MACKAY ANTISYMMETRY SPACE GROUPS *

LJILJANA RADOVIĆ†

The Faculty of Mechanical Engineering, Beogradska 14, 18000 Niš, Serbia

E-mail: liki@masfak.ni.ac.yu

SLAVIK JABLAN‡

The Mathematical Institute, Knez Mihailova 35, P.O.Box 367, 11001 Belgrade, Serbia

E-mail: jablans@mi.sanu.ac.yu

By using the antisymmetry characteristic method implemented in computer programs written in *Mathematica 4*, from 230 space symmetry groups are derived 1191 Mackay groups of the type M^1, 5005 groups of the type M^2, 19467 groups of the type M^3, 72587 groups of the type M^4, 191728 groups of the type M^5, and 598752 groups of the type M^6. Mackay groups are the minimal representation of Zamorzaev's multiple antisymmetry groups derived from 230 space groups.

1. Introduction

The concept of antisymmetry was introduced by H.Heesch [1]. The development of the theory of antisymmetry can be followed though the works of A. V. Shubnikov and V. A. Koptsik [2], A. V. Shubnikov and N. V. Belov [3], A. M. Zamorzaev [4], A. M. Zamorzaev and A. F. Palistrant [5,6], and Kishinev school [7]. Its natural generalization, the idea of multiple antisymmetry was suggested by A. V. Shubnikov and introduced by A. M. Zamorzaev in 1956 [8]. Few months later, another concept of multiple antisymmetry was proposed by A. L. Mackay [9]. After that, mainly by the contribution of the Kishinnev school (Zamorzaev, Palistrant, Gal-

* *MSC 2000:* 20H15.

Keywords: antisymmetry, multiple antisymmetry, mackay groups.

† Work supported by the Ministry of Science under contract No *1646.*

‡ Work supported by the Ministry of Science and Environmental Protection under contract No *144032.*

yarskii,...), the theory of multiple antisymmetry was extended to all categories of isometric symmetry groups of the space E^n ($n \leq 3$), different kinds of non-isometric symmetry groups (of the similarity symmetry, conformal symmetry, *etc.*) and P-symmetry groups [4,5,6,8,10]. On the other hand, the investigation of Mackay approach to the multiple antisymmetry [9] was not continued for many years.

In the case of l-multiple antisymmetry we have a discrete symmetry group G with the set of generators $\{S_1, S_2, \ldots, S_r\}$, given by the presentation (generators and defining relations)

$$g_n(S_1, S_2, ..., S_r) = E, \quad n = 1, ..., s$$

and the set of anti-identities $e_1, e_2, \ldots, e_l$ of the first, second, …, lth kind that generate the group C_2^l and satisfy the relations

$$e_i e_j = e_j e_i \quad e_i^2 = E \quad e_i S_q = S_q e_i, \quad i, j = 1, ..., l, \quad q = 1, ..., r.$$

A group that consists of the transformations $S' = e'S$, where e' is the identity, anti-identity, or a product of anti-identities, is called l-multiple antisymmetry group. In particular, for $i = j = l = 1$ we have simple antisymmetry.

All multiple antisymmetry groups can be divided into the groups of S^k ($1 \leq k \leq l$), $S^k M^m$ ($1 \leq k, m$; $k + l \leq m$) and M^m type ($1 \leq m \leq l$). Because the groups of S^k and $S^k M^m$ types can be derived directly from a generating group G and from the groups of the M^m type, only non-trivial problem is the derivation of the M^m type (junior) groups. Hence, in this paper are considered only the junior multiple antisymmetry groups, i.e. the multiple antisymmetry groups isomorphic with their generating symmetry group G, that posses a system of independent antisymmetries of different kinds. The antisymmetries of different kinds are independent if their corresponding anti-identities and their products generate the group $E^{(m)} \cong C_2^m$.

From every symmetry group G can be derived $(2^m - 1)...(2^m - 2^{m-1})$ antisymmetry groups of the type M^m with a fixed (common) subgroup H of the index 2^m, but some of them can be equal. For detecting the equality of multiple antisymmetry groups, different methods and criteria can be used. Each junior multiple antisymmetry group G' of the type M^m can be denoted by a group/subgroup symbol $G/(H_1, H_2, ..., H_m)/H$, where G is the generating (symmetry) group, H_i are its subgroups of the index 2 satisfying the relationships $G/H_i \cong C_2 = \{e_i\}$, and H is the subgroup of the index 2^m– the symmetry subgroup of the group G' ($G/H \cong C_2^m$). A group/subgroup symbol does not uniquely define its corresponding multiple antisymmetry group, so we need to use the extended symbols. For example, an extended symbol for the junior groups of the type M^3 is $G/(H_1, H_2, H_3)/(H_{12}, H_{13}, H_{23}/H$, where $H_{ij} = H_i \cap H_j$ $(1 \leq i < j \leq 3)$.

According to Zamorzaev's approach, two junior multiple antisymmetry groups of the M^m type are equal *iff* their extended group/subgroup symbols coincide. In this case, the order of the subgroups H_i in the extended group/subgroup symbol is important, and the anti-identities e_i $(i = 1, 2, ..., l)$ are treated as non-equivalent and mutually different. They can be interpreted as the representatives of different physical or geometrical bivalent properties (e.g., as a change of the signs of the electrical charges $(+, -)$, magnetic orientations (S, N), *etc.*).

If we accept the equality of those anti-identities– their equal physical or geometrical role, as the result we obtain Mackay l-multiple antisymmetry groups (M-groups). Hence, the difference between M-groups (Mackay groups) and Z-groups (Zamorzaev groups) follows from the equality criterion. In the case of M-groups, two junior multiple antisymmetry groups of the type M^m are equal *iff* their extended symbols are $G/(H_1, H_2, ..., H_m)/(H_{i_1}, H_{i_2}, ..., H_{i_m}/H$, where $(i_1\, i_2\, ...i_m)$ is the permutation of the set $\{1, 2, ..., m\}$. Every Z-group can be obtained from the corresponding M-group by permuting anti-identities, so we can conclude that M-groups are the minimal representation of Z-groups.

The antisymmetry characteristic method (AC-method), introduced by S. Jablan [11] is used for the derivation of multiple antisymmetry groups.

Definition 1.1 Let all products of the generators of a group G, within which every generator participates once at the most, are formed, and then subsets of transformations that are equivalent in the sense of symmetry with regard to the symmetry group G are selected. The resulting system is called the antisymmetry characteristic of the group G, denoted as $AC(G)$.

The reduced AC can be obtained from a complete AC as the minimal number of subsets which can give all the elements in AC by multiplication, having in mind the idempotency.

Example 1.1 If the symmetry group **pm** is given by the generators $\{X, Y, R\}$, $XY = YX$, $RY = YR$, $R^2 = (RX)^2 = E$ the complete AC is $\{R, RX\}\{Y\}\{RY, RXY\}\{X\}\{XY\}$, and the reduced AC is $\{R, RX\}\{Y\}$.

Definition 1.2 Two or more Z- or M-groups belong to a family *iff* they are derived from the same symmetry group G.

There are some useful theorems [12, 13].

Theorem 1.1 *Two Z-groups G' and G'' of the M^m type for fixed m, with a common generating group G are equal iff they posses equal ACs.*

Theorem 1.2 *Two M-groups G' and G'' of the M^m type for fixed m, with a common generating group G, are equal iff there is a permutation of the anti-identities $e_1, e_2, ..., e_m$ transforming $AC(G')$ into the $AC(G'')$.*

Every $AC(G)$ completely defines the series $N_m(G)$ and $M_m(G)$, where $N_m(G)$ and $M_m(G)$ denote, respectively, the number of Z- and M-groups of the M^m type for each particular m ($1 \leq m \leq l$).

Theorem 1.3 *Symmetry groups possessing isomorphic ACs generate the same number of Z- or M-groups of the M^m type for each particular m; groups derived correspond with each other with regard to structure.*

Corollary 1.1 *The derivation of all Z- or M-groups can be completely reduced to the construction of all non-isomorphic ACs and derivation of the corresponding groups from those ACs.*

The papers [12,13] contain the complete list of non-isomorphic ACs with the generators and the comparative list of the numbers N_m and M_m corresponding to those ACs. All the results in [12,13] are obtained "by hand", and our recent results are obtained by the use of the computer programs.

2. Mackay groups and their derivation

In the paper *Mackay groups and their applications* by S. Jablan [13] one can find survey results about Mackay groups and their applications. The open question that remained there was to find effective algorithms for the derivation of Mackay groups from the space groups G_3. Another problem, proposed by A. F. Palistrant and connected with the derivation of Mackay groups was to obtain multi-dimensional symmetry groups of the categories G_{63} and G_{653}. For that, it was necessary to generalize space groups G_3 by using 32 P-symmetries, where P is isomorphic with , and 31 P-symmetries where P is isomorphic with G_{30} [6]. To solve this problem and complete the derivation of the symmetry groups of the categories G_{63} and G_{653}, the only class of P- symmetry groups that remained non derived are $22\underline{1}$-symmetry groups, corresponding to the symmetry group P of the "brick" **mmm**, i.e. Mackay 3-multiple antisymmetry groups derived from the space groups G_3.

In the papers [12,13], Mackay groups are derived from all ACs with $n \leq 4$ generators. Hence, for the complete derivation of Mackay groups from 230 space groups we need to derive M-groups from the seven space symmetry groups from the paper [10]:

$7s$ with the AC: $\{A,B\}\{C,D,E,CDE\}$;

$9s$ with the AC:

$\{\{C\}\{D,DA,DB,DAB\},\{B\}\{E,EA,EC,EAC\},\{A\}\{DE,DEB,DEC,DEBC\}\}$
$\{\{D,E,DE\},\{DA,EA,DE\},\{E,DB,DEB\},\{EA,DAB,DEB\},\{D,EC,DEC\}$
$\{DA,EAC,DEC\},\{DB,EC,DEBC\},\{DAB,EAC,DEBC\}\}$;

$13s$ with the AC: $\{A\}\{\{B,C\},\{D,E\}\}$;

$18s$ with the AC: $\{\{A,B\},\{C,D\},\{E,F\}\}$;

$19s$ with the AC: $\{A\}\{B,C\}\{D,E\}$;

$21s$ with the AC: $\{\{A,B\},\{C,D\},\{AC,E\}\}$; and

$21h$ with the AC: $[A,B][AE,BE]\{[C,CE],[D,DE]\}[A,B][AE,BE]$.

3. Systems of anti-identities

In order to derive M-groups from 230 space groups, first we need to find all non-equivalent (n,m) systems of independent anti-identities e_i $(1 \leq i \leq m)$ and their products, where n is the number of generators, and m indicates the type of antisymmetry. They are the systems from which every anti-identity can be obtained as independent by multiplying suitably chosen elements of the system. For example, the system $\{e_1, e_1e_2, e_1e_2e_3\}$ consists from independent anti-identities or their products that generate the group $E^{(3)} = \{e_1\} \times \{e_2\} \times \{e_3\} \cong C_2^3$, and the system $\{e_1e_2, e_1e_3, e_2e_3\}$ does not satisfy this property. Every system is the set ordered in the lexicographic order, and can be written in a more concise indexed form. In the indexed form the identity E is denoted by 0, and every e_i $(1 \leq i \leq m)$ is denoted by i. E.g., the indexed form of the system $\{e_1, e_1e_2, e_1e_2e_3\}$ is $\{1, 1\,2, 1\,2\,3\}$. From here in the sequel all systems will be written in the indexed form, and the term "system" will have the meaning "indexed system".

Definition 3.1 Two (n,m) systems s_1 and s_2 are equivalent *iff* there exists a permutation p from the permutation group S_n, such that $p(s_1) = s_2$.

The set of all mutually non-equivalent (n,m) systems with independent anti-identities or their products will be denoted by $S_{n,m}$.

In order to generate all such systems, we propose new and very efficient recursive algorithm, implemented in the computer program developed in *Mathematica 4*.

The basic idea of the algorithm is that every anti-identity e_m $(1 \leq m \leq n)$ or a product of the anti-identities, for fixed n (where n is the number of generators of the generating symmetry group G), can be represented as the vector of the length n. E.g., for $e_1 = (1,0,0)$, $e_2 = (0,1,0)$, $e_3 = (0,0,1)$, $e_1e_2 = (1,1,0)$, $e_1e_3 = (1,0,1)$, $e_2e_3 = (0,1,1)$, and $e_1e_2e_3 = (1,1,1)$. The product of anti-identities is defined as the addition of vectors (mod 2).

In order to derive the systems $S_{n+1,m}$ from the systems $S_{n,m}$, to every system from $S_{n,m}$ the anti-identities of the (n+1)th level and their products are added, and then repeated systems (equivalent to some of preceding ones) are deleted. For example, in order to derive the systems $S_{3,2}$ from the $S_{2,2}$ systems $\{1,2\}$ and $\{1,1\,2\}$, we add to them 0, 1, 2, and 1 2, respectively, and then delete all repeated systems. As the final result, we obtain 6 mutually non-equivalent $S_{3,2}$ systems: $\{0,1,2\}$, $\{1,1,2\}$, $\{0,1,1\,2\}$, $\{1,1,1\,2\}$, $\{1,2,1\,2\}$, and $\{1,1\,2,1\,2\}$. Another algorithm is developed for the derivation of (m,m) systems. Combining those two algorithms, the systems of higher levels $(n \geq 5)$ are obtained.

Every system s can be represented as a matrix S, where the rows are anti-identities (as vectors). Anti-identities and their products belonging to a system (n,m) are independent if there is a block in the matrix S of the range m; for a system (m,m) the condition is $det(S) \neq 0 \pmod 2$.

Definition 3.2 The morphism of the system s is the number of different Z-systems that can be obtained from s by all permutations of anti-identities (indexes different from 0) belonging to it.

For example, the morphism of the system $\{1,2,1\,2\}$ is 1, the morphism of the system $\{1,2,3,1\,2\}$ is 3, and the morphism of the system $\{1,2,3,4,1\,2\}$ is 6.

The stabilizer St_s of the system s is:

$$St_s = \{p \in S_m | p(s) = s\},$$

and the orbit of the system s

$$s^{S_m} = \{p(s) | p \in S_m\}$$

represents all different Z-systems. The morphism of the system s is equal to the index of the stabilizer in the permutation group

$$morf(s) = |s^{S_m}| = |S_m : St_s|.$$

Also, because $|S_m| = m!$, it holds

$$m! = |St_s| \cdot morf(s).$$

M- systems are the transversal of the set of Z-systems, so the number of Z- systems is

$$ZS_{n,m} = \sum_{s \in S_{n,m}} |s^{Sm}| = \sum_{s \in S_{n,m}} |S_m : St_s|.$$

We can also define the morphism of AC with respect to the particular system s inserted in it.

Definition 3.3 The morphism of AC with respect to the particular system inserted in it is the number of different ACs which can be obtained from $AC(s)$ by all permutations $p \in S_m$.

This means that ACs of all Z-groups can be obtained as the orbits of ACs of M-groups, and that all Z-groups can be obtained from M-groups by the permutations of anti-identities.

If the number of all non-equivalent systems $S_{n,m}$ is denoted by $M_{m,n}$, for $m = 2$ and $n = 2, ..., 10$ there are 2, 6, 13, 23, 37, 55, 78, 106, and 140 systems, respectively, indicating the general formulas:

(1) $M_{2,n} = \frac{k}{6}(4k^2 + 15k - 7)$ for $n = 2k$,

(2) $M_{2,n} = \frac{k}{6}(4k^2 + 21k + 11)$ for $n = 2k + 1$.

For $m = 3$ and $n = 3, ..., 17$ there are 7, 33, 101, 249, 576, 1099, 1915, 3308, 4565, 8702, 13482, 20168, 29587, 42511, and 59959 systems $S_{n,3}$, respectively. For $m = 4$ and $n = 4, ..., 7$ there are 51, 367, 1731, and 6248 systems; for $m = 5$, $n = 5, 6$ we obtain 885, and 10753 systems $S_{n,6}$, and for $m = 6$ we obtain 44206 systems $S_{6,6}$.

All those systems correspond to the AC of the general form $\{A_1, A_2, ..., A_n\}$ [14]. We already mentioned that for every system (and every Mackay group) we can define its morphism: the number of different Z-systems (Z-groups) that can be obtained from it by permuting anti-identities. If we make all possible permutations in the M-systems, we have the Z-systems obtained from the AC: $\{A_1, A_2, ..., A_n\}$ (corresponding to the symmetry group **mm...m** belonging to the category G_{n0} of the space E^n).

The combinatorial formula [14] for the numbers N_m corresponding to the AC: $\{A_1, A_2, ..., A_n\}$ is corrected:

Theorem 3.1 *The number of all junior Z-groups derived from the AC: $\{A_1, A_2, ..., A_n\}$ is given by the formula*

$$N(n,m) = \sum_{k=m}^{n} C(k,m)\binom{n-1}{k-1}$$

where the coefficients $C(k,m)$ represent the number of all different k-element sets of the generators of the group C_2^m:

$$\text{(1)} \qquad C(m,m) = \frac{\prod_{l=1}^{m}(2^m - 2^{l-1})}{m!} \quad \text{for} \quad k = m,$$

$$\text{(2)} \qquad C(m,k) = \binom{2^n}{k} - \sum_{i=1}^{m-1} k_i^m C(m-i,k) \quad \text{for} \quad k > m,$$

where the coefficients k_i^m are given by: $k_i^m = \prod_{l=1}^{i} \frac{2^m - 2^{l-1}}{2^i - 2^{i-1}}$.

This formula enables us to compute the number of different Z-systems for every n.

We developed the recursive algorithms and the corresponding programs able to generate systems $S_{n,m}$ even for large values of n ($n = 7, 8, 9, ...$). As a double check of the results obtained we used the number of Z-systems (Theorem 3.1).

4. Derivation of Mackay groups from 230 space groups

The derivation of $S_{n,m}$ systems was the first step in solving the general open problem: derivation of all Mackay groups from 230 space groups G_3 [13]. For the derivation of Mackay groups, we used the programs written in *Mathematica 4*. Two different types of programs are used: first, for the derivation of $S_{n,m}$ systems, and the others for the derivation of M-groups for every class of non-isomorphic ACs. In the case of space symmetry groups G_3 there are 34 such classes [11]. For every space symmetry group (this means for each representative of the equivalence class of the space groups according to the AC isomorphism) is written the particular program based on the AC-method for the derivation of Mackay groups.

The numbers M_m of Mackay groups for ACs with $n \leq 4$ generators are given in the papers [12,13]. After the double check, all the results from those papers are confirmed for $m \leq 3$, and some of them are corrected for $m = 4$.

From symmetry groups with n generators we derived all antisymmetry and m-multiple antisymmetry Mackay groups ($1 \leq m \leq n$). For every AC class and fixed m we use the following algorithm:

(1) take the first system from the corresponding list of $S_{n,m}$ systems;
(2) insert the system into the AC in all possible ways according to the AC structure;
(3) for every particular placement, make all possible permutations of anti-identities represented as vectors;
(4) delete all repeated ACs, save different ACs and the data describing their morphism;
(5) repeat the procedure for all systems from the corresponding list of $S_{n,m}$ systems.

As the result is obtained the complete list of M-groups derived from the given AC.

For a relatively small number of generators and low antisymmetry levels, this algorithm is fast enough. Because of a large number of permutations and systems exceeding computer memory, systems $S_{5,5}$, $S_{6,5}$, and $S_{6,6}$ we divided into the specific equivalence classes and worked only with their representatives.

To detect systems that result in the same number of M- (or Z-groups), we need to consider combinatorial placements of elements. For the derivation of Z-groups by using AC-method [11,15], S. Jablan used the type of AC with respect to the decomposition of AC that can occur in the transition to every next antisymmetry level. Because of the action of permutations, it was not possible to use the same idea in the case of Mackay groups, so we modified it for M-groups.

Definition 4.1 Every system s can be divided into lexicographically ordered subsets consisting from equal elements. The list of lengths of those subsets will be called *the set type* of s.

For example, the set type of the system $\{1, 1, 2, 3, 1\,4, 1\,4\}$ is $\{2, 2, 1, 1\}$, and the set type of the system $\{0, 1, 2, 3, 1\,4, 3\,4\,5\}$ is $\{1, 1, 1, 1, 1, 1\}$. The systems of the same set type give the same number of placements in any AC, that correspond to each other with the regard to the structure.

Definition 4.2 Let us consider any given system s ($s \in S_{n,m}$) decomposed into minimal subsets, such that the stabilizer of each subset is St_s. Decomposition of the system s according to St_s will be called *p-decomposition* of s, and denoted by s^p.

All the $S_{n,m}$ systems with the same morphism can be divided according to their set types. For example, $S_{6,5}$ systems of the morphism 60 can be divided according to the set types into two classes: the systems of the set type $\{2,1,1,1,1\}$ and $\{1,1,1,1,1,1\}$.

The representatives of the first set type are the systems:

$s_1 = \{1,1,2,3,1\,4,4\,5\}$, $St_{s_1} = \{I,(2\,3)\}$, $s_1^p = \{1\}\{1\}\{2,3\}\{1\,4\}\{4\,5\}$, and
$s_2 = \{1,1,2,3,2\,4,3\,5\}$, $St_{s_2} = \{I,(2\,3)(4\,5)\}$, $s_2^p = \{1\}\{1\}\{2,3\}\{2\,4,3\,5\}$.

The representatives of the other set type are the systems:

$s_3 = \{0,1,2,3,1\,4,4\,5\}$, $St_{s_3} = \{I,(2\,3)\}$, $s_3^p = \{0\}\{1\}\{2,3\}\{1\,4\}\{4\,5\}$,
$s_4 = \{1\,2,1\,3,2\,4,3\,5,1\,2\,4,1\,3\,5\}$, $St_{s_4} = \{(2\,3)(4\,5)\}$,
$s_4^p = \{1\,2,1\,3\}\{2\,4,3\,5\}\{1\,2\,4,1\,3\,5\}$, and
$s_5 = \{0,1,2,3,1\,4,2\,5\}$, $St_{s_5} = \{(1\,2)(4\,5)\}$, $s_5^p = \{0\}\{1\,2\}\{3\}\{1\,4,2\,5\}$.

In the same way, among $S_{6,5}$ systems of the morphism 30 are distinguished the systems of the set type $\{2,1,1,1,1\}$ with the representative

$s_6 = \{1,1,2,3,1\,4,1\,5\}$, $St_{s_6} = \{I,(2\,3),(4\,5),(2\,3)(4\,5)\}$,
$s_6^p = \{1\}\{1\}\{2\,3\}\{1\,4,1\,5\}$, and

the systems of the set type $\{1,1,1,1,1,1\}$ with the representative

$s_7 = \{0,1,2,3,4,1\,2\,5\}$, $St_{s_7} = \{I,(1\,2),(3\,4),(1\,2)(3\,4)\}$,
$s_7^p = \{0\}\{1\,2\}\{3,4\}\{1\,2\,5\}$.

Definition 4.3 Two $S_{n,m}$ systems s_1 and s_2 that have the same morphism and set type will be of the same p-type if there is a bijection between the corresponding subsets of $s_1^{p_1}$ and $s_1^{p_1}$. Systems of the same p-type will be called M-equivalent.

Theorem 4.1 *All M-equivalent systems give the same number of Mackay groups derived from a given AC, and obtained groups correspond to each other in morphism.*

Working with the symmetry group 18s with the AC:

$$\{\{A,B\},\{C,D\},\{E,F\}\},$$

the system s_1 gives 6 M-groups, s_2 gives 7 M-groups, s_3 gives 9 M-groups, s_4 gives 11, s_5 gives 9, s_6 gives 7, and the system s_7 gives 6 M-groups.

Every AC can be treated as a set of rules that determine the placement of the elements of a system. We recognized systems that will act in the same way, in the combinatorial sense, with regard to an AC. For every system s we can consider the stabilizer of $AC(s)$ obtained by putting the system into the AC in question. The morphism of the $AC(s)$ is equal or greater than the morphism of the system. Every permutation belonging to the stabilizer of $AC(s)$ is the member of St_s, but *vice-versa* is not true. Knowing the stabilizers of M-groups obtained, we can make conclusion about their morphisms.

For example, from the system $s_1 = \{1, 1, 2, 3, 1\,4, 4\,5\}$, from the AC of the group $18s$ we obtain 9 possible placements

(1) $\{\{1, 1\}, \{2, 3\}, \{1\,4, 4\,5\}\}$ (1)
(2) $\{\{1, 2\}, \{1, 3\}, \{1\,4, 4\,5\}\}$ (2)
(3) $\{\{1, 1\,4\}, \{1, 4\,5\}, \{2, 3\}\}$ (3)
(4) $\{\{1, 1\}, \{2, 1\,4\}, \{3, 4\,5\}\}$ (4)
(5) $\{\{1, 1\}, \{2, 4\,5\}, \{3, 1\,4\}\}$ (4)
(6) $\{\{1, 2\}, \{1, 1\,4\}, \{3, 4\,5\}\}$ (5)
(7) $\{\{1, 3\}, \{1, 1\,4\}, \{2, 4\,5\}\}$ (5)
(8) $\{\{1, 2\}, \{1, 4\,5\}, \{3, 1\,4\}\}$ (6)
(9) $\{\{1, 3\}, \{1, 4\,5\}, \{2, 1\,4\}\}$ (6)

The permutation $(2\,3)$ transforms (4) into (5), (6) into (7), and (8) into (9), so we obtain 6 M-groups (1)-(6). For the groups (1)-(3) the stabilizer is $\{I, (2\,3)\}$, so it is equal to St_{s_1}, and the remaining groups (4)-(6) have a trivial stabilizer. Hence, the morphism of the groups (1)-(3) is 60, and the morphism of the groups (3)-(6) is 120. Together, they give $3 \times 60 + 3 \times 120 = 540$ Z-groups.

According to Theorem 4.1, the number of systems necessary for the complete derivation of M-groups is considerably reduced, especially for the systems of a higher order like $S_{6,5}$ and $S_{6,6}$, by using only the representatives of equivalence classes defined by the p-types of systems. In the derivation of M-groups from the systems with the morphism $6! = 720$, there occurs only one type of systems. All of them produce the maximal decomposition in which all subsets are of the length 1, having the trivial stabilizer.

This enabled the derivation of all M-groups from the symmetry group $18s$, the only space group with 6 generators that gives the possibility for the derivation of M-groups of 6-multiple antisymmetry. From the group $18s$ we obtain:

$M_6(18s) = 598\,752$,
$N_6(18s) = 2 \times 15 + 1 \times 30 + 6 \times 45 + 63 \times 90 + 8 \times 120 + 860 \times 180$

$$+10 \times 240 + 29\,468 \times 360 + 568\,334 \times 720 = 419\,973\,120.$$

This strongly confirms that any approach to the derivation of M-groups and Z-groups must be based on the multiple selection of the large equivalence classes– classes of non-isomorphic ACs, or on the types of M-and Z-systems enabling the reduction of the complete derivation to the derivation from the representatives of those classes.

Table 1

AC	**Rep.**	$\mathbf{M_1 = N_1}$	$\mathbf{M_2}$	$\mathbf{M_3}$	$\mathbf{M_4}$	$\mathbf{M_5}$	$\mathbf{M_6}$	**No.**
I	**1**s	1	1	1				1
II	**2**s	2	3	4	4			1
III	**3**s	5	16	39	55			2
IV	**4**s	4	9	10				7
V	**5**s	5	20	56	90			1
VI	**6**s	5	13	16				41
VII	**7**s	8	48	235	909	2160		1
VIII	**8**s	9	45	144	**246**			4
IX	**9**s	5	29	159	702	1914		1
X	**11**s	3	6	7				3
XI	**12**s	3	14	42	77			1
XII	**13**s	11	100	714	3706	10938		2
XIII	**14**s	11	65	236	444			17
XIV	**17**s	9	57	216	426			3
XV	**18**s	9	107	1296	14124	119580	598752	1
XVI	**19**s	17	181	1376	7314	21776		3
XVII	**20**s	7	31	97	**166**			1
XVIII	**21**s	9	94	775	4436	13984		1
XIX	**23**s	3	3					42
XX	**25**s	7	21	28				29
XXI	**27**s	2	2					20
XXII	**28**s	8	41	134	237			8
XXIII	**37**s	15	105	420	840			4
XXIV	**38**s	1						24
XXV	**61**s							2
XXVI	**3**h	7	31	88	138			1
XXVII	**5**h	5	23	70	122			2
XXVIII	**8**h	3	6	6				1
XXIX	**19**h	4	12	26	33			1
XXX	**21**h	15	161	1268	6984	21376		1
XXXI	**1**a	2	3	3				1
XXXII	**8**a	1	1					1
XXXIII	**21**a	5	23	**80**	**50**			1
XXXIV	**29**a	3	7	10				1
Total		**1**191	**5**005	**1**9467	**7**2587	**1**91728	**5**98752	**2**30

5. Concluding results

For all the computations it is used a PC with the Intel Pentium 4 CPU 2.40 GHz with 504 MB of RAM.

The space symmetry groups are first divided into 34 classes according to the isomorphism of *AC*s. For each class representative is written a computer program for the derivation of *M*-groups. The results for $m \leq 4$ from the papers [12,13] are confirmed, and some of them corrected. In the Table 1 those corrections are denoted by the bold numbers. The new results obtained for $m = 5$ and $m = 6$ completed the derivation of *M*-groups from 230 space groups.

Solution of this general problem gives as a particular result the derivation of the junior groups of $22\underline{1}$-symmetry (the problem proposed by A. F. Palistrant) and the complete enumeration of the multi-dimensional subperiodic groups of the categories G_{63} and G_{653} [6]. The number of the junior groups of $22\underline{1}$-symmetry is $M_3 = 19\,467$.

For the double check of all obtained results, combinatorial relationships between *M*-groups and *Z*-groups are used. Knowing the numbers of *Z*-groups calculated before [11], the new results obtained for *M*-groups are completely checked. The complete results for *M*-groups are given in Table 1, where the first two columns contain the data about *AC* class and its representative, the columns 2-7 contain the numbers M_n $(1 \leq n \leq 6)$, and in the last column is given the number of space groups G_3 belonging to the corresponding *AC* equivalence class.

References

1. H. Heesch, *Zur Strukturtheorie der Ebenen Symmetriegruppen*, Z. Kristallogr., **71** (1929), 95–102.
2. A. V. Shubnikov and V. A. Koptsik, *Symmetry in Science and Art*, Plenum Press, New York, 1974.
3. A. V. Shubnikov, N. V. Belov, N. N. Neronova, T. S. Smirnova, T. N. Tarkhova and E. N. Belova, *Colored Symmetry*, Pergamon Press, Oxford, 1964.
4. A. M. Zamorzaev, *Teoriya prostoi i kratnoi antisimmetrii*, Shtiintsa, Kishinev, 1976.
5. A. M. Zamorzaev and A. F. Palistrant, *Antisymmetry, its generalizations and geometrical applications*, Z. Kristallogr. **151** (1980), 231–248.
6. A. M. Zamorzaev and A. F. Palistrant, *O chisle obobschennyh prostranstvennyh Shubnikovskih grupp*, Kristallografiya **9** (1964), 778–782.
7. A. M. Zamorzaev, Yu. S. Karpova, A. P. Lungu and A. F. Palistrant, *P-simmetriya i yeyo dalneishee razvitie*, Shtiintsa, Kishinev, 1986.

8. A. M. Zamorzaev and E. I. Sokolov, *Simmetriya i razlichnogo roda antisimmetriya konecnyh figur*, Kristallografiya, **2**, 1 (1957), 9–14.
9. A. L. Mackay, *Extensions of space-group theory*, Acta Crystall. **10** (1957), 543–548.
10. A. M. Zamorzaev, *Generalized Antisymmetry*, Comput. Math. Applic. **16** (1988), 555–562.
11. S. V. Jablan, *A New Method of Deriving and Cataloguing Simple and Multiple Antisymmetry G_3^l Space Groups*, Acta Crystall. **A43** (1986), 326–337.
12. S. V. Jablan, *Mackay Groups*, Acta Crystall. **A49** (1993), 132–137.
13. S. V. Jablan, *Mackay Groups and their Applications*, J. Struct. Chemistry **3-4** (2002), 259–266.
14. S. V. Jablan, *Kombinatornye rezul'taty v teorii kratnoi antisimmetrii*, DAN Acad Sci. Moldove **2** (1993), 35–48.
15. S. V. Jablan, *Algebra of Antisymmetric Characteristics*, Publ. Inst. Math. **47** (61) (1989), 39–55.