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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 $(P = 23, 26, \overline{4}3, \overline{4}6)$ $(P, 2^l)$-symmetry three-dimensional space groups $G_3^{l,P}$ are derived.

Cubical P-symmetry three-dimensional space groups G_3^P $(P = 23, 26, \overline{4}3, \overline{4}6)$ 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 $G_3^{\overline{4}3}$ and 150 $G_3^{\overline{4}6}$. 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 $G_3^{l,P}$ $(P = 23, 26, \overline{4}3, \overline{4}6)$.

1. Some general remarks on (23)-, (26)-, ($\overline{4}$3)- and ($\overline{4}$6)-symmetry

The cubical symmetries (23)-, (26)-, ($\overline{4}$3)- and ($\overline{4}$6)- (or ($23C_3$)-, ($26C_3$)-, ($\overline{4}3C_{3v}$)- and ($\overline{4}6C_{3v}$)-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 $(\overline{4}3)$-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:

$$c_1^4 = c_2^2 = (c_1c_2)^3 = E.$$

In the case of $(\overline{4}6)$-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:

$$c_1^4 = c_2^2 = (c_1c_2)^3 = E \quad c_3^2 = E \quad c_1, c_2c_3.$$

By introducing l antiidentity transformations $e_1, \dots, e_l$ $(l \in N)$ [5,6] commuting between themeselves 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 $(\overline{4}3, 2^l)$- and $(\overline{4}6, 2^{l-1})$- symmetry. Using that equalities, the problem of the derivation of all cubical $(P, 2^l)$-symmetry groups $(P = 23, 26, \overline{4}3, \overline{4}6)$ is reduced to the derivation of $(P, 2^l)$-symmetry groups $(P = 23, \overline{4}3)$.

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 antisymmetric 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 $(\overline{4}3, 2^l)$- and $(\overline{4}6, 2^{l-1})$-symmetry, the only non-trivial problem is the derivation of $(\overline{4}3, 2^l)$-symmetry groups.

2. $(\overline{4}3, 2^l)$-symmetry three-dimensional space groups $G_3^{l,\overline{4}3}$

The application of the theoretical assumptions given above will be illustrated by example of junior $(\overline{4}3, 2^l)$-symmetry three-dimensional space groups of the M^m-type derived in the family with the common generating symmetry group $G =$**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 $(\overline{4}3)$-symmetry we have two junior $(\overline{4}3)$-symmetry groups [1]:

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

(2) $\{a^{(2}, b^{(2'}, c^{(2"}\}(3^{3)}/4^{\underline{2}")})$.

The AC of the first group is of the form $\{(\overline{4}, (\overline{4}\}$, so from it can be derived $N_1 = 1$ $(\overline{4}3, 2)$-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 $(\overline{4}3)$-symmetry, this AC results in the new AC:$\{\overline{4}\}\{a\}$ belonging to the AC-equivalence class 3.1 and giving $N_1 = 2$ $(\overline{4}3, 2)$-symmetry groups. Because of the equality between $(\overline{4}3, 2)$-symmetry and $(\overline{4}6)$-symmetry, to the three obtained $(\overline{4}3, 2)$-symmetry groups: $\{\underline{a}, \underline{b}, \underline{c}\}(3^{3)}/4^{(\overline{4})}$, $\{\underline{a}^{(2}, \underline{b}^{(2'}, \underline{c}^{(\underline{2}"}\}(3^{3})/4^{\underline{2}")})$ and $\{\underline{a}, \underline{b}, \underline{c}\}(3^{3)}/\underline{4}^{\underline{2}")})$, correspond three $(\overline{4}6)$-symmetry groups: $\{a^{(2)}, b^{(2)}, c^{(2)}\}(3^{3)}/4^{(\overline{4})})$, $\{a^{(\underline{2}}, b^{(\underline{2}'}$, $c^{(\underline{2}"}\}(3^{3)}/4^{\underline{2}")})$ and $\{a^{(\underline{2}}, b^{(\underline{2}'}, c^{(\underline{2}"}\}(3^{3)}/4^{(\overline{4})})$.

In the same manner is realized the partial catalogue of all junior complete $(\overline{4}3, 2^l)$-symmetry three-dimensional space groups of the M^m-type $G_3^{l,3\overline{4}}$, making possibile their complete cataloguation [7] . The final results corresponding respectively to symmorphic, hemisymorphic and asymmorphic $(\overline{4}3, 2^l)$-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

	$(\overline{4}3)$	$(\overline{4}3, 2)$	$(\overline{4}3, 2^2)$	$(\overline{4}3, 2^3)$	$(\overline{4}6)$	$(\overline{4}6, 2)$	$(\overline{4}6, 2^2)$
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 $(\overline{4}3,1)$-symmetry groups we can first conclude that, because of the equality between $(\overline{4}3,1)$- and $(\overline{4}6)$-symmetry, there exist 157 (not 150) [1,2] $(\overline{4}3,1)$-symmetry groups and, consequently, the same number of $(\overline{4}6)$-symmetry groups. Such a disagreement with the results mentioned implies the necessary corrections for the $(\overline{4}6)$-symmetry groups in the families with the generating groups **46s** (R32), **65s** (P43m), **70a** ($P3_121$), **71a** ($P3_221$), **72a** ($P3_112$), **73a** ($P3_212$) and **98a** ($P4_232$). For these families, the correct numbers of $(\overline{4}6)$-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 $(P = 23, 26, \overline{4}3, \overline{4}6)$ are the following:

$N_0^{23} = 35$ $\quad N_0^{\overline{4}3} = 74$
$N_1^{23} = N_0^{26} = 53$ $\quad N_1^{\overline{4}3} = N_0^{\overline{4}6} = 157$
$N_2^{23} = N_1^{26} = 78$ $\quad N_2^{\overline{4}3} = N_1^{\overline{4}6} = 348$
$N_3^{23} = N_2^{26} = 84$ $\quad N_3^{\overline{4}3} = N_2^{\overline{4}6} = 672$

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