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Minor quasi-symmetry (P-symmetry) crystallographic point groups as semi-direct products

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Abstract. Minor quasi-symmetry (P-symmetry) crystallographic point groups associated with all the 23 distinct two-dimensional and 7 distinct three-dimensional irreducible representations generated by the point groups containing degenerate irreducible representations are obtained as semi-direct products and are tabulated.

1. Introduction

Shubnikov (1951) introduced the concept of anti-symmetry into the realm of crystallography and derived the 58 double-coloured (magnetic) point groups. The association of these groups with the 58 distinct one-dimensional (1D) alternating representations of the crystallographic point groups was accomplished by Indenbom (1959), Niggli and Wondratschek (1960), Bertaut (1968) and Krishnamurty and Gopala Krishna Murty (1969). The interpretation of anti-symmetry as two-colour symmetry has led to the idea of polychromatic symmetry (Belov and Tarkhova 1956), and this paved the way to the derivation of the 18 polychromatic point groups (Indenbom *et al* 1960). These groups were associated with the 18 pairs of 1D complex representations of the generating crystallographic point groups using representation theory by Niggli and Wondratschek (1960) and Krishnamurty and Appalanarasimham (1972). Niggli and Wondratschek (1960) derived some more simple crypto-symmetries against the degenerate irreducible representations (IR) of these point groups using the concept of kernel. Zamorzaev (1967) introduced the concept of quasi-symmetry (P-symmetry) and brought all the earlier generalisations, namely anti-symmetry, colour symmetry, including crypto-symmetry, into its fold. It was shown that the 58 magnetic point groups and the 18 polychromatic point groups are nothing but particular realisations of the minor quasi-symmetry groups with an appropriate point group as generator. Recently Krishnamurty *et al* (1978b) developed a general method of obtaining a quasi-symmetry (P-symmetry) group G' generated by the group G as a semi-direct product ($G' = S' \wedge T'$) of the constituent quasi-symmetry groups S' and T' generated by the appropriate normal divisor S and the sub-group T. These authors also described a new method of associating the minor quasi-symmetry groups obtained with the IR of the generator groups using the idea of little groups and their 1D allowable irreducible representations (AIR), which differ from these of Niggli and Wondratschek (1960).

It is well known that the crystallographic point groups are symmetry groups of physical systems. As such, a knowledge of the minor quasi-symmetry groups generated by the physical systems would be useful. The minor quasi-symmetry groups generated and associated with the 1D alternating and 1D complex IR of the crystallographic point groups are available in the literature, though they are not always termed minor quasi-symmetry groups. For example, the 58 magnetic point groups associated with the 1D alternating IR were tabulated by Tavger and Zaitsev (1956), and the 18 polychromatic point groups associated with the 1D complex IR were tabulated by Indenbom *et al* (1960). Shubnikov and Koptsik (1974) obtained these magnetic and polychromatic point groups as colour groups $G^{(p)}$, isomorphic with the crystallographic groups G, by finding the normal sub-group H of G and forming the direct product, semi-direct product or quasi-product of H with the generating coloured groups $G^{(p)*}$ or with the groups $G^{(p)*}(\text{mod } G_1^*)$. But a list of minor quasi-symmetry point groups (obtained as semi-direct products) associated with all the 23 distinct 2D and 7 distinct 3D IR of the generating crystallographic point groups is not available in the literature.

The utility of expressing crystallographic point groups as semi-direct products (Altmann 1963a, b) has gained sufficient importance, and the physical significance of an AIR that induces the degenerate IR of a point group is already appreciated (Krishnamurty *et al* 1978a): hence, in what follows, the minor quasi-symmetry point groups to be associated with all the 2D and 3D IR (with the help of the AIR) are obtained as semi-direct products of the constituent minor quasi-symmetry groups and are tabulated.

2. Minor quasi-symmetry (P-symmetry) crystallographic point groups as semi-direct products

Krishnamurty *et al* (1978b) developed a general method of obtaining a quasi-symmetry (P-symmetry) group G' generated by the group G, via the concept of semi-direct products and the fundamental quasi-symmetry theorem of Zamorzaev (1967). If G can be expressed as a semi-direct product, i.e. $G = S \wedge T$, and if S' and T' are two quasi-symmetry groups with S and T as generators, respectively, then $G' = S' \wedge T'$ (if S' and T' satisfy all the requirements of semi-direct products) can be shown to be a quasi-symmetry group with G as generator. It was also shown that the nature of G' (whether it is a major, minor or intermediate group) depends upon the nature of S' and T'. Section 2 of Krishnamurty *et al* (1978b) deals with the statements and proofs of the various theorems that arise in the construction of P-symmetry groups as semi-direct products. These authors also described a new method of associating the minor groups obtained with the IR of the generator groups using the idea of little groups and their AIR which induce the appropriate degenerate IR. In the case of minor quasi-symmetry groups the method was exemplified with the point group D_3 for a 2D IR and with the point group T for a 3D IR. In the present paper, the construction of minor quasi-symmetry groups generated by all the point groups containing degenerate IR is taken up and, in all, 30 distinct minor quasi-symmetry groups are generated as semi-direct products. The groups obtained are associated with the respective degenerate IR of the appropriate generator groups and are tabulated in tables 1 and 2, with a view that they might be useful in future to physicists in their further investigations, since the crystallographic point groups are symmetry groups of physical systems and hence the minor quasi-symmetry groups generated by them will be useful.

Table 1. Minor quasi-symmetry groups as semi-direct products associated with the 2D IR of the crystallographic point groups.

No	Point group G	2D IR Γ of G	Little group L	1D AIR of L	Minor quasi-symmetry group associated with the 2D IR Γ of G
1	C_{4v}	E	C_4	^1E	$C''_{4v}=4^{(4)}\wedge\tilde{m}^{(2)}$
2	D_{2d}	E	S_4	^1E	$D''_{2d}=\bar{4}^{(4)}\wedge\tilde{\bar{2}}^{(2)}$
3	D_4	E	C_4	^1E	$D''_4=4^{(4)}\wedge\tilde{\bar{2}}^{(2)}$
4	C_{3v}	E	C_3	^1E	$C''_{3v}=3^{(3)}\wedge\tilde{m}^{(2)}$
5	D_3	E	C_3	^1E	$D''_3=3^{(3)}\wedge\tilde{\bar{2}}^{(2)}$
6	D_{3h}	E′	C_{3h}	$^1E'$	$^1D''_{3h}=\bar{6}^{(3)}\wedge\tilde{\bar{2}}^{(2)}$
7	D_{3h}	E″	C_{3h}	$^1E''$	$^2D''_{3h}=\bar{6}^{(6)}\wedge\tilde{\bar{2}}^{(2)}$
8	C_{6v}	E_1	C_6	$^1E_2$	$^1C''_{6v}=6^{(6)}\wedge\tilde{m}^{(2)})$
9	C_{6v}	E_2	C_6	$^1E_1$	$^2C''_{6v}=6^{(3)}\wedge\tilde{m}^{(2)}$
10	D_6	E_1	C_6	$^1E_2$	$^1D''_6=6^{(6)}\wedge\tilde{\bar{2}}^{(2)}$
11	D_6	E_2	C_6	$^1E_1$	$^2D''_6=6^{(3)}\wedge\tilde{\bar{2}}^{(2)}$
12	T_d	E	T	^1E	$T''_d=3^{(3)}/2\wedge\tilde{m}^{(2)}$
13	O	E	T	^1E	$O''=3^{(3)}/2\wedge\tilde{\bar{2}}^{(2)}$
14	D_{4h}	E_u	C_{4h}	^1E_u	$^1D''_{4h}=4^{(4)}/m\wedge\tilde{\bar{2}}^{(2)}$
15	D_{4h}	E_g	C_{4h}	^1E_g	$^2D''_{4h}=4^{(4)}/m'\wedge\tilde{\bar{2}}^{(2)}$
16	D_{3d}	E_g	C_{3i}	^1E_g	$^1D''_{3d}=\bar{3}^{(3)}\wedge\tilde{\bar{2}}^{(2)}$
17	D_{3d}	E_u	C_{3i}	^1E_u	$^2D''_{3d}=\bar{3}^{(6)}\wedge\tilde{\bar{2}}^{(2)}$
18	D_{6h}	E_{2u}	C_{6h}	$^1E_{1u}$	$^1D''_{6h}=6^{(3)}/m'\wedge\tilde{\bar{2}}^{(2)}$
19	D_{6h}	E_{1u}	C_{6h}	$^1E_{2u}$	$^2D''_{6h}=6^{(6)}/m\wedge\tilde{\bar{2}}^{(2)}$
20	D_{6h}	E_{2g}	C_{6h}	$^1E_{1g}$	$^3D''_{6h}=6^{(3)}/m\wedge\tilde{\bar{2}}^{(2)}$
21	D_{6h}	E_{1g}	C_{6h}	$^1E_{2g}$	$^4D''_{6h}=6^{(6)}/m'\wedge\tilde{\bar{2}}^{(2)}$
22	O_h	E_g	T_h	^1E_g	$^1O''_h=\bar{6}^{(3)}/2\wedge\tilde{\bar{2}}^{(2)}$
23	O_h	E_u	T_h	^1E_u	$^2O''_h=\bar{6}^{(6)}/2\wedge\tilde{\bar{2}}^{(2)}$

Notes to table 1

In column (2) the point group G containing a 2D IR Γ is given in Schönflies notation. In column (3) is given the actual 2D IR Γ of G with which a minor quasi-symmetry group is associated. In column (4) is given the little group L, and in column (5) the 1D AIR of L that induces the 2D IR Γ of G.

In column (6) the minor quasi-symmetry group associated with the 2D IR Γ of G—and thus denoted as G'' with *two* primes—is given as the semi-direct product of two minor quasi-symmetry groups. The first of these is associated with the 1D AIR of L (which happens to be the normal sub-group H in the semi-direct product) which induces the 2D IR Γ of G, in the standard notation of coloured symmetry groups (Indenbom *et al* 1960). The second one is also a minor quasi-symmetry group which can be viewed as a double-coloured group of the corresponding point group T in some non-standard setting, depending upon G and S, in the semi-direct product $G=S\wedge T$. For example, consider the point group C_{4v}: $C_{4v}=C_4\wedge\tilde{m}$ and the minor quasi-symmetry group associated with the 1D complex IR ^1E of C_4 is denoted in the standard notation (Indenbom *et al* 1960) as $4^{(4)}$. The minor quasi-symmetry group generated by the point group $\tilde{m}$ (a non-standard setting of the point group m) can be viewed as a double-coloured group E, $R_2\sigma_x$ and is denoted by $\tilde{m}^{(2)}$. The groups $4^{(4)}$ and $\tilde{m}^{(2)}$ satisfy all the requirements of a semi-direct product when expressed as P-symmetry groups, and hence $C''_{4v}=4^{(4)}\wedge\tilde{m}^{(2)}$. Since the 1D complex IR ^1E of C_4 induces the 2D IR E of C_{4v}, we associate C''_{4v} with the 2D IR E of C_{4v}.

Several possible applications of the P-symmetry groups have been mentioned (Zamorzaev 1967, Krishnamurty *et al* 1978b, Rama Mohana Rao 1980). The notation employed in listing the minor quasi-symmetry groups is explained in the notes under each table. The nomenclature for the IR of the point groups is mostly that of Bradley and Cracknell (1972). As an example, the minor quasi-symmetry group C''_{4v} associated with the 2D IR E of the point group C_{4v} is illustrated in the notes under table 1 for completeness.

Table 2. Minor quasi-symmetry groups as semi-direct products associated with the 3D IR of the crystallographic point groups.

No	Point group G	3D IR Γ of G	Little group L (or isomorphic to L)	1D AIR of L	Minor quasi-symmetry group associated with the 3D IR T of G
1	T	T	D_2	B_2	$T''' = D_2^{(2)} \wedge 3^{(3)}$
2	T_h	T_g	D_{2h}	B_{2g}	${}^1T_h''' = {}^1D_{2h}^{(2)} \wedge 3^{(3)}$
3	T_h	T_u	D_{2h}	B_{2u}	${}^2T_h''' = {}^2D_{2h}^{(2)} \wedge 3^{(3)}$
4	O	T_1	D_4	A_2	$O''' = {}^1D_4^{(2)} \times 3^{(3)}$
		T_2	D_4	B_2	$\cong {}^2D_4^{(2)} \times 3^{(3)}$
					$\cong T''' \wedge \tilde{2}^{(2)}$
5	T_d	T_1	D_{2d}	A_2	$T_d''' = {}^1D_{2d}^{(2)} \times 3^{(3)}$
		T_2	D_{2d}	B_2	$\cong {}^2D_{2d}^{(2)} \times 3^{(3)}$
					$\cong T''' \wedge \tilde{m}^{(2)}$
6	O_h	T_{1g}	D_{4h}	A_{2g}	${}^1O_h''' = {}^1D_{4h}^{(2)} \times 3^{(3)}$
		T_{2g}	D_{4h}	B_{2g}	$\cong {}^2D_{4h}^{(2)} \times 3^{(3)}$
					$\cong {}^1T_h''' \wedge \tilde{2}^{(2)}$
7	O_h	T_{1u}	D_{4h}	A_{2u}	${}^2O_h''' = {}^3D_{4h}^{(2)} \times 3^{(3)}$
		T_{2u}	D_{4h}	B_{2u}	$\cong {}^4D_{4h}^{(2)} \times 3^{(3)}$
					$\cong {}^2T_h''' \wedge \tilde{2}^{(2)}$

Notes to table 2

In column (2) is given the crystallographic point group containing a 3D IR Γ. In column (3) is given the actual 3D IR Γ of G with which a minor quasi-symmetry group given in column (6) is associated. In column (4) is given the little group L (or the group isomorphic to L), and in column (5) the 1D AIR of L that induces the 3D IR Γ of G.

In column (6), in the case of the point groups O, T_d and O_h, both ways of expressing the minor quasi-symmetry groups—as an ordinary binary product and as a semi-direct product—are indicated, corresponding to both ways of expressing O and T_d: i.e. $O = D_4 \times C_3$ or $O = T \wedge \tilde{C}_2$, and $T_d = D_{2d} \times C_3$ or $T_d = T \wedge \tilde{m}$. It has already been shown that the minor quasi-symmetry groups obtained in both the ways given above are equivalent (Krishnamurty *et al* 1978b). The minor quasi-symmetry groups obtained as semi-direct products given in column (6) are indicated by G''' so as to denote that they are associated with the 3D IR.

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