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ON THE NEW TYPES OF COLOUR SYMMETRY GROUPS

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The group theoretical methods give strict and universal algorithms for deriving a detailed and rather full information about those properties of the studied systems, which are connected both with the "geometrical" structure symmetry and its movement in space and time and with the "dynamical" symmetry of physical interactions in the system. The university of the symmetry method allows the usage of pure mathematical group theory results in physics, chemistry and crystallography. And vice versa, a great part of most widely used group-theoretical methods are either found by physicists, chemists, crystallographs or they are once more "discovered" by them. Obviously, not only the exceptive abstraction of the contemporary mathematical language is the reason, but also it is due to the different viewpoints. For example, the physicist puts in one and the same abstract concept different concrete contents and can derive important practical results, which are indiscernible for a mathematician. A confirmation of the above-mentioned and a brilliant example for a "physical" group theory is the theory of a "generalized" (colour) symmetry [1,2]. The rapid development of this theory in the last two decades is due to the stimulating physics influence.

A detailed survey of the basic ideas and a profound analysis of the historical development of the theory of colour symmetry are contained in the book of Shubnikov and Koptsik [1] and in the book of Zamorzaev [2]. The new types of colour groups were already applied in the analysis and the classification of magnetic structures [3-7], in description of the symmetry of real crystals [8], and the space modulated crystal structures, etc.

The only purpose of this paper is to underline the characteristic peculiarities in the structures of the corresponding groups by means of a brief survey of the different types of colour symmetry.

The mathematical theory of colour symmetry can be given in the most generalized form using the group extension theory as a base. But the physical character of colour groups is demonstrated in the best way by the consideration of the action of their elements on the "geometrophysical" space, introduced by Shubnikov [1]. We will try to combine these two methods in this report.

The simplest model of the geometrophysical space is a regular system of colour points, defined as follows. A system of n symmetrical equivalent points with coordinates r_i, forming an orbit R of the group G of order $n= |G|$, is given by

$$R=Gr_1 =\{r_i | r_i = g_i r_1, g_i \in G\}. \tag{1}$$

A scalar, vector, or tensorial function is determined on the orbit R. The values f_a of the function $f(r_i) = f_a$ on the points r_i are called "colour" of the point. The set of all f_a

$$F = \{f_a | f_a = f(r_i), r_i \in Gr_1\} \tag{2}$$

formes a "colour subspace".

The ordered pairs (f_a, r_i) are called colour points of the system FR, where

$$FR= \{(f_a, r_i) | f_a \in F, r_i \in R, f_a = f(r_i)\}. \tag{3}$$

Let $P = \{p_i\}$ be a group, transitive to the set F, i.e. such that: a) $p_k f_a = f_b \in F$ for all $f_a \in F$ and $p_k \in P$; b) for all couples $f_a, f_b \in F$ there exists such an element $p_i \in P$, that $f_b = p_k f_a$. Always exists at least one such group - the symmetric group S_p of degree $p=|F|$, where $p_i \in S_p$ are considered as permutations of the indices of the colours f_a. (P is the group of the corresponding chosen operators in all concrete cases, e.g. $P=\infty\infty\infty 1'$ is the group of rotations and antirotations, when $f(\vec{r})= \vec{S}(\vec{r})$ describe the crystal magnetic structure).

It is obvious that the groups of the automorphisms of such systems of colour points (or the symmetry groups of the "geometro-physical objects") should be groups of combined operators $\langle p ; g\rangle = g^{(p)}$, $g \in G$, $p \in P$.

There are 4 possible basic types of colour groups, named groups of P-, Q-, W_p- and W_q-symmetry type, which depend on the coupling way of f_a and r_i in a given system FR, or depending on the definition of the action of the combined operators $g^{(p)}$ on colour points. The characteristic features of every type are given on Fig. 1 and Tabl.1. In all cases the coordinates $r_i \in Gr_1$ of the colour points (f_a, r_i) are transformed only under the action of the group G (for crystals G is one of the 32 point or 230 space groups). Besides, in the P-type colour groups $G^{(p)}$, the components $g \in G$ of the combined elements $g^{(p)} \in G^{(p)}$ do not act on the colours $f_a \in F$ of the points r_i. In the cases, when $g \in G$ act on $r_i \in R$ as well as on $f_a \in F$, the colour groups $G^{(q)}$ belong to the Q-type of symmetry. The action of colour operators of P- and Q-type is determined by the relations:

$$\langle p_i;\ g_i\rangle\ (f_a, r_k) = (p_i f_a,\ g_i r_k) \in FR;\ \langle p_i; g_i\rangle \in G^{(p)}, \tag{4}$$

$$\langle q_i;\ g_i\rangle\ (f_a, r_k) = (q_i [g_i]\ f_a, g_i r_k) \in FR;\ \langle q_i; g_i\rangle \in G^{(q)}, \tag{5}$$

where $[g_i]$ is an operator, corresponding to g_i and acting on the subspace F (For example, if $f_a = \vec{S}_a$, and g_i is an element of the space group, $[g_i]$ is a proper rotation, associated with the element g_i). From a mathematical point of view the P-type groups are defined as subgroups of the direct product ($\otimes$) of P and G,

$$G^{(p)} \subseteq P \otimes G\ , \tag{6}$$

and the groups of Q-type,

$$G^{(q)} \subseteq Q \circledS G\ , \tag{7}$$

are subgroups of the semi-direct product ($\circledS$) of the groups Q and G. The multiplication law of the corresponding colour elements is:

$$\langle p_2;\ g_2\rangle \otimes \langle p_1;\ g_1\rangle\ =\ \langle p_2 p_1;\ g_2 g_1\rangle \in G^{(p)}\ , \tag{8}$$

$$\langle q_2;\ g_2\rangle \circledS \langle q_1;\ g_1\rangle\ =\ \langle q_2 \cdot [g_2] q_1 [g_2^{-1}];\ g_2 g_1\rangle \in G^{(q)}. \tag{9}$$

For the groups of P and Q-type, the following peculiarities are characteristic. The set of colour loads $\{p\} = P'$, associated with the elements $g^{(p)} \in G^{(p)}$ forms a group $P' \subseteq P$, while the corresponding set $\{q\} \subseteq Q$, for $g^{(q)} \in G^{(q)}$ may not form a group at all.

The elements $g \in G$, associated with the unit element of P or Q form the so-called "classical subgroup" $H^{(1)}$ of the colour group.

$$H^{(1)} = \{\langle e; g\rangle \mid g \in H \subset G\} \subset G^{(p)},\ \text{or}\ G^{(q)}. \tag{10}$$

This subgroup is always invariant in P-type symmetry, $H^{(1)} \triangleleft G^{(p)}$, and may not be invariant in Q symmetry, $H^{(1)} \subset G^{(q)}$.

Let us again look at Fig. 1 and Table 1 and discuss the peculiarities of the actions of the components $p \in P$ on the colours $f_a \in F$.

In all cases the "colour loads" $p \in P$ and $q \in Q$ of the combined operators act only on the colours f_a of the points. But in the groups of P- and Q-type p or q transform f_a into f_b independently of the localization of f_a in the space, i.e. independently of the point r_i, with which f_a is associated.

Essentially different is the action of the "combined colour loads" w_i of the elements $\langle w_i;\ g_i\rangle$ of the W-type groups [7]: the transformation of the colour f_a depends on its localization and could be different for one and the same colour f_a, associated in different pairs (f_a, r_i) and (f_a, r_k).

The "loads" w_i of the elements $g_i \in G$ in W-symmetry are polycomponent: they consist of $n = |G|$ ordered elements P_i,

$$w_i = (p_i^{g_1}, p_i^{g_2}, \ldots\ldots, p_i^{g_k}, \ldots\ldots, p_i^{g_n}) \quad (11)$$

where in $p_i^{g_k}$ the lower index "i" specifies its belonging to the element $\langle w_i; g_i \rangle$, and the upper index "g_k" means, that $p_i^{g_k}$ is acting only on the colour, located in the point $r_k = g_k r_1$ and is not acting on the other points. The introduction of such complicated operators may seem rather artificial to a certain extent, but it is completely justified because:

a) There really exist "geometro-physical objects" whose colour symmetry can be described only using groups of W-type (and the number of such objects is large).

b) The operators of the type

$$\langle w_i; g_i \rangle = \langle p_i^{g_1}, \ldots, p_i^{g_k}, \ldots, p_i^{g_n} \; ; \; g_i \rangle, \; g_i \in G, \; p_i \in P, \quad (12)$$

satisfy the group postulates and form colour groups of essentially new type, proposed by Prof. Koptsik and called W-symmetry groups ("W" - from "Wreath product" multiplication low, "$\wr$") [7].

The theory of W-symmetry, developed for the first time in the paper [7], include as a special case all known colour groups. The group structure of W-symmetry theoretically exhausts all possibilities of new types of colour groups (they should be only special cases of W-groups).

c) The W-symmetry is an essentially new concept for the symmetry of "geometro-physical objects". Undoubtedly, the development of the theory, including the representation theory of these groups and the corresponding generalized Curie principle, will give useful results for the practice.

Besides the new type of "combined loads" in W-symmetry, we can determine in two ways the action of the basic elements $g_i \in G$ - as in P- and Q-type symmetry groups [4].

So, there exist two basic types of W-groups which we will conventionally denote as W_p- and W_q-symmetry groups. In our work [7] the theory of W_p-symmetry is given, and all the 73+1 "junior" point groups $G^{(W_p)} \subset S_p \wr G$, $G^{(W_p)} \leftrightarrow G$, are tabulated. In [4] the groups of the W_q-type are discussed in connection with the magnetic symmetry.

The action of the elements of W-symmetry groups on the colour points is defined by relations [7,4]:

$$\langle \ldots, p_i^{g_k}, \ldots; g_i \rangle (f_a, r_k) = (p_i^{g_k} f_a, g_i r_k) \; , \quad (13)$$

$$\langle \ldots, q_i^{g_k}, \ldots; g_i \rangle (f_a, r_k) = (q_i^{g_k} [g_i] f_a, g_i r_k) \; . \quad (14)$$

From mathematically point of view the colour W_p type groups are subgroups of the wreath product ($\wr$) of the group P and G,

$$G^{(W_p)} \subseteq P \wr G = (P^{g_1} \otimes P^{g_2} \otimes \ldots \otimes P^{g_n}) \circledS G , \qquad (15)$$

where in the parenthesis is given a direct product of n isomorphic copies of the group P , $n=|G|$.

The elements of the subgroups are multiplied in conformity with the law, defined by the wreath product

$$\langle \ldots, p_2^{g_k}, \ldots ; g_2 \rangle \wr \langle \ldots, p_1^{g_k}, \ldots ; g_1 \rangle = \langle \ldots, p_2^{g_1 g_k} p_1^{g_k}, \ldots ; g_2 g_1 \rangle , \qquad (16)$$

or,

$$\langle w_2 ; g_2 \rangle \wr \langle w_1 ; g_1 \rangle = \langle w_2^{(g_1)} w_1 ; g_2 g_1 \rangle , \qquad (16')$$

where the automorphisms in $w_2^{(g_i)}$ are left shifts of the components $p_2^{g_k}$:

$$w_2^{(g)} = (p_2^{g g_1}, \ \ldots\ldots, \ p_2^{g g_k}, \ \ldots, \ p_2^{g g_n}). \qquad (17)$$

The W_q-type groups are subgroups of the generalized wreath product or crown product, $\wr$,of G and Q (P is substituted by Q)

$$G^{(w_q)} \subseteq Q \wr G = (Q^{g_1} \otimes \ldots \otimes Q^{g_n}) \ \circledS' \ G \qquad (18)$$

In W_q-groups, the characteristic for W-symmetry polycomponent loads w_i are combined with the basic element action on both subspaces R and F, which is specific for the Q-type groups. So, we get the following multiplication law:

$$\langle \ldots q_2^{g_k} \ldots ; g_2 \rangle \wr \langle \ldots . q_1^{g_k} \ldots ; g_1 \rangle = \langle \ldots g_2^{g_1 g_k} \cdot [g_2] q_1^{g_k} [g_2^{-1}] \ldots ; g_2 g_1 \rangle , \ (19)$$

or,

$$\langle w_2 ; g_2 \rangle \wr \langle w_1 ; g_1 \rangle = \langle w_2^{(g_1)} \cdot [g_2] w_1 [g_2^{-1}] ; g_2 g_1 \rangle . \qquad (19')$$

We will discuss the simplest example of a construction of a family of colour groups - the groups derived by the crystallographic group $G = 3 = \{1, 3_z, 3_z^2\}$ and the time-inversion group $P = Q = 1' = \{1, 1'\}$. In the frameworks of P- and Q-symmetry, using (6) and (7), we get equal families of Shubnikov groups, consisting of the senior group 31' and the unicolour group $3^{(1)} = 3$. Besides the senior group $\tilde{G}^{(w)} = P \wr G$, the family of W-type groups contains more two "junior" groups ($G^{(w)} \leftrightarrow G$) and two "medial" $\overline{G}^{(w)}$ (the last are not isomorphic with G subgroups of the senior group $\tilde{G}^{(w)}$, but include as component all elements of the basic group G). The senior group can be derived from the wreath product (15)

$$\tilde{G}^{(w)} = 1'2\,3 = (1' \otimes 1' \otimes 1') \circledS 3 =$$

$$= \{ \langle 1,1,1;1 \rangle , \langle 1,1,1;3 \rangle , \langle 1,1,1;3^2 \rangle ,$$
$$\langle 1',1',1';1 \rangle, \langle 1',1',1';3 \rangle , \langle 1',1',1';3^2 \rangle ,$$
$$\langle 1,1',1';1 \rangle, \langle 1,1',1';3 \rangle , \langle 1,1',1';3^2 \rangle ,$$
$$\langle 1',1,1';1 \rangle, \langle 1',1,1';3 \rangle , \langle 1',1,1';3^2 \rangle ,$$
$$\langle 1',1',1;1 \rangle, \langle 1',1',1;3 \rangle , \langle 1',1',1;3^2 \rangle ,$$
$$\langle 1',1,1;1 \rangle, \langle 1',1,1;3 \rangle , \langle 1',1,1;3^2 \rangle ,$$
$$\langle 1,1',1;1 \rangle, \langle 1,1',1;3 \rangle , \langle 1,1',1;3^2 \rangle ,$$
$$\langle 1,1,1';1 \rangle, \langle 1,1,1';3 \rangle , \langle 1,1,1';3^2 \rangle \} \leftrightarrow T_h , \quad (20)$$

and is abstractly isomorphic with the group T_h. (For brevity, we will miss the indices of $p_i{}^{g_k} = p_i \in P = \{1,1'\}$.

The following subgroups of (20) belong to the "junior" groups $G^{(w)} \leftrightarrow 3$:

$$G_1^{(w)} = \{ \langle 1,1,1;1 \rangle , \langle 1,1,1;3 \rangle , \langle 1,1,1;3^2 \rangle \} = 3^{(1)} \quad (21)$$

$$G_2^{(w)} = \begin{cases} \{ \langle 1,1,1;1 \rangle , \langle 1,1',1';3 \rangle , \langle 1',1,1';3^2 \rangle \} , \\ \{ \langle 1,1,1;1 \rangle , \langle 1',1,1';3 \rangle , \langle 1',1',1;3^2 \rangle \} , \\ \{ \langle 1,1,1;1 \rangle , \langle 1',1',1;3 \rangle , \langle 1,1',1';3^2 \rangle \} \end{cases} \quad (22)$$

where (21) is "unicolour", and one of the three equivalent two-colour groups (22), e.g. the first, is picked out as $G_2^{(w)}$.

There are three "medial" groups in the family

$$\overline{G}_1^{(w)} = G_1^{(w)} \cup G_1^{(w)} \langle 1',1',1';1 \rangle \leftrightarrow 31' ,$$

$$\overline{G}_2^{(w)} = G_2^{(w)} \cup G_2^{(w)} \langle 1',1',1';1 \rangle \leftrightarrow C_6 ,$$

$$\overline{G}_3^{(w)} = G_1^{(w)} \cup G_1^{(w)} \langle 1,1',1';1 \rangle \cup G_1^{(w)} \langle 1',1,1';1 \rangle \cup G_1^{(w)} \langle 1',1',1;1 \rangle \leftrightarrow T . \quad (23)$$

We will note that the above-discussed groups are essentially different from Zamorzaev's multiple antisymmetry groups [2], which belong to the P-type

$$G^{(p)} = P \otimes G = (1' \otimes 1^* \otimes \hat{1}) \otimes G , \quad P = 1'1^*\hat{1} , \quad (24)$$

although there is a certain outer similarity with (20).

The above example is suitable for explaining the equivalence relations for colour groups. We will consider two groups $G_1^{(w)}$ and $G_2^{(w)}$ as Γ-equivalent if they are conjugated subgroups of a supergroup $\Gamma = \{ \gamma \}$ of the same type

$$G_2^{(w)} = \gamma\, G_1^{(w)} \gamma^{-1} , \quad \gamma \in \Gamma^{(w)} ; \; G_1^{(w)} , G_2^{(w)} \subset \Gamma^{(w)} , \quad (25)$$

but satisfying the additional condition·

$$H_2^{(1)} = \gamma H_1^{(1)} \gamma^{-1} , \quad H_i^{(1)} \subset G_i^{(w)} , (i=1,2) , \quad (26)$$

where $H_i^{(1)}$ are their maximal "classical" (unicolour) subgroups. The condition (26) is of great importance: for example, it gives us the pos-

sibility to define as non-equivalent the evidently different groups (21) and (22), which are conjugated subgroups of (20).
The families $G^{(W_P)}$ with $P \subset S_p$ are another examples for W-symmetry groups. 73 junior point groups of the "regular" type

$$G_R^{(w)} \subset (P)_p \wr G, \quad (P)_p \subseteq S_p , \tag{27}$$

are derived analytically and tabulated in [7]; $(P)_p$ is the group of regular permutations, isomorphic with P. These groups correspond to the groups discussed by Wittke and Garrido[1]. In [7] the groups of the type

$$G_I^{(w)} \subset (P,P')_p \wr G; \quad (P,P')_p \subseteq S_p , \tag{28}$$

where $(P,P')_p$ is a transitive irregular group of permutations, are called "irregular" W-type groups. There is only one possible group (cubic, 12-colour) among the junior point groups $G_I^{(w)} \leftrightarrow G$.
Examples for the practical application of W groups for magnetic structure classification are given in [4,7].
From all of the above-mentioned colour groups, the P-type groups are the mostly studied groups, for which different classes of point and space groups are derived and tabulated [1,2,6,7] .
Complete tables of the 171 "regular" point groups $G_R^{(p)}$ of P-type (6) where $P=(P)_p \subseteq S_p$, and 73 "irregular" point groups $G_I^{(p)}$, with $P=(P,P')_p \subseteq S_p$, are included in [1,7] . Full tables of all 598 spin point groups $G_s^{(p)}$, $P=\infty\infty 1'$, and of 2804 magneto-electric groups $G_{ME}^{(p)}$, $P=\infty\infty\bar{1}\, 1'$, were for the first time published in [6].

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FIG. 1. Four types of colour symmetry groups

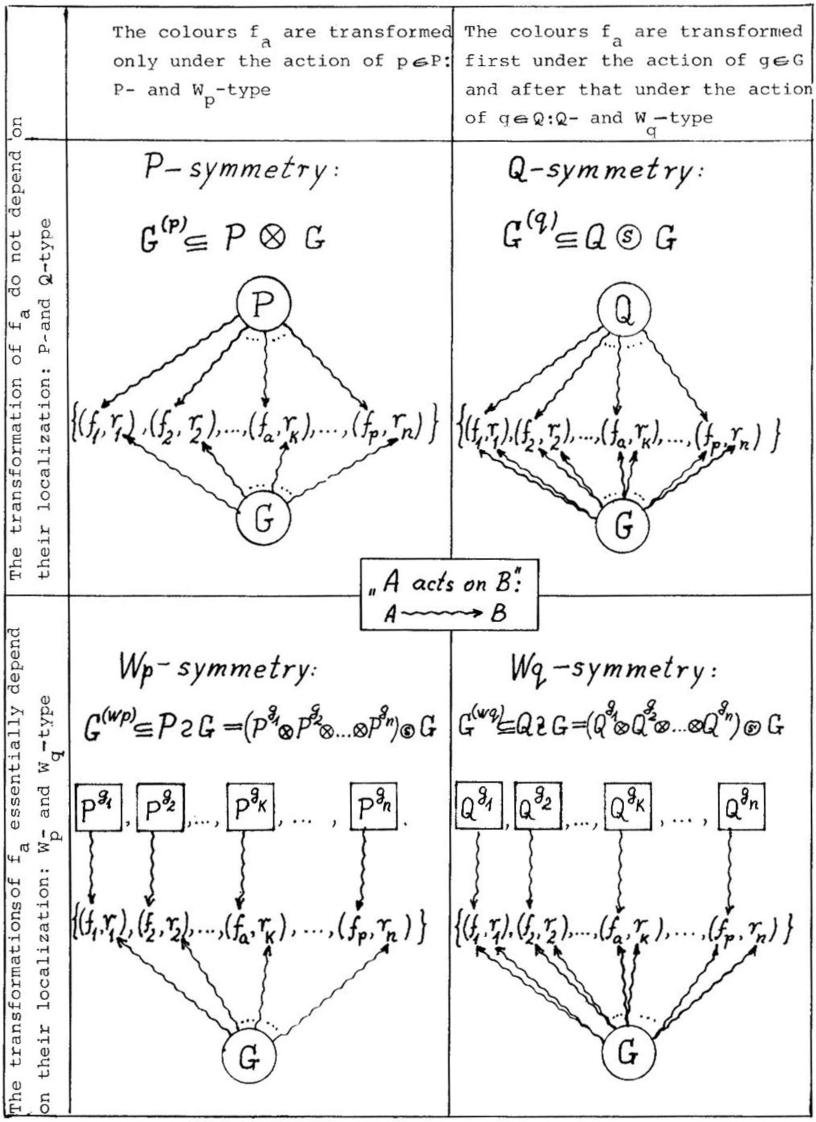

TABLE 1. Comparison between the basic definitions

P-symmetry	*Q-symmetry*
$G^{(p)} \subseteq P \otimes G$ $G^{(p)}=\{\langle p_i;g_i\rangle \mid g_i\in G,\ p_i\in\bar{P}\subseteq P\}$ $H^{(1)}=\{\langle e;g_j\rangle \mid g_j\in H\triangleleft G,\ e\in P\}\triangleleft G^{(p)}$ $\langle p_j;g_j\rangle\langle p_i;g_i\rangle=\langle p_j p_i;\ g_j g_i\rangle$ $\langle p_i;g_i\rangle(f_a,r_k)=(p_i f_a,\ g_i r_k)$	$G^{(q)} \subseteq Q \circledS G$ $G^{(q)}=\{\langle q_i;g_i\rangle \mid g_i\in G,\ q_i\in\bar{Q}\subseteq Q\}$ $H^{(1)}=\{\langle e;g_j\rangle \mid g_j\in H\subset G,\ e\in Q\}\subset G^{(q)}$ $\langle q_j;g_j\rangle\langle q_i;g_i\rangle=\langle q_j[g_j]q_i[g_j]^{-1};\ g_j g_i\rangle$ $\langle q_i;g_i\rangle(f_a,r_k)=(q_i[g_i]f_a,\ g_i r_k)$
W_p-symmetry	*W_q-symmetry*
$G^{(wp)}\subseteq P\wr G=(P^{g_1}\otimes\dots\otimes P^{g_n})\circledS G=$ $=\{\langle p_i^{g_1},\dots,p_i^{g_k},\dots,p_i^{g_n};g_i\rangle \mid g_i\in G,\ p_i^{g_k}\in P^{g_k}\leftrightarrow P\}$ $\langle\dots,p_j^{g_k},\dots;g_j\rangle\langle\dots,p_i^{g_k},\dots;g_i\rangle=$ $=\langle\dots,p_j^{g_i g_k}p_i^{g_k},\dots;\ g_j g_i\rangle$ $g_k r_1=r_k$ $\langle p_i^{g_1},\dots,p_i^{g_k},\dots,p_i^{g_n};g_i\rangle(f_a,r_k)=$ $=(p_i^{g_k}f_a,\ g_i r_k)$	$G^{(wq)}\subseteq Q\wr G=(Q^{g_1}\otimes\dots\otimes Q^{g_n})\circledS G=$ $=\{\langle q_i^{g_1},\dots,q_i^{g_k},\dots,q_i^{g_n};g_i\rangle \mid g_i\in G,\ q_i^{g_k}\in Q^{g_k}\leftrightarrow Q\}$ $\langle\dots,q_j^{g_k},\dots;g_j\rangle\langle\dots,q_i^{g_k},\dots;g_i\rangle=$ $=\langle\dots,q_j^{g_i g_k}[g_j]q_i^{g_k}[g_j]^{-1},\dots;\ g_j g_i\rangle$ $g_k r_1=r_k$ $\langle q_i^{g_1},\dots,q_i^{g_k},\dots,q_i^{g_n};g_i\rangle(f_a,r_k)=$ $=(q_i^{g_k}[g_i]f_a,\ g_i r_k).$

The equivalence relations: $G_2^{(w)}\sim G_1^{(w)}$, *if:* $\begin{cases} G_2^{(w)}=\gamma\, G_1^{(w)}\gamma^{-1}, & \gamma\in\Gamma \\ H_2^{(1)}=\gamma\, H_1^{(1)}\gamma^{-1}, & H_i^{(1)}\subset G_i^{(w)}\subset\Gamma \end{cases}$

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