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Quasisymmetry (*P*-Symmetry) in Crystals†

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Abstract

The concepts of semi-direct product, quasi semi-direct product and the method of constructing quasisymmetry (*P*-symmetry) groups [Krishnamurty, Prasad & Rama Mohana Rao (1978). *J. Phys. A*, **11**, 805–811; (1980). *J. Phys. A*, **13**, 1947–1956] have been explored and a general method of constructing quasisymmetry (*P*-symmetry) groups with the crystallographic space groups as generators is suggested. The study is restricted to only the cubic system for the chosen boundary condition $T_x^2 = T_y^2 = T_z^2 = E$. The minor quasisymmetry cubic space groups so obtained are associated with the one-dimensional complex and two-dimensional real irreducible representations of the generator groups using the ideas of little groups and their one-dimensional allowable irreducible representations. The symmorphic cubic space groups *F*23, *F*432 and the non-symmorphic cubic space groups *Fd*3, *Fd*3*m* are exemplified. For the rest of the cubic space groups the results obtained are tabulated. Some suggestions have been made as to the possible studies in which the groups obtained here can be applied.

1. Introduction

The work of Shubnikov (1951) has made scientists the world over feel that the concept of antisymmetry can be profitably exploited in crystallographic point-group and space-group studies. Zamorzaev (1957) and Belov, Neronova & Smirnova (1955, 1957) have actually translated this feeling into very useful work and consequently the dichromatic space groups were derived. Later the very idea of antisymmetry has been considered from several different points of view and generalizations of this concept have been proposed and worked out. A few instances of these generalizations that emerged are not out of place here, for example, colour symmetry (Belov & Tarkhova, 1956; Belov, 1956; Indenbom, 1959); polychromatic symmetry (Indenbom, Belov & Neronova, 1960); antisymmetry of different kinds (Zamorzaev & Sokolov, 1957; Zamorzaev, 1958, 1962, 1963); cryptosymmetry (Niggli & Wondratschek, 1960, 1961); quasisymmetry (Zamorzaev, 1967), *etc.* The method of constructing different colour symmetry groups in a variety of ways has been discussed and the results tabulated in several Russian publications. For instance, they are tabulated as the antisymmetry point groups and space groups in the Shubnikov groups by Koptsik (1966), as the colour symmetry groups $G^{(p)}$ isomorphic with the crystallographic point groups *G* by finding the normal subgroups *H* of *G* and forming the direct, semi-direct and quasi products of *H* with the generating colour groups $G^{(p)*}$ or with the groups $G^{(p)*}$ (mod G_1^*). A tabular representation of the dichromatic cubic space groups obtained from the non-equivalent alternating representations of the symmorphic space groups that are reciprocal to the underlying point space groups of the considered ones was accomplished by Kirshnamurty & Gopala Krishna Murty (1968, 1969).

Colour symmetry groups of all categories were constructed from the classic ones by means of the one-dimensional (1D) complex representations (Indenbom, 1959) using the tables of the fundamental unitary representations of Fedorov groups (Feddeev, 1964). Zamorzaev (1969, 1971) constructed the Belov groups of index 3, 4 and 6 by restricting himself to the cyclic groups $P = \{p, p^2, \ldots, p^m = 1\}$ isomorphic to the factor groups φ/φ^* by choosing m = 3, 4 or 6 and $p = \begin{pmatrix} 1 & 2 & \ldots & m \\ 2 & 3 & \ldots & 1 \end{pmatrix}$. The theory of group representation was applied by Koptsik & Khuzukeev (1972) to correct the list of Belov groups derived by Zamorzaev (1969, 1971) and to derive the new four- and six-colour space groups with non-cyclic colour permutations $p \leftrightarrow$

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φ/φ^*, $\varphi\Delta\varphi^*$. A one-to-one correspondence between the multiple representations of the Fedorov groups and the Belov groups for any crystallographic number of colours was also established.

Generalizations of Shubnikov's antisymmetry and Belov's colour symmetry were enveloped by the concept of P-symmetry introduced by Zamorzaev (1967) and discussed in detail by Shubnikov & Koptsik (1974). Whenever the generator group G can be expressed as $G = S \wedge T$ of two of its constituent subgroups S and T, Krishnamurty, Prasad & Rama Mohana Rao (1978*a*) established a general method of obtaining quasisymmetry (P-symmetry) groups as semi-direct products. In the case of those generators which can be written as a quasi semi-direct product, *i.e.* $G = H \circ G$ (mod H), similar results as in the case of semi-direct products were obtained (Krishnamurty, Prasad & Rama Mohana Rao, 1980). In either case the obtained minor quasisymmetry groups were associated with the irreducible representations (IRs) of the generator groups using the concept of allowable irreducible representations (AIRs) of the little groups that induce the respective degenerate IRs of the generator groups.

In the present paper, the general method of construction of quasisymmetry groups as semi-direct and quasi semi-direct products (Krishnamurty *et al.*, 1978*a*; 1980) is explored to construct minor quasisymmetry groups with Fedorov groups as generators. In § 2, the connection between the semi-direct and quasi semi-direct products with those of the symmorphic and non-symmorphic groups is briefly dealt with for the sake of completeness. In § 3, the consequent developments of the concept of P-symmetry, the different aspects on the applications of generalized colour symmetry and the position of the P-symmetry groups *vis-a-vis* the Wreath product groups is discussed elaborately. In § 4, the method of construction of minor quasisymmetry space groups is exemplified in the case of both symmorphic and non-symmorphic cubic space groups for the chosen boundary condition $T_x^2 = T_y^2 = T_z^2 = E$, considering the symmorphic cubic space groups $F23$, $F432$ and the nonsymmorphic ones $Fd3$, $Fd3m$. The minor quasisymmetry cubic space groups generated are associated in § 5 with the appropriate 1D complex and 2D real IRs of the generator groups using the ideas of little groups and their 1D AIRs. In § 6, the results obtained are discussed briefly and some suggestions have been made as to the possible studies in which the groups obtained here can be applied.

It is well known that space groups are symmetry groups of crystals. As such, a knowledge of the minor quasisymmetry groups generated by them would be useful. In literature, the minor quasisymmetry groups generated and associated with the 1D alternating IRs of the crystallographic space groups are available, though they are not always termed minor quasisymmetry groups and expressed as semi-direct products. However, a connected account of the minor groups (obtained as semi-direct products) associated with the non-degenerate complex IRs and degenerate IRs of the space groups is not so readily available as far as our knowledge goes.* Hence an extensive tabulation of the minor quasisymmetry cubic space groups associated with the 1D complex and 2D real IRs is undertaken in the present paper, prompted by the feeling that physicists will certainly stand to gain by making extensive use of these groups in their future investigations. The nomenclature adopted for the Fedorov cubic space groups is mostly the International notation (Bradley & Cracknell, 1972; Henry & Lonsdale, 1952).

2. Symmorphic and non-symmorphic groups – semi-direct and quasi semi-direct products

Let H be any subgroup of G, and let $G = Hg_1 \cup Hg_2 \cup \ldots \cup Hg_s$; $g_1 = h_1 = E$ is a decomposition of G into distinct right cosets. In addition, let H be a normal subgroup of G and let $h_1, h_2, \ldots, h_m \in H$. If we introduce in the set $\{g_1, g_2, \ldots, g_s\}$ the law of reduced multiplication (Shubnikov & Koptsik, 1974) then the set $\{g_1, g_2, \ldots, g_s\}$ is said to form a group by modulus and is denoted by G(mod H).

Since the laws of multiplication in the groups G and G(mod H) are different, in general, the group G(mod H) is not a subgroup of G. However, if $H \cap G(\text{mod } H) = h_1 = g_1 = E \in G$, then an extension G of H may be constructed as the product of the groups H and G(mod H) by carrying out the pairwise combination of all the elements $h_1, h_2, \ldots, h_m \in H$ with the elements $g_1, g_2, \ldots, g_s \in G$(mod H) and uniting the results so obtained:

$$G = \{h_1g_1, h_2g_1, \ldots, h_mg_1; h_1g_2, \ldots, h_mg_2; \ldots; h_1g_s, \ldots, h_mg_s\}. \quad (1)$$

If G(mod H) is a subgroup of G, then the extension (1) is an ordinary product and G is called symmorphic. Since G(mod H) is not necessarily a subgroup of G, the extension (1) is called a quasi product (Shubnikov & Koptsik, 1974) and G is called non-symmorphic. The quasi direct product or the quasi semi-direct product is determined by the multiplication law of the binary elements $h_ig_j \in G$.

If G(mod H) happens to be a subgroup of G, then the quasi direct product and quasi semi-direct product reduces to the ordinary direct product and semi-direct product respectively; we write $G = H \wedge K$ for the semi-direct product and $G = H \circ G$ (mod H) for quasi semi-direct product.

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From what has been outlined above, it can be seen that the traditional 230 Fedorov space groups, which were broadly categorized into symmorphic and non-symmorphic groups, can be expressed in terms of the semi-direct and quasi semi-direct products respectively once the constituent normal subgroups H are identified. The symmorphic space group $F432$ and the non-symmorphic one $Fd3m$ necessary for the subsequent discussion are dealt with below.

For the symmorphic space group $F432$, the symmorphic space group $F23$ consisting of the elements:* E; $16C_{3j}^{+}$; $6C_{2m}$; $16C_{3j}^{-}$; $6C_{2m}$; $6T$; $6C_{2m}$; $16C_{3j}^{-}$; $6C_{2m}$; $16C_{3j}^{+}$; T_{123} is a subgroup of index 2 (hence a normal subgroup). Hence with $F23$ as the chosen normal subgroup H, it can be seen that $F432 = EH \cup C_{2a}H$.† The coset representatives $E;C_{2a}$ form a group with the same multiplication law as that of the group $F432$ and we call this group $\tilde{2}$.‡ These groups $F23$ and $\tilde{2}$ satisfy all the requirements of a semi-direct product and we write $F432 = F23 \wedge \tilde{2}$. In the case of the non-symmorphic space group $Fd3m$, the group $Fd3$: E; $16C_{3j}^{-}$; $4i$; $16C_{3j}^{-}$; $16S_{6j}^{+}$; $12C_{2m}$; $16S_{6j}^{+}$; $24\sigma_m$; $6T$; $12C_{2m}$; $16S_{6j}^{-}$; $4i$; $16C_{3j}^{+}$; $16S_{6j}^{-}$; $16C_{3j}^{+}$; T_{123} is a normal subgroup and the factor group $Fd3m/Fd3$ can be expressed as $E\ (Fd3) \cup C_{2a}(Fd3)$.§ Unlike the previous case, the coset representative $E;C_{2a}$ here will not form a group with the induced composition in $Fd3m$. On the other hand, they form a group by modulus and hence $G = Fd3m$ can be expressed as the quasi semi-direct product: $Fd3m = Fd3 \circ Fd3m$ (mod $Fd3$). For the rest of the cubic space groups the results obtained are tabulated in Table 1.

Table 1. *Symmorphic and non-symmorphic cubic space groups as semi-direct and quasi semi-direct products*

Symmorphic cubic space group G as semi-direct product $G = H \wedge K$	Non-symmorphic cubic space group G as quasi semi-direct product $G = H \circ G$ (mod H)
$P432 = P23 \wedge \tilde{2}$	$P4_232 = P23 \circ P4_232$ (mod $P23$)
$F432 = F23 \wedge \tilde{2}$	$F4_132 = F23 \circ F4_132$ (mod $F23$)
$I432 = I23 \wedge \tilde{2}$	$P4_332 = P2_13 \circ P4_332$ (mod $P2_13$)
$P\bar{4}3m = P23 \wedge \tilde{m}$	$P4_132 = P2_13 \circ P4_132$ (mod $P2_13$)
$F\bar{4}3m = F23 \wedge \tilde{m}$	$I4_132 = I2_13 \circ I4_132$ (mod $I2_13$)
$I\bar{4}3m = I23 \wedge \tilde{m}$	$P\bar{4}3n = P23 \circ P\bar{4}3n$ (mod $P23$)
$Pm3m = Pm3 \wedge \tilde{2}$	$F\bar{4}3c = F23 \circ F\bar{4}3c$ (mod $F23$)
$Fm3m = Fm3 \wedge \tilde{2}$	$I\bar{4}3d = I2_13 \circ I\bar{4}3d$ (mod $I2_13$)
$Im3m = Im3 \wedge \tilde{2}$	$Pn3n = Pn3 \circ Pn3n$ (mod $Pn3$)
	$Pm3n = Pm3 \circ Pm3n$ (mod $Pm3$)
	$Pn3m = Pn3 \circ Pn3m$ (mod $Pn3$)
	$Fm3c = Fm3 \circ Fm3c$ (mod $Fm3$)
	$Fd3m = Fd3 \circ Fd3m$ (mod $Fd3$)
	$Fd3c = Fd3 \circ Fd3c$ (mod $Fd3$)
	$Ia3d = Ia3 \circ Ia3d$ (mod $Ia3$)

Note: The symmorphic cubic space groups $Fm3$, $Im3$, $Pm3$, $P23$, $I23$, $F23$ and the non-symmorphic ones $Ia3$, $Pa3$, $Fd3$, $I2_13$, $P2_13$, $Pn3$, with whose 1D complex IRs are associated the minor quasisymmetry groups, are not considered here because, in these cases, the identification of the appropriate normal subgroups H is facilitated by collecting all the elements of G contained in the various conjugate classes in the chosen 1D complex IR with which the character +1 is associated.

3. The *P*-symmetry groups and their extensions

Zamorzaev (1967) introduced the concept of P-symmetry and classified groups as major, minor and intermediate. Let us recall the essentials of the so-called geometric approach to the classification of P-symmetries: To every point of a geometric figure we assign at least one of the indices 1, 2, ..., p and we use the term P-symmetry transformation to denote an isometric transformation of the figure, which transforms each point of the figure with index i into a point with index $k_i \ni$ the permutation of the indices $\begin{pmatrix} 1 & 2 & \dots & p \\ k_1 & k_2 & \dots & k_p \end{pmatrix} \in P$. We shall call a group of P-symmetry transformations a complete P-symmetry group if the group p_1 of permutations of indices involved in the transformation of the group coincides with P. Such groups are divided into major, minor and intermediate groups when the subgroups of the permutations $Q = G \cap P$ coincide with P, consist of identity transformation or are a non-trivial subgroup of P, respectively.

As already explained, the idea of P-symmetry has been extended and generalized by various authors in various ways. Zamorzaev & Palistrant (1980) and Koptsik (1980*a*) developed a geometric approach to the classification of P symmmetries by employing a vector interpretation of the P-symmetries and suggested a method of constructing 122 special types of 4D crystallographic point symmetry groups with a particular 3D plane in the form of symmetry and antisymmetry point groups.

The applications of generalized colour symmetry and the interesting features of n-dimensional crystallography have led to a complete derivation of the p'-symmetry space groups $G_3^{p'}$ for $p = 3,4,6$ (Palistrant, 1980), which, along with the classical Fedorov groups and their generalizations with simple and double antisymmetry, together with P-symmetry groups, was used in the study of 5D crystallographic symmetry groups with a special 3D plane (G_{53}). Palistrant (1981) also made a complete review of the crystallographic

* Throughout this paper, elements in the respective conjugate classes of the space groups are expressed in point-symmetry operation only, dropping the corresponding translational symmetry. These elements should not, however, be misunderstood as simple point-group operations. The suffixes j,m,p used in denoting the elements in the respective conjugate classes stand for one or more of the axes $j = 1,2,3,4$; $m = x,y,z$; $p = a,b,c,d,e,f$.

† The coset representative C_{2a} actually stands for the element $(C_{2a}/000)$.

‡ 2 denotes a space group of the same order as that of the point group 2 with the elements E, $(C_{2a}/000)$.

§ In this case, the coset representative C_{2a} stands for the element $(C_{2a}/\frac{1}{4}\frac{1}{4}\frac{1}{4})$.

point groups of the 32 crystallographic P-symmetries and this review, with an appropriate geometric interpretation of the indices and signs made it possible for him to describe all six-dimensional crystallographic point symmetry groups with a particular three-dimensional plane (G_{630}).

Recently, a geometric method for classifying the crystallographic P-symmetries which makes it possible to describe the essentially new categories of multi-dimensional symmetry groups by means of the P-symmetry groups was presented by Zamorzaev & Palistrant (1981). Shubnikov & Koptsik (1974) and Koptsik (1975) have shown that the interchange of the operators $1' \leftrightarrow 1^*$ places the magnetic and phase-symmetry groups in one-to-one correspondence allowing these magnetic and phase-symmetry groups to be considered physically different interpretations of the colour P-symmetry group and the W_p-symmetry group. A method of defining the space-symmetry group of a model as a semi-direct product was also presented in the novel work of Koptsik (1975, 1980*a*).

It must be emphasized that the P-symmetry groups $G^{(p)}$ are the special case of the wreath product $G^{(W_p)} \subseteq PW \supseteq G$ and that the *IR*s of the generating groups G do not cover all the categories of the $G^{(p)}$ (Koptsik, 1980*a*,*b*,*c*).

4. Construction of minor quasisymmetry space groups as semi-direct and quasi semi-direct products

The fundamental quasisymmetry theorem of Zamorzaev (1967) is taken as defining the concept of major, minor and intermediate quasisymmetry groups. Any symmorphic space group G can be written as the semi-direct product: $G = S \wedge T$ and through the results of Krishnamurty *et al.* (1978*a*), § 2, one obtains the different types of quasisymmetry groups G' generated by G, depending upon the nature of the constituent quasisymmetry groups S' and T' generated by the appropriate normal divisor S and the subgroup T in the semi-direct product $G' = S' \wedge T'$. On the other hand, one can obtain the corresponding quasisymmetry groups with the non-symmorphic space groups as generators invoking Krishnamurty *et al.* (1980). Construction of minor quasisymmetry space groups only is undertaken in this paper, since these groups only can be associated with the IRs of the respective generator groups. The method of construction is exemplified below.

Case 1: *Symmorphic cubic space groups*

As an example the group $F432$ is illustrated for the considered boundary condition, the relevant portion of the character table of which is given in Table 4. From Table 1, $F432 = F23 \wedge \tilde{2}$. Let us consider the group $F23$. For the cubic space group $F23$, the space group $\tilde{F222}$ is a normal subgroup of index 3 and $F23 = F222 \wedge \tilde{3}$. The group $F222'$: $F222\ I$ is a major/minor group with $F222$ as generator and with $\{I\}$ as the permutation group.* Also the group $\tilde{3}^{(3)}$: EI; C_{31}^+ (123); C_{31}^- (132) is a minor quasisymmetry group with the group $\tilde{3}$ consisting of elements E, C_{31}^+, C_{31}^- as generator and with I, (123), (132) as the permutation group. The semi-direct product $F222' \wedge \tilde{3}^{(3)}$: EI; $16C_{3j}^+$ (123); $6C_{2m}$; $16C_{3j}^-$ (132); $6C_{2m}$; $6T$; $6C_{2m}$; $16C_{3j}^-$ (132); $6C_{2m}$; $16C_{3j}^+$ (123); T_{123} is a full minor quasisymmetry group with $F23$ as generator and with A_3 as the permutation group. Denote this group as $F23^{(3)}$. Also, the group $\tilde{2}^{(2)}$: EI; C_{2a} (13) can be seen to be a minor group with $\tilde{2}$ as the generator and P_2: I, (13) as the permutation group. Hence, by Theorem 1 of Krishnamurty *et al.* (1978*a*), the semi-direct product $F23^{(3)} \wedge \tilde{2}^{(2)}$ is a full minor quasisymmetry group with $F432$ as generator and P_3 as the permutation group. We shall denote this group by $F432''$. The minor quasisymmetry groups obtained for the rest of the symmorphic cubic space groups are tabulated in Tables 6 and 7.

Case 2: *Non-symmorphic space groups*

To illustrate the case of non-symmorphic space groups, consider the cubic space group $Fd3m$. From Table 1 we have $Fd3m = Fd3 \circ Fd3m$ (mod $Fd3$). For the non-symmorphic space group $Fd3$, the non-symmorphic groups $Fddd$: E; $4i$; $12C_{2m}$; $24\sigma_m$; $6T$; $12C_{2m}$; $4i$; T_{123} and $Fdd2$: E; $12C_{2m}$; $6T$; $12C_{2m}$; T_{123} from normal subgroups† of index 3 and index 6, respectively. The group $Fd3$ can be expressed as $Fd3 = Fddd \circ Fd3$ (mod $Fddd$) and $Fd3 = Fdd2 \circ Fd3$ (mod $Fdd2$). The group $Fdd2'$: EI; $12C_{2m}I$; $6TI$; $12C_{2m}I$; $T_{123}I$ is a major/minor group with $Fdd2$ as generator. The group $Fd3^{(6)}$ (mod $Fdd2$): EI; S_{61}^+ (123456); C_{31}^+ (135) (246); i (14) (25) (36); C_{31}^- (153) (264); S_{61}^- (165432) is a minor group with $Fd3$ (mod $Fdd2$) as generator. The quasi semi-direct product of these groups $Fdd2' \circ Fd3^{(6)}$ (mod $Fdd2$): EI; $16S_{6j}^+$ (123456); $16S_{6j}^+$ (123456); $16C_{3j}^+$ (135) (246); $16C_{3j}^+$ (135) (246); $8i$ (14) (25) (36); $24\sigma_m$ (14) (25) (36); $16C_{6j}^-$ (153) (264); $16C_{3j}^-$ (153) (264); $16S_{6j}^-$ (165432); $16S_{6j}^-$ (165432); $12C_{2m}I$; $12C_{2m}I$; $6TI$; $T_{123}I$ is a minor quasisymmetry group with $Fd3$ as generator. Denote this group $Fd3^{(6)}$. Similarly, the quasi semi-direct product of the groups $Fddd'$ and $Fd3^{(3)}$ (mod $Fddd$) consisting of elements: EI; $16C_{3j}^-$ (123); $16C_{3j}^-$ (123); $16S_{6j}^+$ (123); $16S_{6j}^+$ (123); $16S_{6j}^-$ (132); $16S_{6j}^-$ (132);

* This group, however, should not be misunderstood as the Shubnikov space group $F222'$ associated with one of the 1D alternating IRs of the group $F222$.

† The actual normal subgroups may be either the groups $Fddd$, $Fdd2$ or groups just isomorphic to them in some non-standard setting.

$16C_{3j}^{+}$ (132); $16C_{3j}^{+}$ (132); $4iI$; $12C_{2m}I$; $24\sigma_m I$; $6TI$; $12C_{2m}I$; $4iI$; $T_{123}I$ also forms a minor group with $Fd3$ as generator and A_3 as the permutation group. Call this group $Fd3^{(3)}$.

With the group formed by the coset representative in the factor group $Fd3m/Fd3$: (E; C_{2a}) as generator, the group EI; C_{2a} (13) $= Fd3m^{(2)}$ (mod $Fd3$) can be seen to be a minor group with P_2 as the permutation group. The quasi semi-direct product: $Fd3^{(3)} \circ Fd3m^{(2)}$ (mod $Fd3$) forms a minor group with $Fd3m$ as generator which we denote by ${}^1Fd3m''$. Similarly, the quasi semi-direct product of the minor group $Fd3^{(6)}$ with the minor group $Fd3m^{(2)}$ (mod $Fd3$) also forms a minor group with $Fd3m$ as generator and it is denoted by the symbol ${}^2Fd3m''$. For the rest of the non-symmorphic cubic space groups, the results obtained are tabulated in Tables 6 and 8.

5. Association of the minor quasisymmetry cubic space groups with the IRs of the generator groups

It is well known that the irreducible representations of the space groups can be obtained from those of the AIRs (G^{k}'s) of the little groups in conjunction with the solvability property (Raghavacharyulu, 1961) using the composition series (Lomont, 1959). The association of the obtained minor quasisymmetry groups with the 1D complex and 2D real IRs of the generator groups is completed in this section with the help of the little groups and their 1D AIRs.

Case (i): *Non-degenerate IRs*

In the case of the non-degenerate IRs of the space groups, it is observed that the little groups (L) always coincide with the generating space group G itself, and the kernels (K) coincide with the chosen normal subgroup H. As the IRs of the factor group $G/H \cong L/K$ engender those of the IRs of the same nature as G, the properly chosen normal subgroup H itself facilitates the required IR of G, which is to be engendered.

The relevant portion of the character table of the symmorphic space group $F23$ for the chosen boundary condition is provided in Table 2. From § 4, the group $F23^{(3)} = F222' \wedge \tilde{3}^{(3)}$. For the group $F23$, the group $F222$ forms a normal subgroup of index 3 and the 1D complex IRs of the factor group $F23/F222$ engender the complex IRs ${}^1E$ and ${}^2E$ of $F23$. Hence we associate $F23^{(3)}$ with the IR ${}^1E$ of $F23$. For non-symmorphic space groups also, as far as the association of minor groups with the non-degenerate IRs, similar results to the case of symmorphic groups are obtained. For example, consider the group $Fd3$. It is seen that the group $Fddd$ forms a normal subgroup of index 3 to $Fd3$ and the 1D complex IR ${}^1E$ of $Fd3/Fddd$ engender the 1D complex IR ${}^1E_1$ of $Fd3$. Hence we associate the minor group $Fd3^{(3)}$: $Fddd' \circ Fd3^{(3)}$ (mod $Fddd$) obtained in § 4 with the 1D complex IR ${}^1E_1$ of the group $Fd3$. By a similar argument the minor group $Fd3^{(6)}$: $Fdd2' \circ Fd3^{(6)}$ (mod $Fdd2$) can be associated with the 1D complex IR ${}^1E_2$ of $Fd3$. The relevant portion of the character table of $Fd3$ is shown in Table 3.

Case (ii): *Degenerate* (2*D*) *IRs*

In the case of 2D real IRs it is observed that the normal subgroup H in the considered semi-direct product as well as in the quasi semi-direct product coincide with the little group (L) and the 1D complex IRs of the normal subgroup induce the appropriate 2D real IRs of the considered generator group. This is illustrated below with the cubic space group $F432 = F23 \wedge \tilde{2}$. It can be seen that $F23$ is a little group of $F432$ and the 1D complex IR ^{1}E of $F23$ is an AIR that induces the 2D real IR E of $F432$ (Tables 2 and 4). The minor group $F23^{(3)}$ generated with $F23$ is associated

Table 2. *Relevant portion of the character table of F*23

$F23$	E	16 C_{3j}^{+}	6 C_{2m}	16 C_{3j}^{-}	6 C_{2m}	6 T	6 C_{2m}	16 C_{3j}^{-}	6 C_{2m}	16 C_{3j}^{+}	1 T
${}^1E$	1	ω	1	ω^2	1	1	1	ω^2	1	ω	1
${}^2E$	1	ω^2	1	ω	1	1	1	ω	1	ω^2	1

Table 3. *Relevant portion of the character table of Fd*3

$Fd3$	E	16 C_{3j}^{-}	16 C_{3j}^{-}	4 i	16 S_{6j}^{+}	16 S_{6j}^{+}	12 C_{2m}	24 σ_m	6 T	12 C_{2m}	16 S_{6j}^{-}	16 S_{6j}^{-}	4 i	16 C_{3j}^{+}	16 C_{3j}^{+}	1 T
${}^1E_1$	1	ω	ω	1	ω	ω	1	1	1	1	ω^2	ω^2	1	ω^2	ω^2	1
${}^2E_1$	1	ω^2	ω^2	1	ω^2	ω^2	1	1	1	1	ω	ω	1	ω	ω	1
${}^1E_2$	1	ω	ω	-1	$-\omega$	$-\omega$	1	-1	1	1	$-\omega^2$	$-\omega^2$	-1	ω^2	ω^2	1
${}^2E2$	1	ω^2	ω^2	-1	$-\omega^2$	$-\omega^2$	1	-1	1	1	$-\omega$	$-\omega$	-1	ω	ω	1

Table 4. *Relevant portion of the character table of F*432

$F432$	E	32 C_{3j}^{+}	24 C_{4m}^{+}	12 C_{2p}	6 C_{2m}	12 C_{2m}	6 T	24 C_{2p}	6 C_{2m}	12 C_{2p}	24 C_{4m}^{-}	32 C_{3j}^{-}	1 T
E	2	-1	0	0	2	2	2	0	2	0	0	-1	2

Table 5. *Relevant portion of the character table of Fd3m*

*Fd*3*m*	E	12 σ_{dp}	32 C_{3j}^{+}	12 C_{2m}	48 $S_{4m}^{\pm}$	4 i	12 C_{2p}	32 S_{6j}^{+}	24 σ_m	48 $C_{4m}^{\pm}$	24 σ_{dp}	12 C_{2m}	24 C_{2p}	6 T	12 σ_{dp}	32 C_{3j}^{-}	4 i	12 C_{2p}	32 S_{6j}^{-}	1 T
E_1	2	0	−1	2	0	2	0	−1	2	0	0	2	0	2	0	−1	2	0	−1	2
E_2	2	0	−1	2	0	−2	0	1	−2	0	0	2	0	2	0	−1	−2	0	1	2

Table 6. *Minor quasisymmetry cubic space groups associated with the* 1D *complex IRs of the cubic space groups containing* 1D *complex IRs*

Cubic space group G	Number of pairs of 1D complex IRs of G	Minor quasisymmetry groups associated with the pairs of 1D complex IRs of G
$P23$	2	$P23^{(3)}$; $P23^{(6)}$
$F23$	1	$F23^{(3)}$
$I23$	2	$I23^{(3)}$; $I23^{(6)}$
$I2_13$	2	$I2_13^{(3)}$; $I2_13^{(6)}$
$P2_13$	2	$P2_13^{(3)}$; $P2_13^{(6)}$
$Pm3$	4	$Pm3^{(3)}$; ${}^1Pm3^{(6)}$; ${}^2Pm3^{(6)}$; ${}^3Pm3^{(6)}$
$Im3$	4	$Im3^{(3)}$; ${}^1Im3^{(6)}$; ${}^2Im3^{(6)}$; ${}^3Im3^{(6)}$
$Pn3$	4	$Pn3^{(3)}$; ${}^1Pn3^{(6)}$; ${}^2Pn3^{(6)}$; ${}^3Pn3^{(6)}$
$Fm3$	2	$Fm3^{(3)}$; $Fm3^{(6)}$
$Fd3$	2	$Fd3^{(3)}$; $Fd3^{(6)}$
$Pa3$	2	$Pa3^{(3)}$; $Pa3^{(6)}$
$Ia3$	4	$Ia3^{(3)}$; ${}^1Ia3^{(6)}$; ${}^2Ia3^{(6)}$; ${}^3Ia3^{(6)}$

Notes: In column 1, the cubic space groups G containing pairs of 1D complex IRs is given in International notation. In column 2 is given the number of pairs of 1D complex IRs contained in G for the considered boundary condition. In column 3, the minor groups obtained as semi-direct or quasi semi-direct products which are associated with the pairs of 1D complex IRs are tabulated.

The minor quasisymmetry groups associated with the 1D complex IRs of the cubic space groups are given International symbols (developed in respect of the colour groups) since these groups denote the polychromatic space groups with colour value given by the number indicated in brackets.

Table 7. *Minor quasisymmetry cubic space groups associated with the* 2D *real IRs of the symmorphic cubic space groups*

Symmorphic cubic space group G	2D IR Γ of G	Little group L (or $\cong L$)	Minor quasisymmetry group associated with the 2D IR Γ of G
$P432$	E_1	$P23$	${}^1P432'' = P23^{(3)} \wedge \mathfrak{2}^{(2)}$
	E_2	$P23$	${}^2P432'' = P23^{(6)} \wedge \mathfrak{2}^{(2)}$
$F432$	E	$F23$	$F432'' = F23^{(3)} \wedge \mathfrak{2}^{(2)}$
$I432$	E_1	$I23$	${}^1I432'' = I23^{(3)} \wedge \mathfrak{2}^{(2)}$
	E_2	$I23$	${}^2I432'' = I23^{(6)} \wedge \mathfrak{2}^{(2)}$
$P\bar{4}3m$	E_1	$P23$	${}^1P\bar{4}3m'' = P23^{(3)} \wedge \tilde{m}^{(2)}$
	E_2	$P23$	${}^2P\bar{4}3m'' = P23^{(6)} \wedge \tilde{m}^{(2)}$
$F\bar{4}3m$	E	$F23$	$F\bar{4}3m'' = F23^{(3)} \wedge \tilde{m}^{(2)}$
$I\bar{4}3m$	E_1	$I23$	${}^1I\bar{4}3m'' = I23^{(3)} \wedge \tilde{m}^{(2)}$
	E_2	$I23$	${}^2I\bar{4}3m'' = I23^{(6)} \wedge \tilde{m}^{(2)}$
$Pm3m$	E_1	$Pm3$	${}^1Pm3m'' = Pm3^{(3)} \wedge \mathfrak{2}^{(2)}$
	E_2	$Pm3$	${}^2Pm3m'' = {}^1Pm3^{(6)} \wedge \mathfrak{2}^{(2)}$
	E_3	$Pm3$	${}^3Pm3m'' = {}^2Pm3^{(6)} \wedge \mathfrak{2}^{(2)}$
	E_4	$Pm3$	${}^4Pm3m'' = {}^3Pm3^{(6)} \wedge \mathfrak{2}^{(2)}$
$Fm3m$	E_1	$Fm3$	${}^1Fm3m'' = Fm3^{(3)} \wedge \mathfrak{2}^{(2)}$
	E_2	$Fm3$	${}^2Fm3m'' = Fm3^{(6)} \wedge \mathfrak{2}^{(2)}$
$Im3m$	E_1	$Im3$	${}^1Im3m'' = Im3^{(3)} \wedge \mathfrak{2}^{(2)}$
	E_2	$Im3$	${}^2Im3m'' = {}^1Im3^{(6)} \wedge \mathfrak{2}^{(2)}$
	E_3	$Im3$	${}^3Im3m'' = {}^2Im^{(6)} \wedge \mathfrak{2}^{(2)}$
	E_4	$Im3$	${}^4Im3m'' = {}^3Im3^{(6)} \wedge \mathfrak{2}^{(2)}$

with the 1D complex IR ${}^1E$ of $F23$ and as this 1D complex IR ${}^1E$ of $F23$ in turn induces the 2D IR E of $F432$, we associated $F432''$ with the 2D real IR E of $F432$.

Similarly, in the case of the non-symmorphic space group $Fd3m$ (Table 5), the group $Fd3$ can be seen to be a subgroup of index 2 and the 1D complex IR ${}^1E_1$ of $Fd3$ is an AIR that induces the 2D IR E_1 of $Fd3m$. From what has been discussed earlier, the minor group associated with the 1D complex IR ${}^1E$ of $Fd3$ is $Fd3^{(3)}$. But this 1D IR ${}^1E$ of $Fd3$ induces the 2D IR E_1 of $Fd3m$. Hence, we associate the minor group ${}^1Fd3m''$: $Fd3^{(3)} \circ Fd3m^{(2)}$ (mod $Fd3$) with the IR E_1 of $Fd3m$. By a similar argument the other minor group ${}^2Fd3m''$: $Fd3^{(6)} \circ Fd3m^{(2)}$ (mod $Fd3$) can be associated with the 2D IR E_2 of $Fd3m$. The results obtained in the case of other cubic space groups are tabulated in Tables 6, 7 and 8.

Notes to Tables 2–5

In Tables 2–5, the numbers given in different columns indicate the order of the various conjugate classes, and the element placed under each number denotes the representative of the respective class of the group G under consideration.

The character tables of all the cubic space groups are constructed by the authors on the basis of the method suggested by Raghavacharyulu (1961) and Bradley & Cracknell (1972), for the boundary condition $T_x^2 = T_y^2 = T_z^2 = E$. For want of space, only the relevant portions of those required for our discussion in §§ 4 and 5 are furnished here.

The symbols j, m, p denote the respective crystallographic axes, they stand for one or more of the following axes: $m = x,y,z$; $j = 1,2,3,4$ and $p = 1,2,3,4,5,6$.

Notes to Tables 7 *and* 8

In column 1 of Table 7, the symmorphic cubic space group G and, in that of Table 8, the non-symmorphic cubic space group G, containing a 2D IR, are given in International notation. In column 2 is given the actual 2D IR Γ of G to which a minor quasisymmetry group is associated and in column 3 is indicated the little

Table 8. *Minor quasisymmetry cubic space groups associated with the* 2D *real IRs of the non-symmorphic cubic space groups*

Non-symmorphic cubic space group G	2D IR Γ or G	Little group L (or L)	Minor quasisymmetry group associated with the 2D IR Γ of G
$Pn3n$	E_1	$Pn3$	$^{1}Pn3n'' = Pn3^{(3)} \circ Pn3n^{(2)}$ (mod $Pn3$)
	E_2	$Pn3$	$^{2}Pn3n'' = {}^{1}Pn3^{(6)} \circ Pn3n^{(2)}$ (mod $Pn3$)
$Fm3c$	E_1	$Fm3$	$^{1}Fm3c'' = Fm3^{(3)} \circ Fm3c^{(2)}$ (mod $Fm3$)
	E_2	$Fm3$	$^{2}Fm3c'' = Fm3^{(3)} \circ Fm3c^{(2)}$ (mod $Fm3$)
$F\bar{4}3c$	E_1	$F23$	$F\bar{4}3c'' = F23^{(6)} \circ F\bar{4}3c^{(2)}$ (mod $F23$)
$F4_132$	E_1	$F23$	$F4_132'' = F23^{(3)} \circ F4_132^{(2)}$ (mod $F23$)
$I\bar{4}3d$	E_1	$I2_13$	$^{1}I\bar{4}3d'' = I2_13^{(3)} \circ I\bar{4}3d^{(2)}$ (mod $I2_13$)
	E_2	$I2_13$	$^{2}I\bar{4}3d'' = I2_13^{(6)} \circ I\bar{4}3d^{(2)}$ (mod $I2_13$)
$P4_332$	E_1	$P2_13$	$^{1}P4_332'' = P2_13^{(3)} \circ P4_332^{(2)}$ (mod $P2_13$)
	E_2	$P2_13$	$^{2}P4_332'' = P2_13^{(6)} \circ P4_332^{(2)}$ (mod $P2_13$)
$P4_132$	E_1	$P2_13$	$^{1}P4_132'' = P2_13^{(3)} \circ P4_132^{(2)}$ (mod $P2_13$)
	E_2	$P2_13$	$^{2}P4_132'' = P2_13^{(6)} \circ P4_132^{(2)}$ (mod $P2_13$)
$Pm3n$	E_1	$Pm3$	$^{1}Pm3n'' = Pm3^{(3)} \circ Pm3n^{(2)}$ (mod $Pm3$)
	E_2	$Pm3$	$^{2}Pm3n'' = {}^{1}Pm3^{(6)} \circ Pm3n^{(2)}$ (mod $Pm3$)
	E_3	$Pm3$	$^{3}Pm3n'' = {}^{2}Pm3^{(6)} \circ Pm3n^{(2)}$ (mod $Pm3$)
$Fd3m$	E_1	$Fd3$	$^{1}Fd3m'' = Fd3^{(3)} \circ Fd3m^{(2)}$ (mod $Fd3$)
	E_2	$Fd3$	$^{2}Fd3m'' = Fd3^{(6)} \circ Fd3m^{(2)}$ (mod $Fd3$)
$Fd3c$	E_1	$Fd3$	$^{1}Fd3c'' - Fd3^{(3)} \circ Fd3c^{(2)}$ (mod $Fd3$)
	E_2	$Fd3$	$^{2}Fd3c'' = Fd3^{(6)} \circ Fd3c^{(2)}$ (mod $Fd3$)
$Ia3d$	E_1	$Ia3$	$^{1}Ia3d'' = Ia3^{(3)} \circ Ia3d^{(2)}$ (mod $Ia3$)
	E_2	$Ia3$	$^{2}Ia3d'' = {}^{1}Ia3^{(6)} \circ Ia3d^{(2)}$ (mod $Ia3$)
	E_3	$Ia3$	$^{3}Ia3d'' = {}^{2}Ia3^{(6)} \circ Ia3d^{(2)}$ (mod $Ia3$)
$P\bar{4}3n$	E_1	$P23$	$^{1}P\bar{4}3n'' = P23^{(3)} \circ P\bar{4}3n^{(2)}$ (mod $P23$)
	E_2	$P23$	$^{2}P\bar{4}3n'' = P23^{(6)} \circ P\bar{4}3n^{(2)}$ (mod $P23$)
$P4_232$	E_1	$P23$	$^{1}P4_232'' = P23^{(3)} \circ P4_232^{(2)}$ (mod $P23$)
	E_2	$P23$	$^{2}P4_232'' = P23^{(6)} \circ P4_232^{(2)}$ (mod $P23$)
$I4_132$	E_1	$I2_13$	$^{1}I4_132'' = I2_13^{(3)} \circ I4_132^{(2)}$ (mod $I2_13$)
	E_2	$I2_13$	$^{2}I4_132'' = I2_13^{(6)} \circ I4_132^{(2)}$ (mod $I2_13$)
$Pn3m$	E_1	$Pn3$	$^{1}Pn3m'' = Pn3^{(3)} \circ Pn3m^{(2)}$ (mod $Pn3$)
	E_2	$Pn3$	$^{2}Pn3m'' = {}^{1}Pn3^{(6)} \circ Pn3m^{(2)}$ (mod $Pn3$)
	E_3	$Pn3$	$^{3}Pn3m'' = {}^{2}Pn3^{(6)} \circ Pn3m^{(2)}$ (mod $Pn3$)
	E_4	$Pn3$	$^{4}Pn3m'' = {}^{3}Pn3^{(6)} \circ Pn3m^{(2)}$ (mod $Pn3$)

group L (or the group $\cong L$), the 1D AIR of which induces the 2D IR Γ of G.

The minor group associated with the 2D IR Γ of G—and thus denoted as G''—is given in the last column as the semi-direct/quasi semi-direct product of two minor groups: the first one a minor group associated with the 1D AIR of the little group L (which happens to be the normal subgroup H in the semi-direct/quasi semi-direct product of G) that induces the 2D IR Γ of G (in the notation developed in Table 6) and the latter also a minor group which can be viewed as a double-coloured group generated by the corresponding symmorphic space group T or the non-symmorphic space group G (mod H) in some non-standard setting which depends upon the groups G and H in the semi-direct/quasi semi-direct products, respectively.

6. Discussion

The minor quasisymmetry cubic space groups constructed as semi-direct products and quasi semi-direct products and associated with the 1D complex IRs of the cubic space groups discussed here are nothing but the polychromatic space groups in which each colour may represent a transformable physical property. Also, the 1191 magnetic space groups associated with distinct alternating IRs of the Fedorov space groups can be seen to be particular realizations of the minor quasisymmetry space groups with a suitable permutation group P_2.

The method of constructing quasisymmetry groups indicated in § 4 and their association with the 1D complex and 2D real IRs of the cubic space groups explained in § 5 can be extended to the rest of the synogonies, and results can be obtained in an analogous manner. In fact, this method can be extended for any other boundary condition.

The concept of semi-direct product and quasi semi-direct product has gained sufficient importance in recent years (Altmann, 1963*a*,*b*; Shubnikov & Koptsik, 1974) and the physical significance of an AIR that induces the degenerate IR of a generator group is already appreciated (Krishnamurty, Prasad & Rama Mohana Rao, 1978*b*). Also it is easier to deal with a 1D IR than with a degenerate IR directly.

Several possible applications of the *P*-symmetry groups have been mentioned (Zamorzaev, 1967; Rama Mohana Rao, 1980). One of these is the use of coloured symmetry space groups in the derivation and description of similarity symmetry space groups as has been done in the case of coloured symmetry point groups. Also, the idea of *P*-symmetry may be useful in the description of stem and layer symmetry groups in higher-dimensional space. An example of physical applications is that of the magnetic symmetry proposed by Naish (1963). The multiplicative groups constructed by Naish are nothing but the quasisymmetry groups. In describing the magnetic symmetry of screw (helicoidal) structures, the periods of which do not coincide with the periods of the atomic structures, the traditional magnetic groups (Shubnikov groups) are not suitable, and these quasisymmetry groups are found to be of much use.

The possible stationary magnetic moment configurations in crystals cannot be completely described by the classical and Shubnikov groups. Only the multi-colour group apparatus of the *P*-symmetry structure alone can adequately cover all the magnetic properties of crystals. A concrete example of this was provided with the help of the antiferromagnetic structure of hematite in the range of $253 < T < 948$ K by Koptsik & Kuzhukeev (1972).

Construction of minor quasisymmetry groups and their association with the 1D complex and 2D real IRs only are dealt with, in this paper, for, in the case of higher-dimensional IRs ($d > 2$), the construction of minor quasisymmetry groups and their association with the degenerate IRs with the help of the 1D AIRs cannot be carried out simultaneously through the present technique.

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