

**SIMPLE AND MULTIPLE ANTISYMMETRY
SPACE GROUPS DERIVED FROM
CUBICAL P -SYMMETRY GROUPS**

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Abstract. By use of antisymmetric characteristic method, from cubical P -symmetry groups G_3^P ($P = 23, 26, \bar{43}, \bar{46}$) ($P, 2^l$)-symmetry three-dimensional space groups $G_3^{l,P}$ are derived.

Cubical P -symmetry three-dimensional space groups G_3^P ($P = 23, 26, \bar{43}, \bar{46}$) are derived by Yu. S. Karpova (Yu. S. Chubarova) [1,2]. From space groups G_3 are derived 35 junior G_3^{23} , 53 G_3^{26} , 74 $G_3^{\bar{43}}$ and 150 $G_3^{\bar{46}}$. By the use of the generalized antisymmetric characteristic method (AC -method) introduced by the author [3], some of the results mentioned will be corrected, and derived all cubical ($P, 2^l$)-symmetry three-dimensional space groups $G_3^{l,P}$ ($P = 23, 26, \bar{43}, \bar{46}$).

1. Some general remarks on (23)-, (26)-, ($\bar{43}$)- and ($\bar{46}$)-symmetry

The cubical symmetries (23)-, (26)-, ($\bar{43}$)- and ($\bar{46}$)- (or $(23C_3)$ -, $(26C_3)$ -, $(\bar{43}C_{3v})$ - and $(\bar{46}C_{3v})$ -symmetry, according [2]) are particular cases of the general P -symmetry [2,4] with $P \simeq T, T_h, O$ and O_h respectively.

In the case of (23)-symmetry $P \simeq A_4$ is the irregular permutation group, generated by the permutations $c_1 = (123)$ and $c_2 = (12)(34)$, satisfying the relations:

$$c_1^3 = c_2^2 = (c_1c_2)^3 = E.$$

In the case of (26)-symmetry $P \simeq T_h \simeq A_4 \times C_2$ is the irregular permutation group, generated by the permutations $c_1 = (123)(567)$, $c_2 = (12)(34)(56)(78)$ and $c_3 = (15)(26)(37)(48)$, satisfying the relations:

$$c_1^3 = c_2^2 = (c_1c_2)^3 = E \quad c_3^2 = E \quad c_1, c_2c_3.$$

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In the case of $(\overline{43})$ -symmetry $P \simeq O \simeq S_4$ is the irregular permutation group, generated by the permutations $c_1 = (1234)$ and $c_2 = (34)$, satisfying the relations:

$$c_1^4 = c_2^2 = (c_1 c_2)^3 = E.$$

In the case of $(\overline{46})$ -symmetry $P \simeq O_h \simeq S_4 \times C_2$ is the irregular permutation group, generated by the permutations $c_1 = (1728)(3645)$, $c_2 = (17)(35)$ and $c_3 = (15)(26)(37)(48)$, satisfying the relations:

$$c_1^4 = c_2^2 = (c_1 c_2)^3 = E \quad c_3^2 = E \quad c_1, c_2 c_3.$$

By introducing l antiidentity transformations e_1, \dots, e_l ($l \in N$) [5,6] commuting between themselves and with the generators of group P we have $(P, 2^l)$ -symmetry, with the group $P' = P \times C_2^l$.

Definition 1.

(a) a $(P, 2^l)$ -symmetry group is called the M^m -type $(P, 2^l)$ -symmetry group, if it is a M^m -type group regarded as a l -multiple antisymmetry group;

(b) a $(P, 2^l)$ -symmetry group $G^{l,P}$ is the group of the complete $(P, 2^l)$ -symmetry, if every e_i -transformation can be obtained in the group $G^{l,P}$ as an independent $(P, 2^l)$ -symmetry transformation. If the condition (b) it is not satisfied, such a group $G^{l,P}$ is the uncomplete $(P, 2^l)$ -symmetry group;

(c) a complete $(P, 2^l)$ -symmetry group $G^{l,P}$ is the junior $(P, 2^l)$ -symmetry group if all the relations given in the presentation of its generating symmetry group G remain satisfied after replacing the generators of the group G by the corresponding $(P, 2^l)$ -symmetry group generators.

In this work will be considered only the junior M^m -type complete $(P, 2^l)$ -symmetry groups.

From the reducibility of the group $T_h \simeq A_4 \times C_2 = \{c_1, c_2\} \times \{c_3\}$ results the equality of $(23, 2^l)$ - and $(26, 2^{l-1})$ -symmetry, and from the reducibility of the group $P \simeq S_4 \times C_2 = \{c_1, c_2\} \times \{c_3\}$ results the equality of $(\overline{43}, 2^l)$ - and $(\overline{46}, 2^{l-1})$ - symmetry. Using that equalities, the problem of the derivation of all cubical $(P, 2^l)$ -symmetry groups ($P = 23, 26, \overline{43}, \overline{46}$) is reduced to the derivation of $(P, 2^l)$ -symmetry groups ($P = 23, \overline{43}$).

The derivation will be realized by the use of generalized AC:

Definition 2. Let all the products of P -symmetry generators of a group G^P , within which every generator participates once at the most, be formed, and then subsets of transformations equivalent with regard to P -symmetry, be separated. The resulting system is called the antisymmetric characteristic of the group G^P and denoted by $AC(G^P)$ [3].

In the case of (23) -symmetry, in every transition from the antisymmetric characteristic $AC(G)$ of a generating group G to the antisymmetric characteristic $AC(G^{23})$ of a (23) -symmetry group G^{23} derived from it, the anti-

symmetric characteristic remains unchanged, and the conditions for $(23, 2^l)$ -symmetry groups of the M^m -type are the same as the conditions for l -multiple antisymmetry groups of the M^m -type. Hence, from every (23) -symmetry group G_3^{23} can be derived N_m junior $(23, 2^l)$ -symmetry groups of the M^m -type, where the number N_m is the same as the number of l -multiple antisymmetry groups of the M^m -type derived from its generating symmetry group G_3 . The corresponding data about $(23, 2^l)$ -symmetry groups and $(26, 2^l)$ -symmetry groups are given in Table 1.

Table 1

	(23)	(23, 2)	(23, 2 ²)	(23, 2 ³)	(26)	(26, 2)	(26, 2 ²)
38s	1	1					
39s	1	1			1		
43s	1	2	3		2	3	
49s	1	3	6		3	6	
51s	1	2	3		2	3	
52s	1	2	3		2	3	
53s	1	5	24	84	5	24	84
59s	3	3			3		
60s	1	1			1		
61s	3						
62s	3	6	9		6	9	
63s	1	3	6		3	6	
64s	3	3			3		
	21	32	54	84	32	54	84
49h	1	2	3		2	3	
50h	1	1					
	2	3	3		2	3	
62a	1	1			1		
69a	1	1			1		
74a	1	1			1		
75a	1	1			1		
76a	1	3	6		3	6	
77a	1	3	6		3	6	
78a	1	1			1		
81a	1	3	6		3	6	
89a	1						
90a	1	1			1		
91a	1	1			1		
92a	1	2	3		2	3	
	12	18	21		18	21	
	35	53	78	84	53	78	84

Having in mind the equality of $(\overline{43}, 2^l)$ - and $(\overline{46}, 2^{l-1})$ -symmetry, the only non-trivial problem is the derivation of $(\overline{43}, 2^l)$ -symmetry groups.

2. $(\overline{43}, 2^l)$ -symmetry three-dimensional space groups $G_3^{l, \overline{43}}$

The application of the theoretical assumptions given above will be illustrated by example of junior $(\overline{43}, 2^l)$ -symmetry three-dimensional space groups of the M^m -type derived in the family with the common generating symmetry group $G = \mathbf{68s}$ (P432), $\{a, b, c\}(3/4)$ with the $AC: \{4, 4a\}$ belonging to the AC -equivalency class 3.2 [3]. In the case of $(\overline{43})$ -symmetry we have two junior $(\overline{43})$ -symmetry groups [1]:

- (1) $\{a, b, c\}(3^3)/4^{\overline{4}}$,
- (2) $\{a^{(2)}, b^{(2')}, c^{(2'')}\}(3^3)/4^{2''}$.

The AC of the first group is of the form $\{\overline{4}, \overline{4}\}$, so from it can be derived $N_1 = 1$ $(\overline{43}, 2)$ -symmetry groups. The AC of the second is of the form $\{\underline{2}''\}, \underline{2}''(2)$. Because of non-equivalence of the transformations $\underline{2}''$ and $\underline{2}''(2) \sim \overline{4}$, in the sense of $(\overline{43})$ -symmetry, this AC results in the new $AC: \{\overline{4}\}\{a\}$ belonging to the AC -equivalence class 3.1 and giving $N_1 = 2$ $(\overline{43}, 2)$ -symmetry groups. Because of the equality between $(\overline{43}, 2)$ -symmetry and $(\overline{46})$ -symmetry, to the three obtained $(\overline{43}, 2)$ -symmetry groups: $\{\underline{a}, \underline{b}, \underline{c}\}(3^3)/4^{\overline{4}}$, $\{\underline{a}^{(2)}, \underline{b}^{(2')}, \underline{c}^{(2'')}\}(3^3)/4^{2''}$ and $\{\underline{a}, \underline{b}, \underline{c}\}(3^3)/4^{2''}$, correspond three $(\overline{46})$ -symmetry groups: $\{a^{(2)}, b^{(2)}, c^{(2)}\}(3^3)/4^{\overline{4}}$, $\{a^{(2)}, b^{(2')}, c^{(2'')}\}(3^3)/4^{2''}$ and $\{a^{(2)}, b^{(2')}, c^{(2'')}\}(3^3)/4^{\overline{4}}$.

In the same manner is realized the partial catalogue of all junior complete $(\overline{43}, 2^l)$ -symmetry three-dimensional space groups of the M^m -type $G_3^{l, \overline{43}}$, making possible their complete catalogation [7]. The final results corresponding respectively to symmorphic, hemisymorphic and asymmorphic $(\overline{43}, 2^l)$ -symmetry groups are summarized in the catalogue, which can be obtained directly from the author. The enumeration results are given in Table 2:

Table 2

	$(\overline{43})$	$(\overline{43}, 2)$	$(\overline{43}, 2^2)$	$(\overline{43}, 2^3)$	$(\overline{46})$	$(\overline{46}, 2)$	$(\overline{46}, 2^2)$
40s	1	2			2		
41s	1	2			2		
42s	1	2			2		
44s	1	1			1		
45s	1	1			1		
46s	1	1			1		
47s	1	4	12		4	12	
48s	1	4	12		4	12	
50s	1	6	24		6	24	
54s	1	4	12		4	12	
55s	1	4	12		4	12	
56s	1	4	12		4	12	
57s	1	4	12		4	12	
58s	1	10	96	672	10	96	672
65s	2	4			4		

66s	1	2			2		
67s	2						
68s	2	3			3		
69s	1	2			2		
70s	2						
71s	2	8	24		8	24	
72s	1	6	24		6	24	
73s	3	6			6		
	30	80	240	672	80	240	672
39h	1						
40h	1						
41h	1						
42h	1	2			2		
43h	1	2			2		
44h	1	2			2		
45h	1	2			2		
46h	1	2			2		
47h	1	2			2		
48h	1	6	24		6	24	
51h	1						
52h	2						
53h	1	2			2		
54h	3	6			6		
	17	26	24		26	24	
70a	1	1			1		
71a	1	1			1		
72a	1	1			1		
73a	1	1			1		
79a	1	2			2		
80a	1	2			2		
82a	1	2			2		
83a	1	2			2		
84a	1	4	12		4	12	
85a	1	4	12		4	12	
86a	1	2			2		
87a	1	6	24		6	24	
88a	1	6	24		6	24	
93a	1						
94a	1						
95a	1						
96a	1	2			2		
97a	3						
98a	2	3			3		
99a	1	2			2		
100a	1	2			2		
101a	1	2			2		
102a	1	2			2		
103a	1	4	12		4	12	

27	51	84		51	84	
74	157	348	672	157	348	672

From the results of the derivation of the $(\overline{43}, 1)$ -symmetry groups we can first conclude that, because of the equality between $(\overline{43}, 1)$ - and $(\overline{46})$ -symmetry, there exist 157 (not 150) $[1, 2]$ $(\overline{43}, 1)$ -symmetry groups and, consequently, the same number of $(\overline{46})$ -symmetry groups. Such a disagreement with the results mentioned implies the necessary corrections for the $(\overline{46})$ -symmetry groups in the families with the generating groups **46s** (R32), **65s** (P43m), **70a** (P3₁21), **71a** (P3₂21), **72a** (P3₁12), **73a** (P3₂12) and **98a** (P4₂32). For these families, the correct numbers of $(\overline{46})$ -symmetry groups are respectively, 1 (not 2), 4 (not 3), 1 (not 0), 1(not 0), 1(not 0), 1(not 0) and 3 (not 0).

3. Conclusion

As the final result, for the junior cubical complete $(P, 2^l)$ - symmetry three-dimensional space groups of the M^m -type the numbers N_m^P ($P = 23, 26, \overline{43}, \overline{46}$) are the following:

$$\begin{aligned} N_0^{23} &= 35 & N_0^{\overline{43}} &= 74 \\ N_1^{23} &= N_0^{26} = 53 & N_1^{\overline{43}} &= N_0^{\overline{46}} = 157 \\ N_2^{23} &= N_1^{26} = 78 & N_2^{\overline{43}} &= N_1^{\overline{46}} = 348 \\ N_3^{23} &= N_2^{26} = 84 & N_3^{\overline{43}} &= N_2^{\overline{46}} = 672 \end{aligned}$$

References

- [1] Chubarova Yu.S., *Derivation of junior space groups of P-simmetry*, Avtoref. dis. ... kand. fiz.-mat. nauk, Shtiintsa, Kishinev, 1983.
- [2] Zamorzaev A.M., Karpova Yu.S., Lungu A.P., Palistrant A.F., *P-symmetry and its further development*, Shtiintsa, Kishinev, 1986.
- [3] Jablan S.V., Algebra of Antisymmetric Characteristics, *Publ. Inst. Math.*, **47** (61) (1990), 39-55.
- [4] Zamorzaev A.M., Galyarskij E.I., Palistrant A.F., *Colored symmetry, its generalizations and applications*, Shtiintsa, Kishinev, 1978.
- [5] Zamorzaev A.M., *Theory of simple and multiple antisymmetry*, Shtiintsa, Kishinev, 1976.
- [6] Zamorzaev A.M., Palistrant A.F., Antisymmetry, its generalizations and geometrical applications, *Z.Kristall.*, **151** (1980), 231-248.
- [7] Jablan S.V., A New Method of Deriving and Cataloguing Simple and Multiple Antisymmetry G_3^l Space Groups, *Acta Cryst.*, **A43** (1987), 326-337.

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