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Images of Physically Irreducible Representations of the 230 Space Groups

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Abstract

Among the 230 crystallographic space groups, we find there are more than 4000 physically irreducible representations (irreps) that arise from **k** points of symmetry. These irreps map the space-group elements onto only 132 different images. These images are listed, and their group–subgroup relations are given. Images which are active in the Landau theory of continuous phase transitions are also indicated.

Group-theoretical methods provide a powerful tool in solid-state physics. The irreducible representations (irreps) of space groups are of central importance in these methods. We recently (Stokes & Hatch, 1984, 1985; Hatch & Stokes, 1984, 1985*a*, 1985*b*, 1985*c*; Kim, Hatch & Stokes, 1986) used group-theoretical methods in the Landau theory (Landau & Lifshitz, 1980) of continuous phase transitions in solids. In this theory, a phase transition is driven by an irrep of the parent space group. We obtained a listing of all possible symmetry changes in such phase transitions to commensurate structures. To do this, we needed the irreps of the space groups.

Each irrep consists of a mapping of space-group elements onto a set of matrices called the *image* of the irrep. Theories which describe physically realizable processes usually require these matrices to be real. If an image cannot be written in real form (*i.e.* it is not equivalent to a set of real matrices), a *physically* irreducible representation can be formed from the direct sum of each matrix and its complex conjugate. The resulting matrices are equivalent to a set of real matrices. In this paper, *irrep* refers to physically irreducible representations.

Each irrep of a space group is associated with some **k** vector in the first Brillouin zone. We have considered all of the irreps which arise from **k** *points* of symmetry (points **k** in the first Brillouin zone which have higher symmetry than any other point in the neighborhood of **k**; see Bradley & Cracknell, 1972). There are more than 4000 of these irreps among the 230 three-dimensional space groups.

We sorted out the images of these irreps and found that there are only 132 different images. We list these in Table 1. We introduce here our labeling of these images (*A*1*a*, *A*2*a*, *B*3*a*, *etc.*; this labeling is in principle similar to that in Gufan & Chechin, 1980) and also give the label used by Tolédano & Tolédano (1980) and by Mozrzymas & Solecki (1975). We have selected an irrep as an example of each image. Each irrep is identified by a space-group number, a space-group symbol, and an irrep label which follows the convention of Miller & Love (1967) (see also Cracknell, Davies, Miller & Love, 1979). If the irrep is not real, a direct sum is indicated, showing the physically irreducible representation. A physically irreducible representation which is formed from a complex irrep which is equivalent to its own complex conjugate is indicated by, for example, $P_2 \oplus (P_2)^*$. A physically irreducible representation which is formed from a complex irrep which is equivalent to the complex conjugate of *another* irrep is indicated by, for example, $\Gamma_2 \oplus \Gamma_3$, where Γ_3 is equivalent to the complex conjugate of Γ_2.

Although we use the irrep labelling of Miller & Love (1967), the matrices we choose for the images are different from their choice in many cases (but still *equivalent* to their choice). An explicit listing of our generating matrices of these images will be given in a later publication. We have chosen matrices which give rise to the same set of invariant fourth-degree polynomials as those given by Tolédano & Tolédano (1980) and Tolédano, Michel, Tolédano & Brezin (1985).

We show in Figs 1–6 the group–subgroup relations among the images. Solid lines indicate an actual group–subgroup relation for the matrices we have chosen for the images. Dashed lines indicate that an image is only *equivalent* to a subgroup of another image but not an *actual* subgroup for the matrices we have chosen. A different choice of matrices for the images could change some dashed lines to solid lines and some solid lines to dashed lines on these figures.

In Landau theory, an irrep may drive a continuous phase transition only if it satisfies two conditions, called the Landau & Lifshitz conditions (Landau & Lifshitz, 1980). These irreps are said to be *active*. Images of the active irreps are also said to be active, even though irreps which are *not* active may also have that same image. In Table 1, we indicate which

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images are active. For the active images, an example of an active irrep is given.

Our results for active images disagree with Tolédano & Tolédano (1980). They missed five four-dimensional active images (*D*32*e*, *D*64*b*, *D*64*d*, *D*72*a*, and *D*144*a*) and a six-dimensional active image (*E*96*k*). (More details about *E*96*k* can be found in Hatch, Stokes, Kim & Felix, 1986, and in Kim, Hatch & Stokes, 1986.) Also, we do not find the eight-dimensional image labeled M_5 by Tolédano & Tolédano. (*None* of the irreps of $P6_3mc$ are eight-dimensional.)

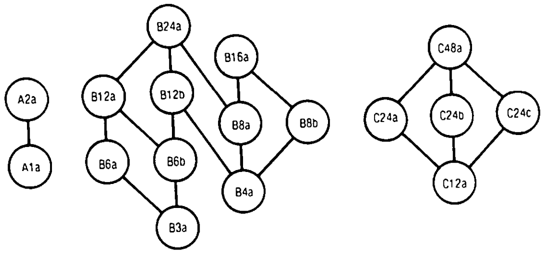

Fig. 1. The group–subgroup relations for the one-, two- and three-dimensional images.

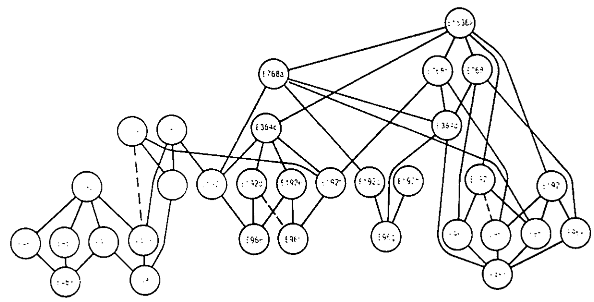

Fig. 4. The group–subgroup relations for the six-dimensional images.

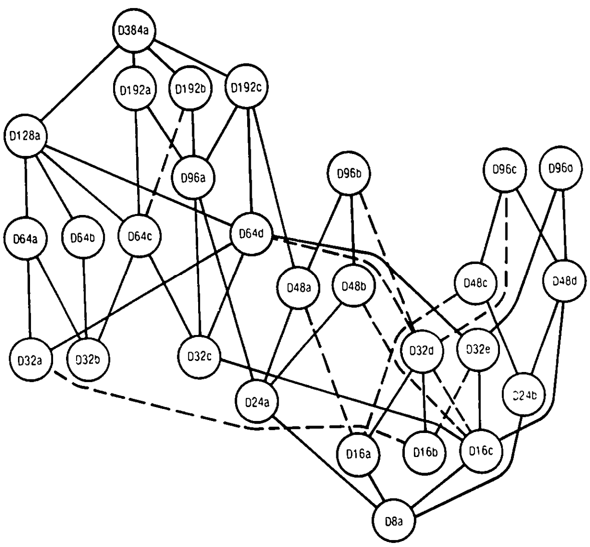

Fig. 2. The group–subgroup relations for some of the four-dimensional images.

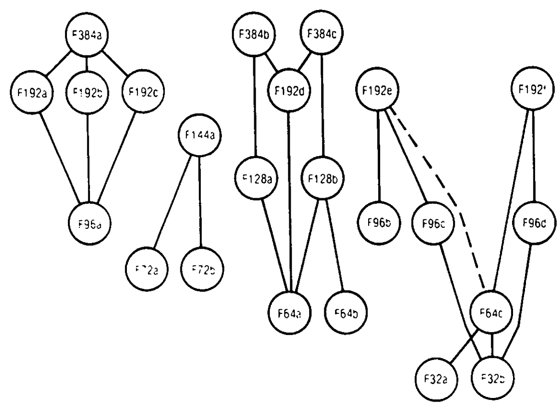

Fig. 5. The group–subgroup relations for the eight-dimensional images.

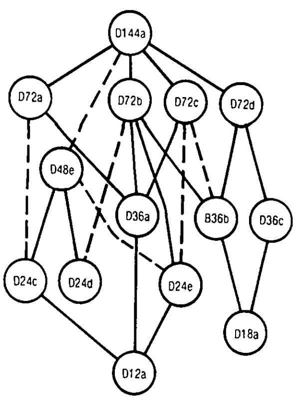

Fig. 3. The group–subgroup relations for the remaining four-dimensional images.

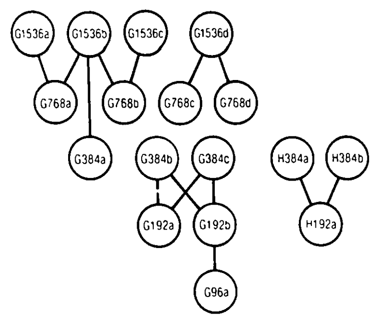

Fig. 6. The group–subgroup relations for the twelve- and sixteen-dimensional images.

Table 1. *The images of the* 230 *space groups*

We give our image label, the dimension (dim.) of the matrices, the order of the image (number of distinct matrices), an example of an irrep with that image, whether or not the image is active, and other labels used for these images in Tolédano & Tolédano (1980) or Mozrzymas & Solecki (1975). If the image is active, the irrep shown is an example of an active irrep.

Image	Dim.	Order	Example irrep	Active	Other label
A1a	1	1	$1P1\ \Gamma_1$	no	C_1
A2a	1	2	$2P\bar{1}\ \Gamma_1^-$	yes	C_2
B3a	2	3	$143P3\ \Gamma_2 \oplus \Gamma_3$	no	C_3
B4a	2	4	$18P2_12_12\ S_1 \oplus S_2$	yes	C_4
B6a	2	6	$149P312\ \Gamma_3$	no	C_{3v}
B6b	2	6	$147P\bar{3}\ \Gamma_2^- \oplus \Gamma_3^-$	yes	C_6
B8a	2	8	$75P4\ X_1$	yes	C_{4v}
B8b	2	8	$76P4_1\ A_1 \oplus A_3$	no	C_8
B12a	2	12	$162P\bar{3}1m\ \Gamma_3^-$	yes	C_{6v}
B12b	2	12	$197I23\ P_2 \oplus (P_2)^*$	yes	C_{12}
B16a	2	16	$91P4_122\ A_1$	no	C_{8v}
B24a	2	24	$211I432\ P_2$	yes	C_{12v}
C12a	3	12	$195P23\ \Gamma_4$	no	T
C24a	3	24	$200Pm^3\ \Gamma_4^-$	yes	T_h
C24b	3	24	$207P432\ \Gamma_5$	no	T_d
C24c	3	24	$207P432\ M_2$	yes	O
C48a	3	48	$221Pm3m\ \Gamma_4^-$	yes	O_h
D8a	4	8	$61Pbca\ R_1^+ \oplus (R_1^+)^*$	yes	13·1
D12a	4	12	$218P\bar{4}3n\ R_3 \oplus (R_3)^*$	yes	21·1
D16a	4	16	$92P4_12_12\ A_1 \oplus A_2$	no	31·1
D16b	4	16	$76P4_1\ R_1 \oplus R_2$	no	29·1
D16c	4	16	$64Cmca\ R_1^+ \oplus R_2^+$	yes	26·1
D18a	4	18	$150P321\ K_3 \oplus (K_3)^*$	no	33·1
D24a	4	24	$205Pa3\ R_1^+ \oplus R_3^+$	yes	49·2
D24b	4	24	$205Pa3\ R_2^+ \oplus (R_2^+)^*$	yes	49·1
D24c	4	24	$217I\bar{4}3m\ P_3 \oplus (P_3)^*$	yes	44·1
D24d	4	24	$204Im3\ P_2 \oplus P_3$	yes	42·1
D24e	4	24	$222Pn3n\ R_2 \oplus R_3$	yes	48·1
D32a	4	32	$80I4_1\ N_1$	yes	59·1
D32b	4	32	$43Fdd2\ L_1$	yes	58·C1
D32c	4	32	$22F222\ L_1$	yes	56·1
D32d	4	32	$91P4_122\ R_1$	no	57·1
D32e	4	32	$92P4_12_12\ R_1 \oplus R_3$	yes	52·1
D36a	4	36	$159P31c\ H_3 \oplus (H_3)^*$	no	62·1
D36b	4	36	$150P321\ H_3 \oplus (H_3)^*$	no	63·1
D36c	4	36	$162P\bar{3}1m\ K_3$	no	64·1
D48a	4	48	$212P4_332\ R_3$	no	77·2
D48b	4	48	$199I2_13\ P_1 \oplus (P_1)^*$	no	
D48c	4	48	$212P4_332\ R_1 \oplus R_2$	no	77·1
D48d	4	48	$199I2_13\ P_2 \oplus (P_2)^*$	no	76·1
D48e	4	48	$299Im3m\ P_3$	yes	74·1
D64a	4	64	$88I4_1/a\ N_1^+$	yes	80·01
D64b	4	64	$122I\bar{4}2d\ N_1$	yes	81·01
D64c	4	64	$70\ Fddd\ L_1^+$	yes	82·01
D64d	4	64	$98I4_122\ N_1$	yes	83·1
D72a	4	72	$186P6_3mc\ H_3$	yes	91·1
D72b	4	72	$190P\bar{6}2c\ H_1 \oplus (H_1)^*$	yes	85·1
D72c	4	72	$163P\bar{3}1c\ H_3$	no	92·1
D72d	4	72	$162P\bar{3}1m\ H_3$	no	88·1
D96a	4	96	$196F23\ L_1$	yes	95·1
D96b	4	96	$214I4_132\ P_1$	no	
D96c	4	96	$214I4_132\ P_2$	no	
D96d	4	96	$220I\bar{4}3d\ P_1 \oplus (P_1)^*$	yes	98·1
D128a	4	128	$141I4_1/amd\ N_1^+$	yes	101.01
D144a	4	144	$194P6_3/mmc\ H_1$	yes	104·1
D192a	4	192	$203Fd3\ L_1^+$	yes	108·01
D192b	4	192	$209F432\ L_1$	yes	109·01
D192c	4	192	$210F4_132\ L_1$	yes	110·1
D384a	4	384	$227Fd3m\ L_1^+$	yes	115·01
E48a	6	48	$197I23\ P_4 \oplus (P_4)^*$	no	
E48b	6	48	$218P\bar{4}3n\ X_1 \oplus X_2$	yes	L_{10}
E48c	6	48	$198P2_13\ M_1 \oplus M_2$	no	
E96a	6	96	$176P6_3/m\ L_1$	no	
E96b	6	96	$178P6_122\ L_1$	no	
E96c	6	96	$217I\bar{4}3m\ P_4 \oplus (P_4)^*$	no	
E96d	6	96	$223Pm3n\ X_3$	yes	L_9
E96e	6	96	$197I23\ N_1$	no	
E96f	6	96	$207P432\ M_5$	no	
E96g	6	96	$198P2_13\ X_1$	no	
E96h	6	96	$212P4_332\ M_1 \oplus M_4$	no	
E96i	6	96	$212P4_332\ M_5$	no	
E96j	6	96	$199I2_13\ N_i$	no	
E96k	6	96	$212P4_332\ M_2 \oplus M_3$	yes	
E192a	6	192	$193P6_3/mcm\ L_1$	no	
E192b	6	192	$218P\bar{4}3n\ X_5$	no	
E192c	6	192	$204Im3\ N_1^-$	yes	L_8
E192d	6	192	$211I432\ N_1$	no	
E192e	6	192	$211I432\ N_2$	yes	L_6
E192f	6	192	$215P\bar{4}3m\ X_5$	yes	L_7
E192g	6	192	$205Pa3\ X_1$	no	
E192h	6	192	$212P4_332\ X_1$	no	
E192i	6	192	$214I4_132\ N_1$	no	
E192j	6	192	$214I4_132\ N_2$	yes	L_5
E384a	6	384	$223Pm3n\ X_1$	no	
E384b	6	384	$222Pn3n\ X_1$	no	
E384c	6	384	$224Pn3mX_3$	yes	L_4
E384d	6	384	$196F23\ W_1$	no	
E768a	6	768	$202Fm3\ W_1$	no	
E768b	6	768	$216F\bar{4}3m\ W_1$	yes	L_3
E768c	6	768	$209F432\ W_1$	yes	L_2
E1536a	6	1536	$225Fm3m\ W_1$	yes	L_1
F32a	8	32	$110I4_1cd\ P_1 \oplus (P_1)^*$	no	
F32b	8	32	$73Ibca\ W_1 \oplus (W_1)^*$	no	
F64a	8	64	$108I4cm\ N_1 \oplus N_2$	no	
F64b	8	64	$110I4_1cd\ N_1 \oplus N_2$	no	
F64c	8	64	$142I4_1/acd\ P_1 \oplus P_2$	no	
F72a	8	72	$184P6cc\ H_3 \oplus (H_3)^*$	no	
F72b	8	72	$165P\bar{3}c1\ H_3 \oplus (H_3)^*$	no	
F96a	8	96	$202Fm3\ L_2^+ \oplus L_3^+$	yes	M_4
F96b	8	96	$220I\bar{4}3d\ P_3 \oplus (P_3)^*$	no	
F96c	8	96	$206Ia3\ P_1 \oplus P_3$	no	
F96d	8	96	$206Ia3\ P_2 \oplus (P_2)^*$	no	
F128a	8	128	$140I4/mcm\ N_1$	no	
F128b	8	128	$142I4_1/acd\ N_1$	no	
F144a	8	144	$192P6/mcc\ H_1 \oplus H_2$	no	
F192a	8	192	$216F\bar{4}3m\ L_3$	yes	M_2
F192b	8	192	$203Fd3\ L_2^+ \oplus L_3^+$	yes	M_3
F192c	8	192	$210F4_132\ L_3$	no	
F192d	8	192	$219F\bar{4}3c\ L_1 \oplus L_2$	no	
F192e	8	192	$230Ia3d\ P_3$	no	
F192f	8	192	$230Ia3d\ P_1 \oplus P_2$	no	
F384a	8	384	$227Fd3m\ L_3^+$	yes	M_1
F384b	8	384	$226Fm3c\ L_3$	no	
F384c	8	384	$228Fd3c\ L_3$	no	
G96a	12	96	$205Pa3\ M_1 \oplus M_2$	no	
G192a	12	192	$220I\bar{4}3d\ N_1$	no	
G192b	12	192	$206Ia3\ N_1$	no	
G384a	12	384	$222Pn3n\ X_3 \oplus X_4$	no	
G384b	12	384	$230Ia3d\ N_1$	no	
G384c	12	384	$230Ia3d\ N_2$	no	
G768a	12	768	$209F432\ W_3 \oplus W_4$	no	
G768b	12	768	$219F\bar{4}3c\ W_1 \oplus W_2$	no	
G768c	12	768	$203Fd3\ W_1$	no	
G768d	12	768	$210F4_132\ W_1$	no	
G1536a	12	1536	$225Fm3m\ W_5$	no	
G1536b	12	1536	$226Fm3c\ W_1 \oplus W_2$	no	
G1536c	12	1536	$226Fm3c\ W_5$	no	
G1536d	12	1536	$227Fd3m\ W_1$	no	
H192a	16	192	$219F\bar{4}3c\ L_3 \oplus (L_3)^*$	no	
H384a	16	384	$226Fm3c\ L_1 \oplus L_2$	no	
H384b	16	384	$228Fd3c\ L_1 \oplus L_2$	no	
K1536a	24	1536	$228Fd3c\ W_1 \oplus W_2$	no	

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Estimation of Quartet Phase Sums from a New Joint Probability Distribution of Normalized Structure Factors

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Abstract

A new joint probability distribution of normalized structure factors is derived for equal-atom structures in space group $P1$. From this general distribution, a series expansion, the conditional joint probability distribution of the quartet phase sum is obtained, when restrictive conditions among the reciprocal vectors are imposed. The main difference from existing quartet distributions is the possibility of enclosing higher-order terms to any given order of N, although an approximation employed in the derivation limits the number of them considerably. The higher-order terms present are easily employed in the series since the determination of their explicit appearance has been automated: a computer program derives the terms up to a desired order and stores them in a coded form. In general, the incorporation of selective terms up to order N^{-3} appears to yield sufficient convergence. Only high $|E|$ values or a low N value may necessitate the use of higher-order terms. Test results show that, in contrast to results from the quartet distributions of Hauptman and Giacovazzo, systematic estimation errors are hardly present, while absolute estimation errors are reduced as well.

1. Introduction

Results of Simerska (1956) and Hauptman & Karle (1953) indicated that the four-phase structure invariant ψ_4,

$$\psi_4 = \varphi_{H_1} + \varphi_{H_2} + \varphi_{H_3} - \varphi_{H_1+H_2+H_3}, \qquad (1)$$

also called the quartet phase sum or simply quartet, lies more probably near zero for larger values of

$$E_4 = |E_{H_1}E_{H_2}E_{H_3}E_{H_1+H_2+H_3}|N^{-1}. \qquad (2)$$

However, in general the triplet relationship

$$\psi_3 = \varphi_{H_1} + \varphi_{H_2} - \varphi_{H_1+H_2} \qquad (3)$$

will be estimated more reliably because the E_3 values, which determine the reliability of the triplet estimation, are in general larger than the E_4 values since they depend on $N^{-1/2}$ only. Therefore, quartets were not used as such for practical purposes. This changed when Schenk (1973*a*) pointed out that quartets can also be formed by summing two triplets with one phase in common and he showed in this way that quartet (1) depends not only on $|E_{H_1}|$, $|E_{H_2}|$, $|E_{H_3}|$ and $|E_{H_1+H_2+H_3}|$ but also on the so-called cross terms $|E_{H_1+H_2}|$, $|E_{H_1+H_3}|$ and $|E_{H_2+H_3}|$. He argued that the larger the E_4 and cross-term magnitudes the more probably ψ_4 lies near zero. Another important result of the introduction of this cross-term principle was that quartets with small cross-term magnitudes could be predicted to lie near π (Schenk & De Jong, 1973; Schenk, 1973*a*, *b*; Hauptman, 1974; Schenk, 1974). This renewed interest in quartets and the cross-term principle led to the development of improved joint probability distributions (j.p.d.'s) for estimating the quartet phase sum (Hauptman, 1975*a*, *b*, 1976; Giacovazzo, 1976*a*, *b*) and initiated the development of the neighbourhood principle (Hauptman, 1975*b*) and the representation theory (Giacovazzo, 1977). The latter theories identify structure factors upon which the phase sum of a structure (sem)invariant most sensitively depends.

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