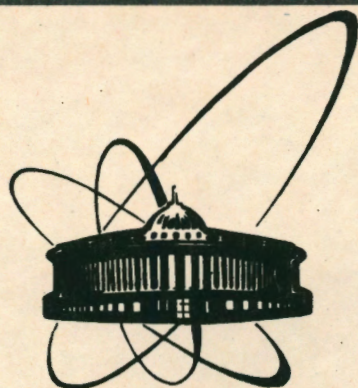


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ДУБНА

E17-90-387

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PERMUTATIONAL MAGNETIC POINT GROUPS  
AND THEIR APPLICATION IN THE LANDAU  
THEORY OF PHASE TRANSITIONS  
General Theory and Chromomorphic Classification

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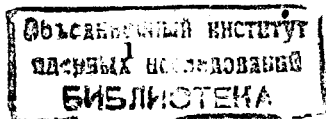
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1990

## 1. Introduction

The symmetry of magnetic structures and the related physical properties of crystals are described by the magnetic (Shubnikov) groups<sup>/1-5/</sup>. They are extensions of classical crystallographic groups by means of time inversion. The structure of the latter implies that they are a specific example of the so called colour groups<sup>/6-10/</sup>. One of the types of the colour groups - the permutational ones is particularly important for solid state physics as they could be effectively applied for a symmetry analysis of phase transition in the framework of Landau theory<sup>/11-17/</sup>. These groups are also an important tool in the description of the vector or tensor properties of the crystals<sup>/18/</sup>, or in the study of Potts models<sup>/19/</sup>. In view of the mentioned application of colour symmetry to the examination of magnetic phase transitions the permutational colour groups, constructed on the basis of magnetic groups (permutational magnetic groups or PMG in what follows), are required. Passing by we note that the so called "groups of colour antisymmetry" (cf. Ref.8) are to some extent similar to the PMG, however our approach, its results and the possible application are quite different.

The idea for a synthesis of magnetic symmetry and polycolor symmetry will be realized in a series of three papers. The present one deals with the general theory and with the classification of PMG in "chromomorphic classes"<sup>/13/</sup>. In the second one<sup>/20/</sup> a subset of the full tables of all Permutational Magnetic Point Groups (PMPG) is shown. The third part<sup>/21/</sup> presents the method of induction and the complete list of all transitive permutational representations of PMPG, as well as an illustration of their efficiency in the analysis of magnetic phase transitions. The present article is organized as follows: in the the next section we remind the basic concepts in the theory of magnetic group and permutational colour groups. In the third section the theory of P-symmetry is applied to the case of permutational magnetic groups, and their chromomorphic classification is discussed. The results are collected in two tables. In the last section some general results concerning the symmetry analysis of phase transitions of the basis of PMPG are briefly discussed.



## 2. Magnetic Groups and Permutational Colour Groups

The magnetic groups<sup>/1-3/</sup> are a particular realization of Shubnikov's antisymmetry<sup>/3,7,8/</sup>, where the operation "anti-identification" is interpreted as time inversion - 1', respectively inversion of magnetic moments,

$$1' \vec{M}(\vec{r}) = - \vec{M}(\vec{r}) . \quad (1)$$

The magnetic groups are direct or subdirect products of a crystallographic group  $G_0$  and the group  $\theta = \langle 1' \rangle$  ( $(1')^2 = 1$ ), generated by the operation of time inverse. In the first case the magnetic group is called a grey one,

$$G(G_0) \cong G_0^* \cong G_0 \times \theta = G \times 1' \quad (2)$$

while in the second case it is a black-and-white group,

$$G(G_0) = G_0 + g'G_0, \quad (g')^2 \in G_0, \quad g' = g1' \notin G_0. \quad (3)$$

In every grey or black-and-white magnetic group the "non primed" operations (the ones that are not products of the form  $g' = g1'$ ) constitute an invariant subgroup  $G_0$  of index 2 with respect to  $G(G_0)$ . (These subgroups we shall denote with a subscript "zero"). The ordinary crystallographic groups are usually added to the set of proper magnetic groups, which are generated by the former. These are colourless groups.

We note that the black-and-white space magnetic groups are classified as antirotational (the respective point group is black-and-white) and antitranslational (the point group is a grey one). The grey space groups describe the symmetry of paramagnetic crystals, while the grey point groups might as well be referred to the antiferromagnetic structures.

In the framework of the theory of the colour symmetry<sup>/6-10/</sup> the magnetic groups might be regarded as "two-colour" ones,  $[G(G_0):G_0] = 2$ , and can be constructed as group extensions of  $G_0$  by means of  $\theta$ . The respective short exact sequence<sup>/22/</sup> is, (cf. Ref.15-17),

$$1 \longrightarrow G_0 \longrightarrow G(G_0) \longrightarrow \theta \longrightarrow 1$$

$$\text{i.e. } G_0 \subset G(G_0), \quad G(G_0)/G_0 \cong \theta, \quad |\theta| = 2. \quad (4)$$

The number of colours however does not coincide with the possible orientations of atom magnetic moments, as the magnetic groups are interpreted as colour Q-type groups<sup>/10/</sup>: Let  $\vec{M}(\vec{r})$  be an axial-vector function of the magnetic density in a crystal with crystallographic group  $G$ , and  $G_M \subset G \times \theta$  is the symmetry group of the function  $\vec{M}(\vec{r})$ . The action of the operators  $g_i \in G \times \theta$  is defined by Eq.(1) and by the forthcoming equality,

$$g_i \vec{M}(\vec{r}) = [g_i] \vec{M}(g_i^{-1} \vec{r}) = \begin{cases} \vec{M}(\vec{r}), & g_i \in G_M \\ \vec{M}_i(\vec{r}) \neq \vec{M}(\vec{r}), & g_i \notin G_M \end{cases} \quad (5)$$

Here  $[g_i]$  is the proper rotational part of  $g_i$ . Therefore the crystallographic part of the colour group elements transforms both the position and the orientation of the magnetic moments (a specific action for Q-type symmetry). The different functions  $\vec{M}_i(\vec{r}), i=1,2,\dots,n, n \leq [G \times \theta : G_M]$  describe the different orientations of the magnetic domains. In general not all of the functions  $\vec{M}_i(\vec{r})$  are linearly independent.

In connection with what we already mentioned, there rises the question in what of the types of colour groups (P- or Q-type) are to be classified the permutational magnetic groups.

The answer is evident: the type of the colour groups is not determined by the group structure alone, but also by the structure of the "colour" system and the definition of the group action on it. In the discussed case the colour group acts on the system of magnetic moments (which can be regarded as axial vectors, localized in atomic positions) as a Q-type group, Eq.(5). This group acts as P-type colour group on the set of  $n = [G:G_M]$  vector functions  $\{\vec{M}_i(\vec{r}), i=1,2,\dots,n\}$ , Eq.(5). The latter correspond to the  $n$  possible domains, i.e. the group acts on the numbers of the domains. The extension from a classical crystallographic group  $G_0$  to colour Q-type group is realized in the form of magnetic group  $G(G_0)$ . The second level of extension from a Shubnikov magnetic group  $G(G_0)$  to permutational magnetic group would be realized as a P-type group. So, let's discuss the basic concepts of permutational P-type colour groups.

The permutational colour groups are defined as direct or sub-direct products of a crystallographic group  $G$  and a group  $P$  which is transitive subgroup of the symmetric group  $S_n$  (see Ref.6-10),

$$G^{(P)} = \left\{ (p; g) \mid p = \pi_G^H(g) \in P, g \in G, \pi_G^H: G \rightarrow P \subseteq S_n \right\} \subset P \times G. \quad (6)$$

The crucial stage of their construction is the determination of the homomorphism  $\pi: G \rightarrow P$ , defining the proper combination of  $g \in G$  and  $p \in P$  in Eq.(6). Following Van-der-Waerden<sup>/6/</sup> we find  $\pi = \pi_G^H$  through a transitive permutational representation  $D_G^{H'}$  of  $G$ , realized by an action from the left (permutation), of the left cosets of  $H'$  in  $G$ ,  $H' \subset G - [G:H'] = n$ ,

$$D_G^{H'}(g) \cong \begin{bmatrix} H', \dots, g_1 H', \dots, g_n H' \\ g H', \dots, g g_1 H', \dots, g g_n H' \end{bmatrix} \in P \subseteq S_n. \quad (7)$$

The kernel of  $D_G^{H'}$ ,  $\text{Ker } D_G^{H'} = \text{ker } \pi_G^H$ , coincides with the invariant subgroup of  $G$  which is an intersection of all conjugated subgroups  $H'_i = g_i H' g_i^{-1}$ , i.e. with the core of the class of conjugated subgroups,

$$\text{Ker } D_G^{H'} = \text{Core } H' = \bigcap_{g \in G} g H' g^{-1} = H \subset G. \quad (8)$$

The subgroup  $H = \text{Core } H'$  determines the maximal "one-colour" (preserving all the colours) subgroup  $H^{(1)} \subset G^{(P)}$ ,  $H^{(1)} \cong H$ . The subgroup  $H'$  determines the maximal subgroup  $H'^{(P)}$ , keeping fixed at least one colour. The homomorphism  $\pi: G \rightarrow P$  is interpreted as a homomorphism  $\phi: G \rightarrow A \cong G/H$  followed by an isomorphism  $A \cong P$  (usually the latter is considered to be a trivial one so  $\phi$  and  $\pi$  are identified). Introducing the abstract groups

$$\begin{aligned} A &\cong G/H \cong P \subseteq S_n \\ A' &\cong H'/H, \quad A' \subset A, \end{aligned} \quad (9)$$

we obtain the following relation between group-subgroup chains

$$\begin{array}{ccccccc} G & \supset & H' & \supset & H & = & \bigcap_{g \in G} (g H' g^{-1}) \\ \phi \downarrow & & \phi \downarrow & & \phi \downarrow & & \\ A & \supset & A' & \supset & C_1 & = & \bigcap_{a \in A} (a A' a^{-1}). \end{array} \quad (10)$$

The transitive permutational representation  $\pi_A^{A'}$  of  $A$  constructed using its decomposition into cosets of  $A'$  is a faithful representation ( $\text{Ker } \pi_A^{A'} = \text{Core } A' = C_1$ ), i.e. the forthcoming isomorphism holds,

$$A \cong P \cong \pi_A^{A'} \cong (A, A')_n \subseteq S_n. \quad (11)$$

The essential information about the colour groups, given in Eqs.(6-11) might be written in a compact form by the so called "three terms symbol"<sup>/7-9/</sup>,

$$G^{(P)} \cong G / H' / H (A, A')_n. \quad (12)$$

The colour group denoted by the symbol (12) is isostructural to  $G$ ,  $[G:H'] = n$ -colour, with one-colour subgroup  $H^{(1)} \cong H$  and a stabilizer of colour number 1,  $H'^{(P)}$  isomorphic to  $H'$ . The image of the permutational representation  $\text{Im } D_G^{H'}$  coincides with the transitive subgroup  $(A, A')_n \subset S_n$ .

It is particularly important that the whole sets of permutational representations  $D_G^{H'}$  and (according to Eq.(6)) the sets of colour groups  $G/H'/H$  have the same image  $(A, A')_n$ . Defining in a proper way the equivalence of the subgroups  $(A, A')_n \subseteq S_n$ , we obtain a finite number of classes, known as "chromomorphic classes"<sup>/1/</sup> and this way we classify all colour groups  $G^{(P)}$  according to these classes.

For the first time such a classification of the colour point groups was presented in Ref.9. Forty five (45) chromomorphic classes were found, denoted for short by the symbol of the group  $(A, A')_n$ . All the 242 colour point groups  $G^{(P)}$  fall in these classes (see Table 1 in Ref.9). The same result was obtained in Ref.23.

As the chromomorphic classification of the colour groups is based on the similarity of the group-subgroup relations, its identical coincidence with the proposed several years later<sup>/24/</sup> "exo-

morphic classification" of group-subgroup relations is not surprising at all. The same is true for the coincidence of the exomorphic classification and the classification of phase transitions given in Ref. (24-30) and Ref. (11-13).

### 3. Permutational Magnetic Point Groups

The permutational magnetic point groups (PMPG) are subdirect products of a magnetic point group  $G(G_0)$  with a transitive subgroup of permutations  $P \subseteq S_n$ :

$$G(G_0)^{(P)} = \left\{ (p; g) \mid p \in P, g \in G, \pi: G(G_0) \rightarrow P \subseteq S_n \right\} \subset P \times G(G_0). \quad (13)$$

The essential difference of these groups from the nonmagnetic ones  $G^{(P)}$ , is the requirement that the homomorphism  $\phi$  in Eq. (10) should perform the same mapping for the corresponding subgroup chains of index 2:

$$\begin{array}{ccccc} A_0 & > & A'_0 & > & C_1 \\ \phi \uparrow & & \phi \uparrow & & \phi \uparrow \\ G_0 & > & H'_0 & > & H_0 \\ \Delta & & \Delta & & \Delta \\ G & > & H' & > & H \\ \phi \downarrow & & \phi \downarrow & & \phi \downarrow \\ A & > & A' & > & C_1 \end{array}, \quad A_0 \cong G_0/H_0, \quad A'_0 \cong H'_0/H_0 \quad (14)$$

$$A \cong G/H, \quad A' \cong H'/H.$$

To take into account the additional information connected with the subgroups  $X_0 \subset X(X_0)$ , the components  $X$  in the "three terms symbols" (12) have to be changed to  $X(X_0)$  (for the cases of black-and-white and grey groups). In the most general situation,

$$G(G_0)^{(P)} = G(G_0)/H'(H'_0)/H(H_0) [A(A_0), A'(A'_0)]_n. \quad (15)$$

In fact this "clumsy" symbol could be significantly simplified. First of all the possible subgroup chains are,

$$G(G_0) > H'(H'_0) > H(H_0) \quad (16a)$$

$$G(G_0) > H'(H'_0) > H_0 \quad (16b)$$

$$G(G_0) > H'_0 > H_0 \quad (16c)$$

$$G_0 > H'_0 > H_0. \quad (16d)$$

The latter case corresponds to colourless magnetic groups and the symbol (15) reduces to (12). The type of the transitive groups  $[A(A_0), A'(A'_0)]_n$  remains to be checked. For this purpose we shall consider  $G(G_0)$  and  $H'(H'_0)$  as group extensions of  $H(H_0)$  or of  $H_0$ . For the case (16a) the following commutative diagrams<sup>15-17</sup> are valid:

$$\begin{array}{ccccccc} C_1 & & C_1 & & C_1 & & C_1 \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ C_1 \rightarrow H_0 & \rightarrow & G_0 & \rightarrow & A_0 & \rightarrow & C_1 \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ C_1 \rightarrow H(H_0) & \rightarrow & G(G_0) & \rightarrow & A(A_0) & \rightarrow & C_1 \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ C_1 \rightarrow C_2 & \rightarrow & C_2 & \rightarrow & C_1 & & C_1 \\ C_1 & & C_1 & & & & C_1 \end{array} \quad \begin{array}{ccccccc} C_1 & & C_1 & & C_1 & & C_1 \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ C_1 \rightarrow H_0 & \rightarrow & H'_0 & \rightarrow & A'_0 & \rightarrow & C_1 \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ C_1 \rightarrow H(H_0) & \rightarrow & H'(H'_0) & \rightarrow & A'(A'_0) & \rightarrow & C_1 \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ C_1 \rightarrow C_2 & \rightarrow & C_2 & \rightarrow & C_1 & & C_1 \\ C_1 & & C_1 & & & & C_1 \end{array} \quad (17)$$

Whereof it follows that  $A(A_0) = A_0$ ,  $A'(A'_0) = A'_0$  and the symbol of the permutational group will be  $P = (A_0, A'_0)_n$ . For the subgroup chain given in Eq. (16b) the diagrams are:

$$\begin{array}{ccccccc} C_1 & & C_1 & & C_1 & & C_1 \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ C_1 \rightarrow H_0 & \rightarrow & G_0 & \rightarrow & A_0 & \rightarrow & C_1 \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ C_1 \rightarrow H_0 & \rightarrow & G(G_0) & \rightarrow & A(A_0) & \rightarrow & C_1 \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ C_1 \rightarrow C_2 & \rightarrow & C_2 & \rightarrow & C_1 & & C_1 \\ C_1 & & C_1 & & & & C_1 \end{array} \quad \begin{array}{ccccccc} C_1 & & C_1 & & C_1 & & C_1 \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ C_1 \rightarrow H_0 & \rightarrow & H'_0 & \rightarrow & A'_0 & \rightarrow & C_1 \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ C_1 \rightarrow H_0 & \rightarrow & H'(H'_0) & \rightarrow & A'(A'_0) & \rightarrow & C_1 \\ \downarrow & & \downarrow & & \downarrow & & \downarrow \\ C_2 & \rightarrow & C_2 & \rightarrow & C_2 & \rightarrow & C_1 \\ & & C_1 & & C_1 & & C_1 \end{array} \quad (18)$$

$$A(A_0) / A_0 \cong C_2 \quad A'(A'_0) / A'_0 \cong C.$$

which implies that now the type of  $P$  is  $[A(A'_0), A'(A'_0)]_n$ . For the chain given in Eq. (16c) we obtain  $P = [A(A'_0), A'_0]_n$ . The symbols  $(A'_0, A'_0)_n$ ,  $[A(A'_0), A'(A'_0)]_n$  and  $[A(A'_0), A'_0]_n$  consist of abstract groups related to the factor-groups of the point groups. The 32 point groups and 115 (out of 122) magnetic groups are isomorphic to 18 abstract groups. This 18 groups  $A$ , and their subgroups  $A'_0$ , with Core  $A'_0 = C_1$ , generate 45 nonequivalent colour groups isomorphic to  $(A, A')_n \subseteq S_n$ ,  $n = [A'_0 : A'_0]$ , which are obtained for the first time in Ref. 9. The remaining 7 grey magnetic groups:  $C_{4h}^*$ ,  $C_{6h}^*$ ,  $D_{2h}^*$ ,  $D_{4h}^*$ ,  $D_{6h}^*$ ,  $T_h^*$ ,  $O_h^*$ , where  $X^* \equiv X \times \theta$  are isomorphic to 7 new abstract groups<sup>/3,31/</sup>. The latter give 23 new permutation groups  $(A'_0, A'_0)_n$  and 2 groups  $[A'_0, A'(A'_0)]_n$ , where  $A'_0 = A'_0 \times \theta$ .

The following equivalence criterion has been accepted for the permutational groups: two groups  $(A_1, A'_1)_{n_1}$  and  $(A_2, A'_2)_{n_2}$  are equivalent (and are considered to be the same group) if they coincide as groups of permutations, i.e. if they are conjugated subgroups of  $S_n$  ( $n_1 = n_2 = n$ ). In Table 1 the symbols  $(A, A')_n$  of all 70 nonequivalent transitive subgroups of  $S_n$ , isomorphic to 25 abstract groups  $A$ , are presented. These groups correspond to 70 classes of chromomorphism of PMPG. Following the symbol of the group  $(A, A')_n$  viewed as a label of the respective chromomorphic class, the quantity of all nonequivalent PMPG belonging to this class is given, i.e. of all PMPG with the corresponding permutation group. For the first 45 classes in the column entitled "OLD" in Table 1 figures stand for the number of the permutation colour point groups generated by the 32 nonmagnetic groups. The number of the PMPG generated from the 122 magnetic point groups is written in column entitled "ALL".

The derivation of the PMPG and the complete lists of their symbols are presented in the next paper<sup>/20,21/</sup>. Here we just note that the equivalence definition we used comprises the following conditions: a) the equivalent groups are isostructural, i.e. they can be generated by the same magnetic point group  $G(G_0)$ ; b) their subgroups  $H'$  ( $H'_0$ ) are conjugated subgroups in  $G(G_0)$ .

We point out, that the problem of the choice of the equivalence criterion for colour groups is rather nontrivial. So we discuss<sup>/32/</sup> four possibilities in the general case and ten modifications for isostructural (with the same  $G$ ) colour groups. Our pre-

sent choice of the mentioned equivalence criterion is based on the presumable application of PMPG in physics: to nonequivalent representations  $D_G^{H'}$  correspond a nonequivalent PMPG (cf. also Ref. 16).

All 1997 PMPG were calculated by means of a designed for this purpose computer program in Turbo-Pascal 5.0 for a personal computer IBM-PC. The following results were obtained:

- A complete list of the subgroups of all 122 magnetic point groups;
- The invariant subgroups and classes of the conjugated noninvariant subgroups as well as the cores of these classes;
- The decomposition of the magnetic groups in left cosets for all the subgroups;
- The transitive permutational representations  $D_G^{H'}$  for each pair group-subgroup  $H' < G$ ;
- The characters and the decomposition of these representations into irreducible components;
- For each colour group a complete list of the combined elements  $(p, g) \in G(G_0)^{(p)}$ .

The comparison of our group-subgroups list with similar ones by other authors<sup>/3,31,33/</sup> proved the effectiveness of the program and brought about the correction of some misprints and omissions in these tables. (For example in the excellent tables of Ascher & Janner<sup>/31/</sup> there are omissions only in two groups: in  $T_h \times \theta$  the 4 subgroups  $S_6 \times \theta$ , and in  $D_{4h} \times \theta$  the 12 noninvariant subgroups of 3 types:  $C_{2v}^* \times \theta$ ,  $D_{2h}(C_{2h}^*)$ ,  $D_{2h}(C_{2v}^*)$ .) We especially note the tables of Ref. 33 that were shown to us by their author after the final termination of our work. The chromomorphic classes of the colour magnetic point groups and the exomorphic classes for the group-subgroup relations for the respective groups completely coincide (in comparison with Ref. 9, 24, here and in Ref. 33 there are 25 new classes, No 46-70). The difference in the number of PMPG - 1997, and the "total number of geometrically nonequivalent symmetry descent" - 1599, is due to the different equivalence criteria. Two subgroups  $H'_1, H'_2 < G$  are considered to be equivalent if they are conjugated by  $g \in G$  in our paper and by  $g \in SO(3)$  (in Ref. 33).

#	P↔G/H	[A,A']n	OLD	ALL	#	P↔G/H	[A,A']n	OLD	ALL	#	P↔G/H	[A,A']n	ALL
1	C <sub>1</sub>	[C <sub>1</sub> ,C <sub>1</sub> ] <sub>1</sub>	32	122	28	O	[O,C <sub>1</sub> ] <sub>24</sub>	3	11	46	C <sub>4h</sub>	[C <sub>4h</sub> ,C <sub>1</sub> ] <sub>16</sub>	1
2	C <sub>2</sub>	[C <sub>2</sub> ,C <sub>1</sub> ] <sub>2</sub>	73	451	29		[O,C <sub>2</sub> ] <sub>12</sub>	3	11	47	C <sub>6h</sub>	[C <sub>6h</sub> ,C <sub>1</sub> ] <sub>24</sub>	1
3	C <sub>3</sub>	[C <sub>3</sub> ,C <sub>1</sub> ] <sub>3</sub>	7	21	30		[O,C <sub>2</sub> ] <sub>12</sub>	3	11	48	D <sub>2h</sub>	[D <sub>2h</sub> ,C <sub>1</sub> ] <sub>16</sub>	3
4	C <sub>4</sub>	[C <sub>4</sub> ,C <sub>1</sub> ] <sub>4</sub>	4	20	31		[O,C <sub>3</sub> ] <sub>8</sub>	3	11	49	D <sub>4h</sub>	[D <sub>4h</sub> ,C <sub>1</sub> ] <sub>32</sub>	1
5	C <sub>6</sub>	[C <sub>6</sub> ,C <sub>1</sub> ] <sub>6</sub>	7	41	32		[O,C <sub>4</sub> ] <sub>6</sub>	3	11	50		[D <sub>4h</sub> ,C <sub>2</sub> ] <sub>16</sub>	8
6	C <sub>4h</sub>	[C <sub>4h</sub> ,C <sub>1</sub> ] <sub>8</sub>	1	12	33		[O,D <sub>2</sub> ] <sub>6</sub>	3	11	51	D <sub>6h</sub>	[D <sub>6h</sub> ,C <sub>1</sub> ] <sub>48</sub>	1
7	C <sub>6h</sub>	[C <sub>6h</sub> ,C <sub>1</sub> ] <sub>12</sub>	1	15	34		[O,D <sub>3</sub> ] <sub>4</sub>	3	11	52		[D <sub>6h</sub> ,C <sub>2</sub> ] <sub>24</sub>	8
8	D <sub>2</sub>	[D <sub>2</sub> ,C <sub>1</sub> ] <sub>4</sub>	34	366	35	O <sub>h</sub>	[O <sub>h</sub> ,C <sub>1</sub> ] <sub>48</sub>	1	9	53	T <sub>h</sub>	[T <sub>h</sub> ,C <sub>1</sub> ] <sub>48</sub>	1
9	D <sub>2h</sub>	[D <sub>2h</sub> ,C <sub>1</sub> ] <sub>8</sub>	3	74	36		[O <sub>h</sub> ,C <sub>2</sub> ] <sub>24</sub>	1	9	54		[T <sub>h</sub> ,C <sub>2</sub> ] <sub>24</sub>	1
10	D <sub>3</sub>	[D <sub>3</sub> ,C <sub>1</sub> ] <sub>6</sub>	10	42	37		[O <sub>h</sub> ,C <sub>3</sub> ] <sub>24</sub>	1	9	55		[T <sub>h</sub> ,C <sub>3</sub> ] <sub>24</sub>	3
11		[D <sub>3</sub> ,C <sub>2</sub> ] <sub>3</sub>	10	42	38		[O <sub>h</sub> ,C <sub>2</sub> ] <sub>24</sub>	2	18	56		[T <sub>h</sub> ,C <sub>3</sub> ] <sub>16</sub>	1
12	D <sub>4</sub>	[D <sub>4</sub> ,C <sub>1</sub> ] <sub>8</sub>	5	32	39		[O <sub>h</sub> ,C <sub>3</sub> ] <sub>16</sub>	1	9	57		[T <sub>h</sub> ,C <sub>2v</sub> ] <sub>12</sub>	3
13		[D <sub>4</sub> ,C <sub>2</sub> ] <sub>4</sub>	10	64	40		[O <sub>h</sub> ,C <sub>4</sub> ] <sub>12</sub>	2	18	58		[T <sub>h</sub> ,C <sub>2v</sub> (C <sub>3</sub> ) <sub>12</sub>	2
14	D <sub>4h</sub>	[D <sub>4h</sub> ,C <sub>1</sub> ] <sub>16</sub>	1	15	41		[O <sub>h</sub> ,C <sub>2v</sub> ] <sub>12</sub>	1	9	59	O <sub>h</sub>	[O <sub>h</sub> ,C <sub>1</sub> ] <sub>96</sub>	1
15		[D <sub>4h</sub> ,C <sub>2</sub> ] <sub>8</sub>	4	60	42		[O <sub>h</sub> ,D <sub>2</sub> ] <sub>12</sub>	2	18	60		[O <sub>h</sub> ,C <sub>2</sub> ] <sub>48</sub>	1
16	D <sub>6</sub>	[D <sub>6</sub> ,C <sub>1</sub> ] <sub>12</sub>	8	62	43		[O <sub>h</sub> ,C <sub>2v</sub> ] <sub>12</sub>	1	9	61		[O <sub>h</sub> ,C <sub>3</sub> ] <sub>48</sub>	3
17		[D <sub>6</sub> ,C <sub>2</sub> ] <sub>6</sub>	16	124	44		[O <sub>h</sub> ,D <sub>3</sub> ] <sub>8</sub>	2	18	62		[O <sub>h</sub> ,C <sub>2</sub> ] <sub>48</sub>	4
18	D <sub>6h</sub>	[D <sub>6h</sub> ,C <sub>1</sub> ] <sub>24</sub>	1	18	45		[O <sub>h</sub> ,C <sub>4v</sub> ] <sub>8</sub>	2	18	63		[O <sub>h</sub> ,C <sub>3</sub> ] <sub>32</sub>	1
19		[D <sub>6h</sub> ,C <sub>2</sub> ] <sub>12</sub>	4	72						64		[O <sub>h</sub> ,C <sub>4</sub> ] <sub>24</sub>	4
20	T	[T,C <sub>1</sub> ] <sub>12</sub>	2	5						65		[O <sub>h</sub> ,C <sub>2v</sub> ] <sub>24</sub>	3
21		[T,C <sub>2</sub> ] <sub>6</sub>	2	5						66		[O <sub>h</sub> ,D <sub>2</sub> ] <sub>24</sub>	4
22		[T,C <sub>3</sub> ] <sub>4</sub>	2	5						67		[O <sub>h</sub> ,C <sub>2v</sub> ] <sub>24</sub>	6
23	T <sub>h</sub>	[T <sub>h</sub> ,C <sub>1</sub> ] <sub>24</sub>	1	6						68		[O <sub>h</sub> ,C <sub>2v</sub> (C <sub>3</sub> ) <sub>24</sub>	1
24		[T <sub>h</sub> ,C <sub>2</sub> ] <sub>12</sub>	1	6						69		[O <sub>h</sub> ,D <sub>3</sub> ] <sub>16</sub>	4
25		[T <sub>h</sub> ,C <sub>3</sub> ] <sub>8</sub>	1	6						70		[O <sub>h</sub> ,C <sub>4v</sub> ] <sub>12</sub>	12
26		[T <sub>h</sub> ,C <sub>3</sub> ] <sub>8</sub>	1	6									
27		[T <sub>h</sub> ,C <sub>2v</sub> ] <sub>6</sub>	1	6									1997

Table No.1

No	[A,A']n	Permutational representation
1	[C <sub>1</sub> ,C <sub>1</sub> ] <sub>1</sub>	$\Gamma_1$
2	[C <sub>2</sub> ,C <sub>1</sub> ] <sub>2</sub>	$\Gamma_1 + \Gamma_2^2$
3	[C <sub>3</sub> ,C <sub>1</sub> ] <sub>3</sub>	$\Gamma_1 + (\Gamma_2 + \Gamma_3)^2$
4	[C <sub>4</sub> ,C <sub>1</sub> ] <sub>4</sub>	$\Gamma_1 + \Gamma_2^2 + (\Gamma_3 + \Gamma_4)^2$
5	[C <sub>6</sub> ,C <sub>1</sub> ] <sub>6</sub>	$\Gamma_1 + \Gamma_2^2 + \Gamma_3^2 + \Gamma_4^2 + (\Gamma_5 + \Gamma_6)^2$
6	[C <sub>4h</sub> ,C <sub>1</sub> ] <sub>8</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 + \Gamma_{1u} + \Gamma_{2u} + \Gamma_{3u} + \Gamma_{4u}$
7	[C <sub>6h</sub> ,C <sub>1</sub> ] <sub>12</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 + \Gamma_5 + \Gamma_6 + \Gamma_{1u} + \Gamma_{2u} + \Gamma_{3u} + \Gamma_{4u} + \Gamma_{5u} + \Gamma_{6u}$
8	[D <sub>2</sub> ,C <sub>1</sub> ] <sub>4</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4$
9	[D <sub>2h</sub> ,C <sub>1</sub> ] <sub>8</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 + \Gamma_{1u} + \Gamma_{2u} + \Gamma_{3u} + \Gamma_{4u}$
10	[D <sub>3</sub> ,C <sub>1</sub> ] <sub>6</sub>	$\Gamma_1 + \Gamma_2 + 2\Gamma_3^2$
11	[D <sub>3</sub> ,C <sub>2</sub> ] <sub>3</sub>	$\Gamma_1 + \Gamma_3^2$
12	[D <sub>4</sub> ,C <sub>1</sub> ] <sub>8</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 + 2\Gamma_5^2$
13	[D <sub>4</sub> ,C <sub>2</sub> ] <sub>4</sub>	$\Gamma_1 + \Gamma_3 + \Gamma_5^2$
14	[D <sub>4h</sub> ,C <sub>1</sub> ] <sub>16</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 + 2\Gamma_5 + \Gamma_{1u} + \Gamma_{2u} + \Gamma_{3u} + \Gamma_{4u} + 2\Gamma_{5u}$
15	[D <sub>4h</sub> ,C <sub>2</sub> ] <sub>8</sub>	$\Gamma_1 + \Gamma_3 + \Gamma_5 + \Gamma_{1u} + \Gamma_{3u} + \Gamma_{5u}$
16	[D <sub>6</sub> ,C <sub>1</sub> ] <sub>12</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 + 2\Gamma_5^2 + 2\Gamma_6$
17	[D <sub>6</sub> ,C <sub>2</sub> ] <sub>6</sub>	$\Gamma_1 + \Gamma_3 + \Gamma_5^2 + \Gamma_6$
18	[D <sub>6h</sub> ,C <sub>1</sub> ] <sub>24</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 + 2\Gamma_5 + 2\Gamma_6 + \Gamma_{1u} + \Gamma_{2u} + \Gamma_{3u} + \Gamma_{4u} + 2\Gamma_{5u} + 2\Gamma_{6u}$
19	[D <sub>6h</sub> ,C <sub>2</sub> ] <sub>12</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 + \Gamma_{1u} + \Gamma_{2u} + \Gamma_{3u} + \Gamma_{4u}$
20	[T,C <sub>1</sub> ] <sub>12</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + 3\Gamma_4^2$
21	[T,C <sub>2</sub> ] <sub>6</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4^2$
22	[T,C <sub>3</sub> ] <sub>4</sub>	$\Gamma_1 + \Gamma_4^2$
23	[T <sub>h</sub> ,C <sub>1</sub> ] <sub>24</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + 3\Gamma_4 + \Gamma_{1u} + \Gamma_{2u} + \Gamma_{3u} + 3\Gamma_{4u}^2$
24	[T <sub>h</sub> ,C <sub>2</sub> ] <sub>12</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 + \Gamma_{1u} + \Gamma_{2u} + \Gamma_{3u} + \Gamma_{4u}^2$
25	[T <sub>h</sub> ,C <sub>3</sub> ] <sub>8</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4 + 2\Gamma_{4u}^2$
26	[T <sub>h</sub> ,C <sub>3</sub> ] <sub>8</sub>	$\Gamma_1 + \Gamma_4 + \Gamma_{1u} + \Gamma_{4u}$
27	[T <sub>h</sub> ,C <sub>2v</sub> ] <sub>8</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_{4u}^2$
28	[O,C <sub>1</sub> ] <sub>24</sub>	$\Gamma_1 + \Gamma_2 + 2\Gamma_3 + 3\Gamma_4^2 + 3\Gamma_5^2$
29	[O,C <sub>2</sub> ] <sub>12</sub>	$\Gamma_1 + \Gamma_2 + 2\Gamma_3 + \Gamma_4^2 + \Gamma_5^2$
30	[O,C <sub>2</sub> ] <sub>12</sub>	$\Gamma_1 + \Gamma_3 + \Gamma_4 + 2\Gamma_5^2$
31	[O,C <sub>3</sub> ] <sub>8</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_4^2 + \Gamma_5^2$
32	[O,C <sub>4</sub> ] <sub>6</sub>	$\Gamma_1 + \Gamma_3 + \Gamma_4^2$
33	[O,D <sub>2</sub> ] <sub>6</sub>	$\Gamma_1 + \Gamma_3 + \Gamma_5^2$
34	[O,D <sub>3</sub> ] <sub>4</sub>	$\Gamma_1 + \Gamma_5^2$
35	[O <sub>h</sub> ,C <sub>1</sub> ] <sub>48</sub>	$\Gamma_1 + \Gamma_2 + 2\Gamma_3 + 3\Gamma_4 + 3\Gamma_5 + \Gamma_{1u} + \Gamma_{2u} + 2\Gamma_{3u} + 3\Gamma_{4u}^2 + 3\Gamma_{5u}^2$
36	[O <sub>h</sub> ,C <sub>2</sub> ] <sub>24</sub>	$\Gamma_1 + \Gamma_2 + 2\Gamma_3 + \Gamma_4 + \Gamma_5 + \Gamma_{1u} + \Gamma_{2u} + 2\Gamma_{3u} + \Gamma_{4u}^2 + \Gamma_{5u}^2$
37	[O <sub>h</sub> ,C <sub>3</sub> ] <sub>24</sub>	$\Gamma_1 + \Gamma_2 + 2\Gamma_3 + \Gamma_4 + \Gamma_5 + 2\Gamma_{4u}^2 + 2\Gamma_{5u}^2$
38	[O <sub>h</sub> ,C <sub>2</sub> ] <sub>24</sub>	$\Gamma_1 + \Gamma_3 + \Gamma_4 + 2\Gamma_5 + \Gamma_{1u} + \Gamma_{3u} + \Gamma_{4u}^2 + 2\Gamma_{5u}^2$
39	[O <sub>h</sub> ,C <sub>3</sub> ] <sub>16</sub>	$\Gamma_1 + \Gamma_2 + \Gamma_4 + \Gamma_5 + \Gamma_{1u} + \Gamma_{2u} + \Gamma_{4u}^2 + \Gamma_{5u}^2$
40	[O <sub>h</sub> ,C <sub>4</sub> ] <sub>12</sub>	$\Gamma_1 + \Gamma_3 + \Gamma_4 + \Gamma_{1u} + \Gamma_{3u} + \Gamma_{4u}^2$
41	[O <sub>h</sub> ,C <sub>2v</sub> ] <sub>12</sub>	$\Gamma_1 + \Gamma_2 + 2\Gamma_3 + \Gamma_{4u}^2 + \Gamma_{5u}^2$
42	[O <sub>h</sub> ,D <sub>2</sub> ] <sub>12</sub>	$\Gamma_1 + \Gamma_3 + \Gamma_5 + \Gamma_{1u} + \Gamma_{3u} + \Gamma_{5u}^2$
43	[O <sub>h</sub> ,C <sub>2v</sub> ] <sub>12</sub>	$\Gamma_1 + \Gamma_3 + \Gamma_5 + \Gamma_{4u}^2 + \Gamma_{5u}^2$
44	[O <sub>h</sub> ,D <sub>3</sub> ] <sub>8</sub>	$\Gamma_1 + \Gamma_5 + \Gamma_{1u} + \Gamma_{5u}^2$
45	[O <sub>h</sub> ,C <sub>4v</sub> ] <sub>8</sub>	$\Gamma_1 + \Gamma_3 + \Gamma_{4u}^2$

Table No.2

No	[A,A']n	Permutational representation
46	$(C_{4h}^1.C_1)_{16}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + \Gamma_{3g}^+ + \Gamma_{4g}^+ + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + \Gamma_{4u}^- + \Gamma_{1g}^- + \Gamma_{2g}^- + \Gamma_{3g}^- + \Gamma_{4g}^- + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + \Gamma_{4u}^-$
47	$(C_{6h}^1.C_1)_{24}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + \Gamma_{3g}^+ + \Gamma_{4g}^+ + \Gamma_{5g}^+ + \Gamma_{6g}^+ + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + \Gamma_{4u}^- + \Gamma_{5u}^- + \Gamma_{6u}^- + \Gamma_{1g}^- + \Gamma_{2g}^- + \Gamma_{3g}^- + \Gamma_{4g}^- + \Gamma_{5g}^- + \Gamma_{6g}^- + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + \Gamma_{4u}^- + \Gamma_{5u}^- + \Gamma_{6u}^-$
48	$(D_{2h}^1.C_1)_{16}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + \Gamma_{3g}^+ + \Gamma_{4g}^+ + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + \Gamma_{4u}^- + \Gamma_{1g}^- + \Gamma_{2g}^- + \Gamma_{3g}^- + \Gamma_{4g}^- + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + \Gamma_{4u}^-$
49	$(D_{4h}^1.C_1)_{32}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + \Gamma_{3g}^+ + \Gamma_{4g}^+ + 2\Gamma_{5g}^+ + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + \Gamma_{4u}^- + 2\Gamma_{5u}^- + \Gamma_{1g}^- + \Gamma_{2g}^- + \Gamma_{3g}^- + \Gamma_{4g}^- + 2\Gamma_{5g}^- + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + \Gamma_{4u}^- + 2\Gamma_{5u}^-$
50	$(D_{4h}^1.C_2)_{18}$	$\Gamma_{1g}^+ + \Gamma_{3g}^+ + \Gamma_{5g}^+ + \Gamma_{1u}^- + \Gamma_{3u}^- + \Gamma_{5u}^- + \Gamma_{1g}^- + \Gamma_{3g}^- + \Gamma_{5g}^- + \Gamma_{1u}^- + \Gamma_{3u}^- + \Gamma_{5u}^-$
51	$(D_{6h}^1.C_1)_{48}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + \Gamma_{3g}^+ + \Gamma_{4g}^+ + 2\Gamma_{5g}^+ + 2\Gamma_{6g}^+ + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + \Gamma_{4u}^- + 2\Gamma_{5u}^- + 2\Gamma_{6u}^- + \Gamma_{1g}^- + \Gamma_{2g}^- + \Gamma_{3g}^- + \Gamma_{4g}^- + 2\Gamma_{5g}^- + 2\Gamma_{6g}^- + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + \Gamma_{4u}^- + 2\Gamma_{5u}^- + 2\Gamma_{6u}^-$
52	$(D_{6h}^1.C_2)_{24}$	$\Gamma_{1g}^+ + \Gamma_{3g}^+ + \Gamma_{5g}^+ + \Gamma_{6g}^+ + \Gamma_{1u}^- + \Gamma_{3u}^- + \Gamma_{5u}^- + \Gamma_{6u}^- + \Gamma_{1g}^- + \Gamma_{3g}^- + \Gamma_{5g}^- + \Gamma_{6g}^- + \Gamma_{1u}^- + \Gamma_{3u}^- + \Gamma_{5u}^- + \Gamma_{6u}^-$
53	$(T_h^1.C_1)_{48}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + \Gamma_{3g}^+ + 3\Gamma_{4g}^+ + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + 3\Gamma_{4u}^- + \Gamma_{1g}^- + \Gamma_{2g}^- + \Gamma_{3g}^- + 3\Gamma_{4g}^- + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + 3\Gamma_{4u}^-$
54	$(T_h^1.C_2)_{24}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + \Gamma_{3g}^+ + \Gamma_{4g}^+ + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + \Gamma_{4u}^- + \Gamma_{1g}^- + \Gamma_{2g}^- + \Gamma_{3g}^- + \Gamma_{4g}^- + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + \Gamma_{4u}^-$
55	$(T_h^1.C_3)_{24}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + \Gamma_{3g}^+ + \Gamma_{4g}^+ + 2\Gamma_{5g}^+ + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{3u}^- + \Gamma_{4u}^- + 2\Gamma_{5u}^-$
56	$(T_h^1.C_3)_{16}$	$\Gamma_{1g}^+ + \Gamma_{4g}^+ + \Gamma_{1u}^- + \Gamma_{4u}^- + \Gamma_{1g}^- + \Gamma_{4g}^- + \Gamma_{1u}^- + \Gamma_{4u}^-$
57	$(T_h^1.C_{2v})_{12}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + \Gamma_{5g}^+ + \Gamma_{4u}^- + \Gamma_{1g}^- + \Gamma_{2g}^- + \Gamma_{5g}^- + \Gamma_{4u}^-$
58	$(T_h^1.C_{2v})_{12}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + \Gamma_{3g}^+ + \Gamma_{4u}^- + \Gamma_{4u}^-$
59	$(O_h^1.C_1)_{96}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + 2\Gamma_{3g}^+ + 3\Gamma_{4g}^+ + 3\Gamma_{5g}^+ + \Gamma_{1u}^- + \Gamma_{2u}^- + 2\Gamma_{3u}^- + 3\Gamma_{4u}^- + 3\Gamma_{5u}^- + \Gamma_{1g}^- + \Gamma_{2g}^- + 2\Gamma_{3g}^- + 3\Gamma_{4g}^- + 3\Gamma_{5g}^- + \Gamma_{1u}^- + \Gamma_{2u}^- + 2\Gamma_{3u}^- + 3\Gamma_{4u}^- + 3\Gamma_{5u}^-$
60	$(O_h^1.C_2)_{48}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + 2\Gamma_{3g}^+ + \Gamma_{4g}^+ + \Gamma_{5g}^+ + \Gamma_{1u}^- + \Gamma_{2u}^- + 2\Gamma_{3u}^- + \Gamma_{4u}^- + \Gamma_{5u}^- + \Gamma_{1g}^- + \Gamma_{2g}^- + 2\Gamma_{3g}^- + \Gamma_{4g}^- + \Gamma_{5g}^- + \Gamma_{1u}^- + \Gamma_{2u}^- + 2\Gamma_{3u}^- + \Gamma_{4u}^- + \Gamma_{5u}^-$
61	$(O_h^1.C_3)_{48}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + 2\Gamma_{3g}^+ + \Gamma_{4g}^+ + \Gamma_{5g}^+ + 2\Gamma_{4u}^- + 2\Gamma_{5u}^- + \Gamma_{1g}^- + \Gamma_{2g}^- + 2\Gamma_{3g}^- + \Gamma_{4g}^- + \Gamma_{5g}^- + 2\Gamma_{4u}^- + 2\Gamma_{5u}^-$
62	$(O_h^1.C_2)_{48}$	$\Gamma_{1g}^+ + \Gamma_{3g}^+ + \Gamma_{4g}^+ + 2\Gamma_{5g}^+ + \Gamma_{1u}^- + \Gamma_{3u}^- + \Gamma_{4u}^- + 2\Gamma_{5u}^- + \Gamma_{1g}^- + \Gamma_{3g}^- + \Gamma_{4g}^- + 2\Gamma_{5g}^- + \Gamma_{1u}^- + \Gamma_{3u}^- + \Gamma_{4u}^- + 2\Gamma_{5u}^-$
63	$(O_h^1.C_3)_{32}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + \Gamma_{4g}^+ + \Gamma_{5g}^+ + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{4u}^- + \Gamma_{5u}^- + \Gamma_{1g}^- + \Gamma_{2g}^- + \Gamma_{4g}^- + \Gamma_{5g}^- + \Gamma_{1u}^- + \Gamma_{2u}^- + \Gamma_{4u}^- + \Gamma_{5u}^-$
64	$(O_h^1.C_4)_{24}$	$\Gamma_{1g}^+ + \Gamma_{3g}^+ + \Gamma_{4g}^+ + \Gamma_{1u}^- + \Gamma_{3u}^- + \Gamma_{4u}^- + \Gamma_{1g}^- + \Gamma_{3g}^- + \Gamma_{4g}^- + \Gamma_{1u}^- + \Gamma_{3u}^- + \Gamma_{4u}^-$
65	$(O_h^1.C_{2v})_{24}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + 2\Gamma_{3g}^+ + \Gamma_{4u}^- + \Gamma_{5u}^- + \Gamma_{1g}^- + \Gamma_{2g}^- + 2\Gamma_{3g}^- + \Gamma_{4u}^- + \Gamma_{5u}^-$
66	$(O_h^1.D_2)_{24}$	$\Gamma_{1g}^+ + \Gamma_{3g}^+ + \Gamma_{5g}^+ + \Gamma_{1u}^- + \Gamma_{3u}^- + \Gamma_{5u}^- + \Gamma_{1g}^- + \Gamma_{3g}^- + \Gamma_{5g}^- + \Gamma_{1u}^- + \Gamma_{3u}^- + \Gamma_{5u}^-$
67	$(O_h^1.C_{2v})_{24}$	$\Gamma_{1g}^+ + \Gamma_{3g}^+ + \Gamma_{5g}^+ + \Gamma_{4u}^- + \Gamma_{5u}^- + \Gamma_{1g}^- + \Gamma_{3g}^- + \Gamma_{5g}^- + \Gamma_{4u}^- + \Gamma_{5u}^-$
68	$(O_h^1.C_{2v})_{24}$	$\Gamma_{1g}^+ + \Gamma_{2g}^+ + 2\Gamma_{3g}^+ + \Gamma_{4u}^- + \Gamma_{5u}^- + \Gamma_{4g}^- + \Gamma_{5g}^- + \Gamma_{4u}^- + \Gamma_{5u}^-$
69	$(O_h^1.D_3)_{16}$	$\Gamma_{1g}^+ + \Gamma_{5g}^+ + \Gamma_{1u}^- + \Gamma_{5u}^- + \Gamma_{1g}^- + \Gamma_{5g}^- + \Gamma_{1u}^- + \Gamma_{5u}^-$
70	$(O_h^1.C_{4v})_{12}$	$\Gamma_{1g}^+ + \Gamma_{3g}^+ + \Gamma_{4u}^- + \Gamma_{1g}^- + \Gamma_{3g}^- + \Gamma_{4u}^-$

Table No.2 (continued)



#### 4. Application of PMPG to the theory of Landau

In Ref.11 it was shown that the colour permutational groups could be very useful in analysis of phase transitions in crystals in the framework of the Landau's theory. This is a consequence of the properties of their transitive permutational representations and also of the well defined relation between groups, subgroups and factor groups. Without repeating the procedures precisely presented in Ref.11-17, we shall just note that in the three-terms symbol (12), or respectively (15), the group  $G$  describes the high symmetry phase,  $H'$  - the low symmetry one and  $H$  is the kernel of the symmetry breaking irreducible representation  $D_G^j$  (related to the order parameter). A necessary condition is that  $D_G^{H'}$  should belong to the decomposition of the permutational representation  $D_G^{H'}$ , where  $\text{Im } D_G^{H'} = (A, A')_n$ .

All the 1977 transitive permutational representations  $D_G^{H'}$  have in total 70 different images  $D_A^{A'} = (A, A')_n$ . The decomposition of  $D_A^{A'}$  to irreducible representations of the abstract group  $A \cong G/H$  are presented in Table 2, where the notations of irreps follow the Ref.35. From the images  $D_A^{A'}$  by engendering<sup>/34/</sup> one obtains all necessary irreducible representations, contained in  $D_G^{H'}$ . The full list of decompositions of  $D_G^{H'}$  to  $G$ -irreducible representations for all PMPG is given in the third part of the present paper.<sup>/21/</sup> Symmetry breaking irreps  $D_G^j$  are engendered only by the faithful irreps  $D_A^j$  of  $A$ .

All faithful representations  $D_A^j \equiv \Gamma_j$ ,  $j=1,2,\dots$  of  $A$  are denoted in Table 2 with an upper index "c", "s" or "\*". The "c" means that the representation  $D_A^j$  of  $G$ , engendered<sup>/34/</sup> by  $D_A^j \equiv \Gamma_j^c$ , does not satisfy the Chain Subduction Criterion (CSC), introduced by Birman<sup>/31,37,12/</sup> and based on the Frobenius Reciprocity Theorem<sup>/34/</sup>; so it is not an active irrep in a phase transition.

The representations with a superscript "s" do not satisfy the Stability Criterion of Landau<sup>/12/</sup> and may drive only first-order transition. The symmetry breaking representations for continuous phase transitions might be engendered only by the faithful irreps, marked in Table 2 with "\*".

The tables allow to reach useful general conclusions on the possibilities concerning equitranslational magnetic phase transitions: all nonequivalent changes of symmetry, described by magnetic groups are 1977, in number equal to the quantity of PMPG and are distributed in 70 classes. All the properties of the groups

in one class are quite similar. Forty one of these classes either have no faithful irreducible representations in  $D_A^{A^*}$  or these representations do not satisfy the CSC (among them are all new 25 classes). Therefore the 912 PMPG belonging to them cannot be connected with any phase transition. Faithful representations with upper index "s" are contained in  $D_A^{A^*}$  of 8 chromomorphic classes total of 142 PMPG and the corresponding phase transitions are from first-order.

All necessary conditions are satisfied for those marked with an asterisk '\*' and fall in 21 classes with a total of 934 groups.

Examples of application of the tables are contained in the forthcoming two parts.

One of the authors (J N K) thanks Dr. V.Kopsky - Czechoslovakian Academy of Sciences, who (after the present work had been already finished) acquainted him with his book<sup>133/</sup>.

#### References :

1. Landau L.D., Lifshitz E.M. Statistical Physics, N.Y. Addison-Wesley, 1958
2. Targer B.A., Zaitsev V.M. - Zh.Eksp.Teor.Fiz., 1956, v.30, p.564
3. Koptsik A.V. Shubnikov Groups, M.:Moscow Univ., 1966 (in Russian)
4. Dzyaloshinski I.E. - Zh.Eksp.Teor.Fiz., 1957, v.32, p.1547
5. Kovalev O.V., Fiz.Tverd.Tela, 1963, v.5, p.3156
6. Waerden B.L. Van der, Burchard J.J. - Z.Kristallogr., 1961, v.115, p.231
7. Shubnikov A.V., Koptsik V.A. Symmetry in Science and Art, N.Y. :Plenum, 1974
8. Zamorzaev A.M., Golyarski E.H., Palistrant A.F., Colour Symmetry, Its Generalization and Applications, Kishinev :Shtiintsa, 1978 (in Russian)
9. Koptsik V.A., Kotzev J.N. -Comm. JINR, 1974, P4-8067 and P4-8068, Dubna
10. Kotzev J.N. - MATCH(Comm.Math.Chem.), 1980, v.9, p.41
11. Kotzev J.N., Litvin D.B., Birman J.L. - Physics A, 1982, v.114A, p.576
12. Litvin D.B., Kotzev J.N., Birman J.L. -Phys.Rev.B, 1982, v26, p.6947

13. Kotzev J.N., Koptsik V.A., Rustamov K.A. - in Group Theoretical Methods in Physics (Proc.Int.Seminar, Zvenigorod, 1982) (ed.by M.A.Markov). M.:Nauka, 1983, v.1, p.332
14. Kotzev J.N., Alexandrova D.A. - in Group Theoretical Methods in Physics, (Proc.Int.Seminar, Yourmala, 1985)
15. Kotzev J.N., Alexandrova D.A. - Lect.Not.Phys., 1988, v.313, p.357
16. Kotzev J.N., Alexandrova D.A. - Acta Cryst.A, 1988, v.A44, p.1082
17. Kotzev J.N., Alexandrova D.A. - Comm. JINR, 1988, P17-88-482, Dubna
18. Berenson R., Kotzev J.N., Litvin D.B., Birman J.L. - Phys.Rev. B, 1982, v.25, p.7523
19. Kotzev J.N., Peev M.K. - Comm.JINR, 1990, E17-90-386, Dubna
20. Kotzev J.N., Tzonev S.S. - Comm.JINR, 1990, E17-90-388, Dubna
21. Kotzev J.N., Tzonev S.S. - Comm.JINR, 1990, E17-90-389, Dubna
22. Michel L., in Particle Symmetries and Axiomatic Field Theory, ed. by M.Chretien, N.Y., 1966, v.1, p.247
23. Zamorzaev A.M., Gusul I.S., Lungu A.P. - in Investigations on the Discrete Geometry (ed. by A.M.Zamorzaev), Kishinev, Shtiintsa, 1974, p.3
24. Kopsky V. - Phys.Let., 1978, v.69A, p.82
25. Ascher E. - J.Phys.C., 1977, v.10, p.1365
26. Gufan Yu.M. - Phys.Tverd.Tela, 1971, v.13, p.225
27. Gufan Yu.M., Sashnenko V.P. - Zh.Eksp.Teor.Fiz., 1972, v.63, p.1909
28. Sirotnin Yu.I., Shaskolskaya M.P. Principles of Crystal Physics, M.:Nauka, 1975, par.66 (in Russian)
29. Michel L., Mozrymas J. - Lect.Not.Phys., 1978, v.279, N.Y.:Springer, p.447
30. Gufan Yu.M. Structural Phase Transitions M.:Nauka, 1982 (in Russian)
31. Ascher E., Janner A. - Acta Cryst., 1965, v.18, p.325
32. Alexandrova D.A., Kotzev J.N. Comm. JINR, 1990, E17-90-291, Dubna
33. Kopsky V. Group Lattices, Subduction of Bases and Fine Domain Structures for Magnetic Crystal Point Groups. Prague: Academia, 1982
34. Jansen L., Boon M. Theory of Finite Groups. Amsterdam:North Holland, 1967
35. Koster G.F., Dimmock J.O., Wheeler R.G., Statz H. Properties of the Thirty-two Point Groups. Cambridge, Mass.: MIT, 1963
36. Birman J.L., Phys.Rev.Lett., 1966, v.17, p.1216
37. Goldrich F.E., Birman J.L. Phys.Rev.Lett., 1968, v.167, p.528

Received by Publishing Department  
on June 6, 1990.

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E17-90-387

Перестановочные магнитные точечные группы  
и их применение в теории фазовых  
переходов Ландау

Общая теория и хромоморфная классификация групп

Магнитные /шубниковские/ точечные группы расширяются с помощью транзитивных подгрупп симметрической группы  $S_n$ . Полученные перестановочные магнитные группы описывают симметрию полидоменных магнитных структур, а также применяются в анализе магнитных фазовых переходов в рамках теории Ландау.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований. Дубна 1990

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E17-90-387

Permutational Magnetic Point Groups  
and Their Application in the Landau Theory  
of Phase Transitions

General Theory and Chromomorphic Classification

Through a two-step extension of point groups by time inversion and transitive permutational groups, new types of colour groups called permutational magnetic groups have been obtained. They describe the symmetry properties of polydomain magnetic crystals and might be applied to symmetry analysis of magnetic phase transitions.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Communication of the Joint Institute for Nuclear Research. Dubna 1990