Group-subgroup structural phase transitions: A comparison with existing tables

Harold T. Stokes and Dorian M. Hatch
Department of Physics and Astronomy, Brigham Young University, Provo, Utah 84602
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We have implemented group-theoretical methods on the computer for the description of possible structural phase transitions. All isotropy groups (corresponding to $\vec{k}$ points of symmetry) for each of the 230 three-dimensional space groups as well as the Landau and Lifshitz conditions for each representation have been obtained. Here we compare our results with previous tables and list the errors and necessary corrections to those tables.

I. INTRODUCTION

Both the theoretical and experimental understanding of phase transitions in solids have greatly benefited from the application of group-theoretical methods. If the space-group symmetry of the phases across the transition have a group-subgroup relationship, much can be said, from group-theoretical considerations alone, about the possible symmetry relationships between the two phases as well as distortions, energy (line) splittings, etc., accompanying the phase transition.

Group-theoretical methods were first applied to phase transitions by Landau[1] for the case of *continuous* phase transitions. In the Landau theory, the free energy F is minimized with respect to an order parameter $\vec{\psi}$ which describes the phase transition. A transition occurs when $\vec{\psi}$ takes on a nonzero value at a minimum of F. It has been shown through extensions of the Landau theory[2–7] that certain *direct* group-theoretical conditions must be satisfied. From these conditions, a heirarchy of constraints is obtained which successively restrict the generality of the phase transition. Even if the phase transition is *discontinuous*, much of the extended Landau theory is applicable if the space-group symmetries of the two phases have a group-subgroup relationship.

A number of authors have systematically applied some or all of the direct group-theoretical conditions (and some have also imposed minimization) and have tabulated for certain space groups the possible subgroups which obey these conditions. In particular, such tabulations have been done for space groups O_h^1 (Goldrich and Birman;[3] Vinberg *et al.*[8]), $D_{2d}^{3,9-12}$ (Zieliński *et al.*[9]), D_{3d}^6 (Hatch[10]), D_{6h}^4 (Pérez-Mato *et al.*[11]), O_h^3 (Jarić[7]), O_h^5 (Sutton and Armstrong;[12] Ghozlen and Mlik[13]), C_{4h}^6 (Deonarine and Birman[14]), and D_{2h}^{25} (Stokes and Hatch[15]). Undoubtedly, the most comprehensive classification has been with respect to the possible species character of the transition (Tolédano and Tolédano[16–19]).

A significant number of these calculations were done primarily by hand and were thus very susceptible to error. We have recently implemented on computer the direct group-theoretical conditions of the Landau theory and have applied them to *all* of the 230 three-dimensional space groups. Details of the procedure and algorithm, as well as a listing of the results, will be given elsewhere. Here, we compare our results with the above-mentioned papers.

II. DIRECT GROUP-THEORETICAL CONDITIONS

We are considering a solid in equilibrium which possesses space-group symmetry G_0 in its high-symmetry phase. The phase transition brings the solid to its low-symmetry phase which possesses space-group symmetry G. We restrict our consideration to cases where G is a subgroup of G_0 and where only *one* irreducible representation (irrep) D of G_0 brings about the transition. The following direct group-theoretical conditions have been discussed elsewhere[4,6] and are only briefly stated here.

(1) *Subduction condition.* The irrep D of G_0 must subduce into the identity irrep of G, that is,

$$i(G)=\frac{1}{|G|}\sum_{g\in G}\chi(g)\neq 0\ ,$$

where $i(G)$ is the subduction frequency, and $\chi(g)$ is the character of D for the element g of G. The summation is taken over all elements g of G.

(2) *Chain condition:* If G is a strict subgroup of another subgroup G' of G_0, then $i(G)$ must be greater than $i(G')$.

(3) *Landau condition:* The symmetrized triple Kronecker product of the irrep D of G_0 does not contain the identity irrep of G_0, that is,

$$\frac{1}{|G_0|}\sum_{g_0\in G_0}\{\tfrac{1}{3}\chi(g_0^3)+\tfrac{1}{2}\chi(g_0)\chi(g_0^2)+\tfrac{1}{6}[\chi(g_0)]^3\}=0\ .$$

The summation is taken over all elements g_0 of G_0.

(4) *Lifshitz condition:* The antisymmetrized double Kronecker product of D does not contain the vector representation of G_0, that is,

$$\frac{1}{|G_0|}\sum_{g_0\in G_0}\tfrac{1}{2}\{[\chi(g_0)]^2-\chi(g_0^2)\}\chi^v(g_0)=0\ ,$$

where $\chi^v(g_0)$ is the character of the vector representation of G_0. Note that in the equations above, χ is the character of a *physically* irreducible representation D of G_0. By physical, we mean that if a representation is complex, we consider the direct sum of it and its complex conjugate.

Conditions (1) and (2) above do not demand that the phase transition be continuous and may therefore be ap-

plied to discontinuous phase transitions. Subgroups G of G_0 which satisfy both conditions (1) and (2) are isotropy subgroups of G. For a continuous phase transition to a commensurate phase, conditions (3) and (4) must also be satisfied.

The four direct group-theoretical conditions listed above are *necessary* conditions in the Landau theory but are not *sufficient* conditions. One must still minimize the free energy F to assure that the conditions of the Landau theory are fully met. However, by first applying the direct group-theoretical conditions, the minimization process is greatly simplified.

In our computer-implemented procedure, for each of the 230 three-dimensional space groups, we calculated all the subgroups which satisfy conditions (1) and (2). (We restricted our considerations to irreps at $\vec{k}$ points of symmetry as listed in Bradley and Cracknell.[20]) As a result, we found 16 280 isotropy subgroups of the 230 space groups. We also applied by computer the conditions (3) and (4) and found that about half of the isotropy subgroups satisfy these conditions as well. We did not minimize the free-energy function, but applied only the *direct* group-theoretical conditions. To completely determine which of these phase transitions are allowed to be continuous by the Landau theory, the free energy F must also be minimized.

III. COMPARISON OF SUBGROUPS WITHOUT MINIMIZATION

Of the papers listed earlier, several considered isotropy subgroups of a given space group without additionally imposing the minimization condition. These allow most directly a comparison with our computer-implemented table.

Goldrich and Birman[3] calculated all possible displacive continuous phase transitions from the perovskite structure (O_h^1) without change of unit cell ($\vec{k}=\vec{0}$). They imposed the Landau and Lifshitz conditions. Because of the particular restrictions imposed by the perovskite structure,

TABLE I. Isotropy subgroups G of O_h^1. Corrections to Tables 2–5 of Vinberg *et al.* (Ref. 8).

Irrep	G
$\frac{2}{5},\frac{2}{6}$	add D_{2h}^3; delete D_{2h}^{25}
$\frac{2}{7},\frac{2}{10}$	add D_{2h}^{28}; delete D_{2h}^{23}
	add C_{2h}^3; delete C_{2h}^6
$\frac{2}{8},\frac{2}{9}$	add D_{2h}^{28}; delete D_{2h}^{23}
$\frac{3}{9},\frac{3}{10}$	add C_{2h}^3
$\frac{4}{9}$	add D_{2h}^{26}; delete D_{2h}^{28}
	add D_{2h}^7; delete D_{2h}^4
$\frac{4}{10}$	add D_{2h}^5; delete D_{2h}^9
	add C_s^3; delete C_2^3
	add C_s^3; delete C_s^1
	add C_{2h}^3

TABLE II. Isotropy subgroups G of D_{3d}^6. Corrections to Table II in Hatch (Ref. 10).

Irrep	$i(G)$	G
$D^{(*F,1)}$	1	add C_{2h}^6; delete C_2^3
	2	delete C_i^1
	3	add C_i^1; delete C_1^1
$D^{(*F,2)}$	1	add C_{2h}^6; delete C_2^3
	2	add C_i^1; delete C_i^2
$D^{(*F,4)}$	1	add C_{2h}^6

TABLE III. Isotropy subgroups G of D_{6h}^4. Corrections to Table 2 in Pérez-Mato *et al.* (Ref. 11).

Irrep	G
M_2^+	T_2: add $Cmca$, $P2_1/b$; delete $B2/b$
M_4^+	T_2: add $Cmca$, $P2_1/b$; delete $C2/m$
M_1^-	T_2: add $Cmca$, $P2_1/b$; delete $Cmc2_1$
M_2^-	T_2: add $Cmcm$, $P2_1/m$; delete $Amm2$
M_3^-	T_2: add $Cmca$, $P2_1/b$; delete $C222_1$
M_4^-	T_2: add $Cmcm$, $P2_1/m$; delete $Ama2$
K_5	add $P\bar{6}2m$, $P\bar{6}$
K_6	add $P321$, $P31m$, $P3$, $P1$
H_1, H_2	add $P\bar{6}2m$, $P\bar{6}2c$, $P\bar{6}$; delete $Ama2$, $Amm2$, Pm
L_1	T_2: add $P1$
	T_3: add $Abm2$, Pb, $P1$
L_2	T_2: add $P1$
	T_3: add $Aba2$, Pb, $P1$

TABLE IV. Isotropy subgroups G of O_h^5. Corrections to Tables III–VI in Sutton and Armstrong (Ref. 12).

Irrep	G
E_g^L	add C_{2h}^6, C_s^1; delete C_s^3
E_u^L	add C_{2h}^3, C_s^1; delete C_s^4

TABLE V. Isotropy subgroups G of O_h^5. Corrections to Tables 3–6 in Ghozlen and Mlik (Ref. 13). Also the tables of Ghozlen and Mlik had 139 omissions. We will indicate those omissions in a separate publication.

Irrep	Cell size	G
A_{1g}^L	8	delete O_h^8
E_g^L	2	delete C_{2h}^3[a]
	8	delete D_{3d}^5, D_{3d}^6[a]
E_u^L	2	delete C_{2h}^6[a]
	8	delete D_{3d}^5, D_{3d}^6[a]
E^W	16	delete D_2^2, D_2^4

[a]These subgroups appear twice in their table as inequivalent subgroups. They only appear once in our table.

TABLE VI. Isotropy subgroups G of C_{4h}^6. Corrections to Tables II–IV of Deonarine and Birman (Ref. 14).

$\vec{k}$	Irrep	$i(G)$	G
$(0\frac{1}{2}0)$	A_g, A_u	1	add S_4^2
		2	add C_2^3
		3	add C_i^1
$(\frac{1}{2}\frac{1}{2}\frac{1}{2})$	τ_{32}	1	add C_4^4

TABLE VII. Correction to the tables of continuous phase transitions published by Tolédano and Tolédano (Refs. 16–19). We list here the low-symmetry space groups which do not appear on our table. They did not use the same labeling of irreps as we did. Therefore, we did not compare *which* irreps for a given $\vec{k}$ gave rise to each low-symmetry space group G.

G_0	$\vec{k}$	G
Improper ferroelectric nonferroelastic transitions		
$P4_2/n$	M	$P4$
$P4_2/ncm$	M	$P4_2cm$, $P4_2nm$
$P\bar{6}m2$	M	$P31m$
$P\bar{6}c2$	M	$P31c$
$P\bar{6}2m$	M	$P3m1$
	K	$P31m$
$P\bar{6}2c$	M	$P3cl$
	K	$P31c$
$P6_3/mcm$	K	$P6_3cm$
$P6_3/mmc$	K	$P6_3mc$
Ferroelastoelectric transitions		
$Pmma$	Γ	$P2_12_12$
$P4/mcc$	Z	a
	A	a
$P4/mnc$	Γ	$P4_22_12$
$P4/nmm$	Γ	$P422$
$P4/ncc$	Γ	$P\bar{4}2c$
$P4_2/nnm$	Γ	$P4_22_12$
$P4_2/mbc$	Z	$P4_122$, $P4_322$
$P4_2/nmc$	Z	$P4_122$, $P4_322$
$P432$	M	$I2_13$
$Fm3c$	X	$P\bar{4}3m$
Ferrobielastic transitions		
$P4/mcc$	Γ	$P4_2/m$
	A	a
	Z	a
$P4/nnc$	Γ	$P4_2/n$
Ferroelastoelectric and ferrobielastic transitions		
$P4_2mc$	A	$I4_1/a$
Higher-order ferroic transitions		
$Ia3d$	H	$P432$
Ferroelastic transitions		
$Pmmn$	R	$B2/m$
$I4_1$	Z	$P2_1$
$P\bar{4}m2$	A	$I222$
$P\bar{4}c2$	A	$I222$
$P\bar{4}b2$	A	$I2_12_12_1$
$P\bar{4}n2$	A	$I2_12_12_1$
$I4_122$	N	$I222$
$P4_2cm$	M	$Cmm2$
	A	$Iba2$
$P4cc$	M	$Cmm2$, $Pma2$
$P4nc$	M	$Pma2$
$P4_2mc$	M	$Pma2$
$P4_2bc$	M	$Pma2$
$I4mm$	A	$Ima2$, $Fdd2$
$P4/mmm$	Γ	$Cmcm$
	M	$Pbam$
	R	$Cmcm$
$P4/mcc$	Γ	$B2/m$
$P4/nbm$	M	$Pmma$
$P4/mbm$	Γ	$B2/b$
$P4/nmm$	M	$Pbam$
$P4_2/mmc$	R	$Cmcm$
$P4_2/mcm$	M	$Pbam$
	A	$Immm$
$P4_2/nnm$	Γ	$B2/b$
$P4_2/nmc$	Z	$Pmma$
$P4_2/ncm$	Γ	$B2/b$
	M	$Pbam$
$I4/mmm$	N	$Cmca$
$I4_1/amd$	N	$Cmmm$
$P6mm$	L	$Pma2$
$P432$	M	$P422$
$P4_232$	M	$P4_222$
$F432$	X	$P4_122$
$I432$	N	$P4_222$
$P\bar{4}3n$	M	$P\bar{4}n2$
$Fm3c$	Γ	$I\bar{4}m2$
$Fd3m$	Γ	$I\bar{4}2m$
$Fd3c$	Γ	$I\bar{4}2m$
	X	$P4_122$, $P4_322$
$Ia3d$	H	$P4_122$, $P4_322$
Nonferroic transitions		
$C222$	Y	$P2_12_12_1$
$Pmm2$	T	$Ama2$
	U	$Ama2$
$Amm2$	Z	$Abm2$
$Ama2$	Y	$Pca2_1$, $Pcc2$, $Pmc2_1$
$Fmm2$	T	b
$P\bar{4}2c$	X	$P\bar{4}2m$, $P\bar{4}2_1m$
$I\bar{4}m2$	X	$P\bar{4}m2$, $P\bar{4}n2$
$P4_2/mmc$	X	$P4_2/mcm$
$P3$	H	a
$P3_1$	H	a
$P3_2$	H	a
$P\bar{3}$	H	a
$P312$	H	a
$P3_112$	H	a
$P3_212$	H	a
$R32$	X	$R32$
$P31m$	H	a
$R3m$	X	$R3m$
$R3c$	X	$R3c$
$R\bar{3}m$	X	$R\bar{3}m$
$R\bar{3}c$	X	$R\bar{3}c$
$P4_232$	X	$P4_232$

[a] All irreps for this $\vec{k}$ fail the Lifshitz condition.

[b] The T point should be the same as the X and Y points.

their list contains only 11 of the 29 possible isotropy subgroups of O_h^1 for $\vec{k}=\vec{0}$. However, all of their subgroups are contained in our table.

Vinberg *et al.*[8] calculated all the isotropy subgroups of O_h^1 (for all $\vec{k}$ points of symmetry) without imposing the Landau and Lifshitz conditions. We compared their list with our table and found 9 errors and 5 omissions (see Table I).

Hatch[10] calculated the isotropy subgroups of D_{3d}^6 for irreps which satisfy the Landau and Lifshitz conditions. We compared his list with our table and found 5 errors and 1 omission (see Table II).

Pérez-Mato *et al.*[11] calculated the isotropy subgroups of D_{6h}^4 for all $\vec{k}$ points of symmetry. We compared their list with our table and found 9 errors and 30 omissions (see Table III). They also applied the Landau and Lifshitz conditions to the irreps of D_{6h}^4. A comparison with our table shows 2 errors there. The Landau condition *is not* satisfied by K_5, and the Lifshitz condition *is* satisfied by H_1+H_2.

Jarić and Birman[5] calculated the isotropy subgroups of O_h^3 for the X and R points. Their work was subsequently subjected to international debate.[21,22,6,7] Jarić[7] recently published an extended list of these isotropy subgroups. We find complete agreement with our table.

Sutton and Armstrong[12] calculated the isotropy subgroups of O_h^5 for *one arm* of the star for each $\vec{k}$ point of symmetry. We compared their list to our table and found 2 errors and 4 omissions (see Table IV). All isotropy subgroups corresponding to the W point arise from multiple-arm contributions and were thus *purposely* omitted.

Recently Ghozlen and Mlik[13] also calculated *all* the isotropy subgroups of O_h^5 (for all $\vec{k}$ points of symmetry). We compared their list to our table and found 9 errors (see Table V). We also found 139 omissions. We will give our results for O_h^5 in a separate publication.

Deonarine and Birman[14] calculated the isotropy subgroups of C_{4h}^6 for irreps which satisfy the Landau and Lifshitz conditions. We compared their list with our table and found 4 omissions (see Table VI). They stated that C_1^1 was purposely omitted.

Neubuser and Wondratschek[23] have widely circulated a list of "translation-equivalent" ("*Zellengleich*") and "class-equivalent" ("*Klassengleich*") maximal subgroups of the 230 space groups. All of the translation-equivalent maximal subgroups in their table are isotropy subgroups ($\vec{k}=\vec{0}$) and are contained in our list. All of the class-equivalent maximal subgroups are also isotropy subgroups ($\vec{k}\neq\vec{0}$), but some of them arise from $\vec{k}$ vectors *not* at points of symmetry. All of the class-equivalent maximal subgroups in their table which *do* arise from $\vec{k}$ points of symmetry are contained in our list.

IV. COMPARISON WHEN MINIMIZATION IS IMPOSED

In this section, we examine published tables which were obtained by minimization of the free energy. All subgroups obtained in this manner, if correct, must be isotropy subgroups listed in our tables. On the other hand, not all of the isotropy subgroups in our table give minima in the free energy for continuous transitions, even after imposing the Landau and Lifshitz conditions. Therefore, we cannot check the tables for subgroups they may have omitted. We can only check for wrong subgroups.

TABLE VIII. Landau condition. Corrections to Table I in Kunert (Ref. 24). He did not use the same labeling of irreps as we did. Therefore, we did not compare *which* irreps (for a given $\vec{k}$) failed the Landau condition. However, we did compare the *number* of irreps which failed the condition. We list here the number of irreps which fail the Landau condition for the cases where our result disagrees. Note that Kunert did not consider irreps of the W point for O_h^{5-8} or the P point for O_h^{9-10}.

G_0	$\vec{k}$	Fail Landau
O_h^1	M	3 irreps
O_h^3	M	3 irreps
O_h^4	M	3 irreps
O_h^9	N	2 irreps

Zieliński *et al.*[9] calculated the lower-symmetry phases for the space groups $D_{2d}^{3,9-12}$. They imposed the Landau and Lifshitz conditions as well as the minimization condition. Upon comparison with our table, we found 1 error in their listing. The space group D_{2d}^9 goes to C_s^3 (not C_s^4 as listed) by irreps 1/1, 1/2.

Tolédano and Tolédano[16–19] published a series of papers giving a list of possible continuous phase transitions of several types. They imposed the Landau and Lifshitz conditions as well as the minimization condition. For the

TABLE IX. Landau and Lifshitz conditions. Corrections to Table I in Tolédano and Pascoli (Ref. 25). They did not use the same labeling of irreps as we did. Therefore, we did not compare *which* irreps (for a given $\vec{k}$) were listed. However, we did compare the *number* of irreps listed. We list here the number of irreps which simultaneously fail the Landau condition and satisfy the Lifshitz condition for the cases where our result disagrees.

G_0	$\vec{k}$	Fail Landau and satisfy Lifshitz
C_3^1	K	none
C_3^2	K	none
C_3^3	K	none
C_{3i}^1	K	none
D_3^1	K	none
D_3^3	K	none
D_3^5	K	none
C_{3v}^1	K	3 irreps
C_{3v}^2	K	none
C_{3v}^3	K	3 irreps
C_{3v}^4	K	none
D_{3d}^3	K	1 irrep
D_{3d}^4	K	1 irrep
C_{3h}^1	K	3 irreps
D_{3h}^1	K	3 irreps
D_{3h}^2	K	3 irreps

TABLE X. Lifshitz condition. Corrections to tables of Tolédano and Tolédano (Tables IV—VI in Ref. 16 and Tables IV—X in Ref. 17). They did not use the same labeling of irreps as we did. Therefore, we did not compare *which* irreps (for a given $\vec{k}$) satisfied the Lifshitz condition. However, we did compare the *number* of irreps which satisfied the condition. We list here the number of irreps which satisfy the Lifshitz condition for the cases where our result disagrees.

G_0	$\vec{k}$	Satisfy Lifshitz
Cmca	*R*	all
*I*4/*m*	*A*	2 irreps
*I*422	*A*	2 irreps
*P*4/*mcc*	*M*	all
	Z	none
	A	none
*I*4/*mmm*	*A*	4 irreps[a]
*P*312	*K*	none
$P3_112$	*K*	none
$P3_212$	*K*	none
*R*32	*H*	none[b]
	K	none[b]
$P\bar{3}ml$	*H*	2 irreps
	K	2 irreps
$P\bar{3}cl$	*K*	2 irreps
$P\bar{6}$	*H*	all
	K	all
$P6_3/m$	*H*	2 irreps
$P\bar{6}m2$	*H*	all
	K	all
$P\bar{6}c2$	*K*	all
$P\bar{6}2c$	*H*	2 irreps
$P6_3/mmc$	*H*	2 irreps
*Pn*3*m*	*R*	all
*Im*3*m*	*H*	all

[a]These errors were in Ref. 1 but were corrected in Ref. 2.
[b]These points are on the surface of the first Brillouin zone of the hexagonal lattice but are in the *interior* of the first Brillouin zone of the trigonal lattice. Therefore, none of the irreps of these points can satisfy the Lifshitz condition.

improper ferroelectric-nonferroelastic transitions,[16] they required that (1) $\vec{k}\neq\vec{0}$, (2) the irrep not be a one-dimensional real irrep, and (3) the crystal classes be restricted to those in Table I of Ref. 16. For the secondary and higher-order ferroic transitions,[17] they required that (1) the irrep not be a one-dimensional real irrep if $\vec{k}\neq\vec{0}$ and (2) the crystal classes be restricted to those of Table I in Ref. 17. For the purely ferroelastic transitions,[18] they required that the crystal classes be restricted to those of Table I in Ref. 18. For the nonferroic transitions,[19] they required that the crystal class not change in the transition. We applied these restrictions to our table and compared our result with their lists. We found 89 errors (see Table VII).

V. COMPARISON OF LANDAU AND LIFSHITZ CONDITIONS

Kunert[24] calculated the Landau and Lifshitz conditions for the irreps of $O_h^{1,3-10}$. We compared our results to his and found additional irreps which do not satisfy the Landau condition (see Table VIII).

Tolédano and Pascoli[25] investigated the irreps of the rhombohedral and hexagonal systems which did not satisfy the Landau condition but did satisfy the Lifshitz condition. We compared their results with our table and found that the errors in their table could be associated with the calculation of the Lifshitz condition, and all were associated with the *K* point. There were 9 irreps which *do not* satisfy the Lifshitz condition as claimed by Tolédano and Pascoli, and 12 irreps that *do* satisfy the Lifshitz condition and are omitted by Tolédano and Pascoli (see Table IX).

Tolédano and Tolédano[16,17] applied the Lifshitz condition to irreps of most of the 230 space groups. We compared their results with our table and found the errors listed in Table X.

VI. CONCLUSION

The calculations required for finding isotropy subgroups are long and tedious. This fact accounts for the many errors which we found in published tables. Computer-implemented calculations are particularly advantageous under these circumstances. Up to the present time, we have found our computer-generated table to be free of any errors. A complete listing of our table will be given in a separate publication.

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