

Symmetry analysis of the microstructure and phase transitions of a crystallographic space group: Applications

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Two tables are presented which result from the symmetry analysis of the microstructure, i.e., atomic site locations, for a system with space-group symmetry $R\bar{3}c$ (D_{3d}^5). The first table contains information about transition order parameters. Representations, allowed subgroup symmetries, Landau and Lifshitz frequencies, changes in primitive-cell size, lattice relationships, etc., are listed. The second table gives the listing of the frequencies of subduction by the representation of the space group $R\bar{3}c$ for the representations of each site point group. After an explanation of the tables, examples are presented which show how the tables are used. Examples include the classification of lattice and magnetic modes, the testing of the tensor field criterion for phase transitions, and the determination of nuclear quadrupole resonance line splitting at phase transitions.

I. INTRODUCTION

The determination of the space-group symmetry G_0 of a crystalline solid conveys a certain level of information about that structure. However in many investigations more detailed microscopic symmetry information is needed. For example, in vibrational considerations the modes are classified¹ by selecting linear combinations of atomic displacements which transform according to an irreducible representation (irrep) of G_0 . This selection depends upon the number and locations of the atoms within the unit cell. Similarly, when magnetic structures are analyzed, linear combinations of the atomic spins (magnetic moments) are selected and classified according to the irreps of G_0 .^{2,3} As with the vibrational modes, the allowed magnetic modes also depend upon the location of the magnetic atoms within the unit cell.

In a slightly different context, the Landau theory of displacive phase transitions interprets a phase transition as taking place due to the growth of a particular crystal displacement. The transformation properties of the displacement must be associated with the irrep inducing the transition. Thus a linear combination of atomic displacements at different sites (the distortion) must be such that it transforms like a vector of this irrep. For order-disorder transitions, the distortion does not result from atomic displacements but from a microscopic probability density change. Again, the density change must transform as the irrep inducing the transition.

The nuclear quadrupole resonance (NQR) frequency is very sensitive to small differences in local field gradients, and the nuclear spins of a particular species will have well-separated resonance frequencies if they occupy inequivalent sites. For a given structure, the resonant atoms will be in a known site (and thus all equivalent sites). If the structure undergoes a phase transition, previously equivalent sites may become inequivalent in the new lower-symmetry phase. Since the sites are now inequivalent, line splitting will result, and the number of lines is equal to the number of inequivalent sites occupied

by the resonant atoms. Thus NQR becomes an important experimental method in analyzing phase transitions.^{4,5}

Recently, Kovalev⁶ emphasized the importance of compiling two lists which would contain sufficient information to exhaustively account for the microstructure and transitions of a given space group. One list would indicate transition subgroup symmetries while the other would indicate site-group subduction frequencies of the space-group irreps. Here we present two tables for the space group $R\bar{3}c$. The table of subgroups (Table I) contains more information than the list suggested by Kovalev. Information of irreps and subgroups, as well as Landau and Lifshitz frequencies, new primitive-cell size, lattice relationships, and irrep subduction frequencies are given. The additional information is extremely important for practical analysis of group-subgroup relationships. The second table (Table II) is the listing of site group subduction frequencies and is essentially the same as that discussed by Kovalev. In Sec. II the method is briefly reviewed by which the subgroup table is obtained. The resulting table is also explained. In Sec. III induced representations of space groups are described and the compilation of the second table is explained. In Sec. IV examples of how to use the two tables are presented. Although there are other situations where the tables are extremely useful (e.g., Raman and infrared activity, Jahn-Teller instabilities, and band representations), only the examples mentioned above will be explicitly given. These examples give ample evidence of the usefulness of the tables.

II. ISOTROPY SUBGROUPS OF SPACE GROUPS

The symmetry change which accompanies transitions between crystalline phases has been a subject of much study, both experimentally and theoretically. These studies are greatly facilitated by a knowledge of the subgroups of the 230 crystallographic space groups. Most existing tables of subgroups⁷⁻¹³ are not very useful for this purpose. They do not provide the space-group representation

which relates the symmetry change to the physical distortion of the crystal. Their approach is based on a mathematical selection without reference to the physical transitions which the symmetry changes represent.

A more useful approach is to first consider the types of possible physical distortions in a crystal and *then* find the corresponding subgroups. The distortions are classified according to representations of the parent space group G_0 . We write a general distortion $\Delta\rho(r)$ as

$$\Delta\rho(\mathbf{r}) = \sum_{i=1}^n \eta_i \phi_i(\mathbf{r}), \quad (1)$$

where $\phi_i(\mathbf{r})$ are basis functions of an n -dimensional representation of G_0 . By a slight extension, particle and/or magnetic moment densities can be included. The symmetry of the distortion is determined by the coefficients η_i which form an n -dimensional vector $\boldsymbol{\eta}$ called the *order parameter*. The subgroup G which results from this distortion consists of all elements $g \in G_0$ which leave the distortion invariant. Such a subgroup is called an *isotropy subgroup*.

By considering all possible distortions of the form given in Eq. (1) (or, equivalently, all possible directions of $\boldsymbol{\eta}$), one can obtain *all* of the distinct isotropy subgroups associated with the representation. The details of this procedure have been given in a series of publications by Hatch and Stokes¹⁴⁻¹⁸ and will not be given here.

In Table I, we list the isotropy subgroups of $R\bar{3}c$ for irreps at \mathbf{k} points of symmetry. The space-group settings given in Ref. 13 are used. For the monoclinic space groups, the setting with "unique axis \mathbf{b} , cell 1" is used. In the trigonal system, the hexagonal axes are used. These settings are the same as those given in the older edition,¹⁹ except for the centered monoclinic space groups.

The irreps are labeled using the convention of Miller and Love.²⁰ Some care must be taken in identifying elements of $R\bar{3}c$ in Miller and Love with elements of $R\bar{3}c$ in Ref. 13. Miller and Love use the "reverse setting" for the rhombohedral lattice, while Ref. 13 uses the "obverse setting." The two settings are related by a sixfold rotation C_6 . We rotate an element g' in Miller and Love by C_6 to obtain the corresponding element g in Ref. 13, i.e., $g = C_6 g' (C_6)^{-1}$.

The meaning of each column of Table I is explained below.

Irrep. The physically irreducible representation. The label follows the convention of Miller and Love.²⁰ In cases where the irrep of Miller and Love is complex, the physically irreducible representation is the direct sum of Miller and Love's irrep with its complex conjugate. This is indicated with *two* irrep labels. For example, $T_1 T_2$ indicates that the irrep is the direct sum of T_1 with its complex conjugate, which is equivalent to T_2 . Unless specifically stated otherwise, the term "irrep" in the following will always refer to physically irreducible representation.

Lan. The "Landau frequency," i.e., the number of times the unit irrep of G_0 is contained in the symmetrized triple Kronecker product of the irrep. If a phase transition is continuous, then Landau theory requires that the

Landau frequency be zero. This is known as the *Landau condition*.^{21,22}

Lif. The "Lifshitz frequency," i.e., the number of times the vector representation of G_0 is contained in the antisymmetrized double Kronecker product of the irrep. If the phase transition is continuous, and the lower-symmetry phase is commensurate, then Landau theory requires that the Lifshitz frequency be zero. This is known as the *Lifshitz condition*.²³

Subgroup. The isotropy subgroups or lower-symmetry space groups G . The space-group number is given, followed by the short Hermann-Mauguin symbol as given in Ref. 13.

Size. The relative size of the *primitive* unit cell in the parent group and subgroup.

Basis. The conventional basis vectors of the lattice of G in terms of the conventional basis vectors of the lattice of G_0 . The conventional basis vectors are the ones to which the x, y, z coordinates refer in Ref. 13. Note that when centered lattices are involved, these are *not* the primitive basis vectors.

Origin. The origin of the space-group setting of the subgroup with respect to the origin of the space-group setting of the parent group. This vector is given in terms of the conventional basis vectors of the lattice of G_0 .

Subduction. The irreps of $R\bar{3}c$ which subduce the identity representation of the given subgroup.

In order to illustrate the meaning of the entries in the table, let us consider the following entry in Table I:

Irrep	F_2^-
Subgroup	14 $P2_1/c$
Size	2
Basis	$(\frac{1}{3}, \frac{2}{3}, \frac{1}{3}), (1, 0, 0), (\frac{2}{3}, \frac{4}{3}, \frac{1}{3})$
Origin	$(\frac{1}{3}, \frac{1}{6}, \frac{1}{6})$

This entry gives a possible phase transition from space group 167 ($R\bar{3}c$) to space group 14 ($P2_1/c$). The conventional basis vectors of the lattice of $R\bar{3}c$ are (using hexagonal axes)

$$\begin{aligned} \mathbf{a}_0 &= \frac{1}{2}\sqrt{3}a\hat{\mathbf{i}} - \frac{1}{2}a\hat{\mathbf{j}}, \\ \mathbf{b}_0 &= a\hat{\mathbf{j}}, \\ \mathbf{c}_0 &= c\hat{\mathbf{k}}. \end{aligned} \quad (2)$$

From the "basis" column in the entry, we find that the conventional basis vectors of the subgroup are

$$\begin{aligned} \mathbf{a} &= -\frac{1}{3}\mathbf{a}_0 - \frac{2}{3}\mathbf{b}_0 + \frac{1}{3}\mathbf{c}_0 = -\frac{1}{6}\sqrt{3}a\hat{\mathbf{i}} - \frac{1}{2}a\hat{\mathbf{j}} + \frac{1}{3}c\hat{\mathbf{k}}, \\ \mathbf{b} &= \mathbf{a}_0 = \frac{1}{2}\sqrt{3}a\hat{\mathbf{i}} - \frac{1}{2}a\hat{\mathbf{j}}, \\ \mathbf{c} &= \frac{2}{3}\mathbf{a}_0 + \frac{4}{3}\mathbf{b}_0 + \frac{1}{3}\mathbf{c}_0 = \frac{1}{3}\sqrt{3}a\hat{\mathbf{i}} + a\hat{\mathbf{j}} + \frac{1}{3}c\hat{\mathbf{k}}. \end{aligned} \quad (3)$$

We see that both \mathbf{a} and \mathbf{c} are perpendicular to \mathbf{b} , as they must be, since the twofold axis is along \mathbf{b} in the space group $P2_1/c$.

Elements of the subgroup $P2_1/c$ are easily identified as elements of the parent group $R\bar{3}c$. For example, we find in Ref. 13 that one of the elements of $P2_1/c$ is $\bar{x}, y + \frac{1}{2}, \bar{z} + \frac{1}{2}$ which is a twofold rotation about \mathbf{b} followed by a fractional translation, $\frac{1}{2}\mathbf{b} + \frac{1}{2}\mathbf{c}$. We see from Eq. (3) that the b axis in $P2_1/c$ is the a_0 axis in $R\bar{3}c$. A twofold

TABLE I. Information about transition order parameters for $R\bar{3}c$. Irreps, allowed subgroup symmetries, Landau and Lifshitz frequencies, new conventional basis vectors and origin (in terms of conventional lattice of $R\bar{3}c$), and the irreps of $R\bar{3}c$ which subduce the identity irrep of each subgroup are shown.

Subgroup	Size	Basis	Origin	Subduction
167 $R\bar{3}c$	1	(1,0,0),(0,1,0),(0,0,1)	Irrep Γ_1^+ , Landau=1, Lifshitz=0 (0,0,0) Γ_1^+	
148 $R\bar{3}$	1	(1,00),(0,1,0),(0,0,1)	Irrep Γ_2^+ , Landau=0, Lifshitz=0 (0,0,0) Γ_1^+, Γ_2^+	
15 $C2/c$	1	(1, $\bar{1}$, 0)(1,1,0), ($\frac{1}{6}, \frac{1}{6}, \frac{1}{3}$)	Irrep Γ_3^+ , Landau=1, Lifshitz=0 ($\frac{1}{3}, \frac{1}{6}, \frac{1}{6}$) Γ_1^+, Γ_3^+	
2 $P\bar{1}$	1	($\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$), ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$), ($\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$)	(0,0,0) $\Gamma_1^+, \Gamma_2^+, \Gamma_3^+$	
155 $R32$	1	(1,0,0),(0,1,0),(0,0,1)	Irrep Γ_1^- , Landau=0, Lifshitz=0 (0,0, $\frac{1}{4}$) Γ_1^+, Γ_1^-	
161 $R3c$	1	(1,0,0),(0,1,0),(0,0,1)	Irrep Γ_2^- , Landau=0, Lifshitz=0 (0,0,0) Γ_1^+, Γ_2^-	
5 $C2$	1	(1, $\bar{1}$, 0)(1,1,0), ($\frac{1}{6}, \frac{1}{6}, \frac{1}{3}$)	Irrep Γ_3^- , Landau=0, Lifshitz=0 ($\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$) $\Gamma_1^+, \Gamma_3^+, \Gamma_1^-, \Gamma_3^-$	
9 Cc	1	(1, $\bar{1}$, 0)(1,1,0), ($\frac{1}{6}, \frac{1}{6}, \frac{1}{3}$)	($\frac{1}{3}, \frac{1}{6}, \frac{1}{6}$) $\Gamma_1^+, \Gamma_3^+, \Gamma_2^-, \Gamma_3^-$	
1 $P1$	1	($\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$), ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$), ($\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$)	(0,0,0) $\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, \Gamma_1^-, \Gamma_2^-, 2\Gamma_3^-$	
13 $P2/c$	2	($\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$), (1,0,0), ($\frac{2}{3}, \frac{4}{3}, \frac{1}{3}$)	Irrep F_1^+ , Landau=1, Lifshitz=0 (0,0,0) $\Gamma_1^+, \Gamma_3^+, F_1^+$	
167 $R\bar{3}c$	4	($\bar{2}$, 0, 0), (0, $\bar{2}$, 0), (0, 0, 1)	(0,0,0) Γ_1^+, F_1^+	
15 $C2/c$	4	($\frac{2}{3}, \frac{2}{3}, \frac{4}{3}$), ($\bar{2}$, $\bar{2}$, 0), ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$)	($\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$) $\Gamma_1^+, \Gamma_3^+, 2F_1^+, F_2^+$	
2 $P\bar{1}$	4	($\frac{4}{3}, \frac{2}{3}, \frac{1}{3}$), ($\frac{2}{3}, \frac{2}{3}, \frac{1}{3}$), ($\frac{2}{3}, \frac{4}{3}, \frac{1}{3}$)	(0,0,0) $\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, 3F_1^+, 3F_2^+$	
14 $P2_1/c$	2	($\frac{2}{3}, \frac{4}{3}, \frac{1}{3}$), ($\bar{1}$, 0, 0), ($\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$)	Irrep F_2^+ , Landau=0, Lifshitz=0 (0,0,0) $\Gamma_1^+, \Gamma_3^+, F_2^+$	
15 $C2/c$	4	($\frac{2}{3}, \frac{2}{3}, \frac{4}{3}$), ($\bar{2}$, $\bar{2}$, 0), ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$)	(0,0,0) $\Gamma_1^+, \Gamma_3^+, 2F_1^+, F_2^+$	
148 $R\bar{3}$	4	($\bar{2}$, 0, 0), (0, $\bar{2}$, 0), (0, 0, 1)	(0,0,0) $\Gamma_1^+, \Gamma_2^+, F_1^+, F_2^+$	
2 $P\bar{1}$	4	($\frac{4}{3}, \frac{2}{3}, \frac{1}{3}$), ($\frac{2}{3}, \frac{2}{3}, \frac{1}{3}$), ($\frac{2}{3}, \frac{4}{3}, \frac{1}{3}$)	(0,0,0) $\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, 3F_1^+, 3F_2^+$	
13 $P2/c$	2	($\frac{2}{3}, \frac{4}{3}, \frac{1}{3}$), ($\bar{1}$, 0, 0), ($\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$)	Irrep F_1^- , Landau=0, Lifshitz=0 ($\frac{1}{3}, \frac{1}{6}, \frac{1}{6}$) $\Gamma_1^+, \Gamma_3^+, F_1^-$	
15 $C2/c$	4	($\frac{2}{3}, \frac{2}{3}, \frac{4}{3}$), ($\bar{2}$, $\bar{2}$, 0), ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$)	($\frac{1}{6}, \frac{1}{6}, \frac{1}{6}$) $\Gamma_1^+, \Gamma_3^+, F_1^+, F_1^-, F_2^-$	
155 $R32$	4	($\bar{2}$, 0, 0), (0, $\bar{2}$, 0), (0, 0, 1)	(0,0, $\frac{1}{4}$) $\Gamma_1^+, \Gamma_1^-, F_1^+, F_1^-$	
2 $P\bar{1}$	4	($\frac{4}{3}, \frac{2}{3}, \frac{1}{3}$), ($\frac{2}{3}, \frac{2}{3}, \frac{1}{3}$), ($\frac{2}{3}, \frac{4}{3}, \frac{1}{3}$)	($\frac{1}{6}, \frac{1}{6}, \frac{1}{6}$) $\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, F_1^+, F_2^+, 2F_1^-, 2F_2^-$	
5 $C2$	4	($\frac{2}{3}, \frac{2}{3}, \frac{4}{3}$), ($\bar{2}$, $\bar{2}$, 0), ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$)	($\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$) $\Gamma_1^+, \Gamma_3^+, \Gamma_1^-, \Gamma_3^-, 2F_1^+, F_2^+, 2F_1^-, F_2^-$	
1 $P1$	4	($\frac{4}{3}, \frac{2}{3}, \frac{1}{3}$), ($\frac{2}{3}, \frac{2}{3}, \frac{1}{3}$), ($\frac{2}{3}, \frac{4}{3}, \frac{1}{3}$)	(0,0,0) $\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, \Gamma_1^-, \Gamma_2^-, 2\Gamma_3^-, 3F_1^+, 3F_2^+, 3F_1^-, 3F_2^-$	
14 $P2_1/c$	2	($\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$), (1,0,0), ($\frac{2}{3}, \frac{4}{3}, \frac{1}{3}$)	Irrep F_2^- , Landau=0, Lifshitz=0 ($\frac{1}{3}, \frac{1}{6}, \frac{1}{6}$) $\Gamma_1^+, \Gamma_3^+, F_2^-$	
15 $C2/c$	4	($\frac{2}{3}, \frac{2}{3}, \frac{4}{3}$), ($\bar{2}$, $\bar{2}$, 0), ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$)	($\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$) $\Gamma_1^+, \Gamma_3^+, F_1^+, F_1^-, F_2^-$	
161 $R3c$	4	($\bar{2}$, 0, 0), (0, $\bar{2}$, 0), (0, 0, 1)	(0,0,0) $\Gamma_1^+, \Gamma_2^-, F_1^+, F_2^-$	
2 $P\bar{1}$	4	($\frac{4}{3}, \frac{2}{3}, \frac{1}{3}$), ($\frac{2}{3}, \frac{2}{3}, \frac{1}{3}$), ($\frac{2}{3}, \frac{4}{3}, \frac{1}{3}$)	($\frac{1}{6}, \frac{1}{6}, \frac{1}{6}$) $\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, F_1^+, F_2^+, 2F_1^-, 2F_2^-$	
9 Cc	4	($\frac{2}{3}, \frac{2}{3}, \frac{4}{3}$), ($\bar{2}$, $\bar{2}$, 0), ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$)	($\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$) $\Gamma_1^+, \Gamma_3^+, \Gamma_2^-, \Gamma_3^-, 2F_1^+, F_2^+, F_1^-, 2F_2^-$	
1 $P1$	4	($\frac{4}{3}, \frac{2}{3}, \frac{1}{3}$), ($\frac{2}{3}, \frac{2}{3}, \frac{1}{3}$), ($\frac{2}{3}, \frac{4}{3}, \frac{1}{3}$)	(0,0,0) $\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, \Gamma_1^-, \Gamma_2^-, 2\Gamma_3^-, 3F_1^+, 3F_2^+, 3F_1^-, 3F_2^-$	
2 $P\bar{1}$	2	($\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$), ($\frac{2}{3}, \frac{2}{3}, \frac{2}{3}$), ($\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$)	Irrep L_1 , Landau=0, Lifshitz=2 (0,0,0) $\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, L_1$	
5 $C2$	2	($\frac{1}{3}, \frac{1}{3}, \frac{2}{3}$), (1,1,0), ($\bar{1}$, 1, 0)	($\frac{1}{8}, \frac{1}{8}, \frac{1}{4}$) $\Gamma_1^+, \Gamma_3^+, \Gamma_1^-, \Gamma_3^-, L_1$	
15 $C2/c$	4	($\frac{4}{3}, \frac{4}{3}, \frac{2}{3}$), ($\bar{4}$, 0, 0), ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$)	($\frac{1}{3}, \frac{1}{6}, \frac{1}{6}$) $\Gamma_1^+, \Gamma_3^+, F_1^-, L_1$	
15 $C2/c$	4	($\frac{4}{3}, \frac{4}{3}, \frac{2}{3}$), ($\bar{4}$, 0, 0), ($\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$)	($\frac{1}{6}, \frac{1}{6}, \frac{1}{6}$) $\Gamma_1^+, \Gamma_3^+, F_1^-, L_1$	
148 $R\bar{3}$	8	(2,0,0)(0,2,0), (0,0,2)	(0,0,0) $\Gamma_1^+, \Gamma_2^+, F_1^+, F_2^+, L_1, T_3$	
155 $R32$	8	(2,0,0), (0,2,0), (0,0,2)	(0,0, $\frac{1}{4}$) $\Gamma_1^+, \Gamma_1^-, F_1^+, F_1^-, L_1, T_3$	

TABLE I. (Continued).

Subgroup	Size	Basis	Origin	Subduction
Irrep L_1 , Landau=0, Lifshitz=2				
1 $P1$	2	$(\frac{2}{3}, \frac{1}{3}, \frac{1}{3}), (\frac{2}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{2}{3}, \frac{1}{3})$	(0,0,0)	$\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, \Gamma_1^-, \Gamma_2^-, 2\Gamma_3^-, 2L_1$
2 $P\bar{1}$	4	$(\frac{4}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{1}{3}, \frac{2}{3}, \frac{1}{3})$	(0,0,0)	$\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, F_1^+, F_2^+, 2L_1$
2 $P\bar{1}$	4	$(\frac{4}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{2}{3}, \frac{1}{3})$	$(\frac{1}{3}, \frac{1}{6}, \frac{1}{6})$	$\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, F_1^-, F_2^-, 2L_1$
2 $P\bar{1}$	4	$(\frac{4}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{1}{3}, \frac{2}{3}, \frac{1}{3})$	$(\frac{1}{6}, \frac{1}{6}, \frac{1}{6})$	$\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, F_1^-, F_2^-, 2L_1$
5 $C2$	4	$(\frac{4}{3}, \frac{4}{3}, \frac{2}{3}), (\bar{4}, 0, 0), (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$	$(\frac{1}{4}, 0, \frac{1}{4})$	$\Gamma_1^+, \Gamma_3^+, \Gamma_1^-, \Gamma_3^-, F_1^+, F_1^-, 2L_1$
9 Cc	4	$(\frac{4}{3}, \frac{4}{3}, \frac{2}{3}), (\bar{4}, 0, 0), (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$	$(\frac{1}{3}, \frac{1}{6}, \frac{1}{6})$	$\Gamma_1^+, \Gamma_3^+, \Gamma_2^-, \Gamma_3^-, F_2^+, F_1^-, 2L_1$
146 $R3$	8	(2,0,0)(0,2,0)(0,0,2)	(0,0,0)	$\Gamma_1^+, \Gamma_2^+, \Gamma_1^-, \Gamma_2^-, F_1^+, F_2^+, F_1^-, F_2^-, 2L_1, 2T_3$
2 $P\bar{1}$	8	$(\frac{4}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{4}{3}, \frac{2}{3})$	(0,0,0)	$\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, 3F_1^+, 3F_2^+, 3L_1, 2T_1T_2, T_3$
2 $P\bar{1}$	8	$(\frac{4}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{4}{3}, \frac{2}{3})$	$(\frac{1}{6}, \frac{1}{3}, \frac{1}{6})$	$\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, F_1^+, F_2^+, 2F_1^-, 2F_2^-, 3L_1, 2T_1T_2, T_3$
5 $C2$	8	(2,2,0)(2,2,0)($\frac{1}{3}, \frac{1}{3}, \frac{2}{3}$)	$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$	$\Gamma_1^+, \Gamma_3^+, \Gamma_1^-, \Gamma_3^-, 2F_1^+, F_2^+, 2F_1^-, F_2^-, 3L_1, 2T_1T_2, T_3$
1 $P1$	4	$(\frac{4}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{1}{3}, \frac{2}{3}, \frac{1}{3})$	(0,0,0)	$\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, \Gamma_1^-, \Gamma_2^-, 2\Gamma_3^-, F_1^+, F_2^+, F_1^-, F_2^-, 4L_1$
1 $P1$	8	$(\frac{4}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{2}{3}, \frac{2}{3}), (\frac{2}{3}, \frac{4}{3}, \frac{2}{3})$	(0,0,0)	$\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, \Gamma_1^-, \Gamma_2^-, 2\Gamma_3^-, 3F_1^+, 3F_2^+, 3F_1^-, 3F_2^-, 6L_1, 4T_1T_2, 2T_3$
Irrep T_1T_2 , Landau=0, Lifshitz=3				
2 $P\bar{1}$	2	$(\frac{2}{3}, \frac{1}{3}, \frac{2}{3}), (\frac{1}{3}, \frac{1}{3}, \frac{2}{3}), (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$	(0,0,0)	$\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, 2T_1T_2, T_3$
5 $C2$	2	(1,1,0)(1,1,0)($\frac{1}{3}, \frac{1}{3}, \frac{2}{3}$)	$(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$	$\Gamma_1^+, \Gamma_3^+, \Gamma_1^-, \Gamma_3^-, 2T_1T_2, T_3$
1 $P1$	2	$(\frac{2}{3}, \frac{1}{3}, \frac{2}{3}), (\frac{1}{3}, \frac{1}{3}, \frac{2}{3}), (\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$	(0,0,0)	$\Gamma_1^+, \Gamma_2^+, 2\Gamma_3^+, \Gamma_1^-, \Gamma_2^-, 2\Gamma_3^-, 4T_1T_2, 2T_3$
Irrep T_3 , Landau=0, Lifshitz=1				
148 $R\bar{3}$	2	(1,1,0)(0,1,0)(0,0,2)	$(0, 0, \frac{1}{2})$	$\Gamma_1^+, \Gamma_2^+, T_3$
155 $R32$	2	(1,0,0)(0,1,0)(0,0,2)	$(0, 0, \frac{3}{4})$	$\Gamma_1^+, \Gamma_1^-, T_3$
146 $R3$	2	(1,0,0)(0,1,0)(0,0,2)	(0,0,0)	$\Gamma_1^+, \Gamma_2^+, \Gamma_1^-, \Gamma_2^-, 2T_3$

rotation about a hexagonal \mathbf{a}_0 axis is denoted by $x - y, \bar{y}, \bar{z}$ (see, for example, p. 37 of Ref. 24). The fractional associated with this rotation in $P2_1/c$ is

$$\frac{1}{2}\mathbf{b} + \frac{1}{2}\mathbf{c} = \frac{5}{6}\mathbf{a}_0 + \frac{2}{3}\mathbf{b}_0 + \frac{1}{6}\mathbf{c}_0. \quad (4)$$

To find the fractional in $R\bar{3}c$, we must move the origin. Consider some symmetry element consisting of a point operation R followed by a fractional translation \mathbf{v} . If we move the origin by an amount $-\tau$, the new fractional translation \mathbf{v}' is given by

$$\mathbf{v}' = \mathbf{v} + \tau - R\tau. \quad (5)$$

From the "origin" column of the entry, we see that the origin of $P2_1/c$ with respect to the origin of $R\bar{3}c$ is at

$$\tau = \frac{1}{3}\mathbf{a}_0 + \frac{1}{6}\mathbf{b}_0 + \frac{1}{6}\mathbf{c}_0. \quad (6)$$

Thus, we want to move the origin by an amount $-\tau$. In this case, $R = x - y, \bar{y}, \bar{z}$ and its fractional with respect to the origin of $R\bar{3}c$ is

$$\begin{aligned} & (\frac{5}{6}\mathbf{a}_0 + \frac{2}{3}\mathbf{b}_0 + \frac{1}{6}\mathbf{c}_0) + (\frac{1}{3}\mathbf{a}_0 + \frac{1}{6}\mathbf{b}_0 + \frac{1}{6}\mathbf{c}_0) \\ & - (\frac{1}{6}\mathbf{a}_0 - \frac{1}{6}\mathbf{b}_0 - \frac{1}{6}\mathbf{c}_0) = \mathbf{a}_0 + \mathbf{b}_0 + \frac{1}{2}\mathbf{c}_0. \end{aligned} \quad (7)$$

Thus the symmetry element in $R\bar{3}c$ is $x - y + 1, \bar{y} + 1, \bar{z} + \frac{1}{2}$.

The index of the subgroup $P2_1/c$ in $R\bar{3}c$ is 6. This result is easily obtained. First, there are 12 elements in the point group $\bar{3}m$ of $R\bar{3}c$, and there are 4 elements in the

point group $2/m$ of $P2_1/c$. Thus the index of $2/m$ in $\bar{3}m$ is $12 \div 4 = 3$. The size of the primitive unit cell in $R\bar{3}c$ is twice as large as that in $P2_1/c$ (see the "size" column in the entry). Thus, the index of the translation group of $P2_1/c$ in the translation group of $R\bar{3}c$ is equal to 2. Combining the point group with the translation group, we obtain the index of the space group $P2_1/c$ in the space group $R\bar{3}c$: $3 \times 2 = 6$.

The number of possible domains in the lower-symmetry phase is given by the index of the subgroup in the parent group. In this case there are six possible domains of $P2_1/c$. Each of the six domains is a different isotropy subgroup of $R\bar{3}c$. But they are equivalent to each other. They are simultaneously minima of the free energy and thus thermodynamically equally probable. They represent the same phase transition²⁵ and thus only one of them is listed in Table I.

In the last column of Table I we list the frequency of subduction, by each irrep of $R\bar{3}c$, of the identity irrep of the given isotropy subgroup. In Sec. IV an example of the use of the subduction frequencies will be given.

III. SITE SYMMETRY SUBDUCTION FREQUENCIES

A crystal with space-group symmetry G_0 can be partitioned into "simple crystals."²⁶ Each simple crystal consists of all atoms obtained from a representative atom by transformations of G_0 . Each simple crystal has all atoms

in equivalent sites. A crystal will then consist of several simple crystals having no atoms in common, and the elements of G_0 permute the atoms of each simple crystal among themselves.

Let us label the primitive cells in the crystal by the lattice translation vectors \mathbf{a} . Considering a simple crystal, label the first primitive cell by $\mathbf{a}=\mathbf{0}$ and suppose it contains m atoms A_r ($r=1, \dots, m$) of type A . Let $G(A_1)$ be the site symmetry group of atom A_1 (the first atom) which is of order n . The elements of the site group $G(A_1)$ are elements of the space group G_0 which leave atom A_1 fixed. We represent these elements as $g_{1p} = \{R_{1p} | \mathbf{a}_{1p}\}$ with $p=1, \dots, n$. (We choose g_{11} to be the identity transformation.) Let g_{r1} be an element of the space group G_0 which takes the atom at position 1 into the atom at position r ($r=1, \dots, m$). Any element of G_0 can then be written in the form, $\{E | \mathbf{a}\}g_{r1}g_{1p}$.

Suppose that the functions $\varphi(\alpha, 1, 0)$, $\alpha=1, \dots, l_j$, of position \mathbf{r} , are basis functions of an irreducible representation (index j) of the site group $G(A_1)$, so that

$$g_{1p}\varphi(\alpha, 1, 0) = \sum_{\beta} \varphi(\beta, 1, 0)d^j(g_{1p})_{\beta\alpha}. \quad (8)$$

Using the transformation property, $g\varphi(\mathbf{r}) = \varphi'(\mathbf{r}) = \varphi(g^{-1}\mathbf{r})$, $l_j(m-1)$ functions are obtained through

$$\varphi(\alpha, r, 0) = g_{r1}\varphi(\alpha, 1, 0). \quad (9)$$

Functions associated with atoms in other cells are obtained through

$$\varphi(\alpha, r, \mathbf{a}) = \{E | \mathbf{a}\}\varphi(\alpha, r, 0). \quad (10)$$

Then for any g in G_0 ,

$$\begin{aligned} g\varphi(\alpha, r, \mathbf{a}) &= g\{E | \mathbf{a}\}g_{r1}\varphi(\alpha, 1, 0) \\ &= \{E | \mathbf{a}'\}g_{s1}g_{1q}\varphi(\alpha, 1, 0), \end{aligned} \quad (11)$$

where $g_{1q} = g_{s1}^{-1}\{E | -\mathbf{a}'\}g\{E | \mathbf{a}\}g_{r1}$. Both $\{E | -\mathbf{a}'\}$ and g_{s1} must be chosen so that g_{1q} is an element of $G(A_1)$. Thus

$$\begin{aligned} g\varphi(\alpha, r, \mathbf{a}) &= \{E | \mathbf{a}'\}g_{s1} \sum_{\beta} \varphi(\beta, 1, 0)d^j(g_{1q})_{\beta\alpha} \\ &= \sum_{\beta} \varphi(\beta, s, \mathbf{a}')d^j(g_{1q})_{\beta\alpha}, \end{aligned} \quad (12)$$

and the functions $\varphi(\alpha, r, \mathbf{a})$ carry a representation $I(d^j)$ of G_0 . $I(d^j)$ is the representation of G_0 induced by the site group representation d^j and is written explicitly as

$$I(d^j, g)_{\beta s \alpha', \alpha r \alpha} = d^j(\bar{g})_{\beta \alpha} \delta(\bar{g} \in G(A_1)), \quad (13)$$

where

$$\bar{g} = g_{s1}^{-1}\{E | -\mathbf{a}'\}g\{E | \mathbf{a}\}g_{r1}.$$

The function δ is equal to one if \bar{g} is in $G(A_1)$ and is equal to zero if not. Note that the dimension of the representation $I(d^j, g)$ is infinite.

Kovalev²⁷ has shown the following result. The irreducible representation D of space group G_0 is contained in the induced representation $I(d^j)$ a total number of times $m(D, d^j)$, given by

$$m(D, d^j) = \frac{1}{n} \sum_{g \in G(A_1)} \chi_D^j(g) \chi_D(g), \quad (14)$$

where χ_D and χ_D^j are the characters of the irrep D and the irrep d^j , respectively. The last expression is just the number of times the irrep D of G_0 subduces the irrep d^j of $G(A_1)$.

Using the full group representation $D^{(**, \gamma)}$, we have calculated the above subduction frequencies for all sites of symmetry (and their irreps) and all irreps for \mathbf{k} points of symmetry of $R\bar{3}c$. This result is shown in Table II. The labeling of point group irreps is that of Bradley and Cracknell.²⁴ In Table III we reproduce those site point group character tables needed for space group $R\bar{3}c$. Also exemplary basis functions are listed for each point group irrep.²⁸

An approach emphasizing color groups was used previously²⁹ to obtain subduction frequency tables for the Γ point ($\mathbf{k}=\mathbf{0}$) space-group irreps. Also, the subduction-

TABLE II. Listing of the frequencies of subduction by each irrep of $R\bar{3}c$ for the irreps of the site point group (see Table III).

Irrep	a (32)	b ($\bar{3}$)	c (3)	d ($\bar{1}$)	e (2)	f (1)
Γ_1^+	A_1	A_g	A	A_g	A	A
Γ_2^+	A_2	A_g	A	A_g	B	A
Γ_3^+	E	E_g^*	E^*	$2A_g$	$A+B$	$2A$
Γ_1^-	A_1	A_u	A	A_u	A	A
Γ_2^-	A_2	A_u	A	A_u	B	A
Γ_3^-	E	E_u^*	E^*	$2A_u$	$A+B$	$2A$
F_1^+	A_1+E	$A_g+E_g^*$	$A+E^*$	A_g+2A_u	$2A+B$	$3A$
F_2^+	A_2+E	$A_g+E_g^*$	$A+E^*$	A_g+2A_u	$A+2B$	$3A$
F_1^-	A_1+E	$A_u+E_u^*$	$A+E^*$	$2A_g+A_u$	$2A+B$	$3A$
F_2^-	A_2+E	$A_u+E_u^*$	$A+E^*$	$2A_g+A_u$	$A+2B$	$3A$
L_1	A_1+A_2+2E	$A_g+E_g^*+A_u+E_u^*$	$2A+2E^*$	$3A_g+3A_u$	$3A+3B$	$6A$
T_1T_2	$2E$	$E_g^*+E_u^*$	$2E^*$	$2A_g+2A_u$	$2A+2B$	$4A$
T_3	A_1+A_2	A_g+A_u	$2A$	A_g+A_u	$A+B$	$2A$

TABLE III. Site point-group character tables for $R\bar{3}c$. For each point-group irrep, exemplary basis functions for that irrep are shown in parentheses.

Irreps	Characters					
Point Group 1	E					
A	1					
Point group $\bar{1}$	E	I				
$A_g(S_x, S_y, S_z)$	1	1				
$A_u(x, y, z)$	1	-1				
Point group 2	E	C_{2z}				
$A(z, S_z)$	1	1				
$B(x, y, S_x, S_y)$	1	-1				
Point group 3	E	C_3^+	C_3^-			
$A(z, S_z)$	1	1	1			
$E^*(x \pm iy, S_x \pm iS_y)$	2	-1	-1			
Point group $\bar{3}$	E	C_3^+	C_3^-	I	S_6^-	S_6^+
$A_g(R, S_z)$	1	1	1	1	1	1
$E_g^*(S_x \pm iS_y)$	2	-1	-1	2	-1	-1
$A_u(z)$	1	1	1	-1	-1	-1
$E_u^*(x \pm iy)$	2	-1	-1	-2	1	1
Point group 32	E	C_3^+	C_3^-	C'_{21}	C'_{22}	C'_{23}
$A_1(R)$	1	1	1	1	1	1
$A_2(z, S_z)$	1	1	1	-1	-1	-1
$E(x, y, S_x \pm iS_y)$	2	-1	-1	0	0	0

frequency table for all \mathbf{k} points of symmetry for the space group $Fd\bar{3}m$ has been previously published.³⁰ These tables yield the same type of information for their space groups as our information in Table II for the space group $R\bar{3}c$.

IV. APPLICATIONS

There are many physical applications where the information contained in Tables I and II is useful. Only four examples will be considered here. These examples, however, will be sufficient to show the extent to which the microstructures of $R\bar{3}c$ are described and the ease with which the information can be obtained from the tables.

A. Lattice distortions

The lattice vibrations of a solid are classified by the irreps of its space group. Specific linear combinations of the atomic displacements are selected such that they transform as the basis functions of the related irrep. Since all atoms in a simple crystal are related by group transformations, the displacement of atom A_1 of cell $\mathbf{a}=\mathbf{0}$ uniquely determines the displacements of all others in the simple crystal. The displacements of atom A_1 transform as a polar vector representation of the site group $G(A_1)$. Thus the displacements of atom A_1 , a vector representation of $G(A_1)$, induce a representation of the space group G_0 . Only the representations of G_0 contained in the induced representation are allowed lattice vibrational modes.

To be specific, consider calcite (CaCO_3). At ambient temperature and pressure, it has a space group symmetry $R\bar{3}c$. The crystal structure consists of three simple crystals. The Ca atoms are at the 6 (b) sites. These positions are generated by $R\bar{3}c$ from the position $(0,0,0)$ and have site symmetry $\bar{3}$. The C atoms are at the 6 (a) sites, which are generated from $(0,0,\frac{1}{4})$ and have site symmetry 32. The O atoms are the 18 (e) sites, which are generated from $(x,0,\frac{1}{4})$, and have site symmetry 2.

For the C atoms (site symmetry 32), a representation $I(d^j)$ will be induced from vector representations d^j of 32. For 32, the vector irreps are A_2 and E (see Table III), corresponding to z and x, y displacements, respectively, i.e., the irreps A_2 of E are contained in the vector irrep each once. From Table II, we see that either the irrep A_2 or E induce representations which contain the following irreps of $R\bar{3}c$: Γ_2^+ , Γ_3^+ , Γ_2^- , Γ_3^- , F_1^+ , $2F_2^+$, F_1^- , $2F_2^-$, $3L_1$, $2T_1T_2$, T_3 . Each of these irreps represents an allowed vibrational mode. Displacements of the C atoms in each of these modes transform as basis functions of the respective irrep. The first four of these irreps represent $\mathbf{k}=\mathbf{0}$ modes (Γ point), and the remainder represent modes for \mathbf{k} on the first Brillouin zone boundary (F , L , and T points). The notation $3L_1$ means that there are three independent sets of modes which transform like the irrep L_1 . One set arises from an A_2 irrep, and two arise from E irreps.

In a similar manner, the vibrational modes for the simple crystal of Ca atoms are seen to be Γ_1^- , Γ_2^- , $2\Gamma_3^-$, $3F_1^-$, $3F_2^-$, $3L_1$, $2T_1T_2$, T_3 . Here, the irrep E_u^* of $\bar{3}$ is reducible, and the basis functions, $x + iy$ and $x - iy$ are independent of each other. (The representation is subduced twice in the vector representation of $\bar{3}$.) Thus we must count E_u^* twice wherever it occurs in Table II. For example, there are two Γ_3^- modes involving the Ca atoms, even though E_u^* occurs only once in Table II for Γ_3^- at the (b) site.

The vibrational modes for the simple crystal of O atoms are Γ_1^+ , $2\Gamma_2^+$, $3\Gamma_3^+$, Γ_1^- , $2\Gamma_2^-$, $3\Gamma_3^-$, $4F_1^+$, $5F_2^+$, $4F_1^-$, $5F_2^-$, $9L_1$, $6T_1T_2$, $3T_3$. Note that in this case, the basis functions of irrep B are x or y , and consequently B is contained in the vector representation twice. Thus we must count B twice wherever it occurs in Table II.

The detailed displacements making up the basis function for each irrep can be obtained by projection operator methods if so desired. For example, the basis functions for the above $\mathbf{k}=\mathbf{0}$ modes are given in Ref. 31.

B. Magnetic distortions

To illustrate the use of the tables for a magnetic structure, consider the ilmenite-type crystals. They have a space-group symmetry $R\bar{3}c$ and include compounds such as CoCO_3 and MnCO_3 . The magnetic atoms are a simple crystal and occupy the six (b) sites with symmetry $\bar{3}$. The magnetic structure corresponds to a "magnetic distortion" of the crystallographic space group $R\bar{3}c$. This magnetic distortion results from associating a dipole moment, an axial vector, at each atomic position. Thus only the induced representations $I(d^j)$ arising from the axial vector irreps of $\bar{3}$ are to be considered.

From Table III the irreps A_g and E_g^* of $\bar{3}$ are the z and x, y components, respectively, of the magnetic moment. Here E_g^* is a reducible representation of $\bar{3}$. Considering the irreps of $R\bar{3}c$, and using Table II, the six (b) sites allow the magnetic distortions Γ_1^+ , Γ_2^+ , $2\Gamma_3^+$, $3F_1^+$, $3F_2^+$, $3L_1$, $2T_1T_2$, T_3 . Since only the (b) sites allow magnetic atoms, these irreps are the only allowed magnetic distortions for CoCO_3 or MnCO_3 at k points of symmetry. The specific atomic dipole distortion can be obtained by projection operator techniques. The basis functions for the above $k=0$ modes are given in Ref. 3.

C. Displacive transitions

The Landau theory of continuous phase transitions classifies allowed transitions from a given higher-symmetry space group. An extension of the Landau theory was used to construct Table I. To apply the information in Table I to a specific crystal, we must use an additional group-theoretical criterion, discussed by Birman,^{32,33} namely, the tensor-field criterion. This criterion states that if a transition is due to a physical property described by an l -component tensor defined on the atoms of a crystal, then the irrep causing the transition must be contained in the representation induced by the tensor field. Thus the irrep must have a nonzero subduction frequency as calculated by Eq. (14).

As an example, consider the transition in CaCO_3 to the $P2_1/c$ phase. The transition is induced by the F_2^- irrep. The relationship of the subgroup to $R\bar{3}c$ has been described in Sec. II. Consider the transition as resulting from a lattice distortion. Then, as was done in Sec. IV A, the (a) sites give rise to two F_2^- displacement modes, the (b) sites give rise to two F_2^- modes, and the (e) sites give rise to five F_2^- modes. Thus the F_2^- does satisfy the tensor field criterion, and we see that all of the atoms can participate in the distortion at the transition. It was shown in Ref. 34 by projection operator techniques that a mode corresponding to an alternate rotation of the CO_3 groups transforms according to F_2^- , and this mode has been observed experimentally³⁵ in the transition to $P2_1/c$.

D. NQR resonance

This section discusses the use of the tables in connection with NQR resonance in phase transitions.^{4,5} As mentioned in the Introduction, nuclear spin resonance is very sensitive to differences of local field gradients and thus exhibits different frequencies at inequivalent sites. Although NQR is taken as the prototypic experimental technique, any spectroscopic technique which is sensitive to inequivalent sites is analyzed in the same manner as described here. If a crystal undergoes a phase transition, the resonant atoms in equivalent sites may occupy inequivalent sites at the transition. This abrupt change in

site symmetry causes a change in the NQR spectrum.

Consider the representation of G_0 induced by the identity representation of site A_1 . A_1 is taken as the atomic site of the resonant atom. The representation $I(d^1)$ induced from the identity irrep d^1 of site A_1 is called the permutation representation and indicates how the atoms of the simple crystal permute under the elements of the space group G_0 . We see from Eq. (14) that when d^j is the identity irrep of the site group [$\chi_d^j(g)=1$], then the identity irrep of G_0 [$\chi_D(g)=1$] is contained in the induced representation once and only once [$m(D, d^1)=1$]. If a phase transition occurs, equivalent sites may become inequivalent with respect to the subgroup G . The single simple crystal in G_0 becomes more than one simple crystal in G . The number of resulting simple crystals in G is simply given by the number of irreps in $I(d^1)$ which subduce the identity irrep of G . This information is easily obtained by combining the information of Tables I, II, and III.

As an example, consider sodium nitrate (NaNO_3) which has a phase with symmetry $R\bar{3}c$. The sodium nuclei are the resonant spins for this structure. They are situated at the six (b) sites. Consider a transition to $R\bar{3}$ induced by irrep Γ_2^+ . This transition is not an actual known transition in NaNO_3 , but we consider it just for illustration of the method. From Table I in the last column, we find that the irreps, Γ_1^+ and Γ_2^+ , each subduce the identity irrep of $R\bar{3}$ once. From Table II, we see that the identity irrep A_g of point group $\bar{3}$ associated with the (b) sites is contained in each of these two irreps once. Therefore, the irrep $I(d^1)$ contains the irreps, Γ_1^+ and Γ_3^+ , each once. There are two irreps in $I(d^1)$ which subduce the identity irrep of G , and consequently, the sodium atoms find themselves in two different simple crystals in $R\bar{3}$. The NQR line arising from the sodium nuclei in $R\bar{3}c$ splits into two distinct lines at the phase transition.

V. CONCLUSION

We have discussed the philosophy of construction and the content of two very useful tables. These tables contain information resulting from the symmetry analysis of the microstructure (atomic site locations) of the space group $R\bar{3}c$. As has been shown, a number of questions can be answered, simply by looking up the information in our listings. Not all possible uses of the tables have been discussed but enough examples to show the variety and significance of the types of questions which can be answered by the information provided. We have obtained similar tables for each of the 230 crystallographic space groups. They will appear in a separate publication.

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