Symmetry analysis of Raman scattering and ir absorption by crystal surfaces

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The allowed transitions for ir absorption and Raman scattering are calculated for all 17 space groups of semi-infinite crystals. Expressions are also given for the Van Hove singularities which arise in the phonon and electron spectra at the surfaces of crystals.

INTRODUCTION

Measurements of the polarization dependence of the optical absorption due to electron transitions and measurements of the polarization dependence of the ir absorption and Raman scattering by phonons at crystal surfaces can be useful for studying the spectrum of excitations at a surface. The polarization dependence reflects the symmetry of the crystal surface and can be useful in identifying various models of surface reconstruction.

Interband electron absorption and ir absorption near the edge can provide useful information on the electron and phonon spectra near singular points. The existence of electron surface states and of surface phonon modes should lead to features in the absorption and scattering spectra which are not found in the bulk spectra. Some questions naturally arise here: Between which surface states (and between which surface states and which bulk states) can transitions occur? How does their intensity depend on the energy and the polarization?

The symmetry of the electron and phonon transitions can be analyzed in a unified way. The phonon and electron surface states should be classified on the basis of irreducible representations of the 17 space groups of semi-infinite crystals. The phonon and electron states (in the spin-zero case) are classified on the basis of vector representations. The electron states are classified on the basis of spinor representations if the spin-orbit interaction is taken into account or on the basis of ordinary vector representations if there is no spin-orbit interaction.

Strictly speaking, the bulk electron and phonon states in the continuous spectrum of a semi-infinite crystal should also be classified on the basis of the irreducible representations of 17 surface groups.

To learn about the possibility of transitions between surface states and bulk states, we should use the representations of the 17 groups of semi-infinite crystals. This is an obvious approach from the physical standpoint, since transitions between bulk states and surface states can occur only within the localization radius of the surface states.

For direct optical transitions between electron states and for ir absorption by phonons, it is sufficient to determine the nonzero matrix elements of the momentum operator.[1] In terms of their transformation properties, these elements are the same as coordinate components. For Raman scattering, the matrix elements are calculated from the product of two components of the momentum operator.[1]

For direct optical transitions and for ir absorption with the photon momentum ignored, the matrix element is nonzero if the product of the representations

$$D=D_\nu^{\mathbf{k}*}\times D_\mu^{\mathbf{k}}\times D_r$$

contains the unit representation. Here $D_\nu^{\mathbf{k}}$, $D_\mu^{\mathbf{k}}$ are representations of energy levels at the $\mathbf{k}$ point of the plane Brillouin zone, and D_r is the representation which transforms the coordinate components. For Raman scattering, the unit representation should be contained in the product of representations

$$D=D_\nu^{\mathbf{k}*}\times D_\mu^{\mathbf{k}}\times D_r^2.$$

The scheme for calculating the nonzero matrix elements is as follows: Select a point in the Brillouin zone. Determine the group of the wave vector and its irreducible representations at the given point. One must then deal with the invariance under time reversal. Three cases can arise:[2]

a) The representation $D_\nu^{\mathbf{k}}$ is itself an irreducible representation of some level.

b) $D_\nu^{\mathbf{k}}$ is a combination of two linearly independent, complex-conjugate representations.

c) $D_\nu^{\mathbf{k}}$ is a combination of two equivalent real representations.

The Herring criterion[3] is used to decide to which case the representation of a given level corresponds. For the final result, the given representation is doubled or not doubled depending on the particular case to which the star $\{\mathbf{k}\}$ of the wave vector corresponds:

1) $\mathbf{k}$ and $-\mathbf{k}$ are equivalent.

2) $\mathbf{k}$ and $-\mathbf{k}$ are not equivalent, but the complete space group contains a symmetry element which sends $\mathbf{k}$ into $-\mathbf{k}$.

3) $\mathbf{k}$ and $-\mathbf{k}$ appear in different stars.

The representation is doubled in cases b and c only in cases 1 and 2. In case 3, the representations are not combined.

SYMMETRY ANALYSIS OF THE MATRIX ELEMENTS

The results calculated for the nonzero matrix elements are given in the Appendix. Figures 1 and 2 show the types of plane lattices with the symmetry elements and the corresponding Brillouin zones. The symmetry points are indicated.

In most cases, representations of a space group are equivalent under projection to representations of point groups. For the representations of the point groups we use the notation of Bir and Pikus.[2] The corresponding characters of the point groups can be found in the same book.

The vibrational degrees of freedom are transformed by ordinary vector representations. The wave functions of electrons in the spin-zero case are transformed by the same representations. The spinor representations and the matrix elements for them belong solely to electron transitions when the spin-orbit interaction is taken into account.

There is a point to be noted here. The form of the electron spectrum near symmetry points was found in Ref. 4.

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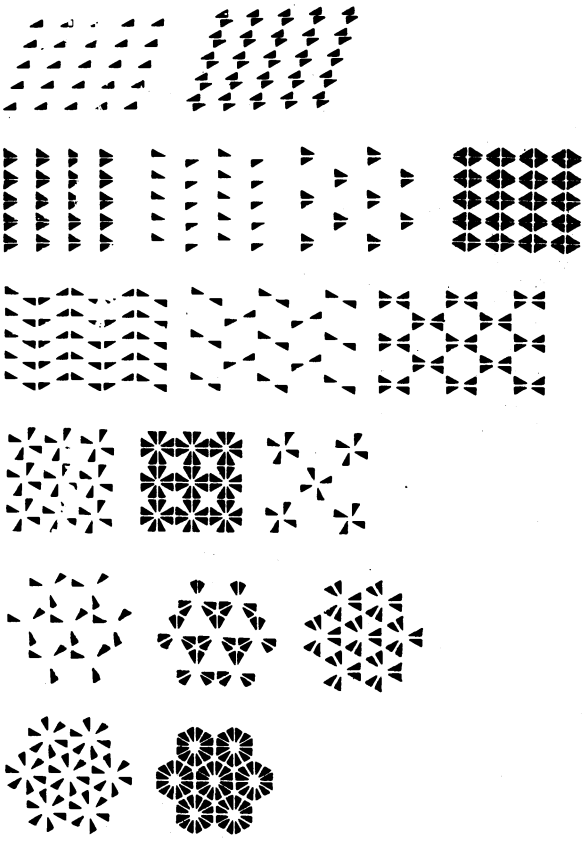

FIG. 1. Examples of the 17 three-dimensional lattices (see Ref. 7; see Ref. 8 for the group notation).

Those results are also valid in the spin-zero case for the phonon branches of the spectrum, with the one difference that $\varepsilon(\mathbf{k})$ should be replaced by $\omega^2(\mathbf{k})$ [here $\varepsilon(\mathbf{k})$ and $\omega(\mathbf{k})$ are the dispersion laws for the electrons and phonons, respectively].

Lattice 1 (p1). In lattice 1 there is only one symmetry element, $\{\varepsilon|\mathbf{R}\}$. In the Brillouin zone, one-dimensional representations A and A' are realized at the symmetry points Γ, A, B, and Y in the wave-vector group in both the spin-zero and spinor cases. In the spin-zero case, the one-dimensional representation corresponds to case a_1. In the spinor case it corresponds to c_1. Accordingly, it should be doubled. All the coordinate components fall in the one representation A. Transitions between levels are possible for any polarization.

Lattice 2 (p2). Lattice 2 has the symmetry elements $\{\varepsilon|\mathbf{R}\}$, $\{C_2|\mathbf{R}\}$. In the spin-zero case, two representations, A and B, are realized at all the symmetry points, Γ, A, B, and Y. The z, xy, xx, and yy components are transformed by the representation A, while the x, y, xz, and yz components are transformed by B. Both representations correspond to case a_1. In the spinor case, the representations A_1' and A_2' have complex-conjugate characters, $\chi(\varepsilon)=1$, $\chi(C_2)=\pm i$, and they belong to case b_1 according to the Herring criterion, since the symmetry points $\mathbf{k}$ and $-\mathbf{k}$ are equivalent. In the spinor case, transitions between levels are allowed for any polarization.

Lattice 3 (p1m1). The analysis of this lattice, in which there are two symmetry elements $\{\varepsilon|\mathbf{R}\}$, $\{\sigma_x|\mathbf{R}\}$ (σ_x is a symmetry plane parallel to the x axis), is analogous to that of the preceding case. There is the difference that the z, x, xz, xx, and yy components are transformed by the single representation A^+, while the y, xy, and yz components are transformed by the odd A^-.

Lattice 4 (p1g1). Lattice 4 contains, in addition to the unit element, a slip plane $\{\sigma_x|\tau+\mathbf{R}\}$ [$\tau=(a_x/2.0)$ is a nonprimitive translation vector which performs a translation of a half-period along the x axis]. The nonzero matrix elements at the Γ and Y points are found by analogy with the $p1m1$ group at point Γ, since the wave-vector group is the same as the point group of directions. To determine the representations at the X and S points, we find the factor system for the two generating elements:

$$\alpha=\omega(\varepsilon,\sigma_x)/\omega(\sigma_x,\varepsilon),\ \alpha=1,$$
$$\omega(\varepsilon,\sigma_x)=\exp[i(\mathbf{k}-\varepsilon^{-1}\mathbf{k})\tau_x]=1,$$
$$\omega(\sigma_x,\varepsilon)=\exp[i(\mathbf{k}-\sigma_x^{-1}\mathbf{k})0]=1.$$

The factor system belongs to class K_0 (Ref. 2), and the representations are under equivalent projection to vector representations. The characters of the representations can be found from the ordinary characters by multiplying the character for element σ_x by $\exp(i\pi/2)$ ($\mathbf{k}$ lies at the boundary of the Brillouin zone). In the spin-zero case, there are two one-dimensional representations with complex-conjugate characters. They correspond to case b_1. In the spinor case the representations belong to case b_1. In both cases the representations combine. The matrix elements are nonzero for any polarization.

At an arbitrary point on side D, the vector $\mathbf{k}$ is not equivalent to $-\mathbf{k}$, but the space group contains an element which sends $\mathbf{k}$ into $-\mathbf{k}$. In each case, we have version c_2, so there is a doubling of the equivalent representations. A degeneracy arises on the entire side. The matrix elements are nonzero for any polarization.

Lattice 5 (c1m1). Lattice 5 has the following symmetry elements: $\{\varepsilon|\mathbf{R}\}$, $\{\sigma_x|\mathbf{R}\}$. The calculation of the matrix elements reduces to the known cases for lattices 1 and 3.

Lattice 6 (p2m1). The symmetry elements of the lattice are $\{\varepsilon|\mathbf{R}\}$, $\{c_2|\mathbf{R}\}$, $\{\sigma_x|\mathbf{R}\}$, $\{\sigma_y|\mathbf{R}\}$. At the symmetry points Γ, X, Y, S we have case a_1 in the spin-zero case, and there are four one-dimensional representations: $A^\pm, B^\pm$. The spinor case also corresponds to a_1. At all points there is one two-dimensional representation, E'. The coordinate components are distributed in accordance with the representations $A^+(z)$, $A^-(xy)$, $B^+(y,yz)$, $B^-(x,xz)$. The vibrational degrees of freedom can be transformed only by the representations A^+, $B^\pm$. The z component of an axial vector is transformed by the representation A^-.

Lattice 7 (p2mg). In space group 7 there is a slip plane. The symmetry elements are $\{\varepsilon|\mathbf{R}\}$, $\{c_2|\mathbf{R}\}$, $\{\sigma_x|\mathbf{R}+\tau\}$, $\{\sigma_y|\mathbf{R}+\tau\}$. [The quantity τ is a translation of half a period along the x axis: $\tau=(a_x/2.0)$.] The calculation of the matrix elements at the Γ and Y points is analogous to the corresponding calculations for group 6. To find the representations at the X and S points, we determine the factor system for the generating elements:

$$\omega(c_2,\sigma_x)=\exp[i(\mathbf{k}-c_2^{-1}\mathbf{k})\tau]=-1,\ \alpha=-1,$$
$$\omega(\sigma_x,c_2)=\exp[i(\mathbf{k}-\sigma_x^{-1}\mathbf{k})0]=1.$$

The factor system belongs to class K_1. In this case the representations of the wave-vector group $D^{\mathbf{k}}(g)$ of the element $g=\{\mathbf{r}|\mathbf{R}+\tau\}$ are found from

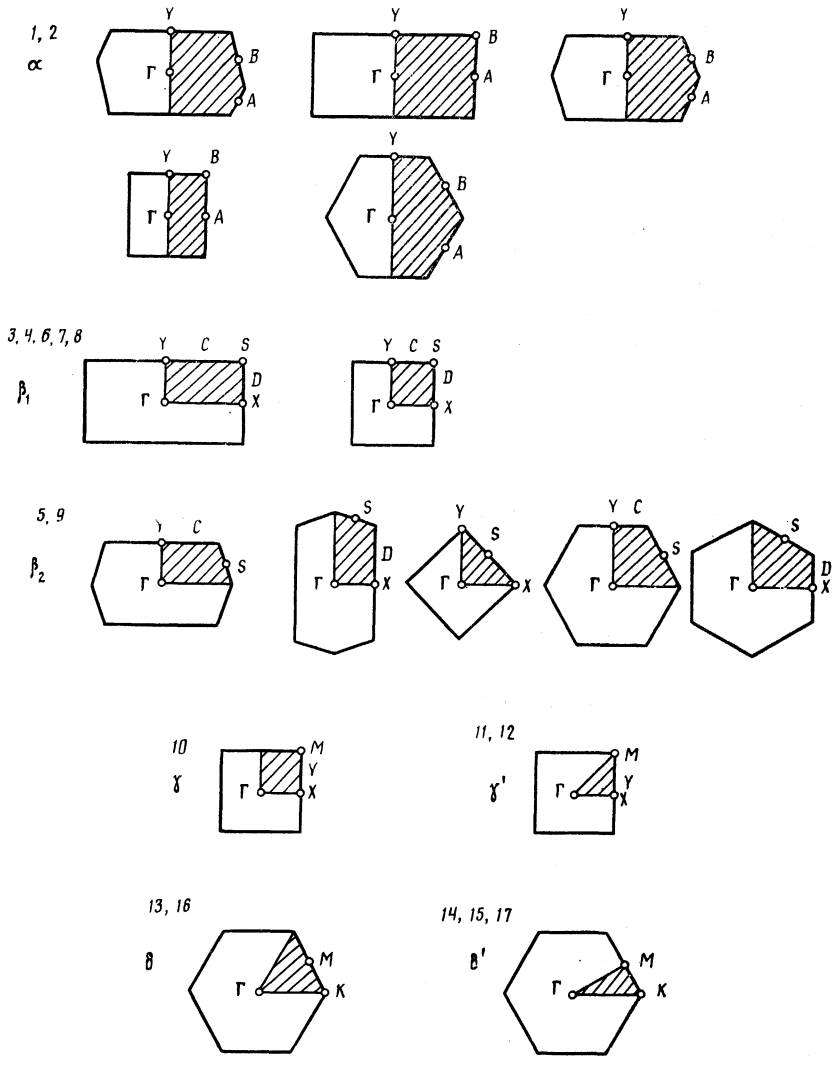

FIG. 2. Types of Brillouin zones for the various lattices. α—1, 2; β_1—3, 4, 6–8; β_2—5, 9; γ—10; γ'—11, 12; δ—13, 16; δ'—14, 15, 17.

$$D^{\mathbf{k}}(g)=\exp[i\mathbf{k}(\mathbf{R}+\boldsymbol{\tau})]u(\mathbf{r})D(\mathbf{r}).$$

Here $D(\mathbf{r})$ is the projection representation corresponding to the standard factor system. If A and B are matrices which correspond to the generating elements of the direction group C_{2v} ($a=c_2$, $b=\sigma_x$), then we have, according to Ref. 2,

$$D(\mathbf{r})=A^mB^n$$

for the standard factor system. For the C_{2v} group there is one two-dimensional projection representation for class K_1 (Ref. 2). Let us determine the factors $u(\mathbf{r})$ which send our factor system into the standard one. For spin-zero representations we have, according to Ref. 2,

$$u(c_2)=\omega\ (c_2,\ c_2)^{1/2}=1,$$
$$u(\sigma_x)=\omega\ \ (\sigma_x,\ \sigma_x)^{1/2}=1$$

for the generating elements. For the other elements we have

$$u(\sigma_y)=u(c_2\sigma_x)=u(c_2)\,u(\sigma_x)/\omega(c_2,\ \sigma_x)=-1.$$

For spinor representations the factor $u(\mathbf{r})$ should be replaced by $u(\mathbf{r})u'(\mathbf{r})$, where

$$u'(c_2)=i,\ \ u'(\sigma_x)=i,$$
$$u'(\sigma_y)=u'(c_2\sigma_x)=-1.$$

In both cases we have case b_1.

At an arbitrary point D on a side perpendicular to the slip plane, the factor system belongs to the class K_0. To demonstrate the point, we write

$$\omega(\varepsilon,\ \sigma_x)=\exp[i(\mathbf{k}-\varepsilon^{-1}\mathbf{k})\tau_x]=1,$$
$$\omega(\sigma_x,\ \varepsilon)=\exp[i(\mathbf{k}-\sigma_x^{-1}\mathbf{k})0]=1.$$

The representations are therefore equivalent under projection to vector representations and can be found from the usual ones by multiplying the character of element σ_x by the factor $\exp(i\mathbf{k}\cdot\boldsymbol{\tau})=\exp(i\pi/2)$. Since $\mathbf{k}$ and $-\mathbf{k}$ are not equivalent, but the space group contains an element which sends $\mathbf{k}$ into $-\mathbf{k}$, we have case c_2 in both cases.

Lattice 8 (p2gg). The symmetry elements of group 8 are $\{\varepsilon|\mathbf{R}\}$, $\{c_2|\mathbf{R}\}$, $\{\sigma_x|\mathbf{R}+\boldsymbol{\tau}\}$, $\{\sigma_y|\mathbf{R}+\boldsymbol{\tau}\}$ [$\boldsymbol{\tau}$ represents a translation of half a period along the x and y axes, $\boldsymbol{\tau}=(a_x/2,a_y/2)$]. The calculation of the nonzero matrix elements at the points Γ, X, Y, D, and C is analogous to the corresponding calculations for group 7.

Let us determine the representations at point S. The factor system for the generating element c_2 and σ_x is

$$\omega(c_2,\ \sigma_x)=\exp[i(\mathbf{k}-l_2^{-1}\mathbf{k})\tau]=1,$$
$$\omega(\sigma_x,\ c_2)=\exp[i(\mathbf{k}-\sigma_x^{-1}\mathbf{k})0]=1.$$

The factor system belongs to class K_0, so the characters of the representations of the wave-vector group can be found

from the characters of the direction group C_{2v}, by multiplying the characters of the elements σ_x, σ_y by i. Since $\mathbf{k}$ and $-\mathbf{k}$ are equivalent, we have case b_1. Consequently, the four one-dimensional representations combine into two two-dimensional representations.

In the spinor case, the factor system belongs to class K_1, where there is one two-dimensional representation, and we have case c_1.

Lattice 9 (c2mm). This lattice has the symmetry elements $\{\varepsilon|\mathbf{R}\}$, $\{c_2|\mathbf{R}\}$, $\{\sigma_x|\mathbf{R}\}$, $\{\sigma_y|\mathbf{R}\}$. The calculation of the matrix elements is analogous to the calculations for groups 2 and 6.

Lattice 10 (p4). In group 10 we have only a fourfold symmetry axis other than the unit element: $\{\varepsilon|\mathbf{R}\}$, $\{c_4|\mathbf{R}\}$. At the Γ and M points, all representations belong to class K_0 in the spin-zero and spinor cases. Representations with real characters belong to case a_1, and those with complex-conjugate characters combine in pairs. The Herring case b_1 is realized. At the X point, the calculations are analogous to the corresponding calculations at the Γ point of group 2 ($p2$).

The characters of the coordinate components and their products are as follows: x, y, xz, $yz-\chi(\varepsilon)=1$, $\chi(c_4)=\chi(c_4^3)=0$, $\chi(c_2)=-1$; $xy-\chi(\varepsilon)=1$, $\chi(c_4)=\chi(c_4^3)=-1, \chi(c_2)=1$. The unit transformation transforms z.

Lattice 11 (p4mm). In group 11 we have the following symmetry elements: $\{\varepsilon|\mathbf{R}\}$, $\{c_4|\mathbf{R}\}$, $\{c_4^3|\mathbf{R}\}$, $\{c_2|\mathbf{R}\}$, $\{\sigma_x|\mathbf{R}\}$, $\{\sigma_y|\mathbf{R}\}$, $\{\sigma_{xy}|\mathbf{R}\}$, $\{\sigma_{yx}|\mathbf{R}\}$ ($\sigma_{xy,yx}$ are diagonal symmetry planes). At the Γ and M points there are four one-dimensional representations and one two-dimensional representation in the spin-zero case. In the spinor case the representations belong to class K_1, where two two-dimensional representations arise. In both cases we have type a_1. The characters of the coordinate components and their products are as follows: x, xz; y, yz $-\chi(\varepsilon)=1$, $\chi(c_2)=1$, $\chi(c_4)=0$, $\chi(\sigma_x,\sigma_y)=1$, -1; -1, 1, $\chi(\sigma_{xy},\sigma_{yx})=0$, $xy-\chi(\varepsilon)=1$, $\chi(c_2)=1$, $\chi(c_4)=-1$, $\chi(\sigma_x,\sigma_y)=-1$, $\chi(\sigma_{xy},\sigma_{yx})=1$, and z is transformed according to the unit representation.

The calculations at the Y and X points reduce to the cases discussed above.

Lattice 12 (p4gm). Group 12 contains the symmetry elements $\{\varepsilon|\mathbf{R}\}$, $\{c_4|\mathbf{R}\}$, $\{c_4^3|\mathbf{R}\}$, $\{c_2|\mathbf{R}\}$, $\{\sigma_x|\mathbf{R}+\tau\}$, $\{\sigma_y|\mathbf{R}+\tau\}$, $\{\sigma_{xy}|\mathbf{R}+\tau\}$, $\{\sigma_{yx}|\mathbf{R}+\tau\}$ [$\tau=(a_x/2,a_y/2)$ is a nontrivial translation vector]. The calculations for the Γ point are analogous to the calculations in group 11. To determine the representations at the M point we find the factor system for the generating elements:

$$\omega(c_4,\sigma_x)=\exp[i(\mathbf{k}-c_4^{-1}\mathbf{k})\tau]=\exp(2ik_y\tau_y)=-1,$$
$$\omega(\sigma_x,c_4)=\exp[i(\mathbf{k}-\sigma_x^{-1}\mathbf{k})0]=1.$$

In the spin-zero case the factor system thus corresponds to class K_1, and projective representations should be used. In the C_{4v} group there are two projective two-dimensional representations with complex-conjugate characters. We can put our factor system in standard form. For this purpose we determine the factors $u(\mathbf{r})$. According to Ref. 2 we have

$$u(c_4)=\omega_{c_4n}^{1/4}(c_4,c_4)\varepsilon,\quad u(\sigma_x)=\omega^{1/2}(\sigma_x,\sigma_x),$$
$$n=4,\ c_4^n=\varepsilon,$$
$$m=2,\ \sigma_x^2=\varepsilon,$$
$$\varepsilon=\varepsilon_n^{m/2}=e^{m\pi i/n}=i.$$

We finally find

$$u(c_4)=1^{1/4}i=-1,$$
$$u(\sigma_x)=(-1)^{1/2}=i,$$
$$u(c_2)=u(c_4^2)=\omega_{c_4n}^{2/n}\varepsilon^2/\omega_{c_42}=-1,$$
$$u(\sigma_{xy})=u(c_4\sigma_x)=u(c_4)u(\sigma_x)/\omega(c_4,\sigma_x)=i.$$

The matrices of the representations for the wave-vector group can be written in the following form, where we are using the factors $u(\mathbf{r})$:

$$D^{\mathbf{k}}(c_4)=-1\begin{pmatrix}\varepsilon_8^3 & 0\\ 0 & \varepsilon_8\end{pmatrix},\quad D^{\mathbf{k}}(\sigma_x)=ie^{i\mathbf{k}\tau}\sigma_x,$$
$$D^{\mathbf{k}}(c_2)=-1\begin{pmatrix}\varepsilon_8^6 & 0\\ 0 & \varepsilon_8^2\end{pmatrix},\quad D^{\mathbf{k}}(\sigma_{xy})=ie^{i\mathbf{k}\tau}\begin{pmatrix}0 & \varepsilon_8^3\\ \varepsilon_8 & 0\end{pmatrix}$$

for the representation $P_1^{(1)}$ (Ref. 2), and for the representation $P_2^{(1)}$ we have

$$D^{\mathbf{k}}(c_4)=-1\begin{pmatrix}\varepsilon_8^{-1} & 0\\ 0 & \varepsilon_8^{-3}\end{pmatrix},\quad D^{\mathbf{k}}(\sigma_x)=ie^{i\mathbf{k}\tau}\sigma_x,$$
$$D^{\mathbf{k}}(c_2)=-1\begin{pmatrix}\varepsilon_8^{-2} & 0\\ 0 & \varepsilon_8^{-6}\end{pmatrix},\quad D^{\mathbf{k}}(\sigma_{xy})=ie^{i\mathbf{k}\tau}\begin{pmatrix}0 & \varepsilon_8^{-1}\\ \varepsilon_8^{-3} & 0\end{pmatrix},$$

where $\varepsilon_8=e^{i\pi/4}$.

To determine the case according to the Herring criterion at the point M, we need to sum over all the elements of the wave-vector group:

$$\Sigma=\sum_{g\mathbf{k}=-\mathbf{k}}\chi(g^2)=\mathrm{Sp}\{D^{\mathbf{k}}(\varepsilon)^2+2D^{\mathbf{k}}(c_4)^2+D^{\mathbf{k}}(c_2^2)^2+2D^{\mathbf{k}}(\sigma_x)^2+2D^{\mathbf{k}}(\sigma_{xy})^2\}$$
$$=2+2\cdot 0-2+2\cdot(-2)+2\cdot(+2)=0.$$

In other words we have case b_1. Consequently, two two-dimensional representations with complex-conjugate characters combine into one four-dimensional representation.

In the spinor case the factor system also belongs to class K_1. For a transition to the standard factor system in the spinor case we need to multiply the factors $u(\mathbf{r})$ found above by an additional factor of $u'(\mathbf{r})$. According to Ref. 2, we find

$$u'(c_4^k)=e^{i\pi k/2},$$
$$u'(\sigma_x)=e^{i\pi/2},$$
$$u'(c_4^k\sigma_x)=u'(c_4^k)u'(\sigma_x)=e^{i\pi(k+1)/2}.$$

In other words, there are two two-dimensional representations with real characters, each of which should be doubled, since we have case c_1 according to the Herring criterion. The calculation of the matrix elements at other points reduces to the cases already considered. The vibrational degrees of freedom cannot be transformed by the representation A_2 for the z component of an axial vector.

Lattice 13 (p3). Group 13 contains the elements $\{\varepsilon|\mathbf{R}\}$, $\{c_3|\mathbf{R}\}$. At the Γ point all representations belong to class K_0. In the spin-zero case one representation, with a real character, belongs to case a_1, while two others, with complex-conjugate characters, belong to case b_1 and combine into a two-dimensional representation. In the spinor case the real representation belongs to case c_1 and should be doubled. The two other one-dimensional representations belong to case b_1. The characters of the coordinate components are $\chi(\varepsilon)=1, \chi(c_3)=\chi(c_3^2)=-\frac{1}{2}$ for x, y, xy, xz, and yz. The z component falls in the unit representation.

The calculations for the M point reduce to known cases. At the K point there is case B_3, since $\Sigma = 0$. The reason is that the group has no element which sends $\mathbf{k}$ into $-\mathbf{k}$ or an equivalent. It is necessary to combine the stars, but not the representations themselves. All the representations are one-dimensional in both cases.

Lattice 14 (p3m1). The symmetry elements are $\{\varepsilon|\mathbf{R}\}$, $\{c_3|\mathbf{R}\}$, $\{c_3^2|\mathbf{R}\}$, $\{\sigma_y|\mathbf{R}\}$, $\{\sigma_1|\mathbf{R}\}$, $\{\sigma_2|\mathbf{R}\}$. At the Γ point in the spin-zero case there are two one-dimensional representations and one two-dimensional representation, which belong to case a_1. In the spinor case the representations belong to class K_0 (Ref. 2). Two one-dimensional representations with complex-conjugate characters combine into one, and we have case b_1 according to the Herring criterion. The two-dimensional representation belongs to case a_1. The characters of the coordinate components and their products are as follows: x, y, xy, xz, $yz - \chi(\varepsilon) = 1$; $\chi(2c_3) = 1$, $\chi(\sigma_{x,1,2}) = 0$; and z is transformed by the unit representation. The vibrational degrees of freedom cannot be transformed by the representation A_2 for the z component of an axial vector.

At the X point the wave-vector group is $p1m1$. In the spin-zero case we have case a_1, and in the spinor case we have b_1. At the K point the wave-vector group is $p3$. Here $\mathbf{k}$ and $-\mathbf{k}$ are not equivalent. However, the space group contains an element, not part of the wave-vector group, which sends $\mathbf{k}$ into $-\mathbf{k}$ from one star to another. We have case a_2 in both situations.

Lattice 15 (p31m). In this group there are the same symmetry elements as in group 14, but the symmetry plane $\{\sigma_x|\mathbf{R}\}$ is replaced by $\{\sigma_y|\mathbf{R}\}$. The calculations at the Γ and M points are analogous to those in the preceding case. At the K point the wave-vector group is $p3m1$. Since $\mathbf{k}$ and $-\mathbf{k}$ are not equivalent, and they are in different stars, we have case b_3.

Lattice 16 (p6). In space group $p6$ we have the symmetry elements $\{\varepsilon|\mathbf{R}\}$, $\{c_6|\mathbf{R}\}$, $\{c_6^5|\mathbf{R}\}$, $\{c_3|\mathbf{R}\}$, $\{c_3^2|\mathbf{R}\}$, $\{c_2|\mathbf{R}\}$. In both cases representations with complex-conjugate characters combine at the Γ point and belong to case b_1.

At the M point we have group $p2$. Since $\mathbf{k}$ and $-\mathbf{k}$ are equivalent, the representations belong to case 2. At the K point the wave-vector group is $p3$; $\mathbf{k}$ and $-\mathbf{k}$ are not equivalent; but the space group has an element which sends $\mathbf{k}$ into $-\mathbf{k}$. We have case 2. The characters of the wave-vector components are as follows: for x, y, xz, yz; $xy - \chi(\varepsilon) = 1$, $\chi(c_3, c_3^2) = -\frac{1}{2}\chi(c_2) = -1$; $1, \chi(c_6, c_6^5) = \frac{1}{2}; -\frac{1}{2}$.

Lattice 17 (p6mn). In group 17 we have the following symmetry elements: $\{\varepsilon|\mathbf{R}\}$, $\{c_6|\mathbf{R}\}$, $\{c_6^5|\mathbf{R}\}$, $\{c_3|\mathbf{R}\}$, $\{c_3^2|\mathbf{R}\}$, $\{c_2|\mathbf{R}\}$, $\{\sigma_x|\mathbf{R}\}$, $\{\sigma_y|\mathbf{R}\}$, $\{\sigma'|\mathbf{R}\}$, $\{\sigma_1|\mathbf{R}\}$, $\{\sigma_2|\mathbf{R}\}$, $\{\sigma_3|\mathbf{R}\}$. At the Γ point all representations belong to case a_1. At the M point the wave-vector group is $p2mm$, and the calculations reduce to those in the preceding cases. At the K point the group is $p31m$, but $\mathbf{k}$ and $-\mathbf{k}$ do not go into the same star. In the space group there is an element which sends $\mathbf{k}$ into $-\mathbf{k}$, so we have case a_2. The characters of the coordinate components and their products are x, y, xz, yz; $xy - \chi(\varepsilon) = 1$, $\chi(2c_3) = -\frac{1}{2}$, $\chi(3\sigma_x) = 0$, $\chi(c_2) = -1; 1, \chi(2c_6) = \frac{1}{2}; -\frac{1}{2}, \chi(3\sigma) = 0$. The z component is transformed by the unit representation. The vibrational degrees of freedom can be transformed by all representations other than A_3.

The results of the calculations are summarized in Table I (see the Appendix). The representations of the energy levels are denoted by the symbols corresponding to the point of the Brillouin zone with either a single index, which indicates the order number of the representation of the wave-vector group, or a double index, which is made up of the indices of the representations which combine due to time reversal. The projection-equivalent representations, if they exist, are shown in parentheses. The designation of the type with respect to time reversal is denoted in accordance with Ref. 2. The last column shows, in parentheses between representations, the coordinate components and their products for which the matrix elements are nonzero. If there are several points with identical symmetry in the Brillouin zone of the given lattice, the allowed transitions are given for only one of them. If there are points with identical symmetry in different lattices, the data are given for only one of them. For a point with symmetry properties which have already been found, we refer the reader to the place in the table where this symmetry was found first.

TWO-DIMENSIONAL VAN HOVE SINGULARITIES

Let us find the behavior of the density of states near the symmetry points. For a nondegenerate zone, spectra of three types are possible: a maximum, a minimum, and a saddle point. In the cases of the electron and phonon spectra we have, for the maximum,

$$\varepsilon(\mathbf{k}),\ \omega^2(\mathbf{k}) = k_x^2 + k_y^2. \tag{1}$$

We are omitting the coefficients of k_x, k_y, since we are interested in only the symmetry properties of the spectrum. The density of states is

$$\rho(\varepsilon) = \int \delta(\varepsilon - \varepsilon(\mathbf{k}))\, dk_x\, dk_y \propto \theta(\varepsilon), \tag{2}$$

$$\rho(\varepsilon) = \int \delta(\varepsilon - \omega(\mathbf{k}))\, dk_x\, dk_y \propto \theta(\varepsilon), \tag{3}$$

where $\theta(\varepsilon)$ is the unit step function.

In the case of a minimum for the electron spectrum, the density of states has the same functional form as for a maximum. For phonons, there cannot be a minimum for ω^2, since this situation would correspond to an instability of the lattice. A saddle point can be realized in a stable system only for the electron spectrum:

$$\rho(\varepsilon) = \int \delta(\varepsilon - (k_x^2 - k_y^2))\, dk_x\, dk_y. \tag{4}$$

A transformation to parabolic coordinates

$$k_x = \rho \operatorname{ch}\varphi, \quad k_y = \rho \operatorname{sh}\varphi$$

leads to

$$\rho(\varepsilon) = \int d\varphi. \tag{5}$$

This integral diverges. Formally, the density of the states is infinite. Physically, this circumstance has an obvious meaning: At energies ε close to zero, the constant-energy cross sections are parabolas, and the area which they bound is infinite. Formally, at a given energy $\varepsilon \neq 0$ it is possible to place an infinite number of particles in the zone since the branches of the parabola are unbounded. The reason is that for the given energy there are states with arbitrarily large values of k_x, k_y.

An infinity in the density of states means that it is necessary to consider the following terms in the expansion in k_x, k_y in the expression for $\varepsilon(\mathbf{k})$ at large $\mathbf{k}$. At small values of ε there is also a well-known logarithmic singularity. To see it explicitly, it is convenient to evaluate the integral (4) without switching to parabolic coordinates. We have

$$\rho(\varepsilon)=\int\delta(\varepsilon-(k_x^2-k_y^2))\,dk_x\,dk_y\propto\int_0^{q_c}dk_y/(\varepsilon+k_y^2)^{1/2}\propto\ln|\varepsilon|,$$

where q_c is a cutoff vector.

The doubly degenerate massless dispersion relation is

$$\varepsilon(\mathbf{k}),\ \omega^2(\mathbf{k})=\text{const}\pm(k_x^2+k_y^2)^{1/2}. \tag{6}$$

For phonons, a spectrum of this sort is possible near certain points on the boundary of the Brillouin zone with const >0. The densities of states for electrons and phonons are, respectively,

$$\rho(\varepsilon)\propto\varepsilon, \tag{7}$$

$$\rho(\varepsilon)\propto\varepsilon^3\theta(|\varepsilon|-\text{const}). \tag{8}$$

A spectrum with cubic splitting is possible only for electrons. This spectrum is

$$\varepsilon(\mathbf{k})=\pm(|k_x^3-3k_y^2k_x|^2)^{1/3},\ \pm(|k_y^3-3k_x^2k_y|^2)^{1/2}. \tag{9}$$

To calculate the density of states we note that

$$\left.\begin{aligned}k_x^3-3k_y^2k_x&=\mathrm{Re}\\ k_y^3-3k_x^2k_y&=\mathrm{Im}\end{aligned}\right\}\{[(k_x+ik_y)^3\pm(k_x-ik_y)^3].$$

It is convenient to introduce the new variables λ_1, λ_2 such that

$$(\lambda_1\pm i\lambda_2)^2=(k_x\pm ik_y)^3.$$

After this substitution, the integral reduces to

$$\rho(\varepsilon)\propto\int\delta(\varepsilon-|\lambda_1^2-\lambda_2^2|)\,(\lambda_1^2+\lambda_2^2)^{-1/3}\,d\lambda_1\,d\lambda_2. \tag{10}$$

The transformation to parabolic coordinates finally leads to

$$\rho(\varepsilon)\propto|\varepsilon|^{-1/3}.$$

In the case of the electron spectrum, the symmetry thus allows singularities of four types in the density of states: $\rho(\varepsilon)\propto$ const, ε, $|\varepsilon|^{-1/3}$, $\propto\ln|\varepsilon|$. In the case of phonons there are two types: $\rho(\varepsilon)\propto\varepsilon$, ε^3.

SOME EXAMPLES

Let us look at two examples of the use of the table (see the Appendix). We wish to determine for which polarization there will be optical transitions in the electron spectrum on Si(001)2×1 and Si(001)2×2 surfaces with asymmetric dimers (the Chadi model[5]). We assume that the axis of the dimers runs along the X axis. In the 2×1 structure, the space group 3 ($p1m1$) corresponds to the lattice symmetry. We know that there are two bands of surface states in the band gap.[5,6] At all the symmetry points of the surface Brillouin zone (see the table for lattice 3), there are two representations if we ignore the spin-orbit interaction (it is in this approximation that the calculations were carried out in Refs. 5 and 6). One representation is even, and the other odd, under reflection in a plane normal to the surface passing through the axis of the dimer. Transitions between these surface bands occur in the case of a polarization perpendicular to the axis of the dimer (x polarization). For the case of an x polarization along the axis of the dimer, transitions are forbidden. When the spin-orbit interaction is taken into account, no transitions are forbidden; transitions are possible for an arbitrary polarization. However, when the spin-orbit interaction is weak (and this is the case in silicon), the transitions occur primarily for the y polarization.

The Si(001)2×2 phase corresponds to space group 7 ($p2gm$), which has a nontrivial translation of half a period in the direction perpendicular to the axis of the dimer. In this group, there are four levels in the band gap at the Γ and Y points.[6] One pair, with approximately the same energies, derives from the level with symmetry A^+ in the Si(001)2×1 structure. The second pair, again with approximately equal energies, derives from the level with symmetry A^- in the Si(001)2×1 phase.

The first pair (with approximately equal energies) corresponds to the representations A^+, B^- (see the accompanying table for lattice 7). At the Γ and Y points, transitions within each pair (transitions with a low photon energy) are possible in the case of the x expolarization along the axis of the dimers. Transitions occur between levels of different pairs (with a higher photon energy) for the y polarization. At the boundary y of the Brillouin zone perpendicular to the grazing plane there is a degeneracy of the bands (see also the calculations of Ref. 6). Two bands in each pair merge, each into a separate degenerate band. Transitions between two degenerate bands are possible along the entire face for an arbitrary polarization of the radiation. When the spin-orbit interaction is taken into account, all selection rules in terms of polarization direction are eliminated.

APPENDIX

In the table below, the columns have the following meaning: 1—Lattice number; 2—lattice symmetry; 3—type of Brillouin zone; 4—symmetry points in the Brillouin zone; 5—wave-vector group; 6—point group corresponding to the wave-vector group if the latter exists; 7—irreducible representations; 8—symmetry under time reversal according to the Herring criterion; 9—nonzero matrix elements.

TABLE I.

1	2	3	4	5	6	7	8	9
1	$p1$	α	Γ, A, B, Y	$p1$	1	Γ_1, A_1, B_1, Y_1 (A) Γ_{11}', A_{11}', B_{11}', Y_{11}' $(A'+A')$	a_1 c_1	Γ_1 (*) Γ_1 Γ_{11}' (*) Γ_{11}'

(*Continued*)

TABLE I. (Cont'd)

1	2	3	4	5	6	7	8	9
2	$p2$	α	Γ, A, B, Y	$p2$	2	$\Gamma_{1,2}$, $A_{1,2}$, $B_{1,2}$, $Y_{1,2}$ (A, B)	a_1	$\Gamma_{1,2}(z, xx, yy, zz)\,\Gamma_{1,2}$; $\Gamma_1(x, y, xy, xz, yz)\,\Gamma_2$
						Γ_{12}', A_{12}', B_{12}', Y_{12}' $(A_1' + A_2')$	b_1	$\Gamma_{12}'(*)\,\Gamma_{12}'$
3	$p1m1$	β_1	Γ, X, Y, S	$p1m1$	$1m$	Γ_1, X_1, Y_1, S_1 (A^+, A^-)	a_1	$\Gamma_{1,2}(x, z, xx, yy, zz, xz)\,\Gamma_{1,2}$; $\Gamma_1(y, xy, yz)\,\Gamma_2$
						Γ_{12}', X_{12}', Y_{12}', S_{12}' $(A_1' + A_2')$	b_1	$\Gamma_{12}'(*)\,\Gamma_{12}'$
4	$p1g1$	β_1	Γ, Y	$p1g1$	$1m$	Γ_1, Y_1 (A^+, A^-)	a_1	№ 3, Γ
						Γ_{12}', Y_{12}' $(A_1' + A_2')$	b_1	
			X, S	$p1g1$		X_{12}, S_{12}	b_1	$X_{12}(*)\,X_{12}$
			D	$p1$		X_{11}', X_{22}', S_{11}', S_{22}'	c_1	$X'_{11,\,22}(*)\,X'_{11,\,22}$;
					1	$D_{11}(A + A)$	c_2	$X_{11}'(*)\,X_{22}'$
						$D_{11}'(A' + A')$	c_2	$D_{11}(*)\,D_{11}$; $D_{11}'(*)\,D_{11}'$
5	$c1m1$	β_2	Γ, X, Y	$c1m1$	$1m$	Γ_1, X_1, Y_1 (A^+, A^-)	a_1	№ 3, Γ
						Γ_{12}', X_{12}', Y_{12}' $(A_1' + A_2')$	b_1	
			S	$p1$	1	$S_1(A)$	a_1	$S_1(*)\,S_1$
						$S_{11}'(A' + A')$	c_1	$S_{11}'(*)\,S_{11}'$
6	$p2mm$	β_1	Γ, X, Y, S	$2mm$	$2mm$	$\Gamma_{1,2}$, $X_{1,2}$, $Y_{1,2}$, $S_{1,2}$ $(A^{\pm}, B^{\pm})$	a_1	$\Gamma_{1,\,2,\,3,\,4}(z, xx, yy, zz)$ $\Gamma_{1,\,2,\,3,\,4}$; $\Gamma_1(xy)\,\Gamma_2$; $\Gamma_1(y, yz)\,\Gamma_3$; $\Gamma_1(x, xz)\,\Gamma_4$; $\Gamma_2(x, xz)\,\Gamma_3$; $\Gamma_2(y, yz)\,\Gamma_4$; $\Gamma_3(xy)\,\Gamma_4$
						Γ_1', X_1', Y_1', S_1' (E')	a_1	$\Gamma_1'(*)\,\Gamma_1'$
7	$p2mg$	β_1	Γ, Y	$p2mg$	$2mm$	$\Gamma_{1,\,2}$, $Y_{1,\,2}(A, B)$	a_1	№ 6, Γ
						Γ_1', $Y_1'(E')$	a_1	
			X, S	$p2mg$		X_1, S_1	a_1	$X_1(*)\,X_1$
						X_{12}', X_{34}', S_{12}', S_{34}'	b_1	$X'_{12,\,34}(*)\,X'_{12,\,34}$; $X_{12}'(*)\,X_{34}'$
			D	$p1m1$	$1m$	$D_{12}(A^+ + A^-)$	b_2	$D_{12}(*)\,D_{12}$
						$D_{12}'(A_1' + A_2')$	b_2	$D_{12}'(*)\,D_{12}'$
8	$p2gg$	β_1	Γ	$p2gg$	$2mm$	$\Gamma_{1,2}(A, B)$	a_1	№ 6, Γ
						$\Gamma_1'(E')$	a_1	
			X, Y	$p2gg$		X_1, Y_1	a_1	$X_{1,\,2}(*)\,X_{1,\,2}$; $X_1(*)\,X_2$
						X_{12}', X_{34}', Y_{12}', Y_{34}'	b_1	$X'_{12,\,34}(*)\,X'_{12,\,34}$; $X_{12}'(*)\,X_{34}'$;
			D, C	$p1g1$		D_{12}, $S_{12}(A^+ + A^-)$	b_2	$D_{12}(*)\,D_{12}$
						D_{12}', C_{12}' $(A_1' + A_2')$	b_2	$D_{12}'(*)\,D_{12}'$
								$S_{12,\,34}(x, z, xx, yy, zz)$ $S_{12,\,34}$
			S	$p2gg$		S_{12} S_{11}'	b_1 c_1	$S_{12}(y, xy, yz)\,S_{34}$; $S_{11}'(*)\,S_{11}'$
9	$c2mm$	β_2	Γ, X, Y	$c2mm$	$2mm$	$\Gamma_{1,\,2}$, $X_{1,\,2}$, $Y_{1,\,2}$ (A, B)	a_1	№ 6, Γ
						Γ_1', X_1', $Y_1'(E')$	a_1	
			S	$p2$	2	$S_{1,\,2}(A, B)$	a_1	№ 2, Γ
						$S_{12}'(A_1' + A_2')$	b_1	
10	$p4$	γ	Γ, M	$p4$	4	$\Gamma_{1,\,2}$, $M_{1,2}(A, B_1)$	a_1	$\Gamma_{1,\,2}(z, xx, yy, zz)\,\Gamma_{1,\,2}$;
						Γ_{34}, $M_{34}(B_2 + B_3)$	b_1	$\Gamma_1(xx, xy, yy)\,\Gamma_2$; $\Gamma_{34}(z, xx, xy, yy, zz)\,\Gamma_{34}$; $\Gamma_{12}(x, y, xz, yz, xy)\,\Gamma_{34}$
						Γ_{12}', $M_{12}'(A_1' + B_2')$	b_1	$\Gamma'_{12,\,34}(x, y, z, xx, yy, zz,$
						Γ_{34}', $M_{34}'(A_2' + B_1')$	b_1	$xz, yz)\,\Gamma'_{12,\,34}$; $\Gamma_{12}'(x, y,$ $xx, yy, xy, xz, yz)\,\Gamma_{34}'$
			X	$p2$	2	$X_{1,2}(A, B)$	a_1	№ 2, Γ
						$X_{12}'(A_1' + A_2')$	b_1	
11	$p4mm$	γ	Γ, M	$p4mm$	$4mm$	$\Gamma_{1,\,2,\,3,\,4}$, $M_{1,\,2,\,3,\,4}$ $(A_{1,\,2}, B_{1,\,2})$	a_1	$\Gamma_{1,\,2,\,3,\,4,\,5}(z, xx, yy, zz)\,\Gamma_{1,\,2,\,3,\,4}$; $\Gamma_1(xx, yy)\,\Gamma_3$;

(*Continued*)

TABLE I. (Cont'd)

1	2	3	4	5	6	7	8	9
						$\Gamma_5 M_5\,(E)$	a_1	$\Gamma_1\,(xy)\,\Gamma_4$; $\Gamma_1\,(x,\ y,\ xz,\ yz)\,\Gamma_5$; $\Gamma_2\,(xy)\,\Gamma_3$; $\Gamma_2\,(x,\ y,\ xz,\ yz)\,\Gamma_5$; $\Gamma_3\,(x,\ y;\ xz,\ yz)\,\Gamma_5$; $\Gamma_4\,(x,\ y,\ xz,\ yz)\,\Gamma_5$; $\Gamma_2\,(xx,\ yy)\,\Gamma_4$
						$\Gamma'_{1,\,2}$, $M'_{1,\,2}$ $(E_1',\ E_2')$	a_1	$\Gamma'_{1,\,2}\,(x, z, xy, xz, yz)\,\Gamma'_{1,\,2}$; $\Gamma_1'\,(x,\ y,\ xx,\ yy,\ xy,\ xz,\ yz)\,\Gamma_2'$
			X	$p2mm$	$2mm$	$X_{1,\,2}\,(A,\ B)$	a_1	№ 6, Γ
						$X_1'\,(E')$	a_1	
12	$p4gm$	γ'	Γ	$p4gm$	$4mm$	$\Gamma_{1,\,2,\,3,\,4}\,(A_{1,2},\ B_{1,2})$	a_1	№ 11, Γ
						$\Gamma_5\,(E)$	a_1	
						$\Gamma'_{1,\,2}$	a_1	
			X	$p2gg$		X_1	a_1	№ 8, X, Y
						X_{12}', X_{34}'	b_1	
			Y	$p1g1$		$Y_{12}\,(A^+ + A^-)$	b_2	№ 8, D, C
						$Y_{12}'\,(A_1' + A_2')$	b_2	
			M	$p4gm$		$M_{11} + M_{22}$	b_1	$M_{11} + M_{22}$ (*) $M_{11} + M_{22}$
						$M_{11}' + M_{22}'$	b_1	$M_{11}' + M_{22}'$ (*) $M_{11}' + M_{22}$
13	$p3$	δ	Γ	$p3$	3	$\Gamma_1\,(A)$	a_1	$\Gamma_1\,(z,\ xx,\ yy,\ zz)\,\Gamma_1$; Γ_{23} (*) Γ_{23};
						$\Gamma_{23}\,(B_1 + B_2)$	b_1	$\Gamma_1\,(x,\ y,\ xy,\ xz,\ yz,\ xx,\ yy)\,\Gamma_{23}$
						$\Gamma_{11}'\,(A' + A')$	c_1	$\Gamma_{11}'\,(z,\ xx,\ yy,\ zz)\,\Gamma_{11}'$; Γ_{22}' (*) Γ_{22}';
						$\Gamma_{22}'\,(B_1' + B_2')$	b_1	$\Gamma_{11}'\,(x,\ y,\ xy,\ xz,\ yz,\ xx,\ yy)\,\Gamma_{22}'$
			M	$p1$	1	$M_1\,(A)$	a_1	№ 1, Γ
						$M_{11}'\,(A' + A')$	c_1	
						$K_{1,\,2,\,3}\,(A,\ B_{1,\,2})$	b_3	$K_{1,\,2,\,3}\,(z,\ zz,\ xx,\ yy)\,K_{1,\,2,\,3}$; $K_1\,(x,\ y,\ xz,\ yz,\ xx,\ yy)\,K_{2,3}$; $K_2\,(z,\ zz,\ xx, yy)\,K_3$, $K'_{1,\,2,\,3}\,(z, zz, xx,\ yy)\,K'_{1,\,2,\,3}$; $K_1'\,(x,\ y,\ xy,\ xz,\ yz,\ xx,\ yy)\,K'_{2,\,3}$; $K_2'\,(x, y, xz, yz, xx, yy)\,K_3'$
			K	$p3$	3	$K'_{1,\,2,\,3}\,(A',\ B'_{1,\,2})$	b_3	
14	$p3m1$	δ'	Γ	$p3m1$	$3m$	$\Gamma_{1,\,2}\,(A_{1,\,2})$	a_1	$\Gamma_{1,\,2}\,(z,\ zz,\ xx,\ yy)\,\Gamma_{1,2}$
						$\Gamma_3\,(E)$	a_1	$\Gamma_{1,\,2}\,(x,\ y,\ xy,\ xz,\ yz,\ xx,\ yy)\,\Gamma_3$; Γ_3 (*) Γ_3
						$\Gamma_{12}'\,(A_1' + A_2')$	b_1	$\Gamma'_{12,\,3}$ (*) $\Gamma'_{12,\,3}$; $\Gamma_{12}'\,(z,\ zz,\ xx,\ yy)\,\Gamma_3'$
						$\Gamma_3'\,(E')$	a_1	
			M	$p1m1$	$1m$	$M_1\,(A^+ + A^-)$	a_1	№ 3, Γ
						$M_{12}'\,(A_1' + A_2')$	b_1	
			K	$p3$	3	$K_{1,\,2,\,3}\,(A_1,\ B_{1,\,2})$	a_2	№ 13, K
						$K'_{1,\,2,\,3}\,(A_1',\ B'_{1,\,2})$	a_2	
15	$p3m1$	δ'	Γ	$p3m1$	$3m$	$\Gamma_{1,\,2}\,(A_{1,\,2})$	a_1	№ 14, Γ
						$\Gamma_3\,(E)$	a_1	
						$\Gamma_{12}'\,(A_1' + A_2')$	b_1	
						$\Gamma_3'\,(E')$	a_1	
			M	$p1m1$	$1m$	$M_{1,\,2}\,(A^+\,A^-)$	a_1	№ 3, Γ
						$M_{12}'\,(A_1' + A_2')$	b_1	
			K	$p31m$	$3m$	$K_{1,\,2}\,(A_1,\ A_2)$	b_3	$K_{1,\,2}\,(z,\ zz,\ xx,\ yy)\,K_{1,\,2}$; K_3 (*) K_3;
						$K_3\,(E)$	b_3	$K_{1,\,2}\,(x,\ y,\ xy,\ xz,\ yz,\ xx,\ yy)\,K_3$
						$K'_{1,\,2}\,(A_1',\ A_2')$	b_3	$K'_{1,\,2}\,(z,\ zz,\ xx,\ yy)\,K'_{1,\,2}$; K_3' (*) K_3'
						K_3', (E')	b_3	$K'_{1,\,2}\,(x,\ y,\ xy,\ xz,\ yz,\ xx,\ yy)\,K_3'$
16	$p6$	δ	Γ	$p6$	6	$\Gamma_{1,\,2}\,(A_{1,\,2})$	a_1	$\Gamma_{1,\,2}\,(z,\ zz,\ xx,\ yy)\,\Gamma_{1,\,2}$;
						Γ_{34}, Γ_{56}	b_1	$\Gamma_{34,\,56}\,(z,\ zz,\ xx,\ yy,\ xy)\,\Gamma_{34,\,56}$; $\Gamma_1\,(xy)\,\Gamma_{34}$;
						$(B_1 + B_3,\ B_2 + B_4)$		$\Gamma_1\,(x,\ y,\ xz,\ yz)\,\Gamma_{56}$; $\Gamma_2\,(x,\ y,\ xz,\ yz)\,\Gamma_{34}$; $\Gamma_2\,(xy,\ xx,\ yy)\,\Gamma_{56}$; $\Gamma_{34}\,(x,\ y,\ xz,\ yz)\,\Gamma_{56}$
						$\Gamma_{12}'\,(A_1' + A_2')$	b_1	$\Gamma_{12}'\,(z,\ zz,\ xx,\ yy)\,\Gamma_{12}'$;
						Γ_{34}', Γ_{56}'	b_1	$\Gamma'_{34,\,56}\,(x,\ y,\ z,\ xz,\ yz,\ zz,\ xx,\ yy)\,\Gamma'_{34,\,56}$; $\Gamma_{12}'\,(x,\ y,$
						$(B_1' + B_4',\ B_2' + B_3')$		

(Continued)

TABLE I. (Cont'd)

1	2	3	4	5	6	7	8	9
								$xz, yz, xy, xx, yy)\,\Gamma'_{34,\,56}$; $\Gamma_{34}'(xx, yy, xy)\,\Gamma_{56}'$
			M	$p2$	2	$M_{1,\,2}(A, B)$ $M_{12}'(A_1' + A_2')$	a_1 b_1	№ 2, Γ
			K	$p3$	3	$K_1(A)$ $K_{23}(B_1 + B_2)$ $K_1'(A')$ $K_{23}'(B_1' + B_2')$	a_2 b_2 a_2 b_2	№ 13, Γ
17	$p6mm$	δ′	Γ	$p6mm$	$6m$	$\Gamma_{1,\,2,\,3,\,4}(A_{1,\,2,\,3,\,4})$ $\Gamma_{5,\,6}(E_{1,\,2})$ $\Gamma'_{1,\,2}(E'_{1,\,2})$	a_1 a_1 a_1	$\Gamma_{1,\,2,\,3,\,4}(z, zz; xx, yy)\,\Gamma_{1,\,2,\,3,\,4}$; $\Gamma_{5,\,6}(z, xy, zz, xx, yy)\,\Gamma_{5,\,6}$; $\Gamma_1(xy)\,\Gamma_5$; $\Gamma_1(x, y, xz, yz)\,\Gamma_6$; $\Gamma_2(x, y, xz, yz)\,\Gamma_5$; $\Gamma_2(xy, xx, yy)\,\Gamma_6$; $\Gamma_3(xy, xx, yy)\Gamma_5$; $\Gamma_3(x, y, xz, yz)\,\Gamma_6$; $\Gamma_4(x, y, xz, yz)\,\Gamma_5$; $\Gamma_4(xy, xx, yy)\,\Gamma_6$
						$\Gamma_3'(E_3')$	a_1	$\Gamma'_{1,\,2}(x, y, z, xz, yz, zz, xx, yy)\,\Gamma'_{1,\,2}$; $\Gamma_3'(z, zz, xx, yy)\,\Gamma_3'$; $\Gamma_1'(xy, xx, yy)\,\Gamma_2'$; $\Gamma'_{1,\,2}(x, y, xz, yz, xy, xx, yy)\,\Gamma_3'$
			M	$p2mm$	$2mm$	$M_{1,\,2}(A, B)$ $M_{12}'(A_1' + A_2')$	a_1 b_1	№ 6, Γ
			K	$p31m$	$3m$	$K_{1,\,2}(A_{1,\,2})$ $K_3(E)$ $K'_{1,\,2}(A'_{1,\,2})$ $K_3'(E')$	a_2 a_2 a_2 a_2	№ 15, K

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