ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ
ДУБНА

E17 - 11920

29/I-79

M.Kucab

359/2-79

COLOUR LATTICES AND SPIN TRANSLATION GROUPS.

GENERAL CASE

1978

E17 - 11920

M.Kucab [*]

COLOUR LATTICES AND SPIN TRANSLATION GROUPS. GENERAL CASE [**]

Submitted to Acta Crystallografica

---

[*] Permanent address: Institute of Nuclear Physics and Techniques, University of Mining and Metallurgy, 30-059, Cracow, Poland.

[**] Presented in part at the 11th International Congress of Crystallography, 3–12 August 1978, Warsaw, Poland.

Куцаб М.

E17 - 11920

Цветные решетки и спиновые трансляционные группы. Общий случай

В работе приводится метод получения цветных d-мерных кристаллографических решеток без наложения условий симметрии на базисные вектора. Найдено число неэквивалентных n-цветных решеток для $d \leq 4$ и любого конечного n. Цветные решетки используются для получения спиновых трансляционных групп. Результаты для триклиновых спиновых трансляционных групп сравниваются с результатами Литвина[10].

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1978

Kucab M.

E17 - 11920

Colour Lattices and Spin Transition Groups. General Case

A method of derivation of colour d-dimensional crystallographic lattices with no symmetry conditions on basis vectors is given. A number of nonequivalent n-colour lattices is evaluated for $d \leq 4$ and any finite n. An application of colour lattices for obtaining spin translation groups is presented. The results for triclinic spin translation groups are compared with those of Litvin[10].

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

Preprint of the Joint Institute for Nuclear Research. Dubna 1978

---

1. INTRODUCTION

Colour groups in crystallography are defined as extensions of classical crystallographic groups. The idea started in works of Belov and Tarkhova[1], Indebom[7], Niggli[13] and others preceded by an idea of antisymmetry (2-colour symmetry) of Heesch and Shubnikov. Colour groups are of interest in the theory of symmetry of compound systems (magnetic crystals, alloys, defect crystals, etc.). It is well known that magnetic groups have appeared in physics as an interpretation of 2-colour groups. The generalized magnetic groups, called spin groups, have been recently introduced as realizations of many-coloured groups.

The different types of colour groups, their properties and bibliography have been reviewed by Shubnikov and Koptsik[15] and Opechowski[14]. Only P-type colour groups (called further colour groups) will be considered here, as usually discussed in connection with magnetic symmetry. Colour point groups have been derived by Koptsik and Kotsev[8] and Harker[4]. Zamorzaev[18] and Shubnikov and Koptsik[15] have listed 2-, 3-, 4- and 6-colour 3-dimensional lattices.

Only very limited classes of colour space groups are known (Zamorzaev[18], Koptsik and Kuzhukeev[19]).Harker[5] has recently proposed a method of derivation of colour lattices with symmetry conditions on basis vectors. He has listed also triclinic colour lattices for $n \leq 16$.

In this paper an algebraic method of derivation of colour d -dimensional lattices in general case, i.e., no symmetry conditions are imposed on basis vectors of a lattice, is presented. The exact formulas for a number of nonequivalent n -colour lattices are given for $d \leq 4$ and any finite n. The results are used for deriving spin translation groups of triclinic system. Preliminary definitions and basic properties of colour groups are briefly presented in Sec. 2. In Sec. 3, after formulation of four group-theoretical lemmas, we develop a method of obtaining n-colour lattices; the main result is given here. The spin translation groups, abbreviated by STG's, are derived and tabulated in Sec. 4. The examples in Table 1 show the distribution of STG's over their isomorphic colour images of lowest n. In Table 2 the symbols of nonequivalent classes of triclinic STG's are given. A specific discussion on the change of basis vectors of a colour lattice is given in the Appendix.

2. COLOUR GROUPS

For a given group $\mathcal{G}$ and a discrete set of points $\mathcal{R} = \{r_1, r_2, \dots\}$ let us consider an orbit $\mathcal{Q}$ in $\mathcal{R}$ relative to $\mathcal{G}$:

$$\mathcal{Q} = \mathcal{G} r_1 = \{r_i \mid r_i = g_i r_1, \ g_i \subset \mathcal{G}\}.$$

Table 1

Examples of colour lattices (CL) and isomorphic to them spin translation groups (STG)

n	CL	STG
1	{111}	111
2	{211}	(211),(2′11),(1′11)
3	{311}	(311)
4	{411}	(411),(4′11)
	{221}	(21′1), $(2_x 2_y 1)$, $(2'_x 2_y 1)$
5	{511}	(511)
6	{611}	(611),(6′11),(3′11)
7	{711}	(711)
8	{811}	(811),(8′11)
	{421}	(41′1)
	{222}	$(2_x 2_y 1')$
36	{36,1,1)}	(36,1,1),(36′,1,1)
	{18,2,1}	(18,1,1)
	{12,3,1}	-
	{6,6,1}	-

Let $f(r)$ be an arbitrary function defined on $\mathcal{G} r_1$. Any value f_i of function $f(r)$ is called a colour. An ordered pair $[f(r_i), r_i]$ is called a colour point. Let $\mathcal{F} = \{f_j\}$ be a set of all n distinct values of a function f(r) and $\mathcal{P} = \{p_i\}$ be a transitive group on $\mathcal{F}$. In particular, $\mathcal{P}$ can be thought as any subgroup of the group $\mathcal{S}_n$ of all permutations of indices of colours f_k. Next, we consider ordered pairs (p_k, g_i), where $p_k \subset \mathcal{P}$ and $g_i \subset \mathcal{G}$, and define their action on colour points $[f_i, r_j]$. We may assume that elements

Table 2

Spin translation groups of triclinic system

$(N\ 1\ 1)$	$(Z\ N\ 1')$*		$(Z_1 Z_2 N)$
$(N'\ 1\ 1)$			$(Z_1' Z_2 N)$
$(N\ 1'1)$*	$(Z\ N\ 1)$		$(Z_1' Z_2' N)$
	$(Z'N\ 1)$		$(Z_1 Z_2 N')$
$(2_x 2_y\ 1)$	$(Z\ N'\ 1)$		$(Z_1' Z_2 N')$
$(2_x' 2_y\ 1)$	$(Z'N'1)$		$(Z_1' Z_2' N')$
$(2_x 2_y\ 1)$			
		$(Z_1 Z_2 Z_3)$	
		$(Z_1' Z_2 Z_3)$	
		$(Z_1' Z_2' Z_3)$	
		$(Z_1' Z_2' Z_3')$	

---

* N even.

of $\mathcal{P}$ act independently relative to elements of $\mathcal{G}$:

$$(p_k, g_i)[f_\ell, r_j] = [p_k f_\ell, g_i\ r_j] = [f_q, r_s];$$

$$f_\ell, f_q \in \mathcal{F};\ r_j, r_s \in \mathcal{Q}.$$

Any subgroup of the group $\widetilde{\mathcal{G}^{\mathcal{P}}} = \mathcal{P} \otimes \mathcal{G}$, where $\otimes$ denotes direct product of groups, is called the colour group (P -type colour group), (van der Waerden and Burckhardt/16/, Zamorzaev/17/). The colour group $\widetilde{\mathcal{G}^{\mathcal{P}}}$ is called senior colour group . Usually we are interested in those subgroups $\mathcal{G}^{\mathcal{P}}$ of $\mathcal{P} \oplus \mathcal{G}$ which are isomorphic to $\mathcal{G}$:

$$\mathcal{G} \cong \mathcal{G}^{\mathcal{P}} \subseteq \mathcal{P} \oplus \mathcal{G}.$$

The subgroups $\mathcal{G}^{\mathcal{P}}$ are called junior or non-trivial colour groups. The set of classical elements (e, g_i), $e \in \mathcal{P}$, $g_i \in \mathcal{G}$, forms a subgroup $\mathcal{H}^1$ of a colour group, called classical subgroup of a colour group. The symmetry group of a system of colour points $\mathcal{K}$ is the colour group leaving $\mathcal{K}$ invariant. A system of colour points with the junior colour group as the symmetry group has selected "colour properties". In particular: (i) A function $f(r)$ is single-valued, i.e., only one colour f_ℓ is paired with each point r_i. (ii) The numbers of colour points $[f_\ell, r_i]$ for each colour f_ℓ of $\mathcal{F}$ are the same; they are equal to the order of the classical subgroup $\mathcal{H}^1$ of $\mathcal{G}^{\mathcal{P}}$.

Only junior colour groups $\mathcal{G}^{\mathcal{P}}$ will be discussed in the next sections.

A method of deriving all subgroups $\mathcal{G}^{\mathcal{P}}$ of $\mathcal{P} \otimes \mathcal{G}$ is based on an "isomorphism theorem" (Zamorzaev/17/).

A set of all elements p_i of $\mathcal{P}$ in a junior group $\mathcal{G}^{\mathcal{P}}$ constitutes a group $\mathcal{P}$ isomorphic to a factor group $\mathcal{G}/\mathcal{H}$. The elements p_i of $\mathcal{P}$ are paired with elements g_k of $\mathcal{G}$ by a homomorphism

$$\mathcal{G} \to \mathcal{G}/\mathcal{H} \cong \mathcal{P}.$$

We need yet the concept of the equivalence of two colour groups.

We have said that two colour groups $\mathcal{G}^{\mathcal{P}}$ and $\overline{\mathcal{G}^{\mathcal{P}}}$ are equivalent if they are conjugate subgroups of a group $\Omega = \{a_j\}$:

$$\overline{\mathcal{G}^{\mathcal{P}}} = a_i \, \mathcal{G}^{\mathcal{P}} a_i^{-1}, \quad a_i \in \Omega \tag{1}$$

and

$$\mathcal{H}^1 = a_i \mathcal{H}^1 a_i^{-1}, \tag{2}$$

where $\mathcal{H}^1$ is the maximal classical subgroup of $\mathcal{G}^{\mathcal{P}}$ and $\overline{\mathcal{G}^{\mathcal{P}}}$. In the following, only crystallographic groups will be taken as groups $\mathcal{G}$ and the equivalence of colour groups will be determined by a group

$$\Omega = \mathcal{P} \otimes \mathcal{A}^+ , \tag{3}$$

where $\mathcal{P}$ is either an abstract group or a concrete group of transformations, $\mathcal{A}^+$ is the proper subgroup of the affine group $\mathcal{A}$.

3. COLOUR LATTICES

Let $\mathcal{G}$ be a d-dimensional crystallographic lattice denoted by $\mathcal{T}$:

$$\mathcal{T} = \{ t;\ t = \sum_{i=1}^{d} n_i a_i , \quad n_i - \text{integers} \},$$

where $a_1, a_2, \dots, a_d$ are d linearly independent vectors in d-dimensional Euclidean space. Vectors $a_1, a_2, \dots, a_d$ form a basis of $\mathcal{T}$. Here we assume that no symmetry conditions are imposed on basis vectors, i.e., any set of d linearly independent vectors of $\mathcal{T}$ stands for the basis of $\mathcal{T}$. The colour lattice $\mathcal{T}^{\mathcal{P}}$ isomorphic to $\mathcal{T}$ will be called general colour lattice. The lattice $\mathcal{T}$ is an abelian group and it can be expressed as a direct product of 1-dimensional lattices:

$$\mathcal{T} = \mathcal{T}_1 \otimes \mathcal{T}_2 \otimes \dots \otimes \mathcal{T}_d ,$$

where all $\mathcal{T}_i$ $(i = 1, 2, \dots, d)$ are infinite cyclic groups. Now we formulate four group-theoretical lemmas which are standard statements in the theory of abelian groups (Fuchs/3/).

L1: Let a lattice $\mathcal{T}^*$ be a d-dimensional subgroup of $\mathcal{T}$. Then there exist basis $a_1, a_2, \dots, a_d$ of the group $\mathcal{T}$ and $b_1, b_2, \dots, b_d$ of the group $\mathcal{T}^*$, respectively, such that

$$b_i = m_i a_i \quad (i = 1, 2, \dots, d), \tag{4}$$

where all m_i are integers.

L2: If $\mathcal{G} \simeq \mathcal{A}_1 \otimes \mathcal{A}_2 \otimes \dots \otimes \mathcal{A}_\ell$

and $\mathcal{A}_i^*$ is an invariant subgroup of $\mathcal{A}_i$, $i = 1, 2, \dots, \ell$, then for some subgroup $\mathcal{H}$ of $\mathcal{G}$ there is

$$\mathcal{H} \simeq \mathcal{A}_1^* \otimes \mathcal{A}_2^* \otimes \dots \otimes \mathcal{A}_\ell^*$$

and

$$\mathcal{G}/\mathcal{H} \simeq (\mathcal{A}_1/\mathcal{A}_1^*) \otimes (\mathcal{A}_2/\mathcal{A}_2^*) \otimes \dots \otimes (\mathcal{A}_\ell/\mathcal{A}_\ell^*).$$

L3: Every finite abelian group $\mathcal{G}$ is a direct product of groups

$$\mathcal{G} = \mathcal{G}_1 \otimes \mathcal{G}_2 \otimes \dots \otimes \mathcal{G}_k , \tag{5}$$

where each $\mathcal{G}_i$ is cyclic of prime power order $p_i^{\lambda_i}$, $\lambda_i > 0$. The orders $p_i^{\lambda_i}$ are called invariants and the groups $\mathcal{G}_i$ are called prime components of the decomposition (5). Two finite abelian groups are isomorphic if and only if they have the same set of elementary divisors.

L4: A direct product

$$\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \dots \otimes \mathcal{H}_q \qquad (6)$$

of cyclic groups, whose orders are powers of distinct primes, is cyclic.

A method of constructing general colour lattices $\mathcal{T}^{\mathcal{P}}$ for a given lattice $\mathcal{T}$ will be based on the following theorem:

T1:

$$\mathcal{T}^{\mathcal{P}} = \mathcal{T}_1^{\mathcal{P}_1} \otimes \mathcal{T}_2^{\mathcal{P}_2} \otimes \dots \otimes \mathcal{T}_d^{\mathcal{P}_d}, \qquad (7)$$

where

$$\mathcal{T}_i^{\mathcal{P}_i} \equiv \mathcal{T}_i \quad (i=1,2,\dots,d)$$

and

$$\mathcal{P} = \mathcal{P}_1 \otimes \mathcal{P}_2 \otimes \dots \otimes \mathcal{P}_d, \qquad (8)$$

where each $\mathcal{P}_i$ is cyclic group of order m_i, $\prod_{i=1}^{d} m_i = n$. The lattice $\mathcal{T}_i\mathcal{P}_i$ $(i=1,2,\dots,d)$ is the group formed by all powers of (p_i, a_i) where p_i is a generating element of $\mathcal{P}_i$, a_i is a basis vector of $\mathcal{T}_i$.

This result follows immediately from the isomorphism theorem, L1 and L2. Since $\mathcal{T}$ is abelian, any subgroup $\mathcal{T}^*$ of $\mathcal{T}$ is normal. The factor group $\mathcal{T}/\mathcal{T}^*$ ever exists and it is also abelian. Thus the group $\mathcal{P}$ of $\mathcal{T}^{\mathcal{P}}$ is an abelian group. In the 1-dimensional case the group $\mathcal{T}_i/\mathcal{T}_i^*$ is a cyclic group of order m_i, so is the group $\mathcal{P}_i$.

Thus, to derive all colour lattices $\mathcal{T}^{\mathcal{P}}$ for a given lattice $\mathcal{T}$ and number n, one needs to find all nonisomorphic abelian groups $\mathcal{P}$ of order n expressed as all possible decompositions (8). We use now L3. Let in the decomposition (11) of the group $\mathcal{G}$ cyclic groups be related to the distinct primes $p_1, p_2, \dots, p_k$. Let the number of prime components related to a prime p_i $(i=1,2,\dots,k)$ is equal to q_i and the prime components are of orders

$$p_i^{\lambda_1}, p_i^{\lambda_2}, \dots, p_i^{\lambda_{q_i}}, \qquad (9)$$

where numbers λ are arranged as follows

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{q_i}; \qquad (10)$$
$$\sum_j \lambda_j = r_i;\ j=1,2,\dots,q_i;\ i=1,2,\dots,k.$$

One obtains in this way from L3 that all nonisomorphic abelian groups of given order $n = p_1^{r_1} p_2^{r_2} \dots p_\ell^{r_\ell}$ can be found by considering all partitions (10) of numbers r_i $(i=1,2,\dots,k)$ with arbitrary numbers q_i. Here we are interested in the decompositions of an abelian groups of order n into d cyclic components with admitted trivial components, i.e., cyclic groups of order 1. It is clear from L3, L4 and Eq. (10) that such decompositions can be found, if numbers q_i are limited to be not larger than d.

A partition of r expressing r as a sum of at most d positive integers is called d-ary partition. The number of d-ary partitions of r will be denote by $\gamma(r)$. All possible decompositions (8) can be then expressed by all d-ary partitions of numbers r_i. The number $\gamma(r)$ can be calculated as a coefficient of x^r in the formal power series expansion of

$$\Phi(x) = \prod_{j=1}^{d} (1-x^{j})^{-1} \equiv \sum_{r=0}^{\infty} \gamma(r)x^{r} ,$$

where $\Phi(x)$ is the Euler generating function (Hall/6/). Thus, we have the following final result:

T2: The number of n-colour d-dimensional lattices for

$$n = p_1^{r_1} p_2^{r_2} \dots p_\ell^{r_\ell} , \tag{11}$$

where all numbers p_i are distinct primes, is equal to

$$\gamma(r_1)\gamma(r_2)\dots\gamma(r_\ell),$$

where $\gamma(r_i)$ can be expressed as:

$$\begin{aligned} &E[\tfrac{1}{144}(r_i+7)^2(r_i+1)+\tfrac{2}{9}] \text{ for } d=4 \text{ and } r_i \text{ odd;} \\ &E[\tfrac{1}{144}\{(r_i+5)^3-3(r_i-7)\}] \text{ for } d=4 \text{ and } r_i \text{ even;} \\ &E[\tfrac{1}{12}(r_i+3)^2+\tfrac{1}{4}] \text{ for } d=3; \\ &E[\tfrac{1}{2}r_i+1] \text{ for } d=2; \ 1 \text{ for } d=1. \end{aligned} \tag{12}$$

Here $E[x]$ denotes the integer part of x; $i=1,2,\dots,\ell$.

A colour lattice $\mathcal{T}^{\mathcal{P}}$ will be represented by basis vectors $a_1, a_2, \dots, a_d$ each vector being paired with an appropriate generating element p_i of $\mathcal{P}_i$ $(i=1,2,\dots,d)$. The symbols $\{a_1^{(p_1)}, a_2^{(p_2)}, \dots, a_d^{(p_d)}\}$ or simply $\{m_1, m_2, \dots, m_d\}$ where m_i is the order of $\mathcal{P}_i$ $(i=1,2,\dots,d)$

are used for denoting the $\mathcal{T}^{\mathcal{P}}$. The number m_i will be also called an order of the vector a_i since $[a_i^{(p_i)}]^{m_i} = b_i^{(1)}$, where $b_i = m_i a_i$ is a classical vector of $\mathcal{T}^{\mathcal{P}}$.

The method of constructing all colour-d-dimensional lattices for given number of colours n will then be as follows.

Start with the decomposition (11) of n and find all d-ary partitions of numbers r_i, $i=1,2,\dots,\ell$. Every set of numbers

$$p_i^{\lambda_j} , \ j=1,2,\dots, \ ; \ 1 \leq j \leq d \tag{14}$$

determines the decomposition of the group $\mathcal{P}$ into cyclic components. For every set of orders (14) one multiplies relatively prime components according to L4. It can be shown that thus obtained orders m_i of cyclic groups $\mathcal{P}_i$ have the property that m_{i+1} divides m_i, $1 \leq i \leq s-1$. We may use this property in establishing the way of associating obtained cyclic groups to the basis vectors $a_1, a_2, \dots, a_s$, where $s \leq d$. If $s < d$, then with vectors $a_{j+1}, a_{j+2}, \dots, a_d$ there are associated cyclic groups of order 1.

As an example, we see that there are two nonequivalent 4-coloured triclinic lattices $\{a_1^{(4)}, a_2^{(1)}, a_3^{(1)}\}$ and $\{a_1^{(2)}, a_2^{(2)}, a_3^{(1)}\}$ but only one 6-coloured triclinic lattice $\{a_1^{(6)}, a_2^{(1)}, a_3^{(1)}\}$. Further examples of colour lattices of lowest n and $d=3$ are given in Table 1.

It should be pointed out that numbers m_i in Eq. (4) of L1 need not be finite. Then the groups $\mathcal{P}_i$ are infinite cyclic groups. In general, the invariants of an abelian group are prime powers and ∞. We will use this fact in the next section.

4. SPIN TRANSLATION GROUPS

Examples of colour groups of physical importance are spin groups. In this interpretation, the function $f(r)$ is meant as a spin density function $\mathcal{S}(r)$ describing the distribution of magnetic moments in a magnetically ordered crystal. The function $\mathcal{S}(r)$ is an axial vector function defined on the set $\mathcal{G}r_1$ which forms a crystal. The symmetry group $\overline{\mathcal{G}^{\mathcal{S}}}$ of such a system can be found to be a subgroup of the group

$$\widetilde{\mathcal{G}^{\mathcal{S}}} = \mathcal{P} \otimes \mathcal{G} , \qquad (15)$$

where $\mathcal{P} = \mathcal{O} \otimes 1'$ is the group of all rotations and axial inversion in the "spin space" and $\mathcal{G}$ is the crystallographic group acting on vectors in the "physical space". The group $\overline{\mathcal{G}^{\mathcal{S}}}$ is called a spin group (Naish/12/, for a review see Litvin and Opechowski/11/). As previously, we are interested in spin groups isomorphic to $\mathcal{G}$, i.e., junior (nontrivial) spin groups, called further spin groups.

The problem of deriving spin groups is simplified if one knows appropriate abstract colour groups. For a given colour group $\mathcal{G}^{\mathcal{P}}$ one needs only to find its isomorphic spin images $\mathcal{G}_1^{\mathcal{S}_1}, \mathcal{G}_2^{\mathcal{S}_2}, \ldots$, where $\mathcal{S}_1, \mathcal{S}_2, \ldots$ are subgroups of $\mathcal{O} \otimes 1'$.

Next, one finds among $\mathcal{G}_1^{\mathcal{S}_1}, \mathcal{G}_2^{\mathcal{S}_2}, \ldots$ nonequivalent groups using Eqs. (1)-(3), where $\mathcal{P} = \mathcal{O} \otimes 1'$. As an illustration, we shall derive here spin translation groups (STG's) with no symmetry conditions on basis vectors. STG's were first tabulated by Litvin/10/. Let $\mathcal{G}$ be assumed to be a lattice $\mathcal{T}$ generated by basis vectors a_i, $i = 1,2,\ldots,d$. First, we find abelian subgroups of $\mathcal{O} \otimes 1'$ which are

point groups of three categories (we use the International notation):

$$\begin{aligned} &1)\ 1,\ 2,\ 3,\ 4,\ \ldots,\ \infty ; \\ &2)\ 1', 2',\ 2 \otimes 1', 3 \otimes 1', 4',\ 4 \otimes 1', \ldots,\ \infty \otimes 1' ; \\ &3)\ 2\ 2\ 2,\ 2'2'2,\ 222 \otimes 1'. \end{aligned} \qquad (16)$$

Thus, a STG is generated by vectors a_i and proper and improper rotations $R_i = R(a_i)$, $i = 1,2,\ldots,d$. Next, for a given colour lattice $\mathcal{T}^{\mathcal{P}}$ we find all spin lattices $\mathcal{T}_1^{\mathcal{S}_1}, \mathcal{T}_2^{\mathcal{S}_2}, \ldots$ and divide them into equivalence classes. The method is explained here by few examples (Table 1). In Table 2, representative STG's of nonequivalent classes of STG's of triclinic system are given. A STG is denoted by (R_1, R_2, R_3). Symbol N denotes a rotation R_i through an angle $2\pi q/N$, where N and q are relatively prime integers and $q < N$. The rotations $2\pi q/N$ are generators of a cyclic group of order N. A rotation R_i through an angle $2\pi/Z$, where Z is an irrational number, is denoted by Z. The rotation Z is a generator of a cyclic group of infinite order. Symbols N′ and Z′ are used for denoting generators of the groups of 2nd category (16) in the case of both even and odd N's, for simplicity. In the symbol (R_1, R_2, R_3) all R_i denote rotations about a single arbitrarily oriented axis, despite rotations belonging to the groups of 3rd category (16). For these groups, subscripts have been added in Table 2 to indicate the mutual orientations of the twofold axes.

The results presented in Table 2 differ from the Litvin's/10/ results given in Table 1 of his work (in the part concerning the triclinic system), as equivalent classes of

STG's are omitted here. For example, the STG denoted by (N_1, N_2, N_3), where corresponding N's are relatively prime, can be found in the class of STG's denoted by $(N,1,1)$, where $N = N_1 N_2 N_3$. The same concerns the groups $(N_1, N_2, 2)$ and $(N,2,1)$, where N_1, N_2, N are odd integers. The discussion of the problem based on very simple number-theoretic considerations is given in the Appendix.

In conclusion, two remarks are made. (i) We can see from an example in Table 1 that not all colour lattices have their spin interpretation; this is not seen in the case of 2-colour and magnetic groups. (ii) One can get another physical interpretation of colour groups by considering a direct product extension of the group $\mathcal{P}$ in Eq. (15) by the group $\bar{I}$ of inversion of polar vector; one arrives in this way at the so-called magnetoelectric groups (Koptsik and Kotsev/9/).

ACKNOWLEDGEMENTS

I would like to thank Professor V.A.Koptsik for many discussions.

APPENDIX

We discuss here in some detail the problem of the change of the basis of a general colour lattice. For simplicity, we consider the case of 2-dimensional lattice. We shall use the symbol $D(X,Y)$ for denoting the greatest common division of two numbers X and Y. Then $D(X,Y)=1$ will denote that two numbers X and Y are relatively prime.

Let $\mathcal{T}^{\mathcal{P}}$ be a colour lattice generated by basis vectors a_1 and a_2 and cyclic elements (N_1) and (N_2) paired with a_1 and a_2, respectively. The lattice T^P is denoted by $\{N_1, N_2\}$. Now let $D(N_1, N_2)$. We shall prove that in this case $\mathcal{T}^{\mathcal{P}}$ can be denoted by $\{N, 1\}$, where $N = N_1 N_2$. This means that in $\mathcal{T}^{\mathcal{P}}$ new basis vectors $\bar{a}_1$ and $\bar{a}_2$ can be chosen with orders N and 1, respectively. The new basis vectors can be found as

$$\begin{aligned} \bar{a}_1 &= X_1 a_1 + X_2 a_2 , \\ \bar{a}_2 &= N_1 a_1 + N_2 a_2 , \end{aligned} \tag{A.1}$$

where coefficients X_1 and X_2 are integers determined by the equation

$$\mathrm{Det} \begin{Vmatrix} X_1 & X_2 \\ N_1 & N_2 \end{Vmatrix} = \pm 1. \tag{A.2}$$

It is clear that the order of $\bar{a}_2$ is equal to 1. The order of $\bar{a}_1$ will be equal to $N_1 N_2$ if

$$D(X_1, N_1) = 1 \quad \text{and} \quad D(X_2, N_2) = 1. \tag{A.3}$$

This is immediate consequence of the following property of cyclic groups:

Let $\mathcal{C}$ be a cyclic group of order k. If $\mathcal{C}$ is generated by g, then $\mathcal{C}$ is also generated by every g^{ℓ}, where $D(k, \ell) = 1$.

We can see that any solution X_1, X_2 of eq. (A2) has the property (A3). Suppose, for example, that $D(X_1, N_1) = c > 1$. Thus it follows from eq. (A2)

$$Y_1 N_2 - X_2 M_1 = \frac{1}{c} < 1$$

what leads to contradiction, as all considered numbers are integers.

The method for solving eq. (A2) is based on an Euclidean algorithm for finding D(X,Y) (Davenport$^{/2/}$). Let us consider the equation

$$N_1X_2 - N_2X_1 = \pm 1. \qquad (A4)$$

The first step is to express N_1/N_2 as a continued fraction

$$\frac{N_1}{N_2} = q_1 + \cfrac{1}{q_2 + \cfrac{1}{q_3 + \ddots \cfrac{1}{q_{m-1} + \cfrac{1}{q_m}}}} . \qquad (A5)$$

Next one calculates numbers called Euler brackets

$$\begin{aligned} \bar{X}_1 &= [q_1, q_2, \ldots, q_{m-1}] \\ \bar{X}_2 &= [q_2, q_3, \ldots, q_{m-1}] \end{aligned} \qquad (A6)$$

by means of the recurrent formulas

$$\begin{aligned} [q_1, q_2, \ldots, q_j] &= q_1[q_2, q_3, \ldots, q_j] + \\ &+ [q_3, q_4, \ldots, q_j], \end{aligned}$$

where

$$[q_i] = q_i, \quad [\quad] = 1, \quad q_1 = E[N_1/N_2].$$

The general solution of eq. (A4) is given by the expressions:

$$\begin{aligned} X_1 &= (-1)^{\delta}\bar{X}_1 + N_1 t, \\ X_2 &= (-1)^{\delta}\bar{X}_2 + N_2 t, \end{aligned} \qquad (A7)$$

where t is any integer, $\delta = m$ for +1 in the right-hand side of eq. (A4), $\delta = m-1$ for -1, respectively. The solution (A7) exists if and only if N_1 and N_2 are relatively prime.

REFERENCES

1. Belov N.V., Tarkova T.N. Kristallografia, 1956, 2, p.619-620.
2. Davenport H. The Higher Arithmetic. An Introduction to the Theory of Numbers. New York: Harper and Brothers, 1962.
3. Fuchs L. Infinite Abelian Groups. Academic Press, New York, 1971, vol. 1.
4. Harker D. Acta Cryst., 1976, A32, p.133-139.
5. Harker D. Preprint of the Center for Crystallographic Research. Biophysics Department, Roswell Park Memorial Institute, Buffalo, New York, USA, 1978.
6. Hall M. (Jr.). Combinatorics. Pergamon Press, New York, 1969.
7. Indebom V.L. Kristallografia, 1959, 4, p.619-621.
8. Koptsik V.A., Kotsev J.N. JINR, P4-8067, Dubna, 1974.
9. Koptsik V.A., Kotsev J.N. JINR, P4-8466, Dubna, 1974.
10. Litvin D.B. Acta Cryst., 1973, A29, p.651-660.

11. Litvin D.B., Opechowski W. Physica, 1974, 76, p.538-554.
12. Naish V.E. Izv. Akad.Nauk SSSR, ser. Fiz., 1963, p.1496-1505.
13. Niggli A. Z.Kristallogr., 1959, 111, p.288-300.
14. Opechowski W. In: Group Theoretical Methods in Physics. Proc. of the Fifth International Colloquium. Sparp R.T. and Kolamn B., eds. Academic Press, New York, 1977.
15. Shubnikov A.V., Koptsik V.A. Symmetry in Science and Art, Plenum Press, New York, 1974.
16. Van der Waerden B.L., Burckhardt J.J. Z.Kristallogr., 1961, 115, p.232-234.
17. Zamorzaev A.M. Kristallografia, 1967, 12, p.819-825.
18. Zamorzaev A.M. Ibid., 1969,14, p.195-199.
19. Koptsik V.A., Kuzhukeev J. N.M., 1972, Kristallografia, 1972, 17, p.705.

Received by Publishing Department
on September 28 1978.