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Colour Lattices and Spin Translation Groups. General Case*

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Abstract

A method of deriving d-dimensional crystallographic colour lattices with no symmetry conditions on the 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 [*Acta Cryst.* (1973), A**29**, 651–660].

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1. Introduction

Colour groups in crystallography are defined as extensions of classical crystallographic groups. The idea started in the works of Below & Tarkhova (1956), Indenbom (1959), Niggli (1959) and others (see also Shubnikov & Koptsik, 1974). Colour groups are of interest in the theory of magnetic crystals, alloys, defect crystals, *etc.* Magnetic groups have been interpreted in terms of two-colour groups. The generalized magnetic groups called spin groups have been recently introduced in the form of many-coloured groups.

Different types of colour groups, their properties and bibliography have been reviewed by Shubnikov & Koptsik (1974) and Opechowski (1977). Only P-type colour groups will be considered here. Colour point groups have been derived by Koptsik & Kotsev (1974*a*) and Harker (1976). Zamorzaev (1969),

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Zamorzaev, Galarskii & Palistrant (1978) and Shubnikov & Koptsik (1974) have listed 2-, 3-, 4- and 6-colour three-dimensional lattices. Only very limited classes of colour space groups are known (Zamorzaev, 1969; Koptsik & Kuzhukeev, 1972). Harker (1978*a*) has recently proposed a method of deriving colour lattices with symmetry conditions on the basis vectors. He has also listed triclinic colour lattices for $n \leq 16$.

In this paper an algebraic method of deriving the colour d-dimensional lattices in a general case is presented, *i.e.* no symmetry conditions are imposed on the basis vectors of a lattice. The exact formulas for a number of non-equivalent n-colour lattices are given for $d \leq 4$ and any finite n. The results are used for deriving spin translation groups in the triclinic system. Preliminary definitions and basic properties of colour groups are briefly presented in § 2. In § 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 (STG's) are derived and tabulated in § 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.*

Table 1. *Examples of colour lattices (CL) and spin translation groups (STG) isomorphic to them*

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_x2_y1), $(2'_x2_y1)$
5	{511}	(511)
6	{611}	(611), (6′11), (3′11)
7	{711}	(711)
8	{811}	(811), (8′11)
	{421}	(41′1)
	{222}	$(2_x2_y1')$
36	{36,1,1}	(36,1,1), (36′,1,1)
	{18,2,1}	(18,1′,1)
	{12,3,1}	–
	{661}	–

Table 2. *Spin translation groups of the triclinic system*

$(N11)$	$(ZN1')$*	(Z_1Z_2N)
$(N'11)$		(Z'_1Z_2N)
$(N1'1)$*	$(ZN1)$	$(Z'_1Z'_2N)$
	$(Z'N1)$	
(2_x2_y1)	$(ZN'1)$	(Z_1Z_2N')
$(2'_x2_y1)$	$(Z'N'1)$	(Z'_1Z_2N')
$(2_x2_y1')$		$(Z'_1Z'_2N')$
	$(Z_1Z_2Z_3)$	
	$(Z'_1Z_2Z_3)$	
	$(Z'_1Z'_2Z_3)$	
	$(Z'_1Z'_2Z'_3)$	

* N even.

2. Colour groups

For a given group G and a discrete set of points $\mathsf{R} = \{\mathbf{r}_1, \mathbf{r}_2, \ldots\}$ consider an orbit Q in R relative to G:

$$\mathsf{Q} = \mathsf{G}\mathbf{r}_1 = \{\mathbf{r}_2 | \mathbf{r}_2 = g_i\,\mathbf{r}_1, g_i \in \mathsf{G}\}.$$

Let $f(\mathbf{r})$ be an arbitrary function defined on $\mathsf{G}\mathbf{r}_1$. Any value f_i of function $f(\mathbf{r})$ is called a *colour*. An ordered pair $[f(\mathbf{r}_i), \mathbf{r}_i]$ is a *colour point*. Let $\mathsf{F} = \{f_i\}$ be a set of all n distinct values of a function $f(\mathbf{r})$ and $\mathsf{P} = \{p_k\}$ a transitive group on F. In particular, P can be thought of as any subgroup of the group S_n of all permutations of colour f_j.

We consider ordered pairs (p_k, g_i), where $p_k \in \mathsf{P}$ and $g_i \in \mathsf{G}$, and define their action on colour points $[f_i, \mathbf{r}_j]$. We assume that elements of P act independently relative to elements of G:

$$(p_k, g_i)[f_l, \mathbf{r}_j] = [p_k f_l, g_i\,\mathbf{r}_j] = [f_q, \mathbf{r}_s];$$
$$f_l, f_q \in \mathsf{F};\ \mathbf{r}_j, \mathbf{r}_s \in \mathsf{Q}.$$

Any subgroup of group $\mathsf{G}^{(\mathsf{P})} = \mathsf{P} \otimes \mathsf{G}$, where $\otimes$ denotes direct product of groups, is a *colour group* (*P-type colour group*) (van der Waerden & Burckhardt, 1961; Zamorzaev, 1967). We are interested in those subgroups $\mathsf{G}^{(\mathsf{P})}$ of $\mathsf{P} \otimes \mathsf{G}$ which are isomorphic to G:

$$\mathsf{G} \simeq \mathsf{G}^{(\mathsf{P})} \subseteq \mathsf{P} \otimes \mathsf{G}.$$

The subgroups $\mathsf{G}^{(\mathsf{P})}$ are *nontrivial* colour groups. The set of classical elements (e, g_i); $e \in \mathsf{P}$, $g_i \in \mathsf{G}$ forms a subgroup $\mathsf{H}^{(1)}$ of a colour group. The symmetry group of a system of colour points K is the colour group leaving K invariant. A system of colour points with the nontrivial colour group as the symmetry group has select 'colour properties'. In particular: (i) a function $f(\mathbf{r})$ is single-valued, *i.e.* only one colour f_i is paired with each point $\mathbf{r}_i$; (ii) the number of colour points $[f_l, \mathbf{r}_l]$ for each colour f_l of F is the same; they are equal to the order of the classical subgroup $\mathsf{H}^{(1)}$ of $\mathsf{G}^{(\mathsf{P})}$.

Only nontrivial colour groups $\mathsf{G}^{(\mathsf{P})}$ are discussed in the following sections.

The method of deriving all subgroups $\mathsf{G}^{(\mathsf{P})}$ of $\mathsf{P} \otimes \mathsf{G}$ is based on the 'isomorphism theorem' of Zamorzaev (1967).

A set of all elements p_l of P in a nontrivial group $\mathsf{G}^{(\mathsf{P})}$ constitutes a group P isomorphic to a factor group G/H. The elements p_l of P are paired with elements g_k of G by the homomorphism

$$\mathsf{G} \rightarrow \mathsf{G}/\mathsf{H} \simeq \mathsf{P}.$$

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Two colour groups $G^{(P)}$ and $\overline{G^{(P)}}$ are equivalent if they are conjugate subgroups of a group $\Omega = \{\alpha_i\}$:

$$\overline{G^{(P)}} = \alpha_i G^{(P)} \alpha_i^{-1}, \quad \alpha_i \in \Omega \tag{1}$$

and

$$H^{(1)} = \alpha_i H^{(1)} \alpha_i^{-1} \tag{2}$$

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

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

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

3. Colour lattices

Let G be a d-dimensional crystallographic lattice denoted by T:

$$T = \left\{ \mathbf{t}; \mathbf{t} = \sum_{i=1}^{d} n_i \mathbf{a}_i, n_i \text{ integers} \right\}$$

where $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_d$ are d linearly independent vectors in d-dimensional Euclidean space. Vectors $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_d$ form a basis of T. We assume that no symmetry conditions are imposed on the basis vectors, *i.e.* any set of d linearly independent vectors of T stands for the basis of T. The colour lattice $T^{(P)}$ isomorphic to T is the *general colour lattice.* The lattice T is an Abelian group and can be expressed as a direct product of d one-dimensional lattices:

$$T = T_1 \otimes T_2 \otimes \ldots \otimes T_d$$

where all T_i ($i = 1, 2, \ldots, d$) are infinite cyclic groups. We now formulate four group-theoretical lemmas which are standard statements in the theory of Abelian groups (Fuchs, 1971).

Lemma 1. Let a lattice T^* be a d-dimensional subgroup of T. Then there exist bases $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_d$ of the group T and $\mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_d$ of the group T^*, respectively, such that

$$\mathbf{b}_i = m_i \mathbf{a}_i \tag{4}$$

where all m_i are integers.

Lemma 2. If

$$G \simeq A_1 \otimes A_2 \otimes \ldots \otimes A_l$$

and A_i^* is an invariant subgroup of A_i, $i = 1, 2, \ldots, l$, then for some subgroup H of G,

$$H \simeq A_1^* \otimes A_2^* \otimes \ldots \otimes A_l^*$$

and

$$G/H \simeq (A_1/A_1^*) \otimes (A_2/A_2^*) \otimes \ldots \otimes (A_l/A_l^*).$$

Lemma 3. Every finite Abelian group G is a direct product of groups

$$G = G_1 \otimes G_2 \otimes \ldots \otimes G_k \tag{5}$$

where each G_i is cyclic of prime power order $p_i^{\lambda_i}$, $\lambda_i > 0$. The orders $p_i^{\lambda_i}$ are *invariants* and the groups are *prime components* of the decomposition (5).

Two finite Abelian groups are isomorphic if and only if they have the same set of elementary divisors.

Lemma 4. A direct product

$$H_1 \otimes H_2 \otimes \ldots \otimes H_q \tag{6}$$

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

A method of constructing general colour lattices $T^{(P)}$ for a given lattice T is based on the following theorem:

Theorem 1.

$$T^{(P)} = T_1^{(P_1)} \otimes T_2^{(P_2)} \otimes \ldots \otimes T_d^{(P_d)} \tag{7}$$

where

$$T_i^{(P_i)} \simeq T_i \; (i = 1, 2, \ldots, d)$$

and

$$P = P_1 \otimes P_2 \otimes \ldots \otimes P_d \tag{8}$$

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

This result follows immediately from the isomorphism theorem, lemma 1 and lemma 2. Since T is Abelian, any subgroup T^* of T is normal. The factor group T/T^* must exist and is also Abelian. Thus the group P of $T^{(P)}$ is an Abelian group. In the one-dimensional case, group T_i/T_i^* is a cyclic group of order m_i, as is the group P_i.

Thus, to derive all colour lattices $T^{(P)}$ for a given lattice T and number n, it is only necessary to find all nonisomorphic Abelian groups P of order n expressed as all possible decompositions (8). We use now lemma 3. In the decomposition (5) of the group G, let the cyclic groups be related to the distinct primes $p_1, p_2, \ldots, p_k$. Let the number of prime components related to a prime p_i ($i = 1, 2, \ldots, k$) be equal to q_i and the prime components of order

$$p_i^{\lambda_1}, p_i^{\lambda_2}, \ldots, p_i^{\lambda_{q_i}} \tag{9}$$

where the numbers λ are arranged as follows:

$$\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_{q_i}; \tag{10}$$

$$\sum_j \lambda_j = r_i; \quad j = 1, 2, \ldots, q_i; \quad i = 1, 2, \ldots, k.$$

In this way, one obtains from lemma 3 all nonisomorphic Abelian groups of given order $n = p_1^{r_1} p_2^{r_2} \ldots p_l^{r_l}$ by considering all partitions (10) of numbers r_i ($i = 1$, 2, ..., k) with arbitrary numbers q_i. Here we are interested in the decomposition of an Abelian group of order n into d cyclic components with admitted trivial components, *i.e.* cyclic groups of order 1. It is clear from lemma 3, lemma 4 and (10) that such decompositions can be found, if the numbers q_i are less than d.

A partition of r as a sum of a maximum of d positive integers is called a d-ary partition. The number of d-ary partitions of r will be denoted by $\gamma(r)$. All possible decompositions (8) can then be expressed by all d-ary partitions of numbers r_i. The numbers $\gamma(r)$ 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, 1969). Thus, we have the following final result:

Theorem 2. The number of n-colour d-dimensional lattices for

$$n = p_1^{r_1} p_2^{r_2} \dots p_l^{r_l} \tag{11}$$

where all numbers p_i are distinct primes, is equal to

$$\gamma(r_1)\, \gamma(r_2) \dots \gamma(r_i) \tag{12}$$

where $\gamma(r_i)$ is expressed as:

$$\begin{gathered} E\{\tfrac{1}{144}(r_i + 7)^2(r_i + 1) + \tfrac{2}{9}\} \text{ for } d = 4 \text{ and } r_i \text{ odd;} \\ E\{\tfrac{1}{144}[(r_l + 5)^3 - 3(r_i - 7)]\} \text{ for } d = 4 \text{ and } r_i \text{ even;} \\ E\{\tfrac{1}{12}(r_i + 3)^2 + \tfrac{1}{4}\} \text{ for } d = 3; \\ E\{(r_l/2) + 1\} \text{ for } d = 2;\ 1 \text{ for } d = 1. \end{gathered} \tag{13}$$

Here $E\{x\}$ denotes the integer part of x; $i = 1, 2, \dots, l$.

A colour lattice $\mathsf{T}^{(\mathsf{P})}$ will be represented by the basis vectors $\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_d$, each vector being paired with an appropriate generating element p_i of P_i ($i = 1, 2, \dots, d$). The symbols $\{\mathbf{a}_1^{(p_1)}, \mathbf{a}_2^{(p_2)}, \dots, \mathbf{a}_d^{(p_d)}\}$ or simply $\{m_1, m_2, \dots, m_d\}$ where m_i is the order of P_i are used for denoting the $\mathsf{T}^{(\mathsf{P})}$. The number m_i is an *order* of the vector $\mathbf{a}_i$ since $[\mathbf{a}_i^{(p_i)}]^{m_l} = \mathbf{b}_i^{(1)}$ where $\mathbf{b}_i = \mathbf{m}_i\, \mathbf{a}_i$ is a classical vector of $\mathsf{T}^{(\mathsf{P})}$.

The method of constructing all colour d-dimensional lattices for a given number of colours n is as follows.

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

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

determines the decomposition of the group P into cyclic components. For every set of order (14) the relatively prime components are multiplied according to lemma 4. It can be shown that the orders thus obtained m_i of cyclic groups P_i have the property that m_{i+1} divides m_i, $1 \leq i \leq s - 1$. We may use this property to establish the associated cyclic groups with the basis vectors $\mathbf{a}_1$, $\mathbf{a}_2$, ..., $\mathbf{a}_s$ where $s \leq d$. If $s < d$, then with vectors $\mathbf{a}_{j+1}$, $\mathbf{a}_{j+2}$, ..., $\mathbf{a}_d$ there are associated cyclic groups of order 1.

For example, we see that there are two non-equivalent 4-coloured triclinic lattices $\{\mathbf{a}_1^{(4)}, \mathbf{a}_2^{(1)}, \mathbf{a}_3^{(1)}\}$ and $\{\mathbf{a}_1^{(2)}, \mathbf{a}_2^{(2)}, \mathbf{a}_3^{(2)}\}$ but only one 6-coloured triclinic lattice $\{\mathbf{a}_1^{(6)}, \mathbf{a}_2^{(1)}, \mathbf{a}_3^{(1)}\}$. Further examples of colour lattices of lowest n and $d = 3$ are given in Table 1.

It is pointed out that the numbers m_i in (4) of lemma 1 need not be finite. It follows that the groups P_i are infinite cyclic groups. In general, the invariants of an Abelian group are prime powers and ∞. We use this fact in the next section.

4. Spin translation groups

Spin groups are examples of colour groups of physical importance. In this interpretation, the function $f(\mathbf{r})$ denotes a spin density function $\mathbf{S}(\mathbf{r})$ describing the distribution of magnetic moments in a magnetically ordered crystal. The function $\mathbf{S}(\mathbf{r})$ is an axial vector function defined on the set $\overline{\mathsf{G}\mathbf{r}_1}$ which forms a crystal. The symmetry group $\overline{\mathsf{G}^\mathsf{S}}$ of such a system is a subgroup of group

$$\tilde{\mathsf{G}}^\mathsf{S} = \mathsf{P} \otimes \mathsf{G} \tag{15}$$

where $\mathsf{P} = \mathsf{O} \otimes 1'$ is the group of all rotations and axial inversion in 'spin space' and G is the crystallographic group $\underline{\text{acting}}$ on the vectors in 'physical space'. The group $\overline{\mathsf{G}^\mathsf{S}}$ is called a spin group (Naish, 1963; for a review see Litvin & Opechowski, 1974). We are interested in spin groups isomorphic to G.

The problem of deriving spin groups is simplified if the appropriate abstract colour group is known. For a given colour group $\mathsf{G}^{(\mathsf{P})}$ one needs only its isomorphic spin images $\mathsf{G}_1^{(\mathbf{S}_1)}, \mathsf{G}_2^{(\mathbf{S}_2)}, \dots$ where $\mathbf{S}_1$, $\mathbf{S}_2$ are subgroups of $\mathsf{O} \otimes 1_0^1$.

The nonequivalent groups among $\mathsf{G}_1^{(\mathsf{S}_1)}, \mathsf{G}_2^{(\mathsf{S}_2)}, \dots$ are found by using (1)–(3) where $\mathsf{P} = \mathsf{O} \otimes 1'$. As an illustration, we derive the STG's with no symmetry conditions on the basis vectors. STG's were first tabulated by Litvin (1973). Assume G to be a lattice T generated by basis vectors $\mathbf{a}_i$, $i = 1, 2, \dots, d$. We find the Abelian subgroups of $\mathsf{O} \otimes 1'$ which are point groups of three categories:

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

Thus, a STG is generated by vectors $\mathbf{a}_i$ and proper and improper rotations $R_i = R(\mathbf{a}_i)$, $i = 1, 2, \dots, d$. For a given colour lattice $\mathsf{T}^{(\mathsf{P})}$ we then find all spin lattices $\mathsf{T}_1^{(\mathsf{S}_1)}$, $\mathsf{T}_2^{(\mathsf{S}_2)}$, ... and divide them into equivalent classes. The method is illustrated by a few examples (Table 1). In Table 2, representative STG's of nonequivalent classes of STG's of the triclinic system are given. A STG is denoted by (R_1, R_2, R_3). The 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 the 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 groups of the second category (16) in the case of both even and odd N. In the symbol (R_1, R_2, R_3) all R_i denote rotations about a single arbitrarily oriented axis, despite rotations belonging to groups of the third category (16). For these groups, subscripts have been added in Table 2 to indicate the mutual orientations of the two-fold axes.

The results presented in Table 2 differ from Litvin's (1973) results given in Table 1 of his work as the 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 $N = N_1 N_2 N_3$. Similarly for 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, we make two remarks. (i) We can see from the example in Table 1 that all colour lattices do not have a spin interpretation; this is not the case with two-colour and magnetic groups. (ii) Another physical interpretation of colour groups follows by considering the direct-product extension of group P in (15) by group $\bar{1}$, which causes inversion of the polar vector; one thus arrives at the so-called magnetoelectric groups (Koptsik & Kotsev, 1974*b*).

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

Note added posthumously: A paper by D. Harker (1978*b*) that appeared after receipt of the present paper presents similar results based on a geometric-algebraic argument. (Note added by Professor A. Oles.)

* See deposition footnote.

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