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Quasi-symmetry and double point groups

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Abstract. The concept of quasi-semi-direct products is explored in order to construct quasi-symmetry groups generated by the double point groups. The minor quasi-symmetry groups so obtained are associated with the irreducible representations of the generator groups using the ideas of little groups and their allowable irreducible representations. The double point groups C_4 and D_3 are illustrated, and the results are tabulated.

1. Introduction

Tavger and Zaitsev (1956) and Bhagavantam and Pantulu (1964) derived the 58 magnetic point groups, and their association with the 58 distinct one-dimensional alternating representations of the crystallographic single point groups, using representation theory, was accomplished by Indenbom (1959), Niggli and Wondratschek (1960), Bertaut (1968) and Krishnamurty and Gopalakrishnamurty (1969). The introduction of anti-symmetry and its interpretation as two-colour symmetry (Shubnikov 1951) has led to the idea of polychromatic symmetry (Belov and Tarkhova 1956, Indenbom et al 1960). Zamorzaev (1967) introduced the concept of quasi-symmetry (P-symmetry) and brought all the earlier generalisations of anti-symmetry and colour symmetry, including crypto-symmetry (Niggli and Wondratschek 1960), into its fold. Krishnamurty et al (1978a) developed an alternative method of obtaining the quasisymmetry (P-symmetry) groups using the concept of semi-direct products. These authors also described a new method of associating the minor quasi-symmetry groups with the irreducible representations (IRs) of the generator groups using the ideas of little groups and their allowable irreducible representations (AIRs), which are different from those of Niggli and Wondratschek (1960). The quasi-symmetry groups generated by single point groups are available in the literature, though they are not always termed quasi-symmetry groups. For example, they are tabulated as crypto-symmetry groups by Niggli and Wondratschek (1960), and some of them appeared in the literature as magnetic point groups (or magnetic variants) of single point groups.

When a system has integral angular momentum, its symmetry group is SO(3) or a subgroup of it. However, spinor wavefunctions of particles with half-odd integral spin angular momenta are multiplied by -1 after a rotation through 2π , and return to their original values only after a rotation through 4π . This means, in the language of group theory, that the symmetry of the wavefunction is governed by the IRs of the corresponding double group rather than those of the original symmetry group. Rudra and Sikdar (1977) have tabulated the Clebsch-Gordan coefficients of the magnetic double point groups which have wider applications. Recently, for double point groups,

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Krishnamurty *et al* (1978b) have developed a method of constructing polychromatic groups (with R_n , n = 3, 4, 6, 8 or 12) by considering subgroups of various indices and associating them with the one-dimensional complex representations of the generating double point groups, using the representation theory. These magnetic double point groups and polychromatic groups generated by double point groups are nothing but quasi-symmetry groups with double point groups as their generators. One can easily see that the isodynamic groups introduced by Altmann (1967) in the discussion on the symmetries of non-rigid molecules are also quasi-symmetry groups. While discussing the symmetry of the dimethylacetylene molecule, where the internal rotation is effectively free, Altmann (1967) has explicitly shown the necessity of introducing the double group of the isodynamic group $(\tilde{\mathscr{C}}_3^I)$ instead of the isodynamic group \mathscr{C}_3^I . Thus the quasi-symmetry groups generated by the double point groups are of physical interest.

In the present paper, a general method of constructing quasi-symmetry groups as quasi-semi-direct products (Shubnikov and Koptsik 1974) is presented. Instead of using the semi-direct product, as was done in our earlier paper (Krishnamurty *et al* 1978a), we have used the quasi-semi-direct product in the construction, since none of the crystallographic double point groups can be expressed as the semi-direct product of two of its subgroups, except the double point group C_3 . Table 1 gives the 32 crystallographic double point groups as quasi-semi-direct products. The minor quasi-symmetry groups (Zamorzaev 1967) generated by the 32 crystallographic double point groups are associated with the IRS of these crystallographic double point groups using the ideas of little groups and their AIRS, as was done in Krishnamurty *et al* (1978a). As the quasi-symmetry groups which we have constructed and associated with the various IRS of the crystallographic double point groups are quite new and are not available in the literature as far as we know, we have given an extensive tabulation of the same in the present paper.

The definitions of quasi-product, minor, intermediate and major quasi-symmetry groups are given in § 2 for the sake of completeness. In § 3 the minor quasi-symmetry

| Double point group G | Normal subgroup H | Double point group G as quasi-semi-direct product $G = H \circ G \pmod{H}$ |
|-------------------------|----------------------|--|
| D ₂ | C ₂ | $\mathbf{D}_2 = \mathbf{C}_2 \circ \mathbf{D}_2 \pmod{\mathbf{C}_2}$ |
| C ₄ | C ₂ | $C_4 = C_2 \circ C_4 \pmod{C_2}$ |
| D_3 | C ₃ | $\mathbf{D}_3 = \mathbf{C}_3 \circ \mathbf{D}_3 \pmod{\mathbf{C}_3}$ |
| D_4 | C ₄ | $\mathbf{D_4} = \mathbf{C_4} \circ \mathbf{D_4} \pmod{\mathbf{C_4}}$ |
| | D_2 | $\mathbf{D}_4 = \mathbf{D}_2 \circ \mathbf{D}_4 \pmod{\mathbf{D}_2}$ |
| D ₆ | D_3 | $\mathbf{D}_6 = \mathbf{D}_3 \circ \mathbf{D}_6 \pmod{\mathbf{D}_3}$ |
| | C ₆ | $\mathbf{D}_6 = \mathbf{C}_6 \circ \mathbf{D}_6 \pmod{\mathbf{C}_6}$ |
| Т | D_2 | $\mathbf{T} = \mathbf{D}_2 \circ \mathbf{T} \pmod{\mathbf{D}_2}$ |
| 0 | Т | $O = T \circ O \pmod{T}$ |
| | D_2 | $O = D_2 \circ O \pmod{D_2}$ |

Table 1. Double point groups as quasi-semi-direct products.

The double point groups C_{2v} , S_4 , C_{3v} , C_{4v} , D_{2d} , C_{6v} , D_{3h} , T_d are omitted because they are isomorphic with those of the groups given above and hence can be easily dealt with. The groups D_{2h} , D_{3d} , D_{4h} , C_{4h} , D_{6h} , T_h , O_h are also omitted since they can be written as the direct product of those of the groups given above with the double group C_i , and hence they too can be easily disposed of.

groups obtained are associated with the IRs of the generating double point groups using the ideas of little groups and their AIRs. The notation for the considered quasi-semidirect product is adopted from Shubnikov and Koptsik (1974), and the nomenclature for the IRs of the crystallographic double point groups is mostly that of Bradley and Cracknell (1972).

2. Construction of quasi-symmetry groups as quasi-semi-direct products

Let H be any subgroup of a group G, and let

$$G = Hg_1 \cup Hg_2 \cup \ldots \cup Hg_s \tag{1}$$

be a decomposition of G into distinct cosets of H. Then G is called an extension of H, and g_1, g_2, \ldots, g_s are called coset representatives. $g_1 = h_1 = e$, the identity element for G. In addition let H be a normal subgroup of G, and let h_1, h_2, \ldots, h_m be the elements comprising H. If we introduce in the set $\{g_1, g_2, \ldots, g_s\}$ the law of reduced multiplication

$$g_j g_l = h_{jl,n} g_n = g_n \pmod{h_{jl,n}}, \qquad h_{jl,n} = h_1, h_2, \dots, h_m \in H, \quad g_n \in \{g_1, g_2, \dots, g_s\},$$

then the set $\{g_1, g_2, \ldots, g_s\}$ is a group by modulus and is denoted as $G(\mod H)$. Since the laws of multiplication in G and $G(\mod H)$ are different, in general, the group $G(\mod H)$ is not a subgroup of G. In particular, if all $h_{jl,n} = h_1 = e$, then the group $G(\mod H)$ is a subgroup of G. If $H \cap G(\mod H) = h_1 = g_1 = e \in G$, then an extension G of H may be constructed as the 'product' of the groups H and $G(\mod H)$ if we carry out 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 unite the results so obtained:

$$G = \{h_1g_1, \ldots, h_mg_1, h_1g_2, \ldots, h_mg_2, \ldots, h_1g_s, \ldots, h_mg_s\}.$$
 (2)

Since $G(\mod H)$ is not necessarily a subgroup of G, the extension (2) is called a 'quasi-product' (Shubnikov and Koptsik 1974), and we write the quasi-semi-direct product as $G = H \circ G(\mod H)$. The difference between the ordinary semi-direct product and quasi-semi-direct product is that in the former the second factor in the product is a subgroup of G, whereas in the latter it need not be.

The following fundamental quasi-symmetry theorem of Zamorzaev (1967) can be taken as defining the concepts of minor, major and intermediate quasi-symmetry groups.

Any group G of full P-symmetry is derivable from its generator S by the following steps: (i) search for normal subgroups, H and Q, of the groups S and P such that $S/H \approx P/Q$; (ii) carry out pairwise multiplication of sH and pQ, the corresponding classes with respect to the isomorphism; and (iii) combine the resulting products. This method gives the major, minor and intermediate quasi-symmetry groups generated by S corresponding to the following cases respectively: (a) Q = P (when H = S); (b) Q = e(when $S/H \approx P$); (c) Q is a non-trivial normal subgroup of P.

In the case of construction of quasi-symmetry groups with the help of quasi-semidirect products, we find that all the results cited and proved in § 2 of Krishnamurty *et al* (1978a) hold good for the quasi-semi-direct products also. One has simply to replace the groups S, T and S', T' by H, $G(\mod H)$ and H', $G'(\mod H)$ respectively, and the corresponding semi-direct product by the quasi-semi-direct product. For example, Krishnamurty *et al* (1978a) have proved that if $G = S \wedge T$, and if S' and T' are two quasi-symmetry groups with S and T as generators respectively, and if $G' = S' \wedge T'$, then G' is a quasi-symmetry group with G as generator. Now in a similar fashion we can prove that, if G is the quasi-semi-direct product of two groups H and $G(\mod H)$, i.e. $G = H \circ G(\mod H)$, and if H' and G'(\mod H) are two quasi-symmetry groups with H and $G(\mod H)$ as generators respectively, and if $G' = H' \circ G'(\mod H)$, then G' is a quasi-symmetry group with G as generator. For the sake of brevity we avoid the statements and proofs of all the results which one can have analogous to those given in § 2 of Krishnamurty *et al* (1978a).

3. Association of the minor quasi-symmetry groups with the IRS of the double point groups

In this section, construction of the minor quasi-symmetry groups is accomplished using the concept of quasi-semi-direct products, and association of the minor groups so obtained with the IRs of the generator groups is completed using the ideas of little groups and their AIRs (Krishnamurty *et al* 1978a). For non-degenerate IRs the group C_4 and for degenerate IRs the group D_3 are illustrated. The results obtained for all the IRs of the double point groups are given in tables 2 and 3.

| Double point group G (1) | Non-degenerate IR Γ of G (2) | Little group L (3) | Chosen normal subgroup H (4) | Quasi-symmetry minor group associated with the IR Γ of G (5) |
|--------------------------------------|------------------------------------|-----------------------------|--|--|
| $\overline{C_1}$ | Ā | C ₁ | Ĉ ₁ | $C_1' = \tilde{C}_1 \circ C_1^{(2)} \pmod{\tilde{C}_1}$ |
| C ₁ | A _u | Ci | C_1 | ${}^{1}C_{i}' = C_{1} \circ C_{i}^{(2)} \pmod{C_{1}}$ |
| | Āg | Ci | C_1^* | ${}^{2}C_{i}' = C_{1}^{*} \circ C_{i}^{(2)} \pmod{C_{1}^{*}}$ |
| | Ā | Ci | C_{1}^{**} | ${}^{3}C_{i}' = C_{1}^{**} \circ C_{i}^{(2)} \pmod{C_{1}^{**}}$ |
| C ₂ | В | C_2 | C_1 | $C'_2 = C_1 \circ C_2^{(2)} \pmod{C_1}$ |
| | ¹ Ē, ² Ē | C ₂ | $\mathbf{\tilde{C}}_1$ | $\mathbf{C}_2^{(4)} = \tilde{\mathbf{C}}_1 \circ \mathbf{C}_2^{(4)} \pmod{\tilde{\mathbf{C}}_1}$ |
| C _{1h} | A″ | C_{1h} | C ₁ | $C'_{1h} = C_1 \circ C^{(2)}_{1h} \pmod{C_1}$ |
| | ¹ Ē, ² Ē | C_{1h} | Č ₁ | $C_{1h}^{(4)} = \tilde{C}_1 \circ C_{1h}^{(4)} \pmod{\tilde{C}_1}$ |
| C_{2h} | Bg | C_{2h} | Ci | ${}_{2}^{1}C'_{2h} = C_{i} \circ C_{2h}^{(2)} \pmod{C_{i}}$ |
| | B _{1u} | C_{2h} | C ₂ | ${}_{2}C'_{2h} = C_2 \circ C_{2h}^{(2)} \pmod{C_2}$ |
| | B _{2u} | C_{2h} | C_{1h} | $C_{2h}' = C_{1h} \circ C_{2h}' \pmod{C_{1h}}$ |
| | E_{g}, E_{g} | C_{2h} | C_1^* | ${}^{1}C_{2h}^{(4)} = C_{1}^{*} \circ C_{2h}^{(4)} \pmod{C_{1}^{*}}$ |
| | E_{u}, E_{u} | C_{2h} | C_{1}^{**} | $^{2}C_{2h}^{(4)} = C_{1}^{**} \circ C_{2h}^{(4)} \pmod{C_{1}^{**}}$ |
| D_2 | B_1, B_2, B_3 | D_2 | C_2 | $D_2' = C_2 \circ D_2' \pmod{C_2}$ |
| C_{2v} | B_1, B_2 | C_{2v} | C_{1h} | $C'_{2v} = C_{1h} \circ C'_{2v} \pmod{C_{1h}}$ |
| _ | A ₂ | C_{2v} | C ₂ | ${}^{2}C'_{2v} = C_{2} \circ C_{2v}^{(2)} \pmod{C_{2}}$ |
| D_{2h} | A _u | D_{2h} | D_2 | $^{2}D_{2h} = D_{2} \circ D_{2h} \pmod{D_{2}}$ |
| | B_{1g}, B_{2g}, B_{3g} | D _{2h} | C _{2h} | $^{2}D_{2h}^{\prime} = C_{2h} \circ D_{2h}^{\prime} \pmod{C_{2h}}$ |
| ~ | B_{3u}, B_{2u}, B_{1u} | D _{2h} | C_{2V} | $D_{2h} = C_{2V} \circ D_{2h}^{(2)} \pmod{C_{2V}}$ |
| C_4 | B 12 | C ₄ | C_2 | $C'_4 = C_2 \circ C'_4 \pmod{C_2}$ |
| | 'E, "E | C ₄ | \mathbf{C}_1 | $C_4^{(4)} = C_1 \circ C_4^{(4)} \pmod{C_1}$ |
| 0 | $E_1, E_1; E_2, E_2$ | C ₄ | C_1 | $C_4^{(2)} = C_1 \circ C_4^{(2)} \pmod{C_1}$ |
| S ₄ | | S4 | C_2 | $S_4 = C_2 \circ S_4^{(2)} \pmod{C_2}$ |
| | E, E | S4 | C_1 | $S_{4}^{(8)} = C_1 \circ S_{4}^{(8)} \pmod{C_1}$ |
| | $E_1, E_1; E_2, E_2$ | S ₄ | C_1 | $\mathbf{S}_4^{\text{cr}} = \mathbf{C}_1 \circ \mathbf{S}_4^{\text{cr}} \pmod{\mathbf{C}_1}$ |

Table 2. Quasi-symmetry minor groups associated with the non-degenerate IRs of the double point groups.

 Table 2—continued

| Double point group G (1) | Non-degenerate IR Γ of G (2) | Little group L (3) | Chosen normal subgroup H (4) | Quasi-symmetry minor group associated with the IR Γ of G (5) |
|--------------------------------------|--|---|--|--|
| C _{4h} | $\begin{array}{c} A_{u} \\ B_{g} \\ B_{u} \\ {}^{1}E_{g}, {}^{2}E_{g} \\ {}^{1}\bar{E}_{1g}, {}^{2}\bar{E}_{1g}; {}^{1}\bar{E}_{2g}, \\ {}^{2}\bar{E}_{2g}, \end{array}$ | C_{4h} C_{4h} C_{4h} C_{4h} C_{4h} | $\begin{array}{c} C_4\\ C_{2h}\\ S_4\\ C_i\\ C_1^* \end{array}$ | $\label{eq:constraint} \begin{array}{l} ^{1}C_{4h}^{\prime} = C_{4} \circ C_{4h}^{(2)} \ (mod \ C_{4}) \\ ^{2}C_{4h}^{\prime} = C_{2h} \circ C_{4h}^{(2)} \ (mod \ C_{2h}) \\ ^{3}C_{4h}^{\prime} = S_{4} \circ C_{4h}^{(2)} \ (mod \ S_{4}) \\ ^{1}C_{4h}^{(4)} = C_{i} \circ C_{4h}^{(4)} \ (mod \ C_{i}) \\ ^{1}C_{4h}^{(4)} = C_{1}^{*} \circ C_{4h}^{(8)} \ (mod \ C_{1}) \end{array}$ |
| | ${}^{1}\bar{E}_{1u}^{2}, {}^{2}\bar{E}_{1u}^{2}; {}^{1}\bar{E}_{2u}^{2}, {}^{2}\bar{E}_{2u}^{2}$ | C_{4h} | C_{1}^{**} | ${}^{2}C_{4h}^{(8)} = C_{1}^{**} \circ C_{4h}^{(8)} \pmod{C_{1}^{**}}$ |
| C ₃ | ${}^{1}E_{u}, {}^{2}E_{u}$ \bar{A} ${}^{1}E, {}^{2}E$ ${}^{1}\bar{E}, {}^{2}\bar{E}$ | C _{4h} C ₃ C ₃ C ₃ | C_{1h} \tilde{C}_3 C_1 \tilde{C}_1 | |
| C _{3i} | $\begin{array}{c} A_{u} \\ \bar{A}_{g} \\ \bar{A}_{u} \\ {}^{1}\bar{E}_{g}, {}^{2}\bar{E}_{g} \\ {}^{1}E_{g}, {}^{2}E_{g} \\ {}^{1}\bar{E}_{u}, {}^{2}\bar{E}_{u} \\ {}^{1}\bar{E}_{u}, {}^{2}\bar{E}_{u} \end{array}$ | $\begin{array}{c} C_{3i}\\ C_{3i}\\$ | C_{3} \tilde{C}_{3i} \tilde{C}_{3i}^{*} C_{1}^{*} C_{i} C_{i}^{**} | ${}^{1}C_{3i}' = C_{3} \circ C_{3i}^{(2)} \pmod{C_{3}}$ ${}^{2}C_{3i}' = \tilde{C}_{3i} \circ C_{3i}^{(2)} \pmod{C_{3i}}$ ${}^{3}C_{3i}' = \tilde{C}_{3i}^{*} \circ C_{3i}^{(2)} \pmod{C_{3i}}$ ${}^{3}C_{3i}' = \tilde{C}_{3i}^{*} \circ C_{3i}^{(2)} \pmod{C_{3i}}$ ${}^{1}C_{3i}^{(6)} = C_{1}^{*} \circ C_{3i}^{(6)} \pmod{C_{1}}$ ${}^{2}C_{3i}^{(3)} = C_{1}^{*} \circ C_{3i}^{(6)} \pmod{C_{1}}$ ${}^{2}C_{3i}^{(6)} = C_{1}^{**} \circ C_{3i}^{(6)} \pmod{C_{1}}$ |
| D ₃ | A_2 ${}^1\bar{E}$, ${}^2\bar{E}$ | D_3 D_3 | C_1 C_3 \tilde{C}_3 | $D'_{3} = C_{3} \circ D'^{(2)}_{3} \pmod{C_{3}}$ $D'_{3} = C_{3} \circ D^{(4)}_{3} \pmod{C_{3}}$ $D^{(4)}_{3} = \tilde{C}_{3} \circ D^{(4)}_{3} \pmod{\tilde{C}_{3}}$ |
| $C_{3\nu}$ | A_2^{1} \bar{E} , $^2\bar{E}$ | C_{3v} C_{3v} | $\begin{array}{c} C_3\\ C_3\end{array}$ | $C'_{3v} = C_3 \circ C^{(2)}_{3v} \pmod{C_3}$ $C^{(4)}_{3v} = \tilde{C}_3 \circ C^{(4)}_{3v} \pmod{C_3}$ |
| D _{3d} | $\begin{array}{c} A_{1u} \\ A_{2g} \\ A_{2u} \\ {}^{1}\bar{E}_{g}, {}^{2}\bar{E}_{g} \\ {}^{1}\bar{E}_{u}, {}^{2}\bar{E}_{u} \end{array}$ | $\begin{array}{c} D_{3d} \\ D_{3d} \\ D_{3d} \\ D_{3d} \\ D_{3d} \\ D_{3d} \end{array}$ | D_{3} C_{3i} C_{3v} \tilde{C}_{3i} \tilde{C}_{3i}^{*} | ${}^{1}\dot{D}'_{3d} = \dot{D}_{3} \circ \dot{D}^{(2)}_{3d} \pmod{D_{3}}$ ${}^{2}\dot{D}'_{3d} = C_{3i} \circ \dot{D}^{(2)}_{3d} \pmod{D_{3}}$ ${}^{3}\dot{D}'_{3d} = C_{3v} \circ \dot{D}^{(2)}_{3d} \pmod{C_{3v}}$ ${}^{1}\dot{D}^{(4)}_{3d} = \tilde{C}_{3i} \circ \dot{D}^{(4)}_{3d} \pmod{\tilde{C}_{3i}}$ ${}^{2}\dot{D}^{(4)}_{3d} = \tilde{C}^{(4)}_{3i} \circ \dot{D}^{(4)}_{3d} \pmod{\tilde{C}^{(4)}_{3i}}$ |
| C ₆ | $B^{1}E_{1}, {}^{2}E_{1} \\ {}^{1}E_{2}, {}^{2}E_{2} \\ {}^{1}\bar{E}_{1}, {}^{2}\bar{E}_{1} \\ {}^{1}\bar{E}_{2}, {}^{2}\bar{E}_{2}; {}^{1}\bar{E}_{3}, \\ {}^{2}\bar{E}_{3}$ | $\begin{array}{c} C_6\\C_6\\C_6\\C_6\\C_6\\C_6\end{array}$ | $C_3 \\ C_2^* \\ C_1 \\ \tilde{C}_3 \\ \tilde{C}_1$ | $\begin{array}{l} C_6' = C_3 \circ C_6^{(2)} \pmod{C_3} \\ C_6^{(3)} = C_2^* \circ C_6^{(3)} \pmod{C_2^*} \\ C_6^{(6)} = C_1 \circ C_6^{(6)} \pmod{C_1} \\ C_6^{(4)} = \tilde{C}_3 \circ C_6^{(4)} \pmod{\tilde{C}_3} \\ C_6^{(12)} = \tilde{C}_1 \circ C_6^{(12)} \pmod{\tilde{C}_1} \end{array}$ |
| C _{3h} | $\begin{array}{c} A'' \\ {}^{1}E', {}^{2}E' \\ {}^{1}E'', {}^{2}E'' \\ {}^{1}\bar{E}_{1}, {}^{2}\bar{E}_{1} \\ {}^{1}\bar{E}_{2}, {}^{2}\bar{E}_{2}; {}^{1}\bar{E}_{3}, \\ {}^{2}\bar{E}_{2} \end{array}$ | C _{3h} C _{3h} C _{3h} C _{3h} C _{3h} | $C_{3} C_{1h}^{*} C_{1} C_{1} C_{3} C_{1}$ | $\begin{array}{l} C_{3h}' = C_{3^{\circ}}C_{3h}^{(2)} \ (mod \ C_{3}) \\ C_{3h}^{(3)} = C_{1h}^{*}\circ C_{3h}^{(3)} \ (mod \ C_{1h}^{*}) \\ C_{3h}^{(6)} = C_{1}\circ C_{3h}^{(6)} \ (mod \ C_{1}) \\ C_{3h}^{(4)} = \tilde{C}_{3}\circ C_{3h}^{(4)} \ (mod \ \tilde{C}_{3}) \\ C_{3h}^{(12)} = \tilde{C}_{1}\circ C_{3h}^{(12)} \ (mod \ \tilde{C}_{1}) \end{array}$ |
| C _{6h} | $ \begin{array}{c} -5 \\ \mathbf{A}_{u} \\ \mathbf{B}_{g} \\ \mathbf{B}_{u} \\ {}^{1}\mathbf{E}_{1g}, {}^{2}\mathbf{E}_{1g} \\ {}^{1}\mathbf{\bar{E}}_{1g}, {}^{2}\mathbf{\bar{E}}_{1g} \\ {}^{1}\mathbf{E}_{2g}, {}^{2}\mathbf{E}_{2g} \\ {}^{1}\mathbf{\bar{E}}_{2g}, {}^{2}\mathbf{\bar{E}}_{2g}, {}^{1}\mathbf{\bar{E}}_{3g}, \\ {}^{2}\mathbf{\bar{E}}_{3g} \end{array} $ | C_{6h} C_{6h} C_{6h} C_{6h} C_{6h} C_{6h} | $\begin{array}{c} C_{6} \\ C_{3i} \\ C_{3h} \\ C_{2h} \\ \tilde{C}_{3i} \\ C_{i} \\ C_{1}^{*} \end{array}$ | $\label{eq:constraint} \begin{array}{l} {}^{1}C_{6h}' = C_{6} \circ C_{6h}^{(2)} \ (mod \ C_{6}) \\ {}^{2}C_{6h}' = C_{3i} \circ C_{6h}^{(2)} \ (mod \ C_{3i}) \\ {}^{3}C_{6h}' = C_{3h} \circ C_{6h}^{(3)} \ (mod \ C_{3h}) \\ {}^{C}C_{6h}' = C_{3i} \circ C_{6h}^{(3)} \ (mod \ C_{2h}) \\ {}^{1}C_{6h}' = \tilde{C}_{3i} \circ C_{6h}^{(6)} \ (mod \ \tilde{C}_{3i}) \\ {}^{1}C_{6h}^{(6)} = C_{i} \circ C_{6h}^{(6)} \ (mod \ C_{i}) \\ {}^{1}C_{6h}^{(6)} = C_{i} \circ C_{6h}^{(1)} \ (mod \ C_{i}) \\ {}^{1}C_{6h}^{(12)} = C_{1}^{*} \circ C_{6h}^{(12)} \ (mod \ C_{1}^{*}) \end{array}$ |
| | ${}^{1}E_{1u}, {}^{2}E_{1u}$ | C_{6h} | C ₂ * | ${}^{2}C_{6h}^{(6)} = C_{2}^{*} \circ C_{6h}^{(6)} \pmod{C_{2}^{*}}$ |

| Double point group G (1) | Non-degenerate IR Γ of G (2) | Little group L (3) | Chosen normal subgroup H (4) | Quasi-symmetry minor group associated with the IR Γ of G (5) |
|--------------------------------------|---|---|---|---|
| C _{6h} | ${}^{1}\bar{E}_{1u}, {}^{2}\bar{E}_{1u}$ ${}^{1}E_{2u}, {}^{2}E_{2u}$ ${}^{1}\bar{E}_{2u}, {}^{2}\bar{E}_{2u}; {}^{1}\bar{E}_{3u},$ ${}^{2}\bar{E}_{3u}$ | C _{6h} C _{6h} C _{6h} | \tilde{C}_{3i}^* C_{1h}^* C_1^{**} | ${}^{2}C_{6h}^{(4)} = \tilde{C}_{3i}^{*} \circ C_{6h}^{(4)} \pmod{\tilde{C}_{3i}^{*}} \\ {}^{3}C_{6h}^{(4)} = C_{1h}^{*} \circ C_{6h}^{(4)} \pmod{C_{1h}^{*}} \\ {}^{2}C_{6h}^{(12)} = C_{1}^{**} \circ C_{6h}^{(12)} \pmod{C_{1}^{**}} $ |
| D ₄ | A_2 B ₁ , B ₂ | D ₄ D ₄ | C ₄ D ₂ | ${}^{1}D'_{4} = C_{4} \circ D_{4}^{(2)} \pmod{C_{4}}$ ${}^{2}D'_{4} = D_{2} \circ D_{4}^{(2)} \pmod{D_{2}}$ |
| C_{4v} | A_2 B_1, B_2 | C_{4v} C_{4v} | C_4 C_{2y} | ${}^{1}C'_{4v} = C_{4} \circ C_{4v}^{(2)} \pmod{C_{4}}$ ${}^{2}C'_{4v} = C_{2v} \circ C_{4v}^{(2)} \pmod{C_{2v}}$ |
| D _{2d} | A_2 B_1 B_2 | D_{2d} D_{2d} | S_4 D_2 C_{2} | ${}^{1}D_{2d} = S_{4} \circ D_{2d}^{(2)} \pmod{S_{4}}$ ${}^{2}D_{2d}^{\prime} = D_{2} \circ D_{2d}^{\prime} \pmod{S_{4}}$ ${}^{3}D_{2d}^{\prime} = C_{2} \circ D_{2d}^{\prime} \pmod{D_{2}}$ |
| D_{4h} | $\begin{array}{c} \mathbf{A}_{1u} \\ \mathbf{A}_{2g} \\ \mathbf{B}_{1g}, \mathbf{B}_{2g} \\ \mathbf{A}_{2u} \\ \mathbf{B}_{1u}, \mathbf{B}_{2v}. \end{array}$ | D_{4h} D_{4h} D_{4h} D_{4h} D_{4h} D_{4h} | $\begin{array}{c} D_4 \\ D_4 \\ D_{2h} \\ C_{4v} \\ D_{2d} \end{array}$ | |
| D_6 | $\begin{array}{c} -10^{2} - 20^{2} \\ A_{2} \\ B_{1}, B_{2} \end{array}$ | D_6 D_6 | C_6 D ₃ | ${}^{1}\mathbf{D}_{6}' = \mathbf{C}_{6} \circ \mathbf{D}_{6}^{(2)} \pmod{\mathbf{C}_{6}}$ ${}^{2}\mathbf{D}_{6}' = \mathbf{D}_{3} \circ \mathbf{D}_{6}^{(2)} \pmod{\mathbf{D}_{3}}$ |
| C _{6v} | $\begin{array}{c} A_2 \\ B_1, B_2 \end{array}$ | C _{6v} C _{6v} | C ₆ C _{3v} | ${}^{1}C_{6v}^{\prime} = C_{6} \circ C_{6v}^{(2)} \pmod{C_{6}}$ ${}^{2}C_{6v}^{\prime} = C_{3v} \circ C_{6v}^{(2)} \pmod{C_{3v}}$ |
| D _{3h} | A ['] ₂ A ^{''} ₁ A ^{''} ₂ | D_{3h} D_{3h} D_{3h} | C _{3h} D ₃ C _{3v} | ${}^{1}D'_{3h} = C_{3h} \circ D_{3h}^{(2)} \pmod{C_{3h}}$ ${}^{2}D'_{3h} = D_{3} \circ D_{3h}^{(2)} \pmod{D_{3}}$ ${}^{3}D'_{2h} = C_{3h} \circ D_{3h}^{(2)} \pmod{D_{3}}$ |
| D _{6h} | $ \begin{array}{c} A_{2g} \\ B_{1g}, B_{2g} \\ A_{1u} \\ A_{2u} \\ B_{2g} \\ B_{2g} \\ A_{2g} \\ A_{2g} \\ $ | $\begin{array}{c} D_{6h} \\ D_{6h} \\ D_{6h} \\ D_{6h} \\ D_{6h} \\ D_{6h} \end{array}$ | $ \begin{array}{c} C_{6h} \\ D_{3d} \\ D_6 \\ C_{6v} \\ D_{v} \end{array} $ | ${}^{1}D_{6h}^{(a)} = C_{6h} \circ D_{6h}^{(2)} \pmod{C_{6h}}$ ${}^{2}D_{6h}^{(a)} = D_{3d} \circ D_{6h}^{(a)} \pmod{D_{3d}}$ ${}^{3}D_{6h}^{(a)} = D_{6} \circ D_{6h}^{(2)} \pmod{D_{6}}$ ${}^{4}D_{6h}^{(a)} = C_{6v} \circ D_{6h}^{(2)} \pmod{C_{6v}}$ ${}^{5}D_{c}^{(a)} = C_{6v} \circ D_{6h}^{(2)} \pmod{D_{6v}}$ |
| т | ${}^{1}E, {}^{2}E$ | D _{6h} T | D_{3h} D_2 | $T^{(3)} = D_2 \circ T^{(3)} \pmod{D_{2}}$ |
| T _h | | T _h T _h T _h | $T D_{2h} D_2$ | $ T'_{h} = T \circ T_{h}^{(2)} \pmod{T} T_{h}^{(3)} = D_{2h} \circ T_{h}^{(3)} \pmod{D_{2h}} T_{h}^{(6)} = D_{2} \circ T_{h}^{(6)} \pmod{D_{2}} $ |
| 0 | A ₂ | 0 | T | $O' = T \circ O^{(2)} \pmod{T}$ |
| I _d O _h | $\begin{array}{c} A_2 \\ A_{1u} \\ A_{2g} \\ A_{2u} \end{array}$ | I _d O _h O _h O _h | I O T _h T _d | $\begin{aligned} \mathbf{I}_{d} &= \mathbf{I} \circ \mathbf{I}_{d}^{*} \pmod{1} \\ \mathbf{O}_{h}^{\prime} &= \mathbf{O} \circ \mathbf{O}_{h}^{(2)} \pmod{0} \\ \mathbf{O}_{h}^{\prime} &= \mathbf{T}_{h} \circ \mathbf{O}_{h}^{(2)} \pmod{T_{h}} \\ \mathbf{O}_{h}^{\prime} &= \mathbf{T}_{d} \circ \mathbf{O}_{h}^{(2)} \pmod{T_{d}} \end{aligned}$ |

Table 2—continued

In column (4) the symbol () on the normal subgroup H (which coincides with the kernel associated with the IR Γ of G) indicates that it is a double point group isomorphic with the corresponding point group. For example, \tilde{C}_1 denotes a double point group with the element $\{E\}$ isomorphic to the point group C_1 , and \tilde{C}_3 a double point group with elements E, \tilde{C}_3^+ and \tilde{C}_3^- which is isomorphic to the point group C_3 . Similarly the symbols () and (*) on the group indicate a double point group isomorphic with the corresponding point group in some non-standard setting. For example, \tilde{C}_{3i}^+ : E, \tilde{C}_3^- , \tilde{C}_3^- , \tilde{I} , IC_3^+ , IC_3^- is a double group isomorphic to a non-standard setting of the point group C_{3i} . Similarly the symbol (*) on the group denotes some non-standard setting of the corresponding double point group. For example C_1^+ is a double point group with the elements E and I, which is isomorphic with the double point group C_1 .

Table 2-continued

In column (5) the symbol (') on the group G denotes a minor quasi-symmetry group (in particular a magnetic double point group) associated with the one-dimensional alternating IR Γ of G with P₂ as the permutation group. For example, C'₂ denotes a minor quasi-symmetry group associated with the one-dimensional alternating IR B of C₂ (which is a magnetic double point group). The number n placed in brackets on the group G indicates a minor quasi-symmetry group (in particular a polychromatic double point group) associated with the one-dimensional complex IR Γ of G whose underlying permutation group is P_n. For example, C'₆ indicates a minor quasi-symmetry group associated with the IR ¹D₂ of C₆ with P₆ as the permutation group.

| Table 3 | . Quas | si-symmetry | minor | groups | associated | with t | the d | egenerate | IRS of | the c | louble |
|----------|--------|-------------|-------|--------|------------|--------|-------|-----------|--------|-------|--------|
| point gi | oups | | | | | | | | | | |

| Double point group G (1) | Degenerate IR Γ of G (2) | Little group L (3) | AIR of <i>L</i> (4) | Minor quasi-symmetry group associated with the IR Γ of G (5) |
|--------------------------------------|--|-----------------------------|--|--|
| D ₂ | Ē | С, | ¹ Ē | $D_2'' = C_2^{(4)} \circ D_2^{(2)} \pmod{C_2}$ |
| C_{2v} | Ē | C ₂ | ¹ Ē | $C_{2y}'' = C_2^{(4)} \circ C_{2y}^{(2)} \pmod{C_2}$ |
| D_{2h} | Ē. | C _{2b} | 1Ē. | ${}^{1}D''_{2h} = {}^{1}C^{(4)}_{2h} \circ D^{(2)}_{2h} \pmod{C_{2h}}$ |
| 2 | Ē | \tilde{C}_{2h} | 1Ē, | ${}^{2}D_{2h}'' = {}^{2}C_{2h}^{(4)} \circ D_{2h}^{(2)} \pmod{C_{2h}^{(2)}}$ |
| D_3 | E | C_3 | ¹ E | ${}^{1}D_{3}'' = C_{3}^{(3)} \circ D_{3}^{(2)} \pmod{C_{3}}$ |
| - | $\bar{\mathbf{E}}_1$ | C_3 | 1Ē | ${}^{2}D_{3}'' = C_{3}^{(6)} \circ D_{3}^{(2)} \pmod{C_{3}}$ |
| C _{3v} | E | C_3 | ¹ E | ${}^{1}C_{3v}'' = C_{3}^{(3)} \circ C_{3v}^{(2)} \pmod{C_{3}}$ |
| | Ēı | C ₃ | ¹ Ē | ${}^{2}C_{3v}'' = C_{3}^{(6)} \circ C_{3v}^{(2)} \pmod{C_{3}}$ |
| D_{3d} | Eg | C_{3i} | ${}^{1}E_{g}$ | ${}^{1}D''_{3d} = C^{(3)}_{3i} \circ D^{(2)}_{3d} \pmod{C_{3i}}$ |
| | Eu | C_{3i} | ¹ E _u | ${}^{2}D''_{3d} = {}^{3}C^{(6)}_{3i} \circ D^{(2)}_{3d} \pmod{C_{3i}}$ |
| | Ēig | C _{3i} | Ëg | ${}^{3}D_{3d}'' = {}^{1}C_{3i}^{(6)} \circ D_{3d}^{(2)} \pmod{C_{3i}}$ |
| | E _{1u} | C_{3i} | ¹ E _u | ${}^{4}D_{3d}'' = {}^{2}C_{3i}^{(6)} \circ D_{3d}^{(2)} \pmod{C_{3i}}$ |
| D_4 | E | C4 | 'E | ${}^{1}D_{4}'' = C_{4}^{(4)} \circ D_{4}^{(2)} \pmod{C_{4}}$ |
| | E_1, E_2 | C ₄ | E_1, E_2 | $^{2}D_{4}^{\prime\prime} = C_{4}^{(4)} \circ D_{4}^{(2)} \pmod{C_{4}}$ |
| C_{4v} | E E E | C_4 | 18 18 18 | $C_{4v}^{*} = C_{4v}^{*} \circ C_{4v}^{*} \pmod{C_{4}}$ |
| D | E_1, E_2 | C4 | E_1, E_2 | $U_{4v} = U_4 \circ U_{4v} \pmod{U_4}$ |
| D_{2d} | | 54 S | 10 10 | $D_{2d} = S_4 \circ D_{2d} \pmod{S_4}$ |
| D | L_1, L_2 | 34 C | $^{1}E_{1}, E_{2}$ | ${}^{1}D''_{2d} = {}^{1}C^{(4)} \circ D_{2d}^{(2)} \pmod{3_4}$ |
| D _{4h} | E E | C _{4h} | | ${}^{2}D''_{4h} = {}^{2}C^{(4)}_{4h} \circ D^{(4)}_{4h} \pmod{C_{4h}}$ |
| | Ē.Ē. | C ₄ h | 1Ē, 1Ē, | ${}^{3}D_{4h}'' = {}^{1}C_{4h}^{(8)} \circ D_{4h}^{(2)} \pmod{C_{4h}}$ |
| | \bar{E}_{1m} , \bar{E}_{2m} | C4h C4h | ${}^{1}\bar{E}_{1}$, ${}^{1}\bar{E}_{2}$ | ${}^{4}D_{4h}'' = {}^{2}C_{4h}^{(8)} \circ D_{4h}^{(2)} \pmod{C_{4h}}$ |
| D۷ | E_1 | C₄n | $^{1}E_{2}$ | ${}^{1}D_{4}^{"} = C_{4}^{(6)} \circ D_{4}^{(2)} \pmod{C_{4}}$ |
| -0 | E_2 | Č, | ¹ E ₁ | ${}^{2}D_{6}'' = C_{6}^{(3)} \circ D_{6}^{(2)} \pmod{C_{6}}$ |
| | $\overline{E}_1, \overline{E}_2$ | C ₆ | ${}^{1}\tilde{E}_{2}, {}^{1}\tilde{E}_{3}$ | ${}^{3}D_{6}'' = C_{6}^{(12)} \circ D_{6}^{(2)} \pmod{C_{6}}$ |
| | \bar{E}_3 | $\tilde{C_6}$ | ${}^{1}\bar{E}_{1}$ | ${}^{4}D_{6}'' = C_{6}^{(4)} \circ D_{6}^{(2)} \pmod{C_{6}}$ |
| C _{6v} | E ₁ | C_6 | ${}^{1}E_{2}$ | ${}^{1}C_{6v}'' = C_{6}^{(6)} \circ C_{6v}^{(2)} \pmod{C_{6}}$ |
| | E ₂ | C ₆ | $^{1}E_{1}$ | ${}^{2}C_{6v}'' = C_{6v}^{(3)} \circ C_{6v}^{(2)} \pmod{C_{6}}$ |
| | Ē3 | C ₆ | ${}^{1}\overline{E}_{1}$ | ${}^{3}C_{6v}'' = C_{6v}^{(4)} \circ C_{6v}^{(2)} \pmod{C_{6}}$ |
| | $\bar{\mathrm{E}}_1, \bar{\mathrm{E}}_2$ | C ₆ | ${}^{1}\bar{E}_{2}, {}^{1}\bar{E}_{3}$ | ${}^{4}C_{6v}'' = C_{6v}^{(12)} \circ C_{6v}^{(2)} \pmod{C_{6}}$ |
| D_{3h} | E" | C_{3h} | ¹ E″ | ${}^{1}D''_{3h} = C^{(6)}_{3h} \circ D^{(2)}_{3h} \pmod{C_{3h}}$ |
| | E′ ≕ | C _{3h} | 'E'1 | $^{2}D_{3h}^{"} = C_{3h}^{(3)} \circ D_{3h}^{(2)} \pmod{C_{3h}}$ |
| | E ₃ | C _{3h} | 'E₁ 1= 1= | ${}^{3}D_{3h}^{"} = C_{3h}^{(4)} \circ D_{3h}^{(2)} \pmod{C_{3h}}$ |
| | E_1, E_2 | C _{3h} | E_{2}, E_{3} | $D_{3h}'' = C_{3h}' \circ D_{3h}^{(2)} \pmod{C_{3h}}$ |
| D_{6h} | E _{2g} | C _{6h} | E_{1g} | $D_{6h}^{"} = C_{6h}^{(3)} \circ D_{6h}^{(2)} \pmod{C_{6h}}$ |
| | E _{3g} | C_{6h} | Elg | $^{-}D_{6h}^{-} = ^{+}C_{6h}^{\vee h} \circ D_{6h}^{\vee h} \pmod{C_{6h}}$ |

| Double point group G (1) | Degenerate IR Γ of G (2) | Little group L (3) | AIR of L (4) | Minor quasi-symmetry group associated with the IR Γ of G (5) |
|--------------------------------------|---|---|---|--|
| D _{6h} | E_{1g} E_{2u} E_{1u} $\bar{E}_{1g}, \bar{E}_{2g}$ \bar{E}_{3u} \bar{E}_{3} \bar{E}_{3} | $\begin{array}{c} C_{6h} \\ C_{6h} \end{array}$ | ${}^{1}E_{2g}$ ${}^{1}E_{1u}$ ${}^{1}E_{2u}$ ${}^{1}\bar{E}_{2g}, {}^{1}\bar{E}_{3g}$ ${}^{1}\bar{E}_{1u}$ ${}^{1}\bar{E}_{2u}, {}^{1}\bar{E}_{2}$ | ${}^{3}D_{6h}'' = {}^{1}C_{6h}^{(6)} \circ D_{6h}^{(2)} \pmod{C_{6h}} + {}^{2}D_{6h}^{(6)} \circ D_{6h}^{(2)} \pmod{C_{6h}} + {}^{2}D_{6h}^{(6)} \circ D_{6h}^{(2)} \pmod{C_{6h}} + {}^{3}D_{6h}^{(4)} \circ D_{6h}^{(2)} \pmod{C_{6h}} + {}^{6}D_{6h}^{(6)} \circ D_{6h}^{(2)} \pmod{C_{6h}} + {}^{2}C_{6h}^{(4)} \circ D_{6h}^{(2)} \pmod{C_{6h}} + {}^{2}C_{6h}^{(4)} \circ D_{6h}^{(2)} \pmod{C_{6h}} + {}^{2}C_{6h}^{(4)} \circ D_{6h}^{(2)} \pmod{C_{6h}} + {}^{2}D_{6h}^{(4)} \circ D_{6h}^{(2)} (2) \otimes D_{6h}^{(2)} \otimes D_{6h}^$ |
| Т | \overline{E} , ${}^{1}\overline{F}$, ${}^{2}\overline{F}$ | D ₂ | Ē Ē | $T'' = D'_{2} \circ T^{(3)} \pmod{D_{2}}$ $T''' = D'_{2} \circ T^{(3)} \pmod{D_{2}}$ |
| T _h | | D_{2h} D_{2h} D_{2h} D_{2h} | \tilde{E}_{g} \tilde{E}_{u} B_{2g} | $ \frac{1}{2} 1$ |
| 0 | $ \begin{array}{c} T_u \\ E \\ \bar{E}_1, \bar{E}_2 \\ T_1, T_2 \end{array} $ | D _{2h} T T T | B _{2u} ¹ E Ē T | ${}^{2}T_{h''}^{m'} = {}^{3}D_{2h}^{\prime}\circ T_{h}^{(3)} \pmod{D_{2h}}$ ${}^{1}O'' = T^{(3)}\circ O^{(2)} \pmod{T}$ ${}^{2}O'' = T''\circ O^{(2)} \pmod{T}$ $O''' = T'''\circ O^{(2)} \pmod{T}$ $O''' = T'''\circ O^{(2)} \pmod{T}$ |
| T _d | F E E_1, E_2 T_1, T_2 \overline{r} | T T T T | ⁴ F, ² F ¹ E Ē T ¹ E ² E | $O''' = T'' \circ O' \circ (mod T)$ ¹ T''_d = T'(3) \circ T'(2) (mod T) ² T''_d = T'' \circ T'(2) (mod T) T'''_d = T'' \circ T'(2) (mod T) T'''_d = T'' \circ T'(2) (mod T) T'''_d = T'' \circ T'(2) (mod T) |
| O _h | $ \begin{array}{c} E_{g} \\ \bar{E}_{1g}, \bar{E}_{2g} \\ T_{1g}, T_{2g} \\ \bar{F}_{g} \\ \bar{E}_{u} \\ \bar{E}_{1u}, \bar{E}_{2u} \\ T_{1u}, T_{2u} \\ \bar{F}_{u} \end{array} $ | $ \begin{array}{c} T_h \\ T_h \end{array} $ | $ \begin{array}{c} \mathbf{r}, \mathbf{r} \\ \mathbf{i} \mathbf{E}_{g} \\ \mathbf{\bar{E}}_{g} \\ \mathbf{T}_{g} \\ \mathbf{i} \mathbf{\bar{F}}_{g}, {}^{2} \mathbf{\bar{F}}_{g} \\ \mathbf{\bar{E}}_{u} \\ \mathbf{\bar{E}}_{u} \\ \mathbf{\bar{E}}_{u} \\ \mathbf{\bar{T}}_{u} \\ \mathbf{\bar{F}}_{u}, {}^{2} \mathbf{\bar{F}}_{u} \end{array} $ | $ \begin{array}{l} {}^{A}_{d} = 1 {}^{A}_{d} (\text{inder } 1') \\ {}^{I}O_{h}'' = T_{h}^{(3)} \circ O_{h}^{(2)} (\text{mod } T_{h}) \\ {}^{2}O_{h}'' = 1 T_{h}'' \circ O_{h}^{(2)} (\text{mod } T_{h}) \\ {}^{I}O_{h}'''' = 1 T_{h}'' \circ O_{h}^{(2)} (\text{mod } T_{h}) \\ {}^{3}O_{h}'' = T_{h}^{(6)} \circ O_{h}^{(2)} (\text{mod } T_{h}) \\ {}^{3}O_{h}'' = T_{h}^{(6)} \circ O_{h}^{(2)} (\text{mod } T_{h}) \\ {}^{4}O_{h}'' = 2 T_{h}'' \circ O_{h}^{(2)} (\text{mod } T_{h}) \\ {}^{2}O_{h}'''' = 2 T_{h}''' \circ O_{h}^{(2)} (\text{mod } T_{h}) \\ {}^{2}O_{h}''''' = 2 T_{h}'' \circ O_{h}^{(2)} (\text{mod } T_{h}) \end{array} $ |

Table 3—continued

In column (5) the number of primes (') on the group G denotes a minor quasi-symmetry group associated with the degenerate IR Γ of G whose dimension is given by that number. For example D_2'' is a minor quasi-symmetry group associated with the two-dimensional IR E of the double point group D_2 . Similarly T'' is a minor quasi-symmetry group associated with the three-dimensional IR T of the double point group T.

In the case of non-degenerate IRS, we have seen that the little groups L always coincide with the group G itself, and the kernels (K) coincide with the chosen normal subgroup H. Since the IRS of the factor group L/K = G/H engender those of the IRS of the same nature of G, the selection of a proper normal subgroup H facilitates the required IR of G which is to be engendered. In table 2 we give the appropriate normal subgroup H (which is in particular the kernel in the process of engendering) associated with the IR Γ of G and for which we associate the minor quasi-symmetry group.

Table 1 gives the double point group G as the quasi-semi-direct product. From table 1 $C_4 = C_2 \circ C_4 \pmod{C_2}$. The group $C'_4 = C_2 \circ C_4^{(2)} \pmod{C_2}$ can be seen to be a minor quasi-symmetry group with the double group C_4 as the generator, since C_2 is a major/minor group with C_2 as generator, and $C_4^{(2)} \pmod{C_2}$ is a minor quasi-symmetry group isomorphic with $C_4 \pmod{C_2}$ with $Q = I_1(1 2)$. Since the kernel associated with

the group C_4 is C_2 , and since the alternating IR of C_4/C_2 engenders the IR B of C_4 , we associate $C'_4 = C_2 \circ C_4^{(2)} \pmod{C_2}$ with the IR B of C_4 . Similarly $C_4^{(4)} = C_1 \circ C_4^{(4)} \pmod{C_1}$ is a minor quasi-symmetry group with C_4 as the generator. Since the one-dimensional complex IRs of the factor group C_4/C_1 engender the IRs ¹E and ²E of C_4 , we associate $C_4^{(4)}$ with ¹E of C_4 .

As an example of degenerate IRs, we consider the double point group D₃. From table 1 D₃ = C₃ \circ D₃(mod C₃). The group ¹D''₃ = C₃⁽³⁾ \circ D₃⁽²⁾(mod C₃) can be seen to be a minor quasi-symmetry group with D₃ as the generator and with P₃ as the group of permutations, since C₃⁽³⁾ and D₃⁽²⁾(mod C₃) are minor quasi-symmetry groups with C₃ and D₃(mod C₃) as generators respectively, and since D''₃ = C₃⁽³⁾ \circ D₃⁽²⁾(mod C₃). From table 2 C₃⁽³⁾ is a quasi-symmetry minor group associated with the IR ¹E of C₃. The group D₃⁽²⁾(mod C₃) is also a minor group isomorphic with the group D₃(mod C₃). Since C₃⁽³⁾ is associated with ¹E of C₃, which induces the IR E of D₃, we associate ¹D''₃ with the IR E of D₃. Similarly ²D''₃ = C₃⁽⁶⁾ \circ D₃⁽²⁾(mod C₃) is also a minor quasi-symmetry group with D₃ as the generator and with P as the group of permutations of order 6 and on 6 symbols. The group C₃⁽⁶⁾ is a minor quasi-symmetry group associated with the IR ¹E of C₃ (table 2). Also the group D₃⁽²⁾(mod C₃) is a minor quasi-symmetry group isomorphic with D₃(mod C₃). Since C₃⁽⁶⁾ is a sasociated with ¹E of C₃, and since this ¹E of C₃ in turn induces the two-dimensional IR E of D₃, we associate the minor group ²D''₃ with the spin IR E of D₃.

In this way we can associate minor groups with all the IRs of the double point groups. Following the definition of equivalence of any two colour groups (Niggli and Wondratschek 1960, Bradley and Cracknell 1972), we see that some of the minor groups associated with various IRs of G are equivalent, and hence only 64 minor groups with the one-dimensional alternating, 41 minor groups with the one-dimensional complex, 53 minor groups with the distinct two-dimensional, 7 minor groups with the distinct three-dimensional, and 4 minor groups with the four-dimensional IRs can be associated for these 32 double point groups.

4. Discussion

The 64 magnetic double point groups, which are obtained as quasi-semi-direct products and associated with the 64 distinct one-dimensional alternating IRs as the quasi-symmetry minor groups, have physical significance (Rudra and Sikdar 1977).

An example of the physical applications of the quasi-symmetry groups is that of magnetic symmetry (Naish 1963, Zamorzaev 1967). In describing the magnetic symmetry of screw (helicoidal) and spiral structures, where the traditional magnetic groups are not suitable, these quasi-symmetry (multiplicative) groups may be of some use (Zamorzaev 1967).

It was verified in the case of double point groups also that, when a set of IRS was induced by a single AIR, the quasi-symmetry minor groups associated with those IRS were isomorphic (Niggli and Wondratschek 1960, Krishnamurty *et al* 1978a). For example, the two-dimensional IR \overline{E} of D_2 induces the three two-dimensional IRS \overline{E} , ${}^1\overline{F}$ and ${}^2\overline{F}$ of T, and hence the minor quasi-symmetry groups associated with those three IRS are mutually isomorphic. This fact that a single minor group can be associated with these three IRS is also justified from the concept of kernels (Niggli and Wondratschek 1960). The kernel (associated) for these three IRS \overline{E} , ${}^1\overline{F}$, ${}^2\overline{F}$ of T is the same, and can be easily seen to be {E}. Also from the fundamental quasi-symmetry theorem (Zamorzaev 1967) the group T has only three normal subgroups D_2 , C_1 and $\{E\}$, and hence only three minor groups can be obtained for T. The minor group with D_2 as the normal subgroup is associated with ¹E and ²E; that with C_1 with T, and hence that with $\{E\}$ is to be associated with the remaining IRS \overline{E} , ¹F and ²F.

It was observed that, when we drop all those elements of the quasi-symmetry minor groups associated with the normal single-valued IRs of the double point groups whose symmetry part is of the form R, we obtain the corresponding quasi-symmetry minor groups derived earlier for the corresponding point groups (Krishnamurty *et al* 1978a).

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