)=(\Gamma^{(15+)}\Delta^{(4)}|\,)$

$(\Gamma^{(15-)}\Delta^{(2)}|\,)=(\Gamma^{(15+)}\Delta^{(3)}|\,)$

$(\Gamma^{(15-)}\Delta^{(3)}|\,)=(\Gamma^{(15+)}\Delta^{(2)}|\,)$

$(\Gamma^{(15-)}\Delta^{(4)}|\,)=(\Gamma^{(15+)}\Delta^{(1)}|\,)$

$(\Gamma^{(15-)}\Delta^{(5)}|\,)=(\Gamma^{(15+)}\Delta^{(5)}|\,)$

$(\Gamma^{(25+)}\Delta^{(1)}|\,)=(\Gamma^{(15+)}\Delta^{(2)}|\,)$

$(\Gamma^{(25+)}\Delta^{(2)}|\,)=(\Gamma^{(15+)}\Delta^{(1)}|\,)$

$(\Gamma^{(25+)}\Delta^{(3)}|\,)=(\Gamma^{(15+)}\Delta^{(4)}|\,)$

$(\Gamma^{(25+)}\Delta^{(4)}|\,)=(\Gamma^{(15+)}\Delta^{(3)}|\,)$

$(\Gamma^{(25+)}\Delta^{(5)}|\,)=(\Gamma^{(15+)}\Delta^{(5)}|\,)$

$(\Gamma^{(25-)}\Delta^{(1)}|\,)=(\Gamma^{(25+)}\Delta^{(4)}|\,)$

$(\Gamma^{(25-)}\Delta^{(2)}|\,)=(\Gamma^{(25+)}\Delta^{(3)}|\,)$

$(\Gamma^{(25-)}\Delta^{(3)}|\,)=(\Gamma^{(25+)}\Delta^{(2)}|\,)$

$(\Gamma^{(25-)}\Delta^{(4)}|\,)=(\Gamma^{(25+)}\Delta^{(1)}|\,)$

$(\Gamma^{(25-)}\Delta^{(5)}|\,)=(\Gamma^{(25+)}\Delta^{(5)}|\,)$

$(\Gamma^{(1+)}\Lambda^{(m)}|\Lambda^{(m)})=1$

$(\Gamma^{(1-)}\Lambda^{(1)}|\Lambda^{(2)})=1$

$(\Gamma^{(1-)}\Lambda^{(2)}|\Lambda^{(1)})=1$

$(\Gamma^{(1-)}\Lambda^{(3)}|\Lambda^{(3)})=1$

$(\Gamma^{(2+)}\Lambda^{(m)}|\,)=(\Gamma^{(1-)}\Lambda^{(m)}|\,)$

$(\Gamma^{(2-)}\Lambda^{(m)}|\,)=(\Gamma^{(1+)}\Lambda^{\ m)}|\,)$

$(\Gamma^{(12+)}\Lambda^{(1)}|\Lambda^{(3)})=1$

$(\Gamma^{(12+)}\Lambda^{(2)}|\,)=(\Gamma^{(12+)}\Lambda^{(1)}|\,)$

$(\Gamma^{(12+)}\Lambda^{(3)}|\Lambda^{(1)})=(|\Lambda^{(2)})=(|\Lambda^{(3)})=1$

$(\Gamma^{(12-)}\Lambda^{(m)}|\,)=(\Gamma^{(12+)}\Lambda^{(m)}|\,)$

$(\Gamma^{(15+)}\Lambda^{(1)}|\Lambda^{(2)})=(|\Lambda^{(3)})=1; \quad (\Gamma^{(15-)}\Lambda^{(2)}|\,)=(\Gamma^{(15+)}\Lambda^{(1)}|\,)$

$(\Gamma^{(15+)}\Lambda^{(2)}|\Lambda^{(1)})=(|\Lambda^{(3)})=1; \quad (\Gamma^{(15-)}\Lambda^{(1)}|\,)=(\Gamma^{(15+)}\Lambda^{(2)}|\,)$

$(\Gamma^{(15\pm)}\Lambda^{(3)}|\Lambda^{(1)})=(|\Lambda^{(2)})=1; \quad (|\Lambda^{(3)})=2; \quad (\Gamma^{(15-)}\Lambda^{(3)}|\,)$

$(\Gamma^{(25\pm)}\Lambda^{(m)}|\,)=(\Gamma^{(15\mp)}\Lambda^{(m)}|\,).$

$(\Delta^{(1)}\Delta^{(1)}|\Gamma^{(1+)})=(|\Gamma^{(12+)})=(|\Gamma^{(15-)})=(|\Sigma^{(1)})=(|\Sigma^{(4)})$
$\quad =(|\Delta'^{(1)})=1$

$(\Delta^{(1)}\Delta^{(2)}|\Gamma^{(2+)})=(|\Gamma^{(12+)})=(|\Gamma^{(25-)})=(|\Sigma^{(1)})=(|\Sigma^{(4)})$
$\quad =(|\Delta'^{(2)})=1$

$(\Delta^{(1)}\Delta^{(3)}|\Gamma^{(2-)})=(|\Gamma^{(12-)})=(|\Gamma^{(25+)})=(|\Sigma^{(2)})=(|\Sigma^{(3)})$
$\quad =(|\Delta'^{(3)})=1$

$(\Delta^{(1)}\Delta^{(4)}|\Gamma^{(1-)})=(|\Gamma^{(12-)})=(|\Gamma^{(15+)})=(|\Sigma^{(2)})=(|\Sigma^{(3)})$
$\quad =(|\Delta'^{(4)})=1$

$(\Delta^{(1)}\Delta^{(5)}|\Gamma^{(15+)})=(|\Gamma^{(15-)})=(|\Gamma^{(25+)})=(|\Gamma^{(25-)})=(|\Sigma^{(1)})$
$\quad =(|\Sigma^{(2)})=(|\Sigma^{(3)})=(|\Sigma^{(4)})=(|\Delta'^{(5)})=1$

$(\Delta^{(5)}\Delta^{(5)}|\Gamma^{(1+)})=(|\Gamma^{(1-)})=(|\Gamma^{(2+)})=(|\Gamma^{(2-)})=(|\Gamma^{(15+)})$
$\quad =(|\Gamma^{(15-)})=(|\Gamma^{(25+)})=(|\Gamma^{(25-)})=(|\Delta'^{(1)})$
$\quad =(|\Delta'^{(2)})=(|\Delta'^{(3)})=(|\Delta'^{(4)})=1;$
$\quad (|\Gamma^{(12+)})=(|\Gamma^{(12-)})=(|\Sigma^{(1)})=(|\Sigma^{(2)})$
$\quad =(|\Sigma^{(3)})=(|\Sigma^{(4)})=2$

$(\Lambda^{(1)}\Lambda^{(1)}|\Gamma^{(1+)})=(|\Gamma^{(2-)})=(|\Gamma^{(15-)})=(|\Gamma^{(25+)})=(|\Lambda'^{(1)})$
$\quad =(|\Sigma'^{(1)})=(|\Sigma'^{(3)})=(|\Delta'^{(1)})$
$\quad =(|\Delta'^{(3)})=(|\Delta'^{(5)})=1$

$(\Lambda^{(1)}\Lambda^{(2)}|\Gamma^{(1-)})=(|\Gamma^{(2+)})=(|\Gamma^{(15+)})=(|\Gamma^{(25-)})=(|\Lambda'^{(2)})$
$\quad =(|\Sigma'^{(2)})=(|\Sigma'^{(4)})=(|\Delta'^{(2)})=(|\Delta'^{(4)})$
$\quad =(|\Delta'^{(5)})=1$

$(\Lambda^{(1)}\Lambda^{(3)}|\Gamma^{(12+)})=(|\Gamma^{(12-)})=(|\Gamma^{(15+)})=(|\Gamma^{(15-)})=(|\Gamma^{(25+)})$
$\quad =(|\Gamma^{(25-)})=(|\Lambda'^{(3)})=(|\Sigma'^{(1)})=(|\Sigma'^{(2)})$
$\quad =(|\Sigma'^{(3)})=(|\Sigma'^{(4)})=(|\Delta'^{(1)})=(|\Delta'^{(2)})$
$\quad =(|\Delta'^{(3)})=(|\Delta'^{(4)})=1; \quad (|\Delta'^{(5)})=2$

$(\Lambda^{(3)}\Lambda^{(3)}|\Gamma^{(1+)})=(|\Gamma^{(1-)})=(|\Gamma^{(2+)})=(|\Gamma^{(2-)})=(|\Gamma^{(12+)})$
$\quad =(|\Gamma^{(12-)})=(|\Lambda'^{(1)})=(|\Lambda'^{(2)})=(|\Lambda'^{(3)})=1;$
$\quad (|\Gamma^{(15+)})=(|\Gamma^{(15-)})=(|\Gamma^{(25+)})=(|\Gamma^{(25-)})=(|\Sigma'^{(1)})$
$\quad =(|\Sigma'^{(2)})=(|\Sigma'^{(3)})=(|\Sigma'^{(4)})=(|\Delta'^{(1)})$
$\quad =(|\Delta'^{(2)})=(|\Delta'^{(3)})=(|\Delta'^{(4)})=2; \quad (|\Delta'^{(5)})=4$

$(\Delta^{(1)}\Delta^{(1)}|\,)=(\Delta^{(2)}\Delta^{(2)}|\,)=(\Delta^{(3)}\Delta^{(3)}|\,)=(\Delta^{(4)}\Delta^{(4)}|\,)$

$(\Delta^{(1)}\Delta^{(2)}|\,)=(\Delta^{(3)}\Delta^{(4)}|\,)$

$(\Delta^{(1)}\Delta^{(3)}|\,)=(\Delta^{(2)}\Delta^{(4)}|\,)$

$(\Delta^{(1)}\Delta^{(4)}|\,)=(\Delta^{(2)}\Delta^{(3)}|\,)$

$(\Delta^{(1)}\Delta^{(5)}|\,)=(\Delta^{(2)}\Delta^{(5)}|\,)=(\Delta^{(3)}\Delta^{(5)}|\,)=(\Delta^{(4)}\Delta^{(5)}|\,)$

$(\Lambda^{(1)}\Lambda^{(1)}|\,)=(\Lambda^{(2)}\Lambda^{(2)}|\,)$

$(\Lambda^{(1)}\Lambda^{(3)}|\,)=(\Lambda^{(2)}\Lambda^{(3)}|\,)$

$(\Delta^{(1)}\Lambda^{(1)}|M^{(1)})=(|\Sigma^{(1)})=(|\Sigma^{(3)})=1;$

$(\Delta^{(3)}\Lambda^{(1)}|\,)=(\Delta^{(2)}\Lambda^{(2)}|\,)=(\Delta^{(4)}\Lambda^{(2)}|\,)=(\Delta^{(1)}\Lambda^{(1)}|\,);$

$(\Delta^{(1)}\Lambda^{(2)}|M^{(2)})=(|\Sigma^{(2)})=(|\Sigma^{(4)})=1;$

$(\Delta^{(3)}\Lambda^{(2)}|\,)=(\Delta^{(2)}\Lambda^{(1)}|\,)=(\Delta^{(4)}\Lambda^{(1)}|\,)=(\Delta^{(1)}\Lambda^{(2)}|\,);$

$(\Delta^{(1)}\Lambda^{(3)}|M^{(1)})=(|M^{(2)})=(|\Sigma^{(1)})=(|\Sigma^{(2)})=(|\Sigma^{(3)})$
$\quad =(|\Sigma^{(4)})=1;$

$(\Delta^{(m)}\Lambda^{(3)}|\,)=(\Delta^{(1)}\Lambda^{(3)}|\,) \quad m=2,\ 3,\ 4;$

$(\Delta^{(5)}\Lambda^{(3)}|M^{(1)})=(|M^{(2)})=(|\Sigma^{(1)})=(|\Sigma^{(2)})=(|\Sigma^{(3)})$
$\quad =(|\Sigma^{(4)})=2.$

[a] Our ${}^\star\Delta^{(3)}$ corresponds to Herrings'[10] Δ_2'; our ${}^\star\Delta^{(4)}$ to his Δ_1'; we reserve primes to denote *different* wave vectors (stars) of a given type, e.g., on a line or plane.

where

$$\{\varepsilon|\mathbf{Q}\}\equiv\{\varepsilon|\mathbf{t}_{xy}+\mathbf{t}_{xz}+\mathbf{t}_{yz}\}.$$

Hence the reduction group $\mathcal{R}$, suitable for reduction of all direct products of type (6.1)–(6.3), consists of $(n_{j''}h)=(8\times48)=384$ elements. To carry out such reductions we need to determine the character of each element in each of the irreducible representations $\Gamma^{(m)}$, ${}^\star X^{(m)}$, ${}^\star L^{(m)}$. The matrix groups involved here are

$$\Gamma^{(m)}/\mathcal{K}_L,\quad {}^\star X^{(m)}/\mathcal{K}_L,\quad {}^\star L^{(m)}/\mathcal{K}_L. \qquad (6.6)$$

We also used the reduction group method to reduce products involving ${}^\star W$ and ${}^\star\Sigma$, the latter for the case of $\Sigma_1=(\pi,\pi,0)(1/a)$. The relevant wave vector selection rules are

$${}^\star W\otimes{}^\star W=6\Gamma\oplus2\,{}^\star X\oplus2\,{}^\star\Sigma \qquad (6.7)$$

and

$$^\star\Sigma\otimes{}^\star\Sigma=12\Gamma\oplus 12\,{}^\star X\oplus 8\,{}^\star\Sigma. \qquad (6.8)$$

In (6.7) and (6.8) we are dealing in all cases with the $^\star\Sigma$ for which $\Sigma_1=(\pi,\pi,0)(1/a)$. The group $\mathcal{T}/\mathcal{K}_W$ is a group of order 32, whose cosets are easily found. The group $\mathcal{T}/\mathcal{K}_\Sigma$ is of order 16 with the specified choice of wave vector. Thus the reduction group for the reduction of (6.7) is or order $(32)\times(48)=1536$; however, most of these cosets have character zero, and far fewer are needed to find the appropriate reduction coefficients. Similarly for (6.8), with 768 cosets in the reduction group; most of these have zero character. In using (6.7) and (6.8), we note that $l_m=2$ for all $^\star W^{(m)}$ and $^\star X^{(m)}$.

Once the cosets, or elements comprising the reduction group, have been determined, the characters of needed symmetry elements in the full space group irreducible representations desired must be given. The character tables in the literature[10] are for the allowable irreducible

TABLE VIII. Reduction coefficients for symmetrized Kronecker square in diamond.

$([\Gamma^{(m)}]_{(2)}|\Gamma^{(1+)})=1;\quad m=1\pm,\ 2\pm$

$([\Gamma^{(m)}]_{(2)}|\Gamma^{(1+)})=(|\Gamma^{(12+)})=1;\quad m=12\pm$

$([\Gamma^{(m)}]_{(2)}|\Gamma^{(1+)})=(|\Gamma^{(12+)})=(|\Gamma^{(25+)})=1;\quad m=15\pm,\ 25\pm$

$([L^{(m)}]_{(2)}|\Gamma^{(1+)})=(|\Gamma^{(25+)})=(|X^{(1)})=1;\quad m=1\pm,\ 2\pm$

$([L^{(m)}]_{(2)}|\Gamma^{(1+)})=(|\Gamma^{(12+)})=(|\Gamma^{(15+)})=(|X^{(2)})=(|X^{(4)})=1;$
$\qquad (|\Gamma^{(25+)})=(|X^{(1)})=2;\quad m=3\pm$

$([X^{(m)}]_{(2)}|\Gamma^{(1+)})=(|\Gamma^{(2-)})=(|\Gamma^{(12+)})=(|\Gamma^{(12-)})=(|\Gamma^{(25+)})$
$\qquad =(|X^{(1)})=(|X^{(4)})=1;\quad m=1,\ 2$

$([X^{(m)}]_{(2)}|\Gamma^{(1+)})=(|\Gamma^{(1-)})=(|\Gamma^{(12+)})=(|\Gamma^{(12-)})=(|\Gamma^{(25+)})$
$\qquad =(|X^{(1)})=(|X^{(4)})=1;\quad m=3,\ 4$

$([\Delta^{(m)}]_{(2)}|\Gamma^{(1+)})=(|\Gamma^{(12+)})=(|\Sigma^{(1)})=(|\Delta'^{(1)})=1\quad m=1,\ 2,\ 3,\ 4$[a]

$([\Delta^{(5)}]_{(2)}|\Gamma^{(1+)})=(|\Gamma^{(1-)})=(|\Gamma^{(2+)})=(|\Gamma^{(12-)})=(|\Gamma^{(25+)})$
$\qquad =(|\Delta'^{(1)})=(|\Delta'^{(2)})=(|\Delta'^{(3)})=(|\Sigma^{(2)})$
$\qquad =(|\Sigma^{(3)})=1;\quad (|\Gamma^{(12+)})=(|\Sigma^{(1)})=2$

$([\Lambda^{(m)}]_{(2)}|\Gamma^{(1+)})=(|\Gamma^{(25+)})=(|\Delta'^{(1)})=(|\Delta'^{(3)})=(|\Lambda'^{(1)})$
$\qquad =(|\Sigma'^{(1)})=1\quad m=1,\ 2$

$([\Lambda^{(3)}]_{(2)}|\Gamma^{(1+)})=(|\Gamma^{(1-)})=(|\Gamma^{(12+)})=(|\Gamma^{(15+)})=(|\Gamma^{(25-)})$
$\qquad =(|\Delta'^{(2)})=(|\Delta'^{(4)})=(|\Delta'^{(5)})=(|\Sigma'^{(2)})$
$\qquad =(|\Sigma'^{(4)})=(|\Lambda'^{(1)})=(|\Lambda'^{(3)})=1;$
$\qquad (|\Gamma^{(25+)})=(|\Delta'^{(1)})=(|\Delta'^{(3)})=(|\Sigma'^{(1)})=2$

$([W^{(m)}]_{(2)}|\Gamma^{(1+)})=(|\Gamma^{(2-)})=(|\Gamma^{(12+)})=(|\Gamma^{(12-)})=(|\Gamma^{(15+)})$
$\qquad =(|\Gamma^{(25+)})=(|X^{(1)})=(|X^{(2)})=(|X^{(4)})$
$\qquad =(|\Sigma^{(2)})=(|\Sigma^{(3)})=1;\quad (|\Sigma^{(1)})=2;\quad m=1,\ 2$[b]

$([\Sigma^{(m)}]_{(2)}|\Gamma^{(1+)})=(|\Gamma^{(12+)})=(|\Gamma^{(25+)})=(|X^{(2)})=(|X^{(4)})$
$\qquad =(|\Sigma^{(2)})=(|\Sigma^{(3)})=1;$
$\qquad (|X^{(1)})=(|\Sigma^{(1)})=2;\quad m=1,\ 2,\ 3,\ 4$[b]

$([k]_{(2)}|\Gamma^{(1+)})=(|\Gamma^{(2+)})=1;\quad (|\Gamma^{(12+)})=2;$
$\qquad (|\Gamma^{(15+)})=(|\Gamma^{(25+)})=3$[c]

[a] See footnote a of Table VII.
[b] See footnote a of Table VI.
[c] Only representations $\Gamma^{(m)}$ were determined, using the basis function method.

[10] C. Herring, J. Franklin Inst. **233**, 525 (1942); W. Döring and V. Zehler, Ann. Physik **13**, 214 (1953). We use essentially the notations of Herring (see also Lax and Hopfield, reference 8, where some errors in Herring's paper are corrected), exceptions are noted in the appropriate table. In labeling representations $^\star L^{(m\pm)}$ we follow Herring (*op. cit.*) and Lax and Hapfield, rather than Döring.

TABLE IX. Reduction coefficients for symmetrized Kronecker cubes in diamond.

$([\Gamma^{(m)}]_{(3)}|\Gamma^{(m)})=1;\quad m=1\pm,\ 2\pm$

$([\Gamma^{(12+)}]_{(3)}|\Gamma^{(1+)})=(|\Gamma^{(2+)})=(|\Gamma^{(12+)})=1$

$([\Gamma^{(12-)}]_{(3)}|\Gamma^{(1-)})=(|\Gamma^{(2-)})=(|\Gamma^{(12-)})=1$

$([\Gamma^{(15+)}]_{(3)}|\Gamma^{(2+)})=(|\Gamma^{(25+)})=1;\quad (|\Gamma^{(15+)})=2$

$([\Gamma^{(15-)}]_{(3)}|\Gamma^{(2-)})=(|\Gamma^{(25-)})=1;\quad (|\Gamma^{(15-)})=2$

$([\Gamma^{(25\pm)}]_{(3)}|\Gamma^{(1\pm)})=(|\Gamma^{(15\pm)})=1;\quad (|\Gamma^{(25\pm)})=2$

$([X^{(1)}]_{(3)}|\Gamma^{(1+)})=(|\Gamma^{(2-)})=(|\Gamma^{(15-)})=(|\Gamma^{(25+)})=(|X^{(3)})$
$\qquad =(|X^{(4)})=1;\quad (|X^{(2)})=2;\quad (|X^{(1)})=4$

$([X^{(3)}]_{(3)}|\Gamma^{(2+)})=(|\Gamma^{(2-)})=(|\Gamma^{(15+)})=(|\Gamma^{(15-)})=(|X^{(1)})$
$\qquad =(|X^{(2)})=1;\quad (|X^{(4)})=2;\quad (|X^{(3)})=4$

$([X^{(4)}]_{(3)}|\Gamma^{(1+)})=(|\Gamma^{(1-)})=(|\Gamma^{(25+)})=(|\Gamma^{(25-)})=(|X^{(1)})$
$\qquad =(|X^{(2)})=1;\quad (|X^{(3)})=2;\quad (|X^{(4)})=4$

$([L^{(1+)}]_{(3)}|L^{(2-)})=(|L^{(3+)})=1;\quad (|L^{(1+)})=2$

$([L^{(2-)}]_{(3)}|L^{(1+)})=(|L^{(3-)})=1;\quad (|L^{(2-)})=2$

$([L^{(3+)}]_{(3)}|L^{(1-)})=(|L^{(2-)})=(|L^{(3-)})=2;\quad (|L^{(1+)})$
$\qquad =(|L^{(2+)})=4;\quad (|L^{(3+)})=7$

$([L^{(3-)}]_{(3)}|L^{(1+)})=(|L^{(2+)})=(|L^{(3+)})=2;\quad (|L^{(1-)})$
$\qquad =(|L^{(2-)})=4;\quad (|L^{(3-)})=7$

$([K^{(1)}]_{(3)}|\Gamma^{(1+)})=(|\Gamma^{(1-)})=(|\Gamma^{(25+)})=(|\Gamma^{(25-)})=1$ [a]

$([K^{(2)}]_{(3)}|\Gamma^{(m)})=([K^{(1)}]_{(3)}|\Gamma^{(m)})$ [a]

$([K^{(3)}]_{(3)}|\Gamma^{(2+)})=(|\Gamma^{(2-)})=(|\Gamma^{(15+)})=(|\Gamma^{(15-)})=1$ [a]

$([K^{(4)}]_{(3)}|\Gamma^{(m)})=([K^{(3)}]_{(3)}|\Gamma^{(m)})$ [a]

[a] For these representations we only obtained coefficients of types $(|\Gamma^{(m)})$, using the basis function method.

TABLE X. Wave vector selection rules in zinc blende.[a]

Ordinary

$(LZ|M)=2;\quad M_1=(\pi,\ \pi,\ -\kappa-\pi)(1/a)$

$(LZ|M')=2;\quad M_1'=(\pi,\ \pi,\ \kappa-\pi)(1/a)$

$(L\Sigma|M)=1;\quad M_1=(\kappa+\pi,\ \kappa+\pi,\ \pi)(1/a)$

$(L\Sigma|M')=1;\quad M_1'=(\kappa-\pi,\ \kappa-\pi,\ \pi)(1/a)$

$(L\Sigma|k)=1;\quad k_1=(\pi+\kappa,\ \kappa-\pi,\ -\pi)(1/a)$

$(L\Delta|M)=1;\quad M_1=(\pi,\ \pi,\ \pi+\kappa)(1/a)$

$(L\Delta|M')=1;\quad M_1=(\pi,\ +\pi,\ \pi-\kappa)(1/a)$

$(\Sigma\Lambda|M)=1;\quad M_1=(\kappa+\kappa',\ \kappa+\kappa',\ \kappa')(1/a)$

$(\Sigma\Lambda|M')=1;\quad M_1'=(\kappa-\kappa',\ \kappa-\kappa',\ \kappa')(1/a)$

$(\Sigma\Lambda|k)=1;\quad k_1=(\kappa+\kappa',\ \kappa-\kappa',\ -\kappa')(1/a)$

$(\Delta\Lambda|M)=1;\quad M_1=(\kappa,\ \kappa,\ \kappa'+\kappa)(1/a)$

$(\Delta\Lambda|M')=1;\quad M_1'=(\kappa,\ \kappa,\ \kappa-\kappa')(1/a)$

$(\Lambda\Lambda'|\Lambda'')=1;\quad \Lambda_1''=(\kappa+\kappa',\ \kappa+\kappa',\ \kappa+\kappa')(1/a)$

$(\Lambda\Lambda'|M)=1;\quad M_1=(\kappa-\kappa',\ \kappa-\kappa',\ \kappa+\kappa')(1/a)$

Symmetrized

$([X]_{(2)}|\Gamma)=3;\quad (|X)=1$

$([\Lambda]_{(2)}|\Lambda')=1;\quad (|\Delta')=1$

$([2\Lambda]_{(2)}|\Lambda')=3;\quad (|\Delta')=4$

$([W]_{(2)}|\Gamma)=3;\quad (|X)=2;\quad (|\Sigma)=1$

$([Z]_{(2)}|\Gamma)=6;\quad (|\Delta)=2;\quad (|\Delta')=1;\quad (|\mathbf{k})=1;$
$\qquad (|X)=2;\quad (|\Sigma)=1;\quad (|\Sigma')=1$

$([\mathbf{k}]_{(2)}|\Gamma)=12;\quad (|\mathbf{k}')=12$

$([X]_{(3)}|\Gamma)=1;\quad (|X)=3$

$([W]_{(3)}|W)=4;\quad (|\Delta)=4;\quad (|L)=2.$

[a] Rules not listed here are identical to those in diamond; see Tables III, IV, and V. When the latter are used for zinc blende, use the appropriate wave vectors (see Table II).

TABLE XI. Reduction coefficients for zinc blende.

$$(\Gamma^{(1)}k_j^{(m)}|k_j^{(m)})=1$$
$$(\Gamma^{(2)}L^{(1)}|L^{(2)})=1$$
$$(\Gamma^{(2)}L^{(2)}|L^{(1)})=1$$
$$(\Gamma^{(2)}L^{(3)}|L^{(3)})=1$$
$$(\Gamma^{(2)}X^{(1)}|X^{(2)})=1$$
$$(\Gamma^{(2)}X^{(2)}|X^{(1)})=1$$
$$(\Gamma^{(2)}X^{(3)}|X^{(4)})=1$$
$$(\Gamma^{(2)}X^{(4)}|X^{(3)})=1$$
$$(\Gamma^{(2)}X^{(5)}|X^{(5)})=1$$
$$(\Gamma^{(12)}L^{(1)}|L^{(3)})=1$$
$$(\Gamma^{(12)}L^{(2)}|L^{(3)})=1$$
$$(\Gamma^{(12)}L^{(3)}|L^{(1)})=(|L^{(2)})=(|L^{(3)})=1$$
$$(\Gamma^{(12)}X^{(1)}|X^{(1)})=(|X^{(2)})=1$$
$$(\Gamma^{(12)}X^{(2)}|X^{(1)})=(|X^{(2)})=1$$
$$(\Gamma^{(12)}X^{(3)}|X^{(3)})=(|X^{(4)})=1$$
$$(\Gamma^{(12)}X^{(4)}|X^{(3)})=(|X^{(4)})=1$$
$$(\Gamma^{(12)}X^{(5)}|X^{(5)})=2$$
$$(\Gamma^{(15)}L^{(1)}|L^{(1)})=(|L^{(3)})=1$$
$$(\Gamma^{(15)}L^{(2)}|L^{(2)})=(|L^{(3)})=1$$
$$(\Gamma^{(15)}L^{(3)}|L^{(1)})=(|L^{(2)})=1;\quad (|L^{(3)})=2$$
$$(\Gamma^{(15)}X^{(1)}|X^{(3)})=(|X^{(5)})=1$$
$$(\Gamma^{(15)}X^{(2)}|X^{(4)})=(|X^{(5)})=1$$
$$(\Gamma^{(15)}X^{(3)}|X^{(1)})=(|X^{(5)})=1$$
$$(\Gamma^{(15)}X^{(4)}|X^{(2)})=(|X^{(5)})=1$$
$$(\Gamma^{(15)}X^{(5)}|X^{(1)})=(|X^{(2)})=(|X^{(3)})=(|X^{(4)})=(|X^{(5)})=1$$
$$(\Gamma^{(25)}L^{(1)}|L^{(2)})=(|L^{(3)})=1$$
$$(\Gamma^{(25)}L^{(2)}|L^{(1)})=(|L^{(3)})=1$$
$$(\Gamma^{(25)}L^{(3)}|L^{(1)})=(|L^{(2)})=1;\quad (|L^{(3)})=2$$
$$(\Gamma^{(25)}X^{(1)}|X^{(4)})=(|X^{(5)})=1$$
$$(\Gamma^{(25)}X^{(2)}|X^{(3)})=(|X^{(5)})=1$$
$$(\Gamma^{(25)}X^{(3)}|X^{(2)})=(|X^{(5)})=1$$
$$(\Gamma^{(25)}X^{(4)}|X^{(1)})=(|X^{(5)})=1$$
$$(\Gamma^{(25)}X^{(5)}|\,)=(\Gamma^{(15)}X^{(5)}|\,)$$

$$(L^{(1)}L^{(1)}|\Gamma^{(1)})=(|\Gamma^{(15)})=(|X^{(1)})=(|X^{(3)})=(|X^{(5)})=1$$
$$(L^{(1)}L^{(2)}|\Gamma^{(2)})=(|\Gamma^{(25)})=(|X^{(2)})=(|X^{(4)})=(|X^{(5)})=1$$
$$(L^{(1)}L^{(3)}|\Gamma^{(12)})=(|\Gamma^{(15)})=(|\Gamma^{(25)})=(|X^{(1)})=(|X^{(2)})$$
$$=(|X^{(3)})=(|X^{(4)})=1;\quad (|X^{(5)})=2$$
$$(L^{(1)}X^{(1)}|L^{(1)})=(|L^{(3)})=1$$
$$(L^{(1)}X^{(2)}|L^{(2)})=(|L^{(3)})=1$$
$$(L^{(1)}X^{(3)}|\,)=(L^{(1)}X^{(1)}|\,)$$
$$(L^{(1)}X^{(4)}|\,)=(L^{(1)}X^{(2)}|\,)$$
$$(L^{(1)}X^{(5)}|L^{(1)})=(|L^{(2)})=1;\quad (|L^{(3)})=2$$
$$(L^{(2)}L^{(2)}|\,)=(L^{(1)}L^{(1)}|\,)$$
$$(L^{(2)}L^{(3)}|\,)=(L^{(1)}L^{(3)}|\,)$$
$$(L^{(2)}X^{(1)}|\,)=(L^{(1)}X^{(2)}|\,)$$
$$(L^{(2)}X^{(2)}|\,)=(L^{(1)}X^{(1)}|\,)$$
$$(L^{(2)}X^{(3)}|\,)=(L^{(1)}X^{(2)}|\,)$$
$$(L^{(2)}X^{(4)}|\,)=(L^{(1)}X^{(1)}|\,)$$
$$(L^{(2)}X^{(5)}|\,)=(L^{(1)}X^{(5)}|\,)$$
$$(L^{(3)}L^{(3)}|\Gamma^{(1)})=(|\Gamma^{(2)})=(|\Gamma^{(12)})=1;\quad (|\Gamma^{(15)})=(|\Gamma^{(25)})$$
$$=(|X^{(1)})=(|X^{(2)})=(|X^{(3)})=(|X^{(4)})=2;$$
$$(|X^{(5)})=4$$
$$(L^{(3)}X^{(1)}|L^{(1)})=(|L^{(2)})=1;\quad (|L^{(3)})=2$$
$$(L^{(3)}X^{(2)}|\,)=(L^{(3)}X^{(1)}|\,)$$
$$(L^{(3)}X^{(3)}|\,)=(L^{(3)}X^{(1)}|\,)$$
$$(L^{(3)}X^{(4)}|\,)=(L^{(3)}X^{(1)}|\,)$$
$$(L^{(3)}X^{(5)}|L^{(1)})=(|L^{(2)})=2;\quad (|L^{(3)})=4$$

$$(X^{(1)}X^{(1)}|\Gamma^{(1)})=(|\Gamma^{(12)})=(|X^{(1)})=(|X^{(2)})=1$$
$$(X^{(1)}X^{(2)}|\Gamma^{(2)})=(|\Gamma^{(12)})=(|X^{(1)})=(|X^{(2)})=1$$
$$(X^{(1)}X^{(3)}|\Gamma^{(15)})=(|X^{(5)})=1$$
$$(X^{(1)}X^{(4)}|\Gamma^{(25)})=(|X^{(5)})=1$$
$$(X^{(1)}X^{(5)}|\Gamma^{(15)})=(|\Gamma^{(25)})=(|X^{(3)})=(|X^{(4)})=(|X^{(5)})=1$$
$$(X^{(2)}X^{(2)}|\,)=(X^{(1)}X^{(1)}|\,)$$
$$(X^{(2)}X^{(3)}|\,)=(X^{(1)}X^{(4)}|\,)$$
$$(X^{(2)}X^{(4)}|\,)=(X^{(1)}X^{(3)}|\,)$$
$$(X^{(2)}X^{(5)}|\,)=(X^{(1)}X^{(5)}|\,)$$
$$(X^{(3)}X^{(3)}|\Gamma^{(1)})=(|\Gamma^{(12)})=(|X^{(3)})=(|X^{(4)})=1$$
$$(X^{(3)}X^{(4)}|\Gamma^{(2)})=(|\Gamma^{(12)})=(|X^{(3)})=(|X^{(4)})=1$$
$$(X^{(3)}X^{(5)}|\Gamma^{(15)})=(|\Gamma^{(25)})=(|X^{(1)})=(|X^{(2)})=(|X^{(5)})=1$$
$$(X^{(4)}X^{(4)}|\,)=(X^{(3)}X^{(3)}|\,)$$
$$(X^{(4)}X^{(5)}|\,)=(X^{(3)}X^{(5)}|\,)$$
$$(X^{(5)}X^{(5)}|\Gamma^{(1)})=(|\Gamma^{(2)})=(|\Gamma^{(15)})=(|\Gamma^{(25)})=(|X^{(1)})$$
$$=(|X^{(2)})=(|X^{(3)})=(|X^{(4)})=1;$$
$$(|\Gamma^{(12)})=(|X^{(5)})=2$$
$$(W^{(1)}W^{(1)}|\Gamma^{(1)})=(|\Gamma^{(12)})=(|\Gamma^{(25)})=(|X^{(1)})=(|X^{(4)})$$
$$=(|\Sigma^{(1)})=(|\Sigma^{(2)})=1$$
$$(W^{(1)}W^{(2)}|\Gamma^{(2)})=(|\Gamma^{(12)})=(|\Gamma^{(15)})=(|X^{(2)})=(|X^{(3)})$$
$$=(|\Sigma^{(1)})=(|\Sigma^{(2)})=1$$
$$(W^{(1)}W^{(3)}|\Gamma^{(15)})=(|\Gamma^{(25)})=(|X^{(5)})=(|\Sigma^{(1)})=(|\Sigma^{(2)})=1$$
$$(W^{(3)}W^{(3)}|\Gamma^{(1)})=(|\Gamma^{(12)})=(|\Gamma^{(25)})=(|X^{(2)})=(|X^{(3)})$$
$$=(|\Sigma^{(1)})=(|\Sigma^{(2)})=1$$
$$(W^{(3)}W^{(4)}|\Gamma^{(2)})=(|\Gamma^{(12)})=(|\Gamma^{(15)})=(|X^{(1)})=(|X^{(4)})$$
$$=(|\Sigma^{(1)})=(|\Sigma^{(2)})=1$$
$$(W^{(1)}W^{(4)}|\,)=(W^{(1)}W^{(3)}|\,)$$
$$(W^{(2)}W^{(2)}|\,)=(W^{(1)}W^{(1)}|\,)$$
$$(W^{(2)}W^{(3)}|\,)=(W^{(1)}W^{(3)}|\,)$$
$$(W^{(4)}W^{(4)}|\,)=(W^{(3)}W^{(3)}|\,)$$

representations of $\mathcal{G}(\mathbf{k}_j)/\mathcal{T}(\mathbf{k}_j)$ for one arm of the star. We must first find the conjugate subgroups for each of the other arms of the star, and then using the general theory we construct the space group irreducible representation as outlined in Sec. 3 above. The case of diamond is troublesome since the same rotational element may be combined with different fractional translation elements in the conjugate subgroups. For example, take wave vector $L_1=(\pi,\pi,\pi)(1/a)$ and $L_2=(\pi,-\pi,-\pi)(1/a)$, both in $\star L$; then $\{\boldsymbol{\delta}_{2y\bar{z}}|\boldsymbol{\tau}_1\}$ in $\mathcal{G}(L_1)/\mathcal{T}(L_1)$ is conjugate to $\{\boldsymbol{\delta}_{2y\bar{z}}|\boldsymbol{\tau}_2\}$ in $\mathcal{G}(L_2)/\mathcal{T}(L_2)$.

In Table VI we give the reduction coefficients for reduction of the ordinary Kronecker product of $\Gamma^{(m)}$ with each of the $\star X^{(m)}$, $\star L^{(m)}$, $\star W^{(m)}$, and $\star\Sigma^{(m)}$, and for the reduction of products of type (6.1), (6.2), (6.3), (6.7), and (6.8). All these coefficients were obtained using the reduction group method.

In Table VII we give the reduction coefficients for ordinary Kronecker products of $\Gamma^{(m)}$ with $\star\Delta^{(m)}$, $\star\Lambda^{(m)}$, and for the products

$$\star\Delta^{(m)}\otimes\star\Delta^{(m')}, \tag{6.9}$$

$$\star\Lambda^{(m)}\otimes\star\Lambda^{(m')}, \tag{6.10}$$

$$\star\Lambda^{(m)}\otimes\star\Delta^{(m')}, \tag{6.11}$$

In this table we have relabeled the representations for certain $\star\Delta^{(m)}$, so as to have a unique meaning for $\star\Delta'^{(m)}$ (see footnote a of Table VII). These coefficients were obtained using direct inspection.

In Table VIII, results for the symmetrized Kronecker square, and in Table IX, results for the cube are given. In certain cases, only the coefficients of types $(|\Gamma^{(m)})$ were obtained, as we have in mind applications to radiative processes; the remaining coefficients can be found, if needed, by our methods.

By way of illustration of the use of the tables consider

TABLE XII. Reduction coefficients in zinc blende.

$(\Gamma^{(2)}\Delta^{(1)}|\Delta^{(2)})=(\Gamma^{(2)}\Delta^{(2)}|\Delta^{(1)})=1$

$(\Gamma^{(2)}\Delta^{(m)}|\Delta^{(m)})=1 \quad m=3,4$

$(\Gamma^{(12)}\Delta^{(1)}|\Delta^{(1)})=(|\Delta^{(2)})=1$

$(\Gamma^{(12)}\Delta^{(2)}|\,)=(\Gamma^{(12)}\Delta^{(1)}|\,)$

$(\Gamma^{(12)}\Delta^{(3)}|\Delta^{(3)})=(|\Delta^{(4)})=1$

$(\Gamma^{(12)}\Delta^{(4)}|\,)=(\Gamma^{(12)}\Delta^{(3)}|\,)$

$(\Gamma^{(15)}\Delta^{(1)}|\Delta^{(1)})=(|\Delta^{(3)})=(|\Delta^{(4)})=1$

$(\Gamma^{(15)}\Delta^{(2)}|\Delta^{(2)})=(|\Delta^{(3)})=(|\Delta^{(4)})=1$

$(\Gamma^{(15)}\Delta^{(3)}|\Delta^{(1)})=(|\Delta^{(2)})=(|\Delta^{(3)})=1$

$(\Gamma^{(25)}\Delta^{(1)}|\,)=(\Gamma^{(15)}\Delta^{(2)}|\,)$

$(\Gamma^{(25)}\Delta^{(2)}|\,)=(\Gamma^{(15)}\Delta^{(1)}|\,)$

$(\Gamma^{(25)}\Delta^{(3)}|\,)=(\Gamma^{(15)}\Delta^{(3)}|\,)$

$(\Gamma^{(2)}\Lambda^{(1)}|\Lambda^{(2)})=1$

$(\Gamma^{(2)}\Lambda^{(2)}|\Lambda^{(1)})=1$

$(\Gamma^{(2)}\Lambda^{(3)}|\Lambda^{(3)})=1$

$(\Gamma^{(12)}\Lambda^{(1)}|\Lambda^{(3)})=1$

$(\Gamma^{(12)}\Lambda^{(2)}|\Lambda^{(3)})=1$

$(\Gamma^{(12)}\Lambda^{(3)}|\Lambda^{(1)})=(|\Lambda^{(2)})=(|\Lambda^{(3)})=1$

$(\Gamma^{(15)}\Lambda^{(1)}|\Lambda^{(1)})=(|\Lambda^{(3)})=1$

$(\Gamma^{(15)}\Lambda^{(2)}|\Lambda^{(2)})=(|\Lambda^{(3)})=1$

$(\Gamma^{(15)}\Lambda^{(3)}|\Lambda^{(1)})=(|\Lambda^{(2)})=1; \quad (|\Lambda^{(3)})=2$

$(\Gamma^{(25)}\Lambda^{(1)}|\Lambda^{(2)})=(|\Lambda^{(3)})=1$

$(\Gamma^{(25)}\Lambda^{(2)}|\Lambda^{(1)})=(|\Lambda^{(3)})=1$

$(\Gamma^{(25)}\Lambda^{(3)}|\,)=(\Gamma^{(15)}\Lambda^{(3)}|\,)$

$(\Delta^{(1)}\Delta^{(1)}|\Gamma^{(1)})=(|\Gamma^{(12)})=(|\Gamma^{(15)})=(|\Sigma^{(1)})=(|\Sigma^{(2)})=(|\Delta'^{(1)})=1$

$(\Delta^{(1)}\Delta^{(2)}|\Gamma^{(2)})=(|\Gamma^{(12)})=(|\Gamma^{(25)})=(|\Sigma^{(1)})=(|\Sigma^{(2)})=(|\Delta'^{(2)})=1$

$(\Delta^{(1)}\Delta^{(3)}|\Gamma^{(15)})=(|\Gamma^{(25)})=(|\Sigma^{(1)})=(|\Sigma^{(2)})=(|\Delta'^{(3)})=1$ [a]

$(\Delta^{(3)}\Delta^{(3)}|\Gamma^{(1)})=(|\Gamma^{(12)})=(|\Gamma^{(15)})=(|\Sigma^{(1)})=(|\Sigma^{(2)})=(|\Delta'^{(2)})=1$ [b]

$(\Delta^{(3)}\Delta^{(3)}|\Gamma^{(2)})=(|\Gamma^{(12)})=(|\Gamma^{(25)})=(|\Sigma^{(1)})=(|\Sigma^{(2)})=(|\Delta'^{(1)})=1$ [b]

$(\Lambda^{(1)}\Lambda^{(1)}|\Delta'^{(1)})=(|\Delta'^{(3)})=(|\Lambda'^{(1)})=1$ [a]

$(\Lambda^{(1)}\Lambda^{(2)}|\Delta'^{(2)})=(|\Delta'^{(3)})=(|\Lambda'^{(2)})=1$ [a]

$(\Lambda^{(1)}\Lambda^{(3)}|\Delta'^{(1)})=(|\Delta'^{(2)})=(|\Delta'^{(3)})=(|\Delta'^{(4)})=(|\Lambda'^{(3)})=1$

$(\Lambda^{(3)}\Lambda^{(3)}|\Lambda'^{(1)})=(|\Lambda'^{(2)})=(|\Lambda'^{(3)})=1; \quad (|\Delta'^{(1)})=(|\Delta'^{(2)})=(|\Delta'^{(3)})=(|\Delta'^{(4)})=2$

$(\Lambda^{(1)}(-\Lambda)^{(1)}|\Gamma^{(1)})=(|\Gamma^{(15)})=(|\Sigma'^{(1)})=1$ [c]

$(\Lambda^{(1)}(-\Lambda)^{(2)}|\Gamma^{(2)})=(|\Gamma^{(25)})=(|\Sigma'^{(2)})=1$

$(\Lambda^{(1)}(-\Lambda)^{(3)}|\Gamma^{(12)})=(|\Gamma^{(15)})=(|\Gamma^{(25)})=(|\Sigma'^{(1)})=(|\Sigma'^{(2)})=1$

$(\Lambda^{(3)}(-\Lambda)^{(3)}|\Gamma^{(1)})=(|\Gamma^{(2)})=(|\Gamma^{(12)})=1; \quad (|\Gamma^{(15)})=(|\Gamma^{(25)})=(|\Sigma'^{(1)})=(|\Sigma'^{(2)})=2$

[a] $\star\Delta^{(3)}$ and $\star\Delta^{(4)}$ are degenerate and interchangeable.
[b] The ambiguity in this reduction arises because of the degeneracy of $\star\Delta^{(3)}$ and $\star\Delta^{(4)}$.
[c] See text, Eqs. (7.1) and (7.2).

TABLE XIII. Reduction coefficients for symmetrized Kronecker square in zinc blende.

$([\Gamma^{(m)}]_{(2)}|\Gamma^{(1)})=1; \quad m=1,2$

$([\Gamma^{(12)}]_{(2)}|\Gamma^{(1)})=(|\Gamma^{(12)})=1$

$([\Gamma^{(m)}]_{(2)}|\Gamma^{(1)})=(|\Gamma^{(12)})=(|\Gamma^{(15)})=1; \quad m=15, 25$

$([L^{(m)}]_{(2)}|\Gamma^{(1)})=(|\Gamma^{(15)})=(|X^{(1)})=(|X^{(3)})=1; \quad m=1,2$

$([L^{(3)}]_{(2)}|\Gamma^{(1)})=(|\Gamma^{(12)})=(|\Gamma^{(25)})=(|X^{(2)})=(|X^{(4)})=(|X^{(5)})=1; \quad (|\Gamma^{(15)})=(|X^{(1)})=(|X^{(3)})=2$

$([X^{(m)}]_{(2)}|\Gamma^{(1)})=(|\Gamma^{(12)})=(|X^{(1)})=1; \quad m=1,2$

$([X^{(m)}]_{(2)}|\Gamma^{(1)})=(|\Gamma^{(12)})=(|X^{(3)})=1; \quad m=3,4$

$([X^{(5)}]_{(2)}|\Gamma^{(1)})=(|\Gamma^{(2)})=(|\Gamma^{(15)})=(|X^{(1)})=(|X^{(3)})=(|X^{(5)})=1; \quad (|\Gamma^{(12)})=2$

$([\Delta^{(m)}]_{(2)}|\Gamma^{(1)})=(|\Gamma^{(12)})=(|\Delta'^{(1)})=(|\Sigma^{(1)})=1; \quad m=1,2$

$([\Delta^{(m)}]_{(2)}|\Gamma^{(2)})=(|\Gamma^{(12)})=(|\Delta'^{(1)})=(|\Sigma^{(1)}); \quad m=3,4$

$([\Lambda^{(m)}]_{(2)}|\Delta'^{(1)})=(|\Lambda'^{(1)})=1; \quad m=1,2$

$([\Lambda^{(3)}]_{(2)}|\Lambda'^{(1)})=(|\Lambda'^{(3)})=(|\Delta'^{(2)})=(|\Delta'^{(3)})=1$ [a]; $(|\Delta'^{(1)})=2$

$([W^{(1)}]_{(2)}|\Gamma^{(1)})=(|\Gamma^{(12)})=(|X^{(1)})=(|X^{(4)})=(|\Sigma^{(1)})=1$

$([W^{(2)}]_{(2)}|\,)=([W^{(1)}]_{(2)}|\,)$

$([W^{(3)}]_{(2)}|\Gamma^{(1)})=(|\Gamma^{(12)})=(|X^{(2)})=(|X^{(3)})=(|\Sigma^{(1)})=1$

$([W^{(4)}]_{(2)}|\,)=([W^{(3)}]_{(2)}|\,)$

$([Z^{(1)}]_{(2)}|\Gamma^{(1)})=(|\Gamma^{(2)})=1; \quad (|\Gamma^{(12)})=2$ [b]

$([Z^{(2)}]_{(2)}|\Gamma^{(m)})=([Z^{(1)}]_{(2)}|\Gamma^{(m)})$ [b]

$([k]_{(2)}|\Gamma^{(1)})=(|\Gamma^{(2)})=1; \; (|\Gamma^{(12)})=2$

$(|\Gamma^{(15)})=(|\Gamma^{(25)})=3$ [b]

[a] $\star\Delta^{(3)}$ and $\star\Delta^{(4)}$ are degenerate and interchangeable.
[b] Only representations $\Gamma^{(m)}$ were obtained, using the basis function method.

the reduction of certain symmetrized Kronecker cubes in diamond (Table IX):

$$[\star X^{(3)}]_{(3)}=\Gamma^{(2+)}\oplus\Gamma^{(2-)}\oplus\Gamma^{(15+)}\oplus\Gamma^{(15-)}\oplus\star X^{(1)}\oplus\star X^{(2)}\oplus 4\,\star X^{(3)}\oplus 2\,\star X^{(4)}, \tag{6.12}$$

$$[\star X^{(4)}]_{(3)}=\Gamma^{(1+)}\oplus\Gamma^{(1-)}\oplus\Gamma^{(25+)}\oplus\Gamma^{(25-)}\oplus\star X^{(1)}\oplus\star X^{(2)}\oplus 2\,\star X^{(3)}\oplus 4\,\star X^{(4)}, \tag{6.13}$$

and

$$[\star X^{(1)}]_{(3)}=\Gamma^{(1+)}\oplus\Gamma^{(2-)}\oplus\Gamma^{(15-)}\oplus\Gamma^{(25+)}\oplus 4\,\star X^{(1)}\oplus 2\,\star X^{(2)}\oplus\star X^{(3)}\oplus\star X^{(4)}. \tag{6.14}$$

7. APPLICATION TO ZINC BLENDE: T_d^2

Zinc blende, T_d^2, is a subgroup[11] of diamond O_h^7. The invariant subgroup of translations (face-centered cubic) is identical in both space groups; the factor group $\mathcal{G}/\mathcal{T}$ now, however, consists of 24 coset representatives, namely, those rotations listed in Table I without fractionals.

The wave vectors and their components are identical in zinc blende and diamond, but the multiplicity s is different for certain **k**, as indicated in Table II. The wave vector selection rules which are different involve the stars $\star\Lambda$, $\star H$, $\star M$. In Table X, those wave vector selection rules for the ordinary Kronecker product,

[11] R. H. Parmenter, Phys. Rev. **100**, 573 (1955). We use essentially the notations of Parmenter; exceptions are noted in the appropriate table.

TABLE XIV. Reduction coefficients for symmerized Kronecker cube in zinc blende.

$$([\Gamma^{(m)}]_{(3)}|\Gamma^{(m)})=1;\quad m=1,2$$
$$([\Gamma^{(12)}]_{(3)}|\Gamma^{(1)})=(|\Gamma^{(2)})=(|\Gamma^{(12)})=1$$
$$([\Gamma^{(15)}]_{(3)}|\Gamma^{(1)})=(|\Gamma^{(25)})=1;\quad (|\Gamma^{(15)})=2$$
$$([\Gamma^{(25)}]_{(3)}|\Gamma^{(2)})=(|\Gamma^{(15)})=1;\quad (|\Gamma^{(25)})=2$$
$$([X^{(1)}]_{(3)}|\Gamma^{(1)})=(|X^{(2)})=1;\quad (|X^{(1)})=2$$
$$([X^{(3)}]_{(3)}|\Gamma^{(1)})=(|X^{(4)})=1;\quad (|X^{(3)})=2$$
$$([X^{(5)}]_{(3)}|\Gamma^{(1)})=(|\Gamma^{(2)})=(|\Gamma^{(15)})=(|\Gamma^{(25)})=(|X^{(1)})$$
$$=(|X^{(2)})=(|X^{(3)})=(|X^{(4)})=1;\quad (|X^{(5)})=6$$
$$([L^{(1)}]_{(3)}|L^{(3)})=1;\quad (|L^{(1)})=3;$$
$$([L^{(3)}]_{(3)}|L^{(1)})=(|L^{(2)})=6;\quad (|L^{(3)})=9.$$

or the symmetrized powers of two stars, which differ in zinc blende from the corresponding rules in diamond, are given.

Note that in T_d^2, $^\star\Lambda$ has 4 arms, and $^\star\Lambda$ and $^\star(-\Lambda)$ are to be considered distinct; $(\kappa,\kappa,\kappa)(1/a)$ and $(-\kappa,-\kappa,-\kappa)\times(1/a)$ are in distinct stars. Time reversal will obviously cause them to be degenerate but at present we consider these two stars distinct. Thus we have

$$^\star\Lambda\otimes{}^\star\Lambda={}^\star\Lambda'\oplus 2\,{}^\star\Delta', \tag{7.1}$$

where

$$\Lambda_1'=(2\kappa,2\kappa,2\kappa)(1/a),$$
$$\Delta_1'=(2\kappa,0,0)(1/a),$$

but

$$^\star\Lambda\otimes{}^\star(-\Lambda)=4\Gamma\oplus{}^\star\Sigma', \tag{7.2}$$

where

$$\Sigma_1'=(2\kappa,2\kappa,0)(1/a).$$

In Table XI we give reduction coefficients for the reduction of those zinc blende ordinary Kronecker products analogous to the diamond products reduced ln Table VI. These were obtained using the appropriate reduction group. In Table XII we give rules analogous to those listed for diamond in Table VII; these were obtained by direct inspection. Because of (7.1) and (7.2) there are two ways of carrying out the direct inspection reduction for products $^\star\Lambda^{(m)}\otimes{}^\star(-\Lambda)^{(m')}$ or $^\star\Lambda^{(m)}\otimes{}^\star\Lambda^{(m')}$; both of these products have identical characters for the 24 cosets in $\mathcal{G}/\mathcal{T}$; no ambiguity arises when we use the correct wave vector selection rules (8.1) or (8.2), depending on which product we mean to reduce. Note also the degeneracy between $^\star\Delta^{(3)}$ and $^\star\Delta^{(4)}$, already pointed out by Parmenter,[11] which means that $^\star\Delta^{(3)}$ and $^\star\Delta^{(4)}$ are interchangeable in the reductions.

In Tables XIII and XIV reduction coefficients are given for symmetrized Kronecker squares and cubes, respectively.

8. SUMMARY

Two general and rigorous methods are discussed for the complete reduction of the ordinary Kronecker products and the symmetrized Kronecker powers of full space group irreducible representations. These are applicable to any space group, and can easily be extended to include time-reversal and spin-orbit effects.

Explicit selection rules are obtained for the diamond and zinc-blende space groups, by applying these methods. A later paper will discuss applications of these rules to physical processes in the two space groups.

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