On exomorphic types of phase transitions

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An algorithmic method is presented to determine the irreducible representations that engender the irreducible representations associated with phase transitions involving a change of symmetry to a subgroup of index n. This method is based on the work of Ascher and Kobayashi [E. Ascher and J. Kobayashi, J. Phys. C **10**, 1349 (1977)] and the derivation of faithful irreducible representations contained in the permutation representation of transitive subgroups of permutation groups S_n. Character tables of all such irreducible representations, and their epikernels, associated with a change in symmetry to a subgroup of index $n = 2, 3, 4, 5$, and 6 are given explicitly. The relationship to exomorphic types of phase transitions is then discussed. The irreducible representations associated with the phase transitions O_h^1 to C_{4v}^1 in $BaTiO_3$ and D_{6h}^4 to D_{2h}^{16} in β-K_2SO_4 are derived and it is shown that these two phase transitions belong to the same exomorphic type.

I. INTRODUCTION

The use of group-theoretical methods to investigate structural phase transitions was introduced by Landau[1] over forty years ago. In the Landau method of determining the change of symmetry accompanying a phase transition, the lower symmetry phase is described by a density function, which is expanded in terms of basis functions of the irreducible representations of the higher symmetry phase. With the coefficients of the density function expansion as variational order parameters, a thermodynamic potential is constructed and minimized to determine the form of the density function and subsequently the symmetry of the lower symmetry phase.[2,3] The most extensive tabulations of changes in symmetry accompanying phase transitions derived using this method have been given by Toledano and Toledano.[4]

A number of necessary group-theoretical criteria have also been derived for use in determining the change in symmetry accompanying a phase transition.[3,5–9] These include the subduction criterion, chain subduction criteria, also called the chain criterion,[8] the Landau criterion for continuous phase transitions, and the Lifshitz homogeneity criterion. Using some or all of these criteria, tabulations of possible lower-phase symmetries have been derived for some phase transitions in crystals. For cases where the higher-phase symmetry group is a cubic space group, such tabulations have been given for O_h^1 by Goldrich and Birman[3] and Vinberg *et al.*,[10] for O_h^3 by Jaric,[9] and for O_h^5 by Sutton and Armstrong[11] and Ghozlen and Mlik.[12] Recently a computer program has been developed by Hatch and Stokes[13] and all the above mentioned criteria have been applied to all 230 space groups.

In parallel with the application of the Landau method with minimization, and the development and application of group-theoretical criteria, investigations into general theorems that apply to the change in symmetry accompanying a phase transition have also been developed. Such general theorems date back to the original papers of Landau.[1] It was shown by Landau that the irreducible representation associated with a phase transition, where the lower-phase symmetry group is a subgroup of index 2 of the higher-phase symmetry group, is a one-dimensional alternating irreducible representation. It was also conjectured that no phase transition between a higher-phase symmetry group and a lower-phase symmetry subgroup of index 3 is continuous. This so-called subgroup of index 3 theorem was shown to be valid for special cases by Anderson and Blout[14] and Boccara.[15] General proofs were subsequently given by Meisel, Gray, and Brown[16] and Brown and Meisel.[17] It has also been shown that the Landau subgroup of index 3 theorem cannot be extended to a subgroup of index n theorem with $n \neq 3$.[18]

Continuing the investigation into the group-theoretical aspects of phase transitions, Ascher and Kobayashi[19] have introduced the so-called "inverse Landau problem." This problem is to determine the irreducible representation associated with a phase transition between a given higher-phase symmetry group and a given lower-phase symmetry group. Following the work of Gufan and Sakhnenko[20] and Ascher and Kobayashi,[19] Kopsky has introduced the concept of "exomorphic" types of phase transitions.[21–24] For example, all phase transitions between a higher-phase symmetry group and lower-phase symmetry subgroup of index 2 belong to a single exomorphic type. Such a concept stresses the mathematical similarity among phase transitions and can be used in the study of the general properties of phase transitions. Two phase transitions belonging to the same exomorphic type have, for example, the same set of order parameters and the same mathematical form of the thermodynamic potential. The transitions can, however, differ in the physical interpretation of the order parameters and corresponding terms in the potential can be of different physical importance.[22] The concept of exomorphic types of phase transi-

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tions can also be used as a basis of proofs of general theorems concerning phase transitions as, for example, in the alternate proof of the subgroup of index 3 theorem.[24]

In this paper we continue the study of exomorphic types of phase transitions. In Sec. II we briefly review the method of Ascher and Kobayashi and its connection to the subduction criterion.[3] We give an algorithmic method to determine the irreducible representations associated with a phase transition between a higher-phase symmetry group and a lower-phase symmetry subgroup of index n. We then determine and tabulate the irreducible representations that engender all irreducible representations associated with phase transitions where the subgroup index $n = 2, 3, 4, 5$, and 6. For each irreducible representation we also determine the epikernels, i.e., the isotropy groups, the subgroups that satisfy the subduction and chain-subduction criteria.

In Sec. III, we apply the results of Sec. II, to determine the irreducible representation associated with each of the two phase transitions O_h^1 to C_{4v}^1 and D_{6h}^4 to D_{2h}^{16}. We also determine the epikernels associated with each of these phase transitions. In Sec. IV we show that these two phase transitions belong to the same exomorphic type. We then derive additional phase transitions, which also belong to this exomorphic type.

II. IRREDUCIBLE REPRESENTATIONS ASSOCIATED WITH A PHASE TRANSITION

We consider a phase transition between a higher-phase symmetry group G and a lower-phase symmetry F, where F is a subgroup of G of index n. Let $D^\alpha(G)$ denote the irreducible representation of G associated with this phase transition. Given the groups G and F we consider the inverse Landau problem, to determine the possible irreducible representations associated with the phase transition.

We apply the subduction criterion

$$(D^\alpha(G)\downarrow F\,|D^1(F))\neq 0. \tag{1}$$

That is, the subduced representation $D^\alpha(G)\downarrow F$, the irreducible representation $D^\alpha(G)$ restricted to the elements of the subgroup F, must contain the identity representation $D^1(F)$ of F a nonzero number of times. Using the Frobenius Reciprocity Theorem,[25] Eq. (1) can be replaced by

$$(D^1(F)\uparrow G\,|D^\alpha(G))\neq 0. \tag{2a}$$

The irreducible representation $D^\alpha(G)$ must be contained a nonzero number of times in the induced representation $D^1(F)\uparrow G$.

We shall use the symbol $D_A^B(A)$ to denote the induced representation $D^1(B)\uparrow A$. Equation (2a) can then be rewritten as

$$(D_G^F(G)\,|D^\alpha(G))\neq 0. \tag{2b}$$

We shall also use the symbol $D_G = D_{G/H}\uparrow\uparrow G$ to denote the representation D_G of G "engendered by the representation $D_{G/H}$ of its factor group G/H. Engendering[26] is defined as follows: Let H be a normal subgroup of G. The cosets g_iH of the coset decomposition of G with respect to H are elements of the factor group G/H. If $D_{G/H}$ is a representation of G/H then to every coset g_iH of the factor group G/H corresponds a matrix $D_{G/H}(g_iH)$. To define the engendered representation $D_G = D_{G/H}\uparrow\uparrow G$, we set all matrices $D_G(g_kh)$, for all h of H, equal to the matrix $D_{G/H}(g_kH)$.

It has been shown [27,28] that

$$D_G^F = D_{G/H}^{F/H}(G/H)\uparrow\uparrow G. \tag{3}$$

The induced representation $D_G^F(G)$ is engendered by the induced representation $D_{G/H}^{F/H}(G/H)$ of the factor group G/H, where

$$H = \text{Core}\, F = \bigcap_{g\in G} gFg^{-1}. \tag{4}$$

From Eqs. (2b) and (3), it follows that an irreducible representation $D^\alpha(G)$ associated with a phase transition between the group G and subgroup F of G is such that

$$D^\alpha(G) = D^\alpha(G/H)\uparrow\uparrow G \tag{5}$$

and

$$(D_{G/H}^{F/H}(G/H)\,|D^\alpha(G/H))\neq 0. \tag{6}$$

That is, the irreducible representation $D^\alpha(G)$ is engendered by an irreducible representation $D^\alpha(G/H)$ of the factor group G/H, and $D^\alpha(G/H)$ must be contained in the induced representation $D_{G/H}^{F/H}(G/H)$ a nonzero number of times. In addition, since the kernel of $D^\alpha(G)$ is equal to the subgroup H (see Refs. 19 and 27), i.e.,

$$\ker D^\alpha(G) = H = \text{Core}\, F, \tag{7}$$

the irreducible representation $D^\alpha(G/H)$, which engenders $D^\alpha(G)$, is a faithful representation of G/H.

A matrix $D_A^B(a)$ of an induced representation $D_A^B(A)$ is also the matrix representing the permutation of the cosets of B in A under multiplication of the cosets by the element a of A (see Refs. 28 and 29). The group of matrices is called a "permutation representation" and represents a group of permutations that is transitive on the cosets of B in A. The dimension of this permutation representation is equal to the number of cosets of B in A. Consequently, the representation $D_{G/H}^{F/H}(G/H)$ is a permutation representation of a transitive subgroup T_n, isomorphic to G/H, of the symmetric group S_n, where n is the index of F in G.

A method to determine all possible irreducible representations $D^\alpha(G)$ associated with a phase transition between a group G and subgroup F of index n in G is based on Eqs. (5)–(7). Such irreducible representations satisfy the subduction criterion and, of course, are further restricted by the use of the chain subduction criterion, Landau criterion, and Lifshitz criterion. We have that an irreducible representation $D^\alpha(G)$ is engendered by a faithful irreducible representation $D^\alpha(G/H)$, which is contained in the permutation representation of a transitive subgroup T_n, isomorphic to G/H, of the symmetric group S_n. A method to determine the irreducible representations $D^\alpha(G)$ is as follows.

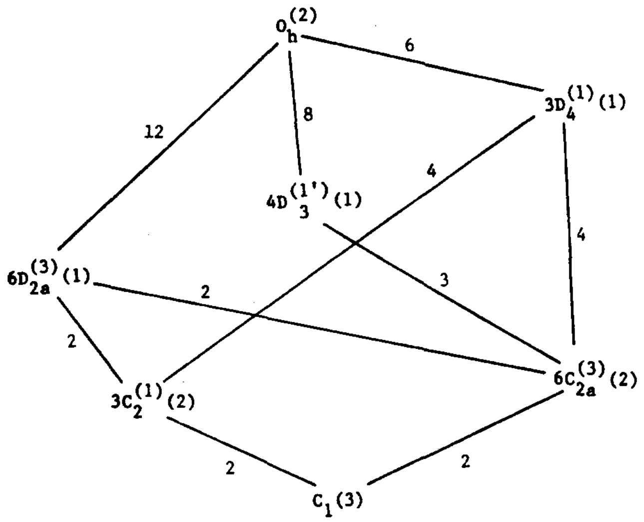
(1) Given the group G and subgroup F of index n, determine the subgroup H, Eq. (4), and the factor group G/H.

(2) Determine the transitive subgroup T_n, isomorphic to G/H, of the symmetric group S_n, and the faithful irreducible representations in the permutation representation of T_n.

(3) Each faithful irreducible representation of the permutation representation determines an irreducible represen-

TABLE I. Character table of the faithful irreducible representation contained in the permutation representation of the transitive subgroup 6/6 of S_6. Above each character is the number and cyclic notation of the elements in each class. The diagram shows the epikernels of the irreducible representation. The generators of each epikernel are listed below the diagram.

$6/6(48)C_2^2\times O^2(O_h^{(2)})$										
1	3	8	6	6	1	3	8	6	6	
(1^6)	$(1^2,2^2)$	(3^2)	(2^3)	$(1^2,4)$	(2^3)	$(1^4,2)$	(6)	$(1^2,2^2)$	$(2,4)$	
3	−1	0	−1	1	−3	1	0	1	−1	(LA)



O_h^2: (3456), (154236)

$3D_4^{(1)}$: (3456), (36)(45); (1426), (16)(24); (1523), (15)(23).

$4D_3^{(1')}$: (134)(256), (13)(25); (136)(254), (16)(24); (145)(263), (15)(23); (156)(234), (16)(24).

$6D_{2a}^{(3)}$: (12), (36) (45); (12), (34)(56); (46), (15)(23); (46), (13)(25); (35), (16)(24); (35), (14)(26).

$6C_{2a}^{(3)}$: (16)(24); (15)(23); (36)(45); (34)(56); (13)(25); (14)(26).

$3C_2^{(1)}$: (12); (46); (35).

tation $D^\alpha(G/H)$, which in turn engenders, Eq. (5), a possible irreducible representation $D^\alpha(G)$ associated with the phase transition between G and subgroup F.

To implement this procedure requires the knowledge of all transitive subgroups T_n of the symmetric groups S_n, and all faithful irreducible representations contained in the permutation representation of each transitive subgroup. We have tabulated all transitive subgroups of the symmetric groups S_n for $n = 2, 3, 4, 5, 6$ and the faithful irreducible representations contained in the permutation representation of each transitive subgroup.[30] In Table I, we give an example from this tabulation. The table contains the following information.

(1) A symbol $n/m(p)$, where n is the degree of the symmetric group S_n, m is a serial number given to a transitive subgroup T_n, and p is the order of the transitive subgroup T_n. This is followed by a symbol or symbols, which denote the group T_n.

(2) The character table of the faithful irreducible representations contained in the permutation representation of T_n is given. The classes of elements are given in cycle length notation with the number of elements in each class given above the class symbol. The symbol "(LA)" is written to the right of the character table if the irreducible representation satisfies the Landau criterion.

(3) Using the lattices of the symmetric groups,[31] we have derived and tabulated the epikernels[24] for each faithful irreducible representation of the transitive subgroup T_n. The subgroup index of the epikernel is given along the line connected each pair of groups and the subduction frequency is given in parenthesis following the subgroup symbol. If there is more than one subgroup of a specific class, the number of such subgroups is given preceding the subgroup symbol.

(4) The generators of at least one epikernel of each class of epikernels is given. When the number of epikernels is not large, as in Table I, the generators of all epikernels in each class are given.

III. EXAMPLES

We shall consider two phase transitions: (1) the equitranslational transition from O_h^1 to C_{4v}^1 in $BaTiO_3$ and (2) the nonequitranslational transition from D_{6h}^4 to D_{2h}^{16} in β-K_2SO_4. We shall determine the irreducible representations associated with these phase transitions and show that the respective irreducible representations are both engendered by the same faithful irreducible representation.

We first consider the phase transition from $G = O_h^1$ to $F = C_{4v}^1$, the equitranslational subgroup of O_h^1 with the point group $C_{4v} = \{E, C_{4z}, C_{2z}, C_{4z}^{-1}, m_x, m_y, m_{xy}, m_{xy}\}$; C_{4v}^1 is a subgroup of index $n = 6$ in O_h^1. The core of $F = C_{4v}^1$, see Eq. (4), is

$$H = \text{Core } C_{4v}^1 = C_1^1,$$

where C_1^1 is the translational subgroup of O_h^1. It follows that $G/H = O_h^1/C_1^1$ and is isomorphic to the point group O_h of order 48. Then $D_{G/H}^{F/H}$ is a permutation representation of a transitive subgroup of order 48 of S_6. There is only one such transitive subgroup of S_6, the group denoted by 6/6(48) given in Table I. This permutation representation contains a single, Landau active, faithful irreducible representation whose character table is given in Table I. This character

TABLE II. Character table of the faithful irreducible representation contained in the permutation representation of the transitive subgroup 6/6 of S^6. In the first and second column are the number and cyclic notation of the elements of each class whose character is given in the third column. In the fourth column, we list in cyclic notation all elements of the transitive subgroup belonging to each class. Below each element we list the cosets of the factor groups O_h^1/C_1^1 and D_{6h}^4/C_2^2 isomorphic to this transitive subgroup of S_6.

1	(1^6)	3	(1)(2)(3)(4)(5)(6) $(E\|000)$ $\{(E\|000),(C_{2z}\|00\frac{1}{2})\}$			
3	$(1^1,2^2)$	−1	(35)(46) $(C_{2x}\|000)$ $\{(E\|010),(C_{2z}\|01\frac{1}{2})\}$	(12)(46) $(C_{2y}\|000)$ $\{(E\|110),(C_{2z}\|11\frac{1}{2})\}$	(12)(35) $(C_{2z}\|000)$ $\{(E\|100),(C_{2z}\|10\frac{1}{2})\}$	
8	(3^2)	0	(145)(263) $(C_{3xyz}\|000)$ $\{(C_3\|010),(C_6^{-1}\|01\frac{1}{2})\}$ (154)(236) $(C_{3xyz}^{-1}\|000)$ $\{(C_3^{-1}\|100),(C_6\|10\frac{1}{2})\}$	(136)(254) $(C_{3\bar{x}yz}\|000)$ $\{(C_3^{-1}\|010),(C_6\|01\frac{1}{2})\}$ (163)(245) $(C_{3\bar{x}yz}^{-1}\|000)$ $\{(C_3\|110),(C_6^{-1}\|11\frac{1}{2})\}$	(134)(256) $(C_{3x\bar{y}z}\|000)$ $\{(C_3^{-1}\|000),(C_6\|00\frac{1}{2})\}$ (143)(265) $(C_{3x\bar{y}z}^{-1}\|000)$ $\{(C_3\|000),(C_6^{-1}\|00\frac{1}{2})\}$	(156)(234) $(C_{3xy\bar{z}}\|000)$ $\{(C_3^{-1}\|110),(C_6\|11\frac{1}{2})\}$ (165)(243) $(C_{3xy\bar{z}}^{-1}\|000)$ $\{(C_3\|100),(C_6^{-1}\|10\frac{1}{2})\}$
6	(2^3)	−1	(15)(23)(46) $(C_{2xy})\|000)$ $\{(C_{2x}\|000),(C_{22}\|00\frac{1}{2})\}$ (13)(25)(46) $(C_{2\bar{x}y}\|000)$ $\{(C_{2x}\|100),(C_{22}\|10\frac{1}{2})\}$	(14)(26)(35) $(C_{2xz}\|000)$ $\{(C_{2xy}\|110),(C_{23}\|11\frac{1}{2})\}$ (16)(24)(35) $(C_{2\bar{x}z}\|000)$ $\{(C_{2xy}\|000)(C_{23}\|00\frac{1}{2})\}$	(12)(36)(45) $(C_{2yz}\|000)$ $\{(C_{2y}\|000),(C_{21}\|00\frac{1}{2})\}$ (12)(34)(56) $(C_{2\bar{y}z}\|000)$ $\{(C_{2y}\|010),(C_{21}\|01\frac{1}{2})\}$	
6	$(1^2,4)$	1	(3456) $(C_{4x}\|000)$ $\{(C_{2y}\|100),(C_{21}\|10\frac{1}{2})\}$ (3654) $(C_{4x}^{-1}\|000)$ $\{(C_{2y}\|110),(C_{21}\|11\frac{1}{2})\}$	(1426) $(C_{4y}\|000)$ $\{(C_{2xy}\|100),(C_{23}\|10\frac{1}{2})\}$ (1624) $(C_{4y}^{-1}\|000)$ $\{(C_{2xy}\|010),(C_{23}\|01\frac{1}{2})\}$	(1325) $(C_{4z}\|000)$ $\{(C_{2x}\|110),(C_{22}\|11\frac{1}{2})\}$ (1523) $(C_{4z}^{-1}\|000)$ $\{(C_{2x}\|010),(C_{22}\|01\frac{1}{2})\}$	
1	(2^3)	−3	(12)(35)(46) $(\bar{1}\|000)$ $\{(\bar{1}\|000),(m_z\|00\frac{1}{2})\}$			
3	$(1^4,2)$	1	(12) $(m_x\|000)$ $\{(\bar{1}\|010),(m_z\|01\frac{1}{2})\}$	(35) $(m_y\|000)$ $\{(\bar{1}\|110),(m_z\|11\frac{1}{2})\}$	(46) $(m_z\|000)$ $\{(\bar{1}\|100),(m_z\|10\frac{1}{2})\}$	
8	(6)	0	(134256) $(S_{6xyz}\|000)$ $\{(S_3^{-1}\|10\frac{1}{2}),(S_6\|100)\}$ (165243) $(S_{6xyz}^{-1}\|000)$ $\{(S_3\|01\frac{1}{2}),(S_6^{-1}\|010)\}$	(143265) $(S_{6\bar{x}yz}\|000)$ $\{(S_3\|11\frac{1}{2}),(S_6^{-1}\|110)\}$ (156234) $(S_{6\bar{x}yz}^{-1}\|000)$ $\{(S_3^{-1}\|01\frac{1}{2}),(S_6\|010)\}$	(163245) $(S_{6x\bar{y}z}\|000)$ $\{(S_3\|00\frac{1}{2}),(S_6^{-1}\|000)\}$ (154236) $(S_{6x\bar{y}z}^{-1}\|000)$ $\{(S_3^{-1}\|00\frac{1}{2}),(S_6\|000)\}$	(145263) $(S_{6xy\bar{z}}\|000)$ $\{(S_3\|10\frac{1}{2}),(S_6^{-1}\|100)\}$ (136254) $(S_{6xy\bar{z}}^{-1}\|000)$ $\{(S_3^{-1}\|11\frac{1}{2}),(S_6\|110)\}$
6	$(1^2,2^2)$	1	(13)(25) $(m_{xy}\|000)$ $\{(m_2\|00\frac{1}{2}),(m_x\|000)\}$ (15)(23) $(m_{\bar{x}y}\|000)$ $\{(m_2\|10\frac{1}{2}),(m_x\|100)\}$	(16)(24) $(m_{xz}\|000)$ $\{(m_3\|11\frac{1}{2}),(m_{xy}\|110)\}$ (14)(26) $(m_{\bar{x}z}\|000)$ $\{(m_3\|00\frac{1}{2}),(m_{xy}\|000)\}$	(34)(56) $(m_{yz}\|000)$ $\{(m_1\|00\frac{1}{2}),(m_y\|000)\}$ (36)(45) $(m_{\bar{y}z}\|000)$ $\{(m_1\|01\frac{1}{2}),(m_y\|010)\}$	
6	(2,4)	−1	(12)(3456) $(S_{4x}\|000)$ $\{(m_1\|11\frac{1}{2}),(m_y\|110)\}$ (12)(3654) $(S_{4x}^{-1}\|000)$ $\{(m_1\|10\frac{1}{2}),(m_y\|100)\}$	(1426)(35) $(S_{4y}\|000)$ $\{(m_3\|01\frac{1}{2}),(m_{xy}\|010)\}$ (1624)(35) $(S_{4y}^{-1}\|000)$ $\{(m_3\|10\frac{1}{2}),(m_{xy}\|100)\}$	(1325)(46) $(S_{4z}\|000)$ $\{(m_2\|01\frac{1}{2}),(m_x\|010)\}$ (1523)(46) $(S_{4z}^{-1}\|000)$ $\{(m_2\|11\frac{1}{2}),(m_x\|110)\}$	

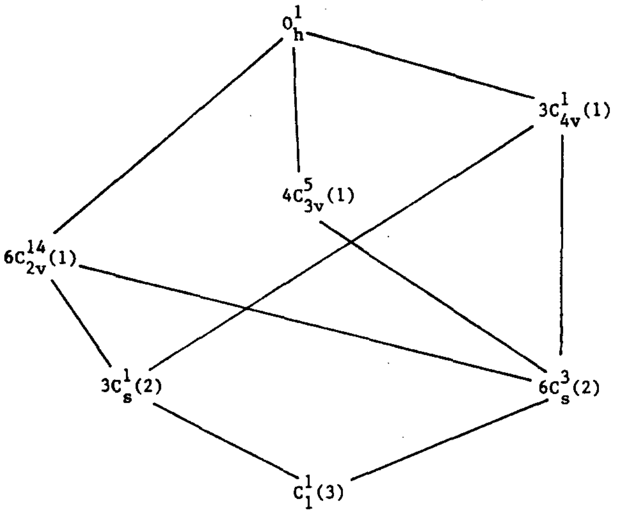


FIG. 1. Epikernels of the irreducible representation $D^{k=(0,0,0),4-}(O_h^1)$.

table is given in detail in Table II. In the first three columns we duplicate the first three rows of the character table given in 6/6(48) of Table I. To the right of each character we list explicitly in cyclic notation the elements of each class of this transitive subgroup of S_6.

The factor group $G/H = O_h^1/C_1^1$ is isomorphic to this transitive subgroup of S_6 denoted by 6/6(48). The isomorphism is between elements P_i of 6/6(48) and cosets $(R_i|000)C_1^1$ of G/H. In Table II we have denoted the coset $(R_i|000)C_1^1$ isomorphic to P_i by listing below the element P_i the coset representative $(R_i|000)$. This isomorphism and the faithful irreducible representation of the transitive subgroup 6/6(48) of S_6 determines the irreducible representation $D^\alpha(O_h^1/C_1^1)$, see Eq. (6), which in turn engenders, Eq. (5), the irreducible representation $D^\alpha(O_h^1)$ associated with the phase transition between O_h^1 and C_{4v}^1. This irreducible representation $D^\alpha(O_h^1)$ is denoted by $D^{(k=0,0,0),4-}(O_h^1)$ in the notation of Cracknell *et al.*[32]

Using the epikernels and generators of the epikernels given in Table I along with the isomorphism between the elements of 6/6(48) and cosets of O_h^1/C_1^1 given in Table II, we can derive the subgroups of O_h^1, which satisfy the chain-subduction criterion for phase transitions from O_h^1 associated with the irreducible representation $D^{(k=0,0,0),4-}(O_h^1)$. These epikernels are given in Fig. 1.

The second example is the phase transition from hexagonal $G' = D_{6h}^4$ to orthorhombic $F' = D_{2h}^{16}$. The subgroup D_{2h}^{16} has the translation subgroup generated by the hexagonal translations $(E|1,0,0)$, $(E|1,2,0)$, and $(E|0,0,1)$. The elements of D_{6h}^4, which are the coset representations of D_{2h}^{16} with respect to its translational subgroup, are

$$(E|0,0,0),\quad (\bar{1}|1,1,0),$$
$$(C_{2z}|0,0,\tfrac{1}{2}),\quad (m_2|1,1,\tfrac{1}{2}),$$
$$(C_{2x}|1,1,0),\quad (m_x|0,0,0),$$
$$(C_{22}|1,1,\tfrac{1}{2}),\quad (m_2|0,0,\tfrac{1}{2}).$$

Now D_{2h}^{16} is a subgroup of index $n = 6$ of D_{6h}^4. The core of $F' = D_{2h}^{16}$, see Eq. (4), is

$$H' = \text{Core}\, D_{2h}^{16} = C_2^2.$$

The group C_2^2 has the translational subgroup generated by the hexagonal translations $(E|2,0,0)$, $(E|0,2,0)$, and $(E|0,0,1)$. The elements of D_{6h}^4, which are the coset representatives of C_2^2 with respect to its translational subgroup, are $(E|0,0,0)$ and $(C_{2z}|0,0,\tfrac{1}{2})$. The factor group $G'/H' = D_{6h}^4/C_2^2$ is isomorphic to the point group O_h of order 48. It follows that $D_{G'/H'}^{F'/H'}$ is then a permutation representation of a transitive subgroup of order 48 of S_6. This is the same transitive group, 6/6(48) given in Table I, as that which arose in the first example given above.

The isomorphism between the elements P_i of 6/6(48) and the cosets $(R_i|\tau_i)C_2^2$ of G'/H' is given in Table II. Two lines below each element P_i of 6/6(48) given in Table II we have denoted the isomorphic coset $(R_i|\tau_i)C_2^2$ of $G'/H' = D_{6h}^4/C_2^2$. Since

$$(R_i|\tau_i)C_2^2 = (R_i|\tau_i)C_1^1 + (R_i|\tau_i)(C_{2z}|0,0,\tfrac{1}{2})C_1^1,$$

where C_1^1 is the translational subgroup of C_2^2, we list the two elements $(R_i|\tau_i)$ and $(R_i|\tau_i)(C_{2z}|0,0,\tfrac{1}{2})$. This isomorphism and the faithful irreducible representation of the transitive subgroup 6/6(48) of S_6 determines the irreducible representation $D^\alpha(D_{6h}^4/C_2^2)$, Eq. (6), which in turn engenders, Eq. (5), the irreducible representation $D^\alpha(D_{6h}^4)$ associated with the phase transition between D_{6h}^4 and D_{2h}^{16}. This irreducible representation $D^\alpha(D_{6h}^4)$ is denoted by $D^{k=(\frac{1}{2},0,0),2-}(D_{6h}^4)$ in the notation of Cracknell *et al.*[32]

Using the epikernels and generators of the epikernels given in Table I along with the isomorphism between elements of 6/6(48) and cosets of D_{6h}^4/C_2^2 given in Table II, we can derive the subgroups that satisfy the chain-subduction criterion for phase transitions from D_{6h}^4 associated with the irreducible representation $D^{k=(\frac{1}{2},0,0),2-}(D_{6h}^4)$. These epikernels are given in Fig. 2.

The above two examples are at first glance quite different, one being an equitranslational phase transition while the second is nonequitranslational. However, as we have seen, these two transitions are mathematically similar; the associated irreducible representations are engendered by the

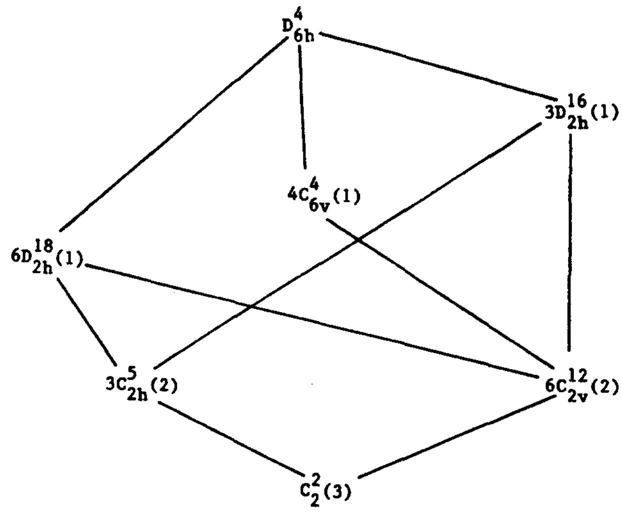


FIG. 2. Epikernels of the irreducible representation $D^{k=(\frac{1}{2},0,0),2-}(D_{6h}^4)$.

TABLE III. Phase transitions O_h^i to C_{4v}^j and O_h^i to D_{2d}^k that belong to the exomorphic type of phase transition characterized by the permutation representation of the transitive subgroup 6/6 of S_6. Here, $H = \text{Core}\, F = C_1^1$ for all cases.

$G = O_h^i$ i	$F = C_{4v}^j$ j	$F = D_{2d}^k$ k
1	1	5
2	6	8
3	7	5
4	4	8
5	9	11
6	10	11
7	11	12
8	12	12
9	9	9
10	12	10

same faithful irreducible representation. This mathematical similarity of different phase transitions has been codified by the concept of exomorphic types of phase transitions.[21–24]

IV. EXOMORPHIC TYPES OF PHASE TRANSITIONS

Two phase transitions, between a higher-phase symmetry group G and lower-phase symmetry F and between a higher-phase symmetry G' and lower-phase symmetry F', are said to be of the same exomorphic types if and only if[21] (1) the factor groups G/H, where $H = \text{Core}\, F$, and G'/H', where $H' = \text{Core}\, F'$, are isomorphic; and (2) there exists an isomorphism that maps the factor group F/H into F'/H'.

Alternatively,[24] we can state that two phase transitions are of the same exomorphic type if and only if a suitable labeling of the cosets $g_i F$ and $g_i' F'$ in the coset decompositions G with respect to F, and G' with respect to F' exists such that the permutation representations $D_{G/H}^{F/H}(G/H)$ and $D_{G'/H'}^{F'/H'}(G'/H')$ are identical groups of permutations.

In the examples of Sec. III, both the transitions $G = O_h^1$ to $F = C_{4v}^1$ and $G' = D_{6h}^4$ to $F' = D_{2h}^{16}$ are of the same exomorphic type. The factor groups $G/H = O_h^1/C_1^1$ and $G'/H' = D_{6h}^4/C_2^2$ are isomorphic with the isomorphism given in Table II, where we find that $F/H = C_{4v}^1/C_1^1$ is isomorphic to $F'/H' = D_{2h}^{16}/C_2^2$. The permutation representations $D_{G/H}^{F/H}(G/H)$ and $D_{G'/H'}^{F'/H'}(G'/H')$ are identical groups of permutations isomorphic to the transitive subgroup 6/6(48) of S_6.

It follows from the above and Eqs. (1)–(6) that if the phase transitions from G to F and G' to F' are of the same exomorphic type, then the irreducible representations $D^\alpha(G)$ and $D^\alpha(G')$, which can be associated with the respective phase transitions, are each engendered by faithful irreducible representations contained in a single permutation representation. This is the permutation representation denoted by $D_{G/H}^{F/H}(G/H)$ and $D_{G'/H'}^{F'/H'}(G'/H')$, and is a permutation representation of a transitive subgroup, isomorphic to G/H and G'/H', of the symmetric group S_n.

If the permutation representation contains a single faithful irreducible representation then this faithful irreducible representation engenders the irreducible representations associated with all phase transitions belonging to the exo-

TABLE IV. Phase transitions D_{6h}^i to D_{2h}^j that belong to the exomorphic type of phase transition characterized by the permutation representation of the transitive subgroup 6/6 of S_6. Here Ch. 1 and Ch. 2 refer to the alternative choice of origins as given in the *International Tables for Crystallography*.[33] The shift in origin, with respect to the translational subgroup of D_{6h}^i is also given. Here, $H = \text{Core}\, F$ is given to the right on the same row as F.

G			F		H
D_{6h}^1	$D_{2h}^{13}\left(P\frac{2_1}{m}\frac{2_1}{m}\frac{2}{n}\right)$	Ch.1	$D_{2h}^4\left(P\frac{2}{b}\frac{2}{a}\frac{2}{n}\right)$	$(\frac{1}{2},\frac{1}{2},0)$Ch.1	C_2^1
	$D_{2h}^7\left(P\frac{2_1}{b}\frac{2}{m}\frac{2}{n}\right)$		$D_{2h}^7\left(P\frac{2}{m}\frac{2_1}{a}\frac{2}{n}\right)$		C_i^1
	$D_{2h}^5\left(P\frac{2_1}{c}\frac{2}{a}\frac{2}{m}\right)$	$(\frac{1}{2},\frac{1}{2},0)$	$D_{2h}^5\left(P\frac{2}{b}\frac{2_1}{m}\frac{2}{m}\right)$		C_s^1
D_{6h}^2	$D_{2h}^{10}\left(P\frac{2_1}{c}\frac{2_1}{c}\frac{2}{n}\right)$	$(\frac{1}{2},\frac{1}{2},0)$	$D_{2h}^2\left(P\frac{2}{n}\frac{2}{n}\frac{2}{n}\right)$	(0,0,1) Ch.1	C_2^1
	$D_{2h}^6\left(P\frac{2_1}{n}\frac{2}{c}\frac{2}{n}\right)$		$D_{2h}^6\left(P\frac{2}{c}\frac{2_1}{n}\frac{2}{n}\right)$		C_i^1
	$D_{2h}^7\left(P\frac{2_1}{c}\frac{2}{n}\frac{2}{m}\right)$	$(\frac{1}{2},\frac{1}{2},0)$	$D_{2h}^7\left(P\frac{2}{n}\frac{2_1}{c}\frac{2}{m}\right)$	$(\frac{1}{2},\frac{1}{2},0)$	C_s^1
D_{6h}^3	$D_{2h}^{16}\left(P\frac{2_1}{m}\frac{2_1}{n}\frac{2_1}{b}\right)$	$(\frac{1}{2},\frac{1}{2},0)$	$D_{2h}^6\left(P\frac{2}{b}\frac{2}{n}\frac{2_1}{n}\right)$	$(\frac{1}{2},\frac{1}{2},0)$	C_2^2
	$D_{2h}^{14}\left(P\frac{2_1}{b}\frac{2}{c}\frac{2_1}{n}\right)$		$D_{2h}^{12}\left(P\frac{2}{m}\frac{2_1}{n}\frac{2_1}{n}\right)$		C_i^1
	$D_{2h}^{13}\left(P\frac{2_1}{m}\frac{2}{n}\frac{2_1}{m}\right)$	$(\frac{1}{2},\frac{1}{2},0)$Ch. 2	$D_{2h}^{11}\left(P\frac{2}{b}\frac{2_1}{c}\frac{2_1}{m}\right)$		C_s^1
D_{6h}^4	$D_{2h}^{16}\left(P\frac{2_1}{c}\frac{2_1}{m}\frac{2_1}{n}\right)$	$(\frac{1}{2},\frac{1}{2},0)$	$D_{2h}^6\left(P\frac{2}{n}\frac{2}{a}\frac{2_1}{n}\right)$	$(\frac{1}{2},\frac{1}{2},0)$	C_2^2
	$D_{2h}^{12}\left(P\frac{2_1}{n}\frac{2}{m}\frac{2_1}{n}\right)$		$D_{2h}^{14}\left(P\frac{2}{c}\frac{2_1}{a}\frac{2_1}{n}\right)$		C_i^1
	$D_{2h}^{11}\left(P\frac{2_1}{c}\frac{2}{a}\frac{2_1}{m}\right)$		$D_{2h}^{13}\left(P\frac{2}{n}\frac{2_1}{m}\frac{2_1}{m}\right)$	$(0,\frac{1}{2},0)$ Ch. 2	C_s^1

morphic type. In the examples of the previous sections the irreducible representations $D^{k=(0,0,0),4-}(O_h^1)$ and $D^{k=(\frac{1}{2},0,0),2-}(D_{6h}^4)$ are associated with the phase transitions from $G=O_h^1$ to $F=C_{4v}^1$ and $G'=D_{6h}^4$ to $F'=D_{2h}^{16}$, respectively. These two phase transitions belong to the same exomorphic type, and both irreducible representations are engendered by the same faithful irreducible representation, denoted by $D^\alpha(O_h^1/C_1^1)$ and $D^\alpha(D_{6h}^4/C_2^2)$, the only faithful irreducible representation contained in the permutation representation of the transitive subgroup 6/6(48) of S_6.

The two phase transitions $G=O_h^1$ to $F=C_{4v}^1$ and $G'=D_{6h}^4$ to $F'=D_{2h}^{16}$ belong to the same exomorphic type whose permutation representation is the permutation representation of the transitive subgroup 6/6(48) of S_6. Additional equitranslational phase transitions belonging to this exomorphic type with $G=O_h^i$ and $F=C_{4v}^j$ and $F=D_{2d}^k$ as given in Table III. In Table IV we give the phase transitions between $G=D_{6h}^i$ and $F=D_{2h}^j$ that belong to this exomorphic type.

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