

## Physical applications of crystallographic color groups: Tensor fields in crystals

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The theory of permutational crystallographic color groups is used to construct tables of the  $k=0$  irreducible representations whose basis functions are linear combinations of the components of tensor fields defined on the atoms of an arbitrary crystal. As examples of their use, these tables are shown to be applicable in determining the  $k=0$  vibrational and magnetic modes of a crystal, the infrared and Raman-active vibrational modes, in testing the validity of the Jahn-Teller theorem in crystals, and in applying the tensor-field criterion in the Landau theory of continuous phase transitions in crystals.

### I. INTRODUCTION

In many problems in solid-state physics it is often necessary to determine the irreducible representations of the symmetry group of the crystal whose basis functions are linear combinations of components of tensors defined on the atoms of the crystal. In lattice vibrational problems, one determines the irreducible representations whose basis functions are combinations of components of a three-component tensor, the displacements, of each of the atoms.<sup>1-4</sup> These irreducible representations of the symmetry group  $G$  of the crystal are contained in the direct product of the polar vector representation  $D_G^V$  and the permutation representation  $D_G^{\text{perm}}$  of the atoms of the crystal. The permutation representation characterizes how the atoms of the crystal permute under elements of the symmetry space group of the crystal. In determining possible types of magnetic ordering in crystals, one can determine the irreducible representations of the nonmagnetic symmetry group of the crystal whose basis functions, the magnetic modes, are linear combinations of the atomic spins.<sup>5-8</sup> These irreducible representations are contained in the direct product of the axial vector representation  $D_G^A$  and

the permutation representation  $D_G^{\text{perm}}$  of the magnetic atoms. In the general case, the problem is to determine the irreducible representations contained in the direct product of a tensor representation  $D_G^T$ , whose basis functions are the components of the tensor defined on the atoms, and the permutation representation  $D_G^{\text{perm}}$  of the atoms of the crystal. We refer to this direct product representation as the tensor field representation  $D_G^{\text{TF}}$  of the crystal.

Central in determining the irreducible representations contained in the tensor field representation, is the problem of determining the irreducible representations contained in the permutation representation  $D_G^{\text{perm}}$ . Using the theory of permutational color groups, Litvin, Kotzev, and Birman<sup>9</sup> have derived and tabulated all  $k=0$  irreducible representations contained in the permutation representation  $D_G^{\text{perm}}$  for all possible crystals of all space-group symmetry  $G$ . In Sec. II we briefly review the method of Litvin, Kotzev, and Birman.<sup>9</sup> We then derive and tabulate all  $k=0$  irreducible representations contained in the tensor-field representation  $D_G^{\text{TF}}$ , for all possible crystals of all space-group symmetry, in the cases where the tensor representation  $D_G^T$  is  $D_G^V$ , the polar vector representation,  $D_G^A$ , the axial vector representation,  $D_G^A \times D_G^V$ , and

$(D_G^V)_{[2]}$ . Applications of these tables in determining lattice vibrational modes, infrared and Raman-active lattice vibrations, in the Jahn-Teller theorem in crystals, magnetic modes, and equitranslational phase transitions are given in Sec. III.

## II. TENSOR-FIELD REPRESENTATION

Let  $T_\alpha$ ,  $\alpha=1,2,\dots,q$  be the  $q$  components of a tensor  $T$  defined on the atoms, at position  $r_{ij}$ , of a crystal of space-group symmetry  $G$ . Let  $D_G^T$  be the tensor representation of  $G$  whose basis functions are the  $q$  components of the tensor  $T$ , and  $D_G^{\text{TF}}$  the tensor-field representation of  $G$  whose basis functions are the components of the tensor field  $T_{i\alpha} \equiv T(r_i)_\alpha$ ,  $\alpha=1,2,\dots,q$ ,  $i=1,2,\dots$  defined on the atoms of the crystal. The tensor-field representation  $D_G^{\text{TF}}$  is related to the tensor representation  $D_G^T$  by

$$D_G^{\text{TF}} = D_G^{\text{perm}} \times D_G^T, \quad (1)$$

where  $D_G^{\text{perm}}$  is the permutation representation of  $G$ , representing how the atoms of the crystal permute under elements of the space group  $G$ .

A crystal of space-group symmetry  $G$  can be partitioned into "simple crystals."<sup>10</sup> Each simple crystal consists of all atoms of the crystal whose position vectors can be obtained by applying all elements of the space group  $G$  to any one position vector  $r$ , and is said to be generated by  $G$  from  $r$ . A crystal can be considered as consisting of a certain number of simple crystals, no two simple crystals having atoms in common, and the elements of  $G$  permute the atoms of each simple crystal among themselves.

For a single simple crystal generated by  $G$  from  $r$ , the permutation representation  $D_G^{\text{perm}}$  is given by<sup>9</sup>

$$D_G^{\text{perm}} = D_G^{S(r)} \equiv D_{S(r)}^1 \uparrow G, \quad (2)$$

where  $S(r)$  is the subgroup of all elements of  $G$  such that  $gr=r$ , and  $D_{S(r)}^{S(r)}$  is the representation of  $G$  induced by the identity representation  $D_{S(r)}^1$  of  $S(r)$ . The tensor-field representation, Eq. (1), can then be written as

$$D_G^{\text{TF}} = D_G^{S(r)} \times D_G^T. \quad (3)$$

The tensor-field representation is in general reducible, and in this paper we are interested in determining the  $k=0$  irreducible representations contained in this representation.

Because the tensor representation  $D_G^T$  describes the rotational properties of the components of the

tensor  $T$ , it contains only  $k=0$  irreducible representations  $D_G^{(0,\nu)}$  of the space group  $G$ . From Eq. (3) it follows that the  $k$  dependence of the irreducible representations contained in the tensor-field representation  $D_G^{\text{TF}}$  depends only on the  $k$  dependence of the irreducible representations contained in the permutation representation  $D_G^{S(r)}$ , Eq. (2). Consequently, to determine the  $k=0$  irreducible representations in  $D_G^{\text{TF}}$  one needs to know the  $k=0$  irreducible representations contained in the permutation representation  $D_G^{S(r)}$ .

Litvin, Kotzev, and Birman<sup>9</sup> have derived and tabulated the  $k=0$  irreducible representations in all permutation representations  $D_G^{S(r)}$ : The permutation representation  $D_G^{S(r)}$  is, in general, reducible,

$$D_G^{S(r)} = \sum_{(k,\nu)} (D_R^{S(r)} | D_G^{(k,\nu)}) D_G^{(k,\nu)}, \quad (4)$$

where  $(D_G^{S(r)} | D_G^{(k,\nu)})$  is the number of times the  $(k,\nu)$ th irreducible representation of the space group  $G$  is contained in  $D_G^{S(r)}$ . It has been shown<sup>9</sup> that

$$(D_G^{S(r)} | D_G^{(0,\nu)}) = (D_{\hat{G}}^{S(r)} | D_{\hat{G}}^\nu), \quad (5)$$

where  $D_{\hat{G}}^\nu \equiv \Gamma_\nu$  is the  $\nu$ th irreducible representation of the point group  $\hat{G}$  of the space group  $G$ . The permutation representation

$$D_{\hat{G}}^{S(r)} = D_{S(r)}^1 \uparrow \hat{G}$$

is the representation of  $\hat{G}$  induced by the identity representation  $D_{S(r)}^1$  of the site point group  $\hat{S}(r)$  of the atom at position  $r$ . All possible permutation representations  $D_{\hat{G}}^{S(r)}$  are in a one-to-one correspondence with all permutational color point groups. Using the "short" notation for permutational color group, the permutation representation  $D_{\hat{G}}^{S(r)}$  corresponds to the permutational color point  $\hat{G}(\hat{S}(r))$ . A list of all classes of permutational color point groups is given in Table I. The number  $(D_{\hat{G}}^{S(r)} | \Gamma_\nu)$  of times each irreducible representation  $\Gamma_\nu = D_{\hat{G}}^\nu$  is contained in each permutation representation  $D_{\hat{G}}^{S(r)}$ , and, by Eq. (5), equal to the number of times  $D_G^{(0,\nu)}$  is contained in  $D_G^{S(r)}$ , has been derived by Litvin, Kotzev, and Birman.<sup>9</sup> Their results are found in the first line of each subtable of Table II.

The tensor-field representation is in general reducible:

$$D_G^{\text{TF}} = \sum_{(k,\nu)} (D_G^{\text{TF}} | D_G^{(k,\nu)}) D_G^{(k,\nu)}. \quad (7)$$

For the  $k=0$  irreducible representations  $D_G^{(0,\nu)}$

$$(D_G^{\text{TF}} | D_G^{(0,\nu)}) = (D_G^{\text{TF}} | \Gamma_\nu), \quad (8)$$

where  $D_G^{\text{TF}}$  is defined by

$$D_G^{\text{TF}} = D_G^{\hat{S}(r)} \times D_G^T. \quad (9)$$

That is, the number  $(D_G^{\text{TF}} | D_G^{(0,\nu)})$  of times the  $k=0$  irreducible representation  $D_G^{(0,\nu)}$  of the space group  $G$  is contained in  $D_G^{\text{TF}}$  is equal to the number  $(D_G^{\text{TF}} | \Gamma_\nu)$  of times the irreducible representation  $\Gamma_\nu$  of the point group  $\hat{G}$  is contained in  $D_G^{\text{TF}}$  defined by Eq. (9). Consequently, determining the irreducible representations  $\Gamma_\nu$  of the point group  $\hat{G}$  in  $D_G^{\text{TF}}$  determines, by Eq. (8), the  $k=0$  irreducible representations  $D_G^{(0,\nu)}$  contained in  $D_G^{\text{TF}}$ . We have calculated the coefficients  $(D_G^{\text{TF}} | \Gamma_\nu)$  for all  $D_G^{\text{TF}}$  for tensor representations  $D_G^T = D_G^V$ , the polar vector representation,  $D_G^A$ , the axial vector representation,  $D_G^A \times D_G^V$ , and  $(D_G^V)_{[2]}$ , the symmetrized square of the polar, or axial, vector representation. These coefficients are tabulated in lines two to four, respectively, of the subtables of Table II.

### III. APPLICATIONS

#### A. Lattice vibrations

The  $k=0$  irreducible representations of a space group  $G$ , whose basis functions are linear combinations of atomic displacements of the atoms of a simple crystal generated by  $G$  from  $r$ , are determined using Eq. (8) by finding the irreducible representation  $\Gamma_\nu$  of the point group  $\hat{G}$  contained in Eq. (9),

$$D_G^{\text{TF}} = D_G^{\hat{S}(r)} \times D_G^V, \quad (10)$$

where  $D_G^V$  is the polar vector representation of the point group  $\hat{G}$  and  $\hat{S}(r)$  is the site point group of  $r$ .

As an example, consider the rutile structure of  $\text{TiO}_2$ .<sup>11</sup> This crystal is of space-group symmetry  $G = D_{4h}^{14}$  and consists of two simple crystals. The simple crystal of Ti atoms, at the  $2(a)$  positions,<sup>12</sup> is generated by  $D_{4h}^{14}$  from  $r_1 = 000$ , and the simple crystal of O atoms, at the  $4(f)$  positions, is generated by  $D_{4h}^{14}$  from  $r_2 = xx0$ . The point group of  $D_{4h}^{14}$  is  $\hat{G} = D_{4h}$ , and the site point groups of the simple crystals are  $\hat{S}(r_1) = D_{2h}^{(z,xy,\bar{xy})}$  and  $\hat{S}(r_2) = C_{2v}^{(xy)}$ .

For the Ti atom simple crystal, irreducible representations contained in the representation  $D_G^{\text{TF}}(r)$ , Eq. (10) for the simple crystal generated by  $G$  from  $r$ , are found as follows: In Table I, the permuta-

tional color point group  $\hat{G}(\hat{S}(r_1)) = D_{4h}(D_{2h}^{(z,xy,\bar{xy})})$  is listed as group 15.15a. In Table II, subtable 15.15a, line two, one finds the irreducible components of the representation, Eq. (10):

$$D_G^{\text{TF}}(r_1) = \Gamma_2^- + \Gamma_3^- + 2\Gamma_5^-. \quad (11)$$

In the same manner, for the O atom simple crystal one finds from subtable 15.5b of Table II:

$$D_G^{\text{TF}}(r_2) = \Gamma_1^+ + \Gamma_2^+ + \Gamma_3^+ + \Gamma_4^+ + \Gamma_5^+ \\ + \Gamma_2^- + \Gamma_3^- + 2\Gamma_5^-. \quad (12)$$

Consequently, the  $k=0$  irreducible representations  $D_G^{(0,\nu)}$  of  $D_{4h}^{14}$  whose basis functions are linear combinations of the atomic displacements of atoms of the  $\text{TiO}_2$  crystals are, combining Eqs. (11) and (12), and using Eq. (8):

$$D_G^{(0,1+)}, D_G^{(0,2+)}, D_G^{(0,3+)}, D_G^{(0,4+)}, \\ D_G^{(0,5+)}, 2D_G^{(0,2-)}, 2D_G^{(0,3-)}, 4D_G^{(0,5-)}. \quad (13)$$

#### B. Infrared and Raman-active lattice vibrations

A  $k=0$  irreducible representation  $D_G^{(0,i)}$  of the space group  $G$  of a crystal whose basis functions are linear combinations of the atomic displacements of the crystal, is said to be infrared active if

$$\Gamma_i \in D_G^V \quad (14)$$

if it is contained in the polar vector representation of the point group  $\hat{G}$ . The irreducible representation  $D_G^{(0,i)}$  is Raman active if

$$\Gamma_i \in (D_G^V)_{[2]} \quad (15)$$

if it is contained in the symmetrized square of the polar vector representation of  $\hat{G}$ .<sup>13</sup>

The  $k=0$  irreducible representations  $D_G^{(0,i)}$  are, for each simple crystal, determined as in the above example, using Tables I and II. For the  $\text{TiO}_2$  crystal, of space-group symmetry  $D_{4h}^{14}$ , these irreducible representations are listed in Eq. (13).

Because the representation  $D_G^{\hat{S}(r)}$ , for  $\hat{S}(r) = \hat{G}$ , is the identity irreducible representation of  $\hat{G}$ , the irreducible components of  $D_G^V$  and  $(D_G^V)_{[2]}$  can also be determined from Table II: In Table II, in the subtable corresponding to the permutational color point group  $\hat{G}(\hat{G})$ , the listed irreducible components of the second and fifth rows, respectively, are the irreducible components of  $D_G^V$  and  $(D_G^V)_{[2]}$ . In the example of the  $\text{TiO}_2$  crystal,  $\hat{G} = D_{4h}$ , the

TABLE I. Permutational color point groups  $\hat{G}(\hat{S})$  are listed using the numbering of Ref. 9. Column 1 lists the group's number, column 2, the point group  $\hat{G}$ , and column 3, the subgroup  $\hat{S}$  of  $\hat{G}$ .

1.1	$C_1$	$C_1$	8.7b	$D_{2h}$	$C_{2h}^z$	14.3	$D_{2d}$	$C_s^{xy}$	17.1	$C_{3i}$	$C_1$
2.1	$C_i$	$C_1$	8.7c		$C_{2h}^y$	14.4		$C_2^z$	17.2		$C_i$
2.2		$C_i$	8.8		$D_{2h}$	14.5		$C_{2v}$	17.3		$C_3$
3.1	$C_2$	$C_1$	9.1	$C_4$	$C_1$	14.6		$D_2$	17.4		$C_{3i}$
3.2		$C_2$	9.2		$C_2$	14.7		$S_4$	18.1	$D_3$	$C_1$
4.1	$C_s$	$C_1$	9.3		$C_4$	14.8		$D_{2d}$	18.2		$C_2$
4.2		$C_s$	10.1	$S_4$	$C_1$	15.1	$D_{4h}$	$C_1$	18.3		$C_3$
5.1	$C_{2h}$	$C_1$	10.2		$C_2$	15.2a		$C_2^x$	18.4		$D_3$
5.2		$C_s$	10.3		$S_4$	15.2b		$C_2^{xy}$	19.1	$C_{3v}$	$C_1$
5.3		$C_2$	11.1	$C_{4h}$	$C_1$	15.3a		$C_s^x$	19.2		$C_s$
5.4		$C_i$	11.2		$C_2$	15.3b		$C_s^{xy}$	19.3		$C_3$
5.5		$C_{2h}$	11.3		$C_s$	15.4		$C_s^z$	19.4		$C_{3v}$
6.1	$D_2$	$C_1$	11.4		$C_i$	15.5a		$C_{2v}^x$	20.1	$D_{3d}$	$C_1$
6.2a		$C_2^x$	11.5		$S_4$	15.5b		$C_{2v}^{xy}$	20.2		$C_2$
6.2b		$C_2^z$	11.6		$C_4$	15.6		$C_i$	20.3		$C_s$
6.2c		$C_2^y$	11.7		$C_{2h}$	15.7a		$C_{2h}^x$	20.4		$C_i$
6.3		$D_2$	11.8		$C_{4h}$	15.7b		$C_{2h}^{xy}$	20.5		$C_{2h}$
7.1	$C_{2v}$	$C_1$	12.1	$D_4$	$C_1$	15.8		$C_2^z$	20.6		$C_3$
7.2		$C_2$	12.2a		$C_2^z$	15.9		$C_{2h}^z$	20.7		$C_{3v}$
7.3a		$C_s^x$	12.2b		$C_2^{xy}$	15.10a		$D_2^{(z,x,y)}$	20.8		$D_3$
7.3b		$C_s^y$	12.3		$C_2^z$	15.10b		$D_2^{(z,xy,xy)}$	20.9		$C_{3i}$
7.4		$C_{2v}$	12.4a		$D_2^{(z,xy,xy)}$	15.11a		$C_{2v}^{(z,x,y)}$	20.10		$D_{3d}$
8.1	$D_{2h}$	$C_1$	12.4b		$D_2^{(z,x,y)}$	15.11b		$C_{2v}^{(z,xy,xy)}$	21.1	$C_6$	$C_1$
8.2		$C_i$	12.5		$C_4$	15.12		$C_4$	21.2		$C_2$
8.3a		$C_2^y$	12.6		$D_4$	15.13		$S_4$	21.3		$C_3$
8.3b		$C_2^z$	13.1	$C_{4v}$	$C_1$	15.14a		$D_{2d}^{(z,xy,xy)}$	21.4		$C_6$
8.3c		$C_2^x$	13.2a		$C_s^x$	15.14b		$D_{2d}^{(z,x,y)}$	22.1	$C_{3h}$	$C_1$
8.4a		$C_s^y$	13.2b		$C_s^{xy}$	15.15a		$D_{2h}^{(z,xy,xy)}$	22.2		$C_s$
8.4b		$C_s^z$	13.3		$C_2$	15.15b		$D_{2h}^{(z,x,y)}$	22.3		$C_3$
8.4c		$C_s^x$	13.4a		$C_{2v}^{(z,xy,xy)}$	15.16		$C_{4v}$	22.4		$C_{3h}$
8.5a		$C_{2v}^x$	13.4b		$C_{2v}^{(z,x,y)}$	15.17		$C_{4h}$	23.1	$C_{6h}$	$C_1$
8.5b		$C_{2v}^z$	13.5		$C_4$	15.18		$D_4$	23.2		$C_i$
8.5c		$C_{2v}^y$	13.6		$C_{4v}$	15.19		$D_{4h}$	23.3		$C_2$
8.6		$D_2$	14.1	$D_{2d}$	$C_1$	16.1	$C_3$	$C_1$	23.4		$C_s$
8.7a		$C_{2h}^x$	14.2		$C_2^z$	16.2		$C_3$	23.5		$C_{2h}$

permutational color point group  $D_{4h}(D_{4h})$  is listed in Table I as group 15.19, and from subtable 15.19 of Table II, we have

$$D_{\hat{G}}^V = \Gamma_2^- + \Gamma_5^- , \quad (16)$$

$$(D_{\hat{G}}^V)_{[2]} = 2\Gamma_1^+ + \Gamma_3^+ + \Gamma_4^+ + \Gamma_5^+ . \quad (17)$$

Consequently, for the  $\text{TiO}_2$  crystal, the lattice vibrations [see Eq. (13)] corresponding to the  $k=0$  irreducible representations  $D_{\hat{G}}^{(0,2-)}$  and  $D_{\hat{G}}^{(0,5-)}$  are

infrared active, and  $D_{\hat{G}}^{(0,1+)}$ ,  $D_{\hat{G}}^{(0,3+)}$ ,  $D_{\hat{G}}^{(0,4+)}$ , and  $D_{\hat{G}}^{(0,5+)}$  are Raman active.

### C. Jahn-Teller theorem in crystals

The Jahn-Teller theorem, which states that degenerate electronic states give rise to configurational instabilities that lower the symmetry and split the electronic degeneracy, has been shown to be

TABLE I. (Continued.)

23.6	$C_{6h}$	$C_3$	27.1	$D_{6h}$	$C_1$	28.4	$T$	$D_2$	31.11	$T_d$	$T_d$
23.7		$C_{3i}$	27.2a		$C_2^x$	28.5		$T$	32.1	$O_h$	$C_1$
23.8		$C_6$	27.2b		$C_2^y$	29.1	$T_h$	$C_1$	32.2		$C_2^z$
23.9		$C_{3h}$	27.3a		$C_s^x$	29.2		$C_s$	32.3		$C_s^z$
23.10		$C_{6h}$	27.3b		$C_s^y$	29.3		$C_2$	32.4		$C_2^{xy}$
24.1	$D_6$	$C_1$	27.4		$C_s^z$	29.4		$C_3$	32.5		$C_s^{xy}$
24.2a		$C_2^y$	27.5a		$C_{2v}^x$	29.5		$C_{2v}$	32.6		$C_3$
24.2b		$C_2^x$	27.5b		$C_{2v}^y$	29.6		$D_2$	32.7		$C_4$
24.3		$C_2^z$	27.6		$C_i$	29.7		$T$	32.8		$S_4$
24.4		$D_2$	27.7a		$C_{2h}^x$	29.8		$C_i$	32.9		$C_{2v}^{(z,x,y)}$
24.5		$C_3$	27.7b		$C_{2h}^y$	29.9		$C_{2h}$	32.10		$D_2^{(z,xy,\bar{y})}$
24.6a		$D_3^{(z,x,x')}$	27.8		$C_2^z$	29.10		$C_{3i}$	32.11		$C_{2v}^{(z,xy,\bar{y})}$
24.6b		$D_3^{(z,y,y')}$	27.9		$D_2$	29.11		$D_{2h}$	32.12		$C_{2v}^{(xy,\bar{y},z)}$
24.7		$C_6$	27.10		$C_{2v}^z$	29.12		$T_h$	32.13		$D_3$
24.8		$D_6$	27.11		$C_{2h}^z$	30.1	$O$	$C_1$	32.14		$C_{3v}$
25.1	$C_{6v}$	$C_1$	27.12		$D_{2h}$	30.2		$C_2^z$	32.15		$C_{4v}$
25.2a		$C_s^y$	27.13		$C_3$	30.3		$C_2^{xy}$	32.16		$D_{2d}^{(z,x,y)}$
25.2b		$C_s^x$	27.14		$C_{3i}$	30.4		$C_3$	32.17		$C_i$
25.3		$C_2$	27.15		$C_6$	30.5		$D_2^{(z,xy,\bar{y})}$	32.18		$C_{2h}^z$
25.4		$C_{2v}$	27.16		$C_{3h}$	30.6		$C_4$	32.19		$C_{2h}^{xy}$
25.5		$C_3$	27.17a		$D_3^{(z,x,x')}$	30.7		$D_3$	32.20		$C_{3i}$
25.6a		$C_{3v}^{(z,x,x')}$	27.17b		$D_3^{(z,y,y')}$	30.8		$D_2^{(z,x,y)}$	32.21		$C_{4h}$
25.6b		$C_{3v}^{(z,y,y')}$	27.18a		$C_{3v}^{(z,x,x')}$	30.9		$D_4$	32.22		$D_{2h}^{(z,xy,\bar{y})}$
25.7		$C_6$	27.18b		$C_{3v}^{(z,y,y')}$	30.10		$T$	32.23		$D_{3d}$
25.8		$C_{6v}$	27.19a		$D_{3h}^{(z,y,y')}$	30.11		$O$	32.24		$D_2^{(z,x,y)}$
26.1	$D_{3h}$	$C_1$	27.19b		$D_{3h}^{(z,x,x')}$	31.1	$T_d$	$C_1$	32.25		$D_4$
26.2		$C_2^y$	27.20a		$D_{3d}^{(z,x,x')}$	31.2		$C_2$	32.26		$D_{2d}^{(z,xy,\bar{y})}$
26.3		$C_s^x$	27.20b		$D_{3d}^{(z,y,y')}$	31.3		$C_s$	32.27		$D_{2h}^{(z,x,y)}$
26.4		$C_s^z$	27.21		$C_{6v}$	31.4		$C_3$	32.28		$D_{4h}$
26.5		$C_{2v}$	27.22		$C_{6h}$	31.5		$C_{2v}$	32.29		$T$
26.6		$C_3$	27.23		$D_6$	31.6		$S_4$	32.30		$T_d$
26.7		$C_{3v}$	27.24		$D_{6h}$	31.7		$C_{3v}$	32.31		$O$
26.8		$D_3$	28.1	$T$	$C_1$	31.8		$D_2$	32.32		$T_h$
26.9		$C_{3h}$	28.2		$C_2$	31.9		$D_{2d}$	32.33		$O_h$
26.10		$D_{3h}$	28.3		$C_3$	31.10		$T$			

valid for all molecules.<sup>14-17</sup> Examples in crystals where the Jahn-Teller theorem is not valid have been given by Birman.<sup>18</sup> We shall discuss here the use of Tables I and II in determining whether or not a  $k=0$  degenerate electronic state in a crystal gives rise to a configurational instability.

Let  $D_G^{(0,e)}$  be a degenerate "single"  $k=0$  irreducible representation of the space group  $G$  of a crystal, corresponding to a degenerate electronic state. This degenerate electronic state gives rise to a con-

figurational instability if there is at least one irreducible representation  $D_G^{(0,i)}$ , corresponding to a lattice vibrational mode, such that

$$\Gamma_i \in (\Gamma_e)_{[2]}, \quad (18)$$

that is,  $\Gamma_i$  is contained in the symmetrized square of  $\Gamma_e$  and where the following conditions apply.

(1)  $\Gamma_i$  is not the identity irreducible representation  $\Gamma_1$ .



TABLE II. (Continued.)

	8.5c	8.6	8.7a	8.7b	8.7c	
	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	
$P$	1	1	1	1	1	
$P \otimes V$	1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1	1 2 1 2	1 1 2 2	
$P \otimes A$	1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1	1 2 2 1	1 2 1 2	1 1 2 2	
$P \otimes V \otimes A$	2 3 2 2 3 2 2 2	3 2 2 2 3 2 2 2	5 4 4 5	5 4 5 4	5 5 4 4	
$P \otimes [V]^2$	3 1 1 1 3 1 1 1	3 1 1 1 3 1 1 1	4 2 2 4	4 2 4 2	4 4 2 2	
	8.8	9.1	9.2	9.3	10.1	10.3
	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$
$P$	1	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1
$P \otimes V$	1 1 1 1	3 3 3 3	1 1 2 2	1 1 1 1	1 1 1 1	3 3 3 3
$P \otimes A$	1 1 1 1	3 3 3 3	1 1 2 2	1 1 1 1	1 1 1 1	3 3 3 3
$P \otimes V \otimes A$	3 2 2 2	9 9 9 9	5 5 4 4	3 2 2 2	9 9 9 9	5 5 4 4
$P \otimes [V]^2$	3 1 1 1	6 6 6 6	4 4 2 2	2 2 1 1	6 6 6 6	4 4 2 2
	11.2	11.3	11.4	11.5	11.6	
	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	
$P$	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1	
$P \otimes V$	1 1 2 2 1 1 2 2	2 2 1 1 1 1 2 2	3 3 3 3	1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1	
$P \otimes A$	1 1 2 2 1 1 2 2	1 1 2 2 2 2 1 1	3 3 3 3	1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1	
$P \otimes V \otimes A$	5 5 4 4 5 5 4 4	4 4 5 5 5 5 4 4	9 9 9 9	2 3 2 2 3 2 2 2	3 2 2 2 3 2 2 2	
$P \otimes [V]^2$	4 4 2 2 4 4 2 2	4 4 2 2 2 2 4 4	6 6 6 6	2 2 1 1 2 2 1 1	2 2 1 1 2 2 1 1	
	11.7	11.8	12.1	12.2a	12.2b	12.3
	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$
$P$	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1
$P \otimes V$	1 1 2 2 1 1 2 2	2 2 1 1 1 1 2 2	3 3 3 3	1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1	1 1 1 1
$P \otimes A$	1 1 2 2 1 1 2 2	1 1 2 2 2 2 1 1	3 3 3 3	1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1	1 1 1 1
$P \otimes V \otimes A$	5 5 4 4 5 5 4 4	4 4 5 5 5 5 4 4	9 9 9 9	2 3 2 2 3 2 2 2	3 2 2 2 3 2 2 2	3 2 2 2
$P \otimes [V]^2$	4 4 2 2 4 4 2 2	4 4 2 2 2 2 4 4	6 6 6 6	2 2 1 1 2 2 1 1	2 2 1 1 2 2 1 1	2 2 1 1
	12.4a	12.4b	12.4c	12.4d	12.4e	12.4f
	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$	$\Gamma_1^- \Gamma_2^- \Gamma_3^- \Gamma_4^-$
$P$	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1
$P \otimes V$	1 1 2 2	1 1 2 2	1 2 2 3	1 2 2 3	1 2 2 3	1 1 1 4
$P \otimes A$	1 1 2 2	1 1 1 1	3 3 3 6	1 2 2 3	1 2 2 3	1 1 1 4
$P \otimes V \otimes A$	5 5 4 4	3 2 2 2	9 9 9 18	5 4 5 4 9	5 4 4 5 9	5 5 5 8
$P \otimes [V]^2$	4 4 2 2	2 2 1 1	6 6 6 12	4 2 4 2 6	4 2 2 4 6	4 4 4 4 4

TABLE II. (Continued.)

	12.4b	12.5	12.6	13.1	13.2a	13.2b	13.3	13.4a
	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$
$P$	1 1	1 1	1	1 1 1 1 2	1 1 1 1	1 1 1 1	1 1 1 1 1	1 1
$P \otimes V$	1 1 2	1 1	1	3 3 3 3 6	2 1 2 1 3	2 1 1 2 3	1 1 1 1 4	1 1 2
$P \otimes A$	1 1 2	1 1	1	3 3 3 3 6	1 2 1 2 3	1 2 2 1 3	1 1 1 1 4	1 1 2
$P \otimes V \otimes A$	3 2 3 2 4	3 3 2 2 4	2 1 1 1 2	9 9 9 9 18	4 5 4 5 9	4 5 5 4 9	5 5 5 5 8	2 3 3 2 4
$P \otimes [V]^2$	3 1 3 1 2	2 2 2 2 2	2 1 1 1	6 6 6 6 12	4 2 4 2 6	4 2 2 4 6	4 4 4 4 4	3 1 1 3 2
	13.4b	13.5	13.6	14.1	14.2	14.3	14.4	14.5
	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$
$P$	1 1	1 1	1	1 1 1 1 2	1 1 1 1	1 1 1 1	1 1 1 1 1	1 1
$P \otimes V$	1 1 2	1 1	1	3 3 3 3 6	1 2 1 2 3	2 1 1 2 3	1 1 1 1 4	1 1 2
$P \otimes A$	1 1 2	1 1	1	3 3 3 3 6	1 2 1 2 3	1 2 2 1 3	1 1 1 1 4	1 1 2
$P \otimes V \otimes A$	2 3 2 3 4	3 3 2 2 4	1 2 1 1 2	9 9 9 9 18	5 4 5 4 9	4 5 5 4 9	5 5 5 5 8	2 3 3 2 4
$P \otimes [V]^2$	3 1 3 1 2	2 2 2 2 2	2 1 1 1	6 6 6 6 12	4 2 4 2 6	4 2 2 4 6	4 4 4 4 4	3 1 1 3 2
	14.6	14.7	14.8	15.1	15.2a			
	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$
$P$	1 1	1 1	1	1 1 1 1 2	1 1 1 1 1 2	1 1 1 1 1 2	1 1 1 1 1	1 1
$P \otimes V$	1 1 2	1 1 2	1 1	3 3 3 3 6	3 3 3 3 6	3 3 3 3 6	1 2 1 2 3 1 2 1 2 3	1 2 3
$P \otimes A$	1 1 2	1 1 2	1 1	3 3 3 3 6	3 3 3 3 6	3 3 3 3 6	1 2 1 2 3 1 2 1 2 3	1 2 3
$P \otimes V \otimes A$	3 2 3 2 4	2 2 3 3 4	1 1 2 1 2	9 9 9 9 18	9 9 9 9 18	9 9 9 9 18	5 4 5 4 9 5 4 5 4 9	4 9
$P \otimes [V]^2$	3 1 3 1 2	2 2 2 2 2	2 1 1 1	6 6 6 6 12	6 6 6 6 12	6 6 6 6 12	4 2 4 2 6 4 2 4 2 6	4 6
	15.2b	15.3a	15.3b	15.4				
	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$
$P$	1 1	1 1	1 1	1 1 1 1 1 1 2	1 1 1 1 1 1 2	1 1 1 1 1 1	1 1 1 1 1	1 1 1 1 1
$P \otimes V$	1 1 2	1 1 2	1 1 1	3 3 3 3 6 3 3 3 6	3 3 3 3 6	3 3 3 3 6	1 2 1 2 3 1 2 1 2 3	1 2 3
$P \otimes A$	1 1 2	1 1 2	1 1	3 3 3 3 6 3 3 3 6	3 3 3 3 6	3 3 3 3 6	1 2 1 2 3 1 2 1 2 3	1 2 3
$P \otimes V \otimes A$	3 2 3 2 4	2 2 3 3 4	1 1 2 1 2	9 9 9 9 18 9 9 9 18	9 9 9 9 18	9 9 9 9 18	5 4 5 4 9 5 4 5 4 9	4 9
$P \otimes [V]^2$	3 1 3 1 2	2 2 2 2 2	2 1 1 1	6 6 6 6 12 6 6 6 12	6 6 6 6 12	6 6 6 6 12	4 2 4 2 6 4 2 4 2 6	4 6
	15.4							
	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$
$P$	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1 1 1 1	1 1 1 1 1 1 1	1 1 1 1 1	1 1 1 1 1	1 1 1 1 1
$P \otimes V$	1 2 2 1 3 1 2 2 1 3	2 1 2 1 3 1 2 1 2 3	2 1 1 2 3 1 2 2 1 3	2 1 1 2 3 1 2 2 1 3	2 1 1 2 3 1 2 2 1 3	2 1 1 2 3 1 2 2 1 3	2 2 2 2 2 1 1 1 1 4	2 2 2 2 2 1 1 1 1 4
$P \otimes A$	1 2 2 1 3 1 2 2 1 3	1 2 1 2 3 2 1 2 1 3	1 2 2 1 3 2 1 2 1 3	1 2 2 1 3 2 1 2 1 3	1 2 2 1 3 2 1 2 1 3	1 1 1 1 1 4 2 2 2 2 2	1 1 1 1 1 4 2 2 2 2 2	1 1 1 1 1 4 2 2 2 2 2
$P \otimes V \otimes A$	5 4 4 5 9 5 4 4 5 9	4 5 4 5 9 5 4 5 4 9	4 5 4 5 9 5 4 5 4 9	4 5 5 4 9 5 4 4 5 9	4 5 5 4 9 5 4 4 5 9	4 4 4 4 10 5 5 5 5 8	4 4 4 4 10 5 5 5 5 8	4 4 4 4 10 5 5 5 5 8
$P \otimes [V]^2$	4 2 2 4 6 4 2 2 4 6	4 2 4 2 6 2 4 2 4 6	4 2 2 4 6 2 4 2 4 6	4 2 2 4 6 2 4 2 4 6	4 2 2 4 6 2 4 2 4 6	4 4 4 4 4 2 2 2 2 2	4 4 4 4 4 2 2 2 2 2	4 4 4 4 4 2 2 2 2 2



TABLE II. (Continued.)

15.5a		15.5b		15.6		15.7a	
$\Gamma$	$\Gamma^2$	$\Gamma$	$\Gamma^2$	$\Gamma$	$\Gamma^2$	$\Gamma$	$\Gamma^2$
1	1	1	1	1	1	1	1
$P \otimes V$	1 1 1 1 1	1 1 1 1 1	1 1 1 1 2	1 1 1 1 2	3 3 3 3 6	1 1 1	1 1 1
$P \otimes A$	1 1 2 1 1 1 1	1 1 1 1 1 1 1	1 1 1 1 1	3 3 3 3 6	1 2 1 2 3	1 2 1 2 3	1 2 1 2 3
$P \otimes V \otimes A$	2 2 2 5 3 2 3 2 4	2 2 2 5 3 2 2 3 4	2 2 2 5 3 2 2 3 4	9 9 9 9 18	5 4 5 4 9	5 4 5 4 9	5 4 5 4 9
$P \otimes [V]^2$	3 1 3 1 2 1 1 1 4	3 1 1 3 2 1 1 1 4	6 6 6 6 12	4 2 4 2 6			
15.7b		15.8		15.9		15.10a	
$\Gamma$	$\Gamma^2$	$\Gamma$	$\Gamma^2$	$\Gamma$	$\Gamma^2$	$\Gamma$	$\Gamma^2$
1	1 1	1 1 1 1 1	1 1 1 1 1	1 1 1 1 1	1 1 1 1 1	1 1 1	1 1 1
$P \otimes V$	1 1 1 1 1 1 1 1 1	1 1 1 1 4 1 1 1 4	1 1 1 1 4	1 1 1 1 4	1 1 2 1 1 2	1 1 2 1 1 2	1 1 2 1 1 2
$P \otimes A$	1 2 2 1 3	1 1 1 4 1 1 1 4	1 1 1 4 1 1 1 4	1 1 1 4	1 1 2 1 1 2	1 1 2 1 1 2	1 1 2 1 1 2
$P \otimes V \otimes A$	5 4 4 5 9	5 5 5 8 5 5 5 8	5 5 5 8 5 5 5 8	5 5 5 8	3 2 3 2 4 3 2 3 2 4	3 2 3 2 4 3 2 3 2 4	3 2 3 2 4 3 2 3 2 4
$P \otimes [V]^2$	4 2 2 4 6	4 4 4 4 4 4 4 4 4	4 4 4 4 4 4 4 4 4	4 4 4 4 4	3 1 3 1 2 3 1 3 1 2	3 1 3 1 2 3 1 3 1 2	3 1 3 1 2 3 1 3 1 2
15.10b		15.11a		15.11b		15.12	
$\Gamma$	$\Gamma^2$	$\Gamma$	$\Gamma^2$	$\Gamma$	$\Gamma^2$	$\Gamma$	$\Gamma^2$
1	1 1 1 1 1	1 1 1 1 1 1 1	1 1 1 1 1 1 1	1 1 1 1 1 1 1	1 1 1 1 1 1 1	1 1 1	1 1 1
$P \otimes V$	1 1 2 1 1 2	1 1 1 2 1 1 1 2	1 1 2 1 1 2	1 1 2 1 1 2	1 1 1 2 1 1 1	1 1 1	1 1 1
$P \otimes A$	1 1 2 1 1 2	1 1 2 1 1 2	1 1 2 1 1 2	1 1 2 1 1 2	1 1 2 1 1 2	1 1 1	1 1 1
$P \otimes V \otimes A$	3 2 2 3 4 3 2 2 3 4	2 3 2 3 4 3 2 3 2 4	2 3 2 3 4 3 2 3 2 4	2 3 2 3 4 3 2 3 2 4	3 3 2 2 4 3 2 2 3 4	3 3 2 2 4 3 3 2 2 4	3 3 2 2 4 3 3 2 2 4
$P \otimes [V]^2$	3 1 1 3 2 3 1 1 3 2	3 1 3 1 2 1 3 1 3 2	3 1 3 1 2 1 3 1 3 2	3 1 1 3 2 1 3 3 1 2	2 2 2 2 2 2 2 2 2 2	2 2 2 2 2 2 2 2 2 2	2 2 2 2 2 2 2 2 2 2
15.13		15.14a		15.14b		15.15a	
$\Gamma$	$\Gamma^2$	$\Gamma$	$\Gamma^2$	$\Gamma$	$\Gamma^2$	$\Gamma$	$\Gamma^2$
1	1 1 1 1 1 1 1	1 1 1 1 1 1 1	1 1 1 1 1 1 1	1 1 1 1 1 1 1	1 1 1 1 1 1 1	1 1 1	1 1 1
$P \otimes V$	1 1 1 2 1 1 2	1 1 1 1 1 1 1	1 1 1 1 1 1 1	1 1 1 1 1 1 1	1 1 1 1 1 1 1	1 1 1	1 1 1
$P \otimes A$	1 1 2 1 1 2	1 1 1 1 1 1 1	1 1 1 1 1 1 1	1 1 1 1 1 1 1	1 1 1 1 1 1 1	1 1 1	1 1 1
$P \otimes V \otimes A$	2 2 3 3 4 3 3 2 2 4	1 1 1 2 2 2 1 1 2	1 1 1 2 2 2 1 1 2	1 1 2 2 1 1 1 2	1 1 2 2 1 1 1 2	3 2 2 3 4	3 2 2 3 4
$P \otimes [V]^2$	2 2 2 2 2 2 2 2 2	2 1 1 1 1 1 2 1	2 1 1 1 1 1 2 1	2 1 1 1 1 1 2 1	3 1 1 1 3 2	3 1 1 3 2	3 1 1 3 2

TABLE II. (Continued.)

15.15b		15.16		15.17		15.18											
$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$										
P	1	1	1	1	1	1	1										
$P \otimes V$	1	1	1	1	1	1	1										
$P \otimes A$	1	1	1	1	1	1	1										
$P \otimes V \otimes A$	3	2	3	2	4	2	1										
$P \otimes [V]^2$	3	1	3	1	2	2	1										
15.19		16.1		16.2		17.1		17.2		17.3		17.4					
$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$				
P	1	1	1	1	1	1	1	1	1	1	1	1	1				
$P \otimes V$	1	3	3	3	3	3	3	3	3	3	3	3	3				
$P \otimes A$	1	3	3	3	3	3	3	3	3	3	3	3	3				
$P \otimes V \otimes A$	2	1	1	1	2	9	9	9	9	9	9	9	9				
$P \otimes [V]^2$	2	1	1	1	2	6	6	6	6	6	6	6	6				
18.1		18.3		18.4		19.1		19.2		19.3		19.4		20.1		20.2	
$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+$	
P	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
$P \otimes V$	3	3	6	1	2	3	3	6	2	1	3	3	6	3	3	6	
$P \otimes A$	3	3	6	1	2	3	3	6	1	2	3	3	6	1	2	3	
$P \otimes V \otimes A$	9	9	18	5	4	9	9	18	4	5	9	9	18	1	2	3	
$P \otimes [V]^2$	6	6	12	4	2	6	6	12	4	2	6	6	12	4	2	6	
20.3		20.4		20.5		20.6		20.7		20.8		20.9					
$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$				
P	1	1	1	1	1	1	1	1	1	1	1	1	1				
$P \otimes V$	2	1	3	1	2	3	3	6	1	2	3	3	6				
$P \otimes A$	1	2	3	2	1	3	3	6	1	2	3	3	6				
$P \otimes V \otimes A$	4	5	9	5	4	9	9	18	5	4	9	9	18				
$P \otimes [V]^2$	4	2	6	2	4	6	6	12	4	2	6	6	12				



TABLE II. (Continued.)

23.9	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$	23.10	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$	24.1	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	24.2a	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	24.2b	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$
P	1	1	1	1	1 1 1 1 2 2	1	1 1 1 1	1	1 1 1 1
P⊗V	1 1 1 1	1 1 1 1	1	1 1 1	3 3 3 3 6 6	1	2 1 2 3 3	1	2 2 1 3 3
P⊗A	1	1 1 1 1 1	1 1 1	1 1 1	3 3 3 3 6 6	1	2 1 2 3 3	1	2 2 1 3 3
P⊗V⊗A	2 2 3 1 1 3 1 1	2 2	3 1 1	2 2	9 9 9 9 18 18	5	4 5 4 9 9	5	4 4 5 9 9
P⊗[V] <sup>2</sup>	2 1 1 1 1	1 1 2 1 1	2 1 1 1 1	1 1 1	6 6 6 6 12 12	4	2 4 2 6 6	4	2 2 4 6 6
24.3	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	24.4	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	24.5	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	24.6a	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	24.6b	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$
P	1 1	2 1	1 1 1 1 1	1	1 1 1 1	1	1 1 1	1	1 1 1
P⊗V	1 1 2 2 4 2	1 1 1 2 1	1 1 1 1 2 2	1 1 1 1	1 1 1 1 1	1 1 1	1 1 1	2	1 1 1
P⊗A	1 1 2 2 4 2	1 1 1 2 1	1 1 1 1 2 2	1 1 1 1	1 1 1 1 1	1 1 1	1 1 1	2	1 1 1
P⊗V⊗A	5 5 4 4 8 10	3 2 2 2 4 5	3 3 3 3 6 6	2 1 1 2 3 3	2 1 2 1 3 3	3 3	4 2	2 1	2 1
P⊗[V] <sup>2</sup>	4 4 2 2 4 8	3 1 1 1 2 4	2 2 2 2 4 4	2 2 2 2	2 2 2 2	2 2	2 2	2 2	2 2
25.1	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	25.2a	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	25.2b	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	25.3	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	25.4	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$
P	1 1 1 1 2 2	1 1 1 1 1	1 1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1
P⊗V	3 3 3 3 6 6	2 1 2 1 3 3	2 1 1 2 3 3	1 1 2 2 4 2	1 1 2 2 4 2	1 1 2 1	1 1 1 1 2 2	1 1 1 1 2 2	1 1 1 1
P⊗A	3 3 3 3 6 6	1 2 1 2 3 3	1 2 2 1 3 3	1 1 2 2 4 2	1 1 2 2 4 2	1 1 1 2 1	1 1 1 1 2 2	1 1 1 1 2 2	1 1 1 1
P⊗V⊗A	9 9 9 9 18 18	4 5 4 5 9 9	4 5 5 4 9 9	5 5 4 4 8 10	5 5 4 4 8 10	2 3 2 2 4 5	3 3 3 3 6 6	1 2 2 1 3 3	1 2 2 1 3 3
P⊗[V] <sup>2</sup>	6 6 6 6 12 12	4 2 4 2 6 6	4 2 2 4 6 6	4 4 2 2 4 8	4 4 2 2 4 8	3 1 1 1 2 4	2 2 2 2 2 4	2 2 2 2 2 4	2 2 2 2
25.6a	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	25.6b	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	25.6c	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	25.6d	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	25.6e	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$
P	1 1 1 1 2 2	1 1 1 1 1	1 1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1
P⊗V	3 3 3 3 6 6	2 1 2 1 3 3	2 1 1 2 3 3	1 1 2 2 4 2	1 1 2 2 4 2	1 1 2 1	1 1 1 1 2 2	1 1 1 1 2 2	1 1 1 1
P⊗A	3 3 3 3 6 6	1 2 1 2 3 3	1 2 2 1 3 3	1 1 2 2 4 2	1 1 2 2 4 2	1 1 1 2 1	1 1 1 1 2 2	1 1 1 1 2 2	1 1 1 1
P⊗V⊗A	9 9 9 9 18 18	4 5 4 5 9 9	4 5 5 4 9 9	5 5 4 4 8 10	5 5 4 4 8 10	2 3 2 2 4 5	3 3 3 3 6 6	1 2 2 1 3 3	1 2 2 1 3 3
P⊗[V] <sup>2</sup>	6 6 6 6 12 12	4 2 4 2 6 6	4 2 2 4 6 6	4 4 2 2 4 8	4 4 2 2 4 8	3 1 1 1 2 4	2 2 2 2 2 4	2 2 2 2 2 4	2 2 2 2
25.66	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	25.7	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	25.8	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	26.1	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$	26.2	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5 \Gamma_6$
P	1 1 1 1	1 1 1	1 1 1	1 1 1 1 2 2	1 1 1 1 2 2	1 1 1 1 1 1	1 1 1 1	1 1 1 1	1 1 1 1
P⊗V	1 1 1 1	1 1 1	1 1 1	3 3 3 3 6 6	1 2 1 2 3 3	1 2 1 2 3 3	2 1 1 2 3 3	2 2 1 1 2 4	2 2 1 1 2 4
P⊗A	1 1 1 1	1 1 1	1 1 1	3 3 3 3 6 6	1 2 1 2 3 3	1 2 1 2 3 3	1 2 1 2 3 3	1 1 2 2 4 2	1 1 2 2 4 2
P⊗V⊗A	1 2 1 2 3 3	3 3 3 3	4 2 1 2	9 9 9 9 18 18	5 4 5 4 9 9	5 4 5 4 9 9	4 5 4 9 9	4 4 5 5 10 8	4 4 5 5 10 8
P⊗[V] <sup>2</sup>	2 2 2 2	2 2 2	2 2 2	6 6 6 6 12 12	4 2 4 2 6 6	4 2 4 2 6 6	4 2 4 2 6 6	4 2 4 2 6 6	4 2 4 2 6 6





TABLE II. (Continued.)

	27.17b	27.18a	27.18b			
	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$		
P	1	1	1	1		
P $\otimes$ V	1	1	1	1		
P $\otimes$ A	1	1	1	1		
P $\otimes$ V $\otimes$ A	2	1	1	1		
P $\otimes$ [V] <sup>2</sup>	2	2	2	2		
	27.19a	27.19b	27.20a			
	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$			
P	1	1	1	1		
P $\otimes$ V	1	1	1	1		
P $\otimes$ A	1	1	1	1		
P $\otimes$ V $\otimes$ A	1	1	1	1		
P $\otimes$ [V] <sup>2</sup>	2	2	2	2		
	27.20b	27.21	27.22			
	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$			
P	1	1	1	1		
P $\otimes$ V	1	1	1	1		
P $\otimes$ A	1	1	1	1		
P $\otimes$ V $\otimes$ A	2	1	1	1		
P $\otimes$ [V] <sup>2</sup>	2	2	2	2		
	27.23	27.24	28.1	28.2	28.3	28.4
	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_6^+$
P	1	1	1	1	1	1
P $\otimes$ V	1	1	1	1	1	1
P $\otimes$ A	1	1	1	1	1	1
P $\otimes$ V $\otimes$ A	2	1	1	1	1	1
P $\otimes$ [V] <sup>2</sup>	2	2	2	2	2	2

TABLE II. (Continued.)

28.5	29.1	29.2	29.3	29.4	29.5	
$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+$	
P	1 1 1 3 1 1 1 1	2 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1	
$P \otimes V$	1 3 3 3 9 3 3 9	2 2 2 4 1 1 1 5	1 1 1 5 1 1 1 5	1 1 1 3 1 1 1 3	1 1 1 2 1 1 1 2	
$P \otimes A$	1 3 3 3 9 3 3 9	1 1 1 5 2 2 4 1	1 1 1 5 1 1 1 5	1 1 1 3 1 1 1 3	3 1 1 2 3 1 1 2	
$P \otimes V \otimes A$	1 1 1 2 9 9 9 27 9 9 27	4 4 4 14 5 5 13 5 5 13	5 5 5 13 5 5 13 5 5 13	3 3 3 9 3 3 9 3 3 9	2 2 2 7 3 3 6 2 2 7 3 3 6	
$P \otimes [V]^2$	1 1 1 1 6 6 6 18 6 6 18	4 4 4 8 2 2 2 10 4 4 8 4 4 8	4 4 4 8 2 2 2 10 4 4 8 4 4 8	2 2 2 6 2 2 2 6 2 2 2 6 2 2 6	3 3 3 3 3 1 1 5 3 3 3 3 1 1 5	
29.6	29.7	29.8	29.9	29.10		
$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+$		
P	1 1 1 1 1 1 1 1	1 1 1 1 3 1 1 1 1 1	1 1 1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1 1 1		
$P \otimes V$	3 3 3 3 9 3 3 9	1 1 1 3 3 3 3 9 1 1 1 3	3 3 3 9 1 1 1 3 3 3 9	1 1 1 3 1 1 1 3 1 1 1 3		
$P \otimes A$	3 3 3 3 9 3 3 9	1 1 1 3 3 3 3 9 1 1 1 3	1 1 1 3 3 3 3 9 1 1 1 3	1 1 1 3 1 1 1 3 1 1 1 3		
$P \otimes V \otimes A$	3 3 3 6 3 3 3 6 1 1 1 2 1 1 2	1 1 1 2 1 1 1 2 9 9 9 27 1 1 1 2	9 9 9 27 1 1 1 2 5 5 5 13 1 1 1 2	3 3 3 9 3 3 3 9 2 2 2 6 2 2 2 6		
$P \otimes [V]^2$	3 3 3 3 3 3 3 3 1 1 1 1 1 1 1	6 6 6 18 1 1 1 1 1 1 1 1 1 1 1	4 4 4 8 1 1 1 1 1 1 1 1 1 1 1	2 2 2 6 2 2 2 6 2 2 2 6 2 2 2 6		
29.11	29.12	30.1	30.2	30.3	30.4	30.5
$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4$
P	1 1 1 1 1 1 1 1	1 1 2 3 3 1 1 2 1 1 1	1 1 2 3 3 1 1 2 1 1 1	1 1 2 3 3 1 1 2 1 1 1	1 1 2 3 3 1 1 2 1 1 1	1 1 2 3 3 1 1 2 1 1 1
$P \otimes V$	3 3 3 3 9 3 3 9	1 3 3 6 9 9 1 3 3 6 9 9	1 1 2 5 5 1 1 2 5 5 1 1 2 5 5	1 1 2 5 5 1 1 2 5 5 1 1 2 5 5	1 1 2 3 3 1 1 2 3 3 1 1 2 3 3	1 1 2 3 3 1 1 2 3 3 1 1 2 3 3
$P \otimes A$	3 3 3 3 9 3 3 9	1 3 3 6 9 9 1 3 3 6 9 9	1 1 2 5 5 1 1 2 5 5 1 1 2 5 5	1 1 2 5 5 1 1 2 5 5 1 1 2 5 5	1 1 2 3 3 1 1 2 3 3 1 1 2 3 3	1 1 2 3 3 1 1 2 3 3 1 1 2 3 3
$P \otimes V \otimes A$	3 3 3 6 3 3 3 6 1 1 1 2 1 1 2	9 9 18 27 27 9 9 18 27 27 9 9 18 27	5 5 10 13 13 5 5 10 13 13 5 5 10 13 13	5 4 9 13 14 5 4 9 13 14 5 4 9 13 14	3 3 6 9 9 3 3 6 9 9 3 3 6 9 9	3 2 5 6 7 3 2 5 6 7 3 2 5 6 7
$P \otimes [V]^2$	3 3 3 3 3 3 3 3 1 1 1 1 1 1 1	6 6 12 18 18 6 6 12 18 18 6 6 12 18 18	4 4 8 8 8 4 4 8 8 8 4 4 8 8 8	4 2 6 8 10 4 2 6 8 10 4 2 6 8 10	2 2 4 6 6 2 2 4 6 6 2 2 4 6 6	3 1 4 3 5 3 1 4 3 5 3 1 4 3 5
30.6	30.7	30.8	30.9	30.10	30.11	30.12
$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4$	$\Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4$
P	1 1 1 1 1 1 1 1	1 1 2 1 2 1 1 1 2 1 1 1	1 1 2 1 2 1 1 1 2 1 1 1	1 1 2 1 2 1 1 1 2 1 1 1	1 1 2 1 2 1 1 1 2 1 1 1	1 1 2 1 2 1 1 1 2 1 1 1
$P \otimes V$	1 1 3 2 1 1 2 1 1 1 2 1 1	3 3 3 3 9 3 3 3 3 3 3 3 3	2 1 2 1 2 1 2 1 2 1 2 1 2 1	3 3 3 3 9 3 3 3 3 3 3 3 3	1 1 2 3 3 1 1 2 3 3 1 1 2 3 3	1 1 2 5 5 1 1 2 5 5 1 1 2 5 5
$P \otimes A$	1 1 3 2 1 1 2 1 1 1 2 1 1	3 3 3 3 9 3 3 3 3 3 3 3 3	2 1 2 1 2 1 2 1 2 1 2 1 2 1	3 3 3 3 9 3 3 3 3 3 3 3 3	1 1 2 3 3 1 1 2 3 3 1 1 2 3 3	1 1 2 5 5 1 1 2 5 5 1 1 2 5 5
$P \otimes V \otimes A$	3 2 5 7 6 2 1 3 4 5 2 1 3 4 5	3 3 6 6 6 3 3 6 6 6 3 3 6 6 6	2 1 3 3 3 2 1 3 3 3 2 1 3 3 3	3 3 6 6 6 3 3 6 6 6 3 3 6 6 6	1 1 2 2 2 1 1 2 2 2 1 1 2 2 2	9 9 18 27 27 9 9 18 27 27 9 9 18 27
$P \otimes [V]^2$	2 2 4 4 4 2 2 2 4 2 2 2 4 2 2	3 3 6 3 3 3 3 6 3 3 3 6 3 3	2 1 3 1 2 2 1 3 1 2 2 1 3 1 2	3 3 6 3 3 3 3 6 3 3 3 6 3 3	1 1 2 1 1 1 1 2 1 1 1 2 1 1	6 6 12 18 18 6 6 12 18 18 6 6 12 18 18



TABLE II. (Continued.)

31.3		31.4		31.5		31.6		31.7		31.8		31.9		31.10																		
$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$													
P	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1													
P $\otimes$ V	2	1	3	4	5	1	1	2	3	1	1	1	2	3	1	1	2	3	4	5												
P $\otimes$ A	1	2	3	5	4	1	1	2	3	1	1	3	3	3	2	1	2	3	5	4												
P $\otimes$ V $\otimes$ A	4	5	9	14	13	3	3	6	9	2	3	5	6	7	1	2	3	3	3	3												
P $\otimes$ [V] <sup>2</sup>	4	2	6	8	10	2	2	4	6	3	3	6	6	3	2	1	3	3	3	3												
31.11		32.1		32.2		32.3		32.4		32.5		32.6		32.7		32.8		32.9		32.10												
$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$								
P	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1							
P $\otimes$ V	1	3	3	6	9	3	3	6	9	9	1	1	2	5	5	2	2	4	4	4	1	2	5	5	1	2	3	5	4			
P $\otimes$ A	1	3	3	6	9	3	3	6	9	9	1	1	2	5	5	1	1	2	5	5	2	2	4	4	1	2	3	5	4			
P $\otimes$ V $\otimes$ A	1	1	1	9	18	27	27	9	18	27	5	5	10	13	13	4	4	8	14	14	5	5	10	13	5	4	9	13	14	14		
P $\otimes$ [V] <sup>2</sup>	1	1	1	6	12	18	18	6	12	18	4	4	8	8	8	4	4	8	8	8	2	2	4	4	2	2	4	4	4	4	4	
32.5		32.6		32.7		32.8		32.9		32.10		32.11		32.12		32.13		32.14		32.15		32.16		32.17								
$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$								
P	1	1	1	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1							
P $\otimes$ V	2	1	3	4	5	1	2	3	5	4	1	1	2	3	3	1	1	3	2	1	1	3	2	1	1	2	3					
P $\otimes$ A	1	2	3	5	4	2	1	3	4	5	1	1	2	3	3	1	1	3	2	1	1	3	2	1	1	2	3					
P $\otimes$ V $\otimes$ A	4	5	9	14	13	5	4	9	13	14	3	3	6	9	9	3	2	5	7	6	3	2	5	7	6	2	3	5	7	6		
P $\otimes$ [V] <sup>2</sup>	4	2	6	8	10	2	4	6	10	8	2	2	4	6	2	2	2	4	6	2	2	4	6	2	2	4	6	2	2	4	6	
32.9		32.10		32.11		32.12		32.13		32.14		32.15		32.16		32.17		32.18		32.19		32.20		32.21								
$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$	$\Gamma_1$	$\Gamma_2$	$\Gamma_3$	$\Gamma_4$	$\Gamma_5$								
P	1	1	2	2	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1							
P $\otimes$ V	1	1	2	2	2	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1							
P $\otimes$ A	3	3	1	1	2	2	2	2	2	2	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3							
P $\otimes$ V $\otimes$ A	2	2	4	7	7	3	3	6	6	6	3	2	5	6	7	3	2	5	6	7	2	2	4	7	7							
P $\otimes$ [V] <sup>2</sup>	3	3	6	3	3	1	1	2	5	5	3	1	4	3	3	1	4	3	5	3	3	1	4	3	5							

TABLE II. (Continued.)

32.13	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	32.14	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	32.15	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	32.16	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$
P	1 1 1	1	1 1 1	1	1 1 1	1	1 1 1
$P \otimes V$	1 1 2 1 1 1 2 1	1	1 1 2 1 1 2 1	1	1 1 1 1 2 1	1 1 1 1 1	1 1 1 1 1 2 1
$P \otimes A$	1 1 2 1 1 1 2 1	1	1 1 2 1 1 1 2	1	2 1 1 1 1 1	2 1 1 1 1 1	2 1 1 1 1 1
$P \otimes V \otimes A$	2 1 3 4 5 2 1 3 4 5	1	2 3 5 4 2 1 3 4 5	1	1 2 4 3 2 1 3 3 3	1 1 2 3 4 2 1 3 3 3	1 1 2 3 4 2 1 3 3 3
$P \otimes [V]^2$	2 2 2 4 2 2 2 4	2	2 2 4 2 2 4 2	2	1 3 1 2 1 1 3 2	2 1 3 1 2 1 1 2 3	2 1 3 1 2 1 1 2 3
32.17	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	32.18	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	32.19	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	32.20	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$
P	1 1 2 3 3	1	1 1 2 1 1	1	1 1 1 2	1 1 1 1	1 1 1 1
$P \otimes V$	3 3 6 9 9	1	1 1 2 5 5	1	1 2 3 5 4	1 1 2 3 3	1 1 2 3 3
$P \otimes A$	3 3 6 9 9	1	1 2 5 5	1	2 3 5 4	1 1 2 3 3	1 1 2 3 3
$P \otimes V \otimes A$	6 6 12 18 18	4	4 8 8 8	4	4 2 6 8 10	2 2 4 6 6	2 2 4 6 6
$P \otimes [V]^2$							
32.21	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	32.22	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	32.23	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	32.24	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$
P	1 1 1	1	1 1 1	1	1 1 1	1 1 1 2	1 1 2
$P \otimes V$	1 1 3 2	1	1 1 3 2	1	1 1 2 1	3 3	3 3
$P \otimes A$	1 1 3 2	1	1 1 3 2	1	1 1 2 1	3 3	3 3
$P \otimes V \otimes A$	2 2 4 4 4	3	3 2 5 7 6	2	2 2 4	3 3 6 6 6	3 3 6 6 6
$P \otimes [V]^2$							
32.25	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	32.26	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	32.27	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$	32.28	$\Gamma^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+ \Gamma_1 \Gamma_2 \Gamma_3 \Gamma_4 \Gamma_5$
P	1 1 1	1	1 1 1	1	1 1 2	1 1 1	1 1 1
$P \otimes V$	2 1 2 1	1	1 2 2 1	1	3 3	3 3	2 1
$P \otimes A$	2 1 2 1	1	2 1 1 2	1	3 3	3 3	2 1
$P \otimes V \otimes A$	2 1 3 3 3 2 1 3 3 3	1	2 3 3 3 2 1 3 3 3	3	3 3 6 6 6	2 1 3 3 3	2 1 3 3 3
$P \otimes [V]^2$	2 1 3 1 2 2 1 3 1 2	2	2 1 3 1 2 1 2 3 2 1	3	3 6 3 3	2 1 3 1 2	2 1 3 1 2

TABLE II. (Continued.)

	32.29	32.30	32.31	32.32
	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$
$P$	1 1	1	1	1 1
$P \otimes V$	1 1	1	1	1 1
$P \otimes A$	1 1	1	1	1 1
$P \otimes V \otimes A$	1 1 2 2	1 1 1 1	1 1 1 1	1 1 2 2
$P \otimes [V]^2$	1 1 2 1 1 1 2 1 1	1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1	1 1 2 1 1

  

	32.33
	$\Gamma_1^+ \Gamma_2^+ \Gamma_3^+ \Gamma_4^+ \Gamma_5^+$
$P$	1
$P \otimes V$	1
$P \otimes A$	1
$P \otimes V \otimes A$	1 1 1 1
$P \otimes [V]^2$	1 1 1

(2) If  $\Gamma_i$  is contained  $m$  times in  $D_G^V$ ,  $\Gamma_i$  is contained  $M > m$  times in  $D_G^{TF}$ , Eq. (10). If  $\Gamma_i = \Gamma_1$ , the symmetry of the crystal is not lowered, and the degeneracy of the electronic state is not split. Condition (2) takes into account that a rigid translation of the crystal also does not lower the symmetry of the crystal and split the electronic degeneracy.

(3) If  $\Gamma_i$  is contained  $m$  times in  $D_G^A$  and  $\Gamma_i$  corresponds to a rigid rotational lattice vibrational mode of the atoms in the unit cell of the crystal,  $\Gamma_i$  is contained  $M > m$  times in Eq. (10). If there is only one atom per unit cell of the crystal, condition (3) may be deleted. The symmetrized squares of all degenerate point-group irreducible representations are given in Table III.

In the TiO<sub>2</sub> crystal of space-group symmetry  $D_{4h}^{14}$ , the symmetrized squares  $(\Gamma_e)_2$  of irreducible representations  $\Gamma_e$  corresponding to  $k=0$  degenerate irreducible representations  $D_G^{(0,e)}$  are (see  $D_{4h}$  in Table III)

$$(\Gamma_5^+)_{[2]} = (\Gamma_5^-)_{[2]} = \Gamma_1^+ + \Gamma_4^+ . \tag{19}$$

The irreducible representations  $\Gamma_i$  corresponding to  $k=0$  irreducible representations of lattice vibrations in TiO<sub>2</sub> are given in Eqs. (11) and (12), and from subtable 15.19 of Table II we have, for the point group  $D_{4h}$

$$D_G^V = \Gamma_2^- + \Gamma_5^- , \tag{20}$$

$$D_G^A = \Gamma_2^+ + \Gamma_3^+ . \tag{21}$$

The irreducible representation  $\Gamma_4^+$  is contained in both Eqs. (19) and (12), i.e.,  $\Gamma_i = \Gamma_4^+$  is contained in  $(\Gamma_e)_{[2]}$ , and is not contained in either  $D_G^V$  or  $D_G^A$ , Eqs. (20) and (21). Consequently, both the  $k=0$  degenerate electronic states  $D_G^{(0,5^+)}$  and  $D_G^{(0,5^-)}$  of TiO<sub>2</sub> give rise to configurational instabilities. Since  $\Gamma_4^+$  is contained in Eq. (12), we have that these configurational instabilities are associated with the oxygen atoms of the crystal.

In the diamond structure, the space group is  $O_h^7$ , and the crystal consists of a single simple crystal generated by  $O_h^7$  from  $r=000$ , the  $8(a)$  atomic positions, with site point group  $\hat{S}(r) = T_d$ . The symmetrized squares of irreducible representations  $\Gamma_e$  corresponding to  $k=0$  degenerate electronic states  $D_G^{(0,e)}$  are (see Table III)

$$(\Gamma_3^+)_{[2]} = (\Gamma_3^-)_{[2]} = \Gamma_1^+ + \Gamma_3^+ , \tag{22}$$

$$(\Gamma_4^+)_{[2]} = (\Gamma_4^-)_{[2]} = (\Gamma_5^+)_{[2]} = (\Gamma_5^-)_{[2]} = \Gamma_1^+ + \Gamma_3^+ + \Gamma_5^+ . \tag{23}$$

The irreducible representations  $\Gamma_i$  contained in Eq.

TABLE III. Symmetrized squares of degenerate point-group irreducible representations. The notation for the point-group irreducible representations is that of Ref. 25.

Point group	$\Gamma$	$(\Gamma)_{[2]}$
$D_4, C_{4v}, D_{2d}$	$\Gamma_5$	$\Gamma_1 + \Gamma_4$
$D_{4h}$	$\Gamma_5^\pm$	$\Gamma_1^\pm + \Gamma_4^\pm$
$D_3, C_{3v}$	$\Gamma_3$	$\Gamma_1 + \Gamma_3$
$D_{3d}$	$\Gamma_3^\pm$	$\Gamma_1^\pm + \Gamma_3^\pm$
$D_6, C_{6v}, D_{3h}$	$\Gamma_5, \Gamma_6$	$\Gamma_1 + \Gamma_6$
$D_{6h}$	$\Gamma_5^\pm, \Gamma_6^\pm$	$\Gamma_1^\pm + \Gamma_6^\pm$
$T$	$\Gamma_4$	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4$
$T_h$	$\Gamma_4^\pm$	$\Gamma_1^\pm + \Gamma_2^\pm + \Gamma_3^\pm + \Gamma_4^\pm$
$O, T_d$	$\Gamma_3$	$\Gamma_1 + \Gamma_3$
	$\Gamma_4, \Gamma_5$	$\Gamma_1 + \Gamma_3 + \Gamma_5$
$O_h$	$\Gamma_3^\pm$	$\Gamma_1^\pm + \Gamma_3^\pm$
	$\Gamma_4^\pm, \Gamma_5^\pm$	$\Gamma_1^\pm + \Gamma_3^\pm + \Gamma_5^\pm$

(10) are found in subtable 32.30 of Table II:

$$D_G^{\text{TF}} = \Gamma_5^+ + \Gamma_4^- \quad (24)$$

and from subtable 32.33, for the point group  $O_h$ :

$$D_G^V = \Gamma_4^- , \quad (25)$$

$$D_G^A = \Gamma_4^+ . \quad (26)$$

Since the irreducible representation  $\Gamma_i = \Gamma_5^+$ , Eq. (24), is contained in  $(\Gamma_e^-)_{[2]}$ , Eq. (23), for  $\Gamma_e = \Gamma_4^+$ ,  $\Gamma_4^-$ ,  $\Gamma_5^+$ ,  $\Gamma_5^-$ , but not in Eqs. (25) and (26), the  $k=0$  degenerate electronic states  $D_G^{(0,4+)}$ ,  $D_G^{(0,4-)}$ ,  $D_G^{(0,5+)}$ , and  $D_G^{(0,5-)}$  all give rise to configurational instabilities. Since no  $\Gamma_i$  of Eq. (24) is contained in Eq. (22), the  $k=0$  degenerate electronic states  $D_G^{(0,3+)}$  and  $D_G^{(0,3-)}$  do not give rise to configurational instabilities.<sup>18</sup>

#### D. Magnetic modes

The  $k=0$  irreducible representations of a space group  $G$ , whose basic functions are linear combinations of the spins of the magnetic atoms of a simple crystal generated by  $G$  from  $r$ , are determined using Eq. (8) by finding the irreducible representations  $\Gamma_\nu$  of the point group  $\hat{G}$  contained in

$$D_G^{\text{TF}} = D_G^{\hat{S}(r)} \times D_G^A \quad (27)$$

where  $D_G^A$  is the axial vector representation of the point group  $\hat{G}$  and  $\hat{S}(r)$  is the site point group of  $r$ .

As an example, we consider the crystal of  $\text{TbCrO}_3$  of space-group symmetry  $D_{2h}^{16}$ .<sup>7</sup> The terbium atom simple crystal is generated by  $D_{2h}^{16}$

from  $r_1 = xy\frac{1}{2}$ ,  $4(c)$  atomic positions,<sup>12</sup> and the site point group  $\hat{S}(r_1) = C_3^z$ . The permutational color point group  $D_{2h}(C_3^z)$  is listed as group 8.4b in Table I, and in line three, subtable 8.4b of Table II one finds the irreducible representations  $\Gamma_\nu$ , contained in Eq. (27):

$$D_G^{\text{TF}}(r_1) = \Gamma_1^+ + 2\Gamma_2^+ + \Gamma_3^+ + 2\Gamma_4^+ \\ + 2\Gamma_1^- + \Gamma_2^- + 2\Gamma_3^- + \Gamma_4^- . \quad (28)$$

The chromium simple crystal is generated by  $D_{2h}^{16}$  from  $r_2 = 0\frac{1}{2}0$ , the  $4(b)$  atomic positions, and the site point group  $\hat{S}(r_2) = C_i$ . The permutational color point group  $D_{2h}(C_i)$  is listed as group 8.2 in Table I, and in line three subtable 8.2 of Table II one finds the irreducible representations  $\Gamma_\nu$ , contained in Eq. (27):

$$D_G^{\text{TF}}(r_2) = 3\Gamma_1^+ + 3\Gamma_2^+ + 3\Gamma_3^+ + 3\Gamma_4^+ . \quad (29)$$

Consequently, the terbium  $k=0$  magnetic modes are associated with the irreducible representations  $D_G^{(0,\nu)}$  with  $\nu$  of the representations  $\Gamma_\nu$ , given in Eq. (28), and the chromium magnetic modes to those given in Eq. (29).

#### E. Equitranslational phase transitions

In the Landau theory of continuous phase transitions one of the several group theoretical criteria used<sup>19-23</sup> is the tensor-field criterion. As reformulated by Litvin, Kotzev, and Birman,<sup>9</sup> this criterion, for equitranslational phase transitions is as follows. If the phase transition is due to a physical property described by a  $q$ -component tensor  $T$  de-

fined on the atoms of a crystal of space-group symmetry  $G$ , then a  $k=0$  irreducible representation  $D_G^{(0,\nu)}$  of  $G$  is associated with a phase transition from a high-symmetry phase  $G$  is  $\Gamma_\nu$  is contained in  $D_G^{\text{TF}}$  defined by Eq. (9).

As an example, consider  $\text{UBi}_2$  whose nonmagnetic space group is  $D_{4h}^7$  with the uranium atoms forming a single simple crystal, the  $2(c)$  atomic positions, generated by  $D_{4h}^7$  from  $r=0\frac{1}{2}z$ .<sup>24</sup> The site point group  $\hat{S}(r)=C_{4v}$ . For the magnetic phase transition in  $\text{UBi}_2$ , to find the  $k=0$  irreducible representations which satisfy the tensor-field criterion, one uses Eq. (9) with  $D_G^{\text{TF}}=D_G^A$ , the axial vector representation. From line three, subtable 15.16, of Table II one finds that

$$D_G^{\text{TF}} = \Gamma_2^+ + \Gamma_5^+ + \Gamma_1^- + \Gamma_5^- . \quad (30)$$

Consequently, the  $k=0$  irreducible representations  $D_G^{(0,2^+)}$ ,  $D_G^{(0,5^+)}$ ,  $D_G^{(0,1^-)}$ , and  $D_G^{(0,5^-)}$  satisfy the tensor-field criterion for equitranslational magnetic phase transitions in  $\text{UBi}_2$ . Using the additional

group theoretical criteria as formulated in Ref. 9, the magnetic phase transition associated with the irreducible representation  $D_G^{(0,1^-)}$  gives rise to the low-symmetry phase of space-group symmetry  $D_4^2$  with a spin arrangement generated by  $D_4^2$  from  $\bar{S}(0, \frac{1}{2}, z) = (0, 0, w)$ . This is the spin arrangement of the uranium atoms in the magnetic phase of  $\text{UBi}_2$ .

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