COLOUR SPACE GROUPS OF ALL CUBIC CHROMOMORPHIC CLASSES AND THEIR APPLICATION

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ABSTRACT
The method and the derivation of the full tables of 2801 permutational colour groups,isomorphic to the crystallographic space groups,with the colour permutation groups,isomorphic to the cubic point groups, are given.The application of these groups and their permutational representations in the Landau theory of phase transitions is discussed.

1.Introduction

In this paper we shall consider only the permutational colour groups G^P of P-type, isomorphic to the classical crystallographic space groups G. A detailed information about the structure of these groups,henceforth named for short "colour groups", is contained in their full symbols

$$G^P \equiv G/H'/H(A,A')_n \qquad (1)$$

and can be found in Ref.1-6. We shall remind only that in (1) H′is a subgroup of G of index n (n is the number of permutated colours); it is isomorphic to the maximal subgroup of G^P which preserves at least one of the colours. The group H is the maximal invariant subgroup of G contained in H′and it is isomorphic to the maximal subgroup of G^P which does not change any colour.The subgroup P of the symmetric group S_n,transitive on the set of n colours, is denoted by the symbol $(A,A')_n$. Here the abstract groups A and $A'\subset A$ are isomorphic to the factor-groups G/H and H′/H,respectively. The subgroup chains of G and A are related by the homomorphism with Kerφ=H:

$$\begin{array}{ccccccc} G & \supset & H' & \triangleright & H & = & \bigcap_{g\in G} gH'g^{-1} \\ \varphi\downarrow & & \varphi\downarrow & & \varphi\downarrow & & \\ A & \supset & A' & \triangleright & C_1 & = & \bigcap_{a\in A} aA'a^{-1} \end{array} \qquad (2)$$

Due to the homomorphism φ the group P constructed as an image of the transitive permutation representation[4-6] $\pi_G^{H'}$ of G, coincides with the representation $\pi_A^{A'}$ of A:

$$P = \mathrm{Im}\,\pi_G^{H'} = \pi_A^{A'} = (A,A')_n \cong A \qquad (3)$$

All the colour groups $G/H'/H(A,A')_n$ with the same group $(A,A')_n$ of colour permutations belong to the same chromomorphic class[2,7], labeled by the symbol of the group $(A,A')_n$.

In the present paper all the 2801 colour space groups G^P of the cubic chromomorphic classes (i.e. A in (1) are isomorphic to the cubic point groups T, O, T_h or O_h) and the associated with them permutation representations $D_G^{H'}$ (see Ref. 2,5-7) are derived. The application of these groups in the classification and symmetry analysis of phase transitions(PT) in the frame of Landau theory is discussed following Ref.5-8.

2. Colour space groups of cubic chromomorphic classes.

The colour space groups G^P of all the 26 cubic chromomorphic classes[2,7] $(A,A')_n$, where $A \cong T, O, T_h$ or O_h, and their permutation representations $D_G^{H'}$ have been derived using the general algorithm proposed in our recent reports[8-10]. It is based on the theory of zentral extensions of groups and the corresponding representations of space groups. In our case the groups H in the symbol (1) appear as kernels of three dimensional physically irreducible representations (irreps) of the 230 space groups G due to the following statement, that will be proved elsewhere[11]. The group H is an invariant subgroup of the space group G, such that $G/H \cong T, O, T_h$ or O_h iff H is a kernel of some three dimensional physically irreducible representation $D_j^{[k]}$ of G (the vector k corresponds to a Lifshitz point[12] of the first Brillouin zone).

As an example in Table1 the 7 color groups G^P isomorphic to the space group $G = O_h^5$ with the same $H = \mathrm{Ker}D_G^{H'} = \mathrm{Ker}D_7^{[k10]}$, $\dim D_7^{[k10]} = 3$, are given. They belong to the 7 classes $(A,A')_n$, where $A \cong O$. For each group $O_h^5/H'/D_{2h}^2(O,A')_n$ the subgroup H'is specified by[13]: i)the matrix $m = \|m_{ij}\|$, connecting the generators $\{a'_j \mid j=1,2,3\}$ and $\{a_i \mid i=1,2,3\}$ of the translation subgroups T'and T of the space groups H'and H, respectively ($a'_j = a_i m_{ij}$); ii)the additional translations $t_i \in T$, assigned to the corresponding generators h_i of the point group $\hat{H}'$ of H'; iii)the origin shift $\mathfrak{T}$ of T'with respect to T. On the right hand side of Table1 the permutational representations $D_G^{H'}$ are given by the multiplicity $(D_G^{H'} \mid D_j^{[k]})$ of their ir-

Table1. Colour groups $G^P \cong O_h^5$ witu H=Ker $D_7^{[k10]}$.

$G/H'/H(A,A')_n$	m	t_i	τ	${}^sD_1^{[k11]}$	$D_3^{[k11]}$	${}^sD_5^{[k11]}$	${}^sD_3^{[k10]}$	$D_7^{[k10]}$
$O_h^5/D_{2h}^2(0,C_1)_{24}$	m_1	$t_2=(100)$ $t_4=(001)$	$(\frac{3}{4},\frac{3}{4},\frac{3}{4})$	1	1	2	3^*	3^*
$O_h^5/D_{2h}^{20}/D_{2h}^2(0,C_2)_{12}$	m_2	$t_2=(100)$ $t_4=(000)$	$(\frac{3}{4},\frac{3}{4},-\frac{1}{4})$	1	1	2	1	1
$O_h^5/D_{4h}^{12}/D_{2h}^2(0,C_2')_{12}$	m_1	$t_{14}=(100)$ $t_2=(100)$	$(1\frac{1}{4},\frac{1}{4},\frac{1}{4})$	1	.	1	2^*	1^*
$O_h^5/T_h^2/D_{2h}^2(0,C_3)_8$	m_1	$t_9=(010)$ $t_2=(100)$	$(\frac{3}{4},\frac{3}{4},-\frac{1}{4})$	1	1	.	1	1^*
$O_h^5/D_{4h}^9/D_{2h}^2(0,D_2')_6$	m_2	$t_{14}=(100)$ $t_2=(100)$	$(\frac{1}{2},\frac{1}{2},0)$	1	.	1	1^*	.
$O_h^5/D_{4h}^6/D_{2h}^2(0,C_4)_6$	m_2	$t_{14}=(000)$ $t_2=(100)$ $t_{16}=(100)$	$(\frac{1}{4},1\frac{1}{4},-\frac{1}{4})$	1	.	1	.	1^*
$O_h^5/O_h^4/D_{2h}^2(0,D_3)_4$	m_1	$t_{14}=(100)$ $t_9=(010)$	$(\frac{3}{4},\frac{3}{4},-\frac{1}{4})$	1		.	1^*	
		$t_{25}=(000)$						

$$m_1=\begin{pmatrix}-1 & 1 & 1\\ 1 & -1 & 1\\ 1 & 1 & -1\end{pmatrix} \qquad m_2=\begin{pmatrix}-1 & 0 & 1\\ 1 & 0 & 1\\ 0 & 1 & -1\end{pmatrix}$$

reducible components $D_j^{[k]}$. The choice of a_i , the notation of h_i and $D_j^{[k]}$ and identification of the space groups have been made according Ref.12.

All the derived 2801 colour space groups G^P are classified in

Table2.The total number of G^P is presented as a sum of the numbers of groups with monochromatic lattice $T^{(1)}\hat{G}^{(p)}$ and polychromatic lattice ,respectively, for each cubic chromomorphic class $(A,A')_n$. The space groups G,isomorphic to them, are also given.

We have considered two colour groups,belonging to the family of G as equivalent iff H_1' and H_2' are conjugated subgroups of G (in their symbols $G/H_1'/H_1$ and $G/H_2'/H_2$).

3.Application in the Landau theory.

The reformulation of the group-theoretical criteria of the Landau theory in therms of colour groups allows to consider the algorithm for derivating G^P and their representations $D_G^{H'}$ as an effective procedure for getting necessary information for PT analysis(see Ref.5-7). Each PT from prototype phase G to the low-symmetry phase $H' \subset G$,i.e. $G \to H'$, may be associated with the colour group $G/H'/H(A,A')_n$.The basises of irreps $D_G^j \in D_G^{H'}$ contribute the primary order parameters and the secondary ones to the low-symmetry phase.The investigation of this PT and a great number of other ones,classified by the colour groups G^P with common $(A,A')_n$, is reduced to the investigation of only one PT $A \to A'$. The irreps D_G^j responsible for the PT $G \to H'$ should be engendered by the faithful irreps $D_A^j \in D_A^{A'}$ of A and all the triads (G,H',D_G^j) satisfy the Birman-Jarič chain-subduction criteron (CSC) iff the corresponding triads (A,A',D_A^j) do it.The Landau stability criterion (LSC) $[D_G^j]^3_{sym} \not\ni D_G^1$ is satisfied iff $[D_A^j]^3_{sym} \not\ni D_A^1$. All the corresponding PT may be continuous.The colour groups of cubic chromomorphic classes describe all possible triads (G,H',D_G^j) with three dimensional physically irreducible representations of the 230 space groups. The corresponding 26 representations $D_A^{A'}$ have been analysed in Ref.7. Only for the groups of 19 chromomorphic classes the CSC is satisfied.

For example (see Table2) there are 85 possible PT of the chromomorphic class $(O,C_4)_6$. Their permutational representations $D_G^{H'}$ are engendered by the same representation $D_A^{A'} = D_O^{C4} = \Gamma_1^s + \Gamma_3 + \Gamma_4^f$. The active irreps D_G^j in the PT for the 85 groups $G/H'/H(O,C_4)_6$ are engendered by the same faithful irrep Γ_4^f of O, which satisfies the above mentioned criteria.Therefore all the 85 chromomorphic

Table2. Classification of G^P

$(A,A')_n$	G^P	G
$(T,C_1)_{12}$	43= 12+ 31	$C_3^{1-4}, S_6^{1,2}, C_6^{1-6}$
$(T,C_2)_6$	43= 12+ 31	$C_{3h}^1, C_{6h}^{1,2}, T^{1-5}, T_h^{1-7}$
$(T,C_3)_4$	43= 12+ 31	
$(T_h,C_1)_{24}$	73= 7+ 66	$C_3^{1-4}, S_6^{1-2}, C_{3h}^1$
$(T_h,C_2)_{12}$	73= 7+ 66	$C_6^{1-6}, C_{6h}^{1-2},$
$(T_h,C_s)_{12}$	73= 7+ 66	$T^{1,3,5}, T_h^{1-7}$
$(T_h,C_3)_8$	73= 7+ 66	
$(T_h,C_{2v})_6$	73= 7+ 66	
$(O,C_1)_{24}$	85= 24+ 61	D_3^{1-7}, C_{3v}^{1-6}
$(O,C_2)_{12}$	85= 24+ 61	D_{3d}^{1-6}, D_6^{1-6}
$(O,C_2')_{12}$	85= 24+ 61	$C_{6v}^{1-4}, D_{3h}^{1-4}$
$(O,C_3)_8$	85= 24+ 61	D_{6h}^{1-4}, O^{1-8}
$(O,C_4)_6$	85= 24+ 61	T_d^{1-6}, O_h^{1-10}
$(O,D_2')_6$	85= 24+ 61	
$(O,D_3)_4$	85= 24+ 61	
$(O_h,C_1)_{48}$	107= 10+ 97	$D_3^{1-7},$
$(O_h,C_2)_{24}$	107= 10+ 97	$C_{3v}^{1,2,5,6}$
$(O_h,C_s)_{24}$	107= 10+ 97	$D_{3d}^{1-6}, D_{3h}^{1-4}$
$(O_h,C_2')_{24}$	214= 20+194	D_6^{1-6}, C_{6v}^{1-4}
$(O_h,C_3)_{16}$	107= 10+ 97	$D_{6h}^{1-4},$
$(O_h,C_4)_{12}$	214= 20+194	$T_d^{1,3,4}$
$(O_h,C_{2v})_{12}$	107= 10+ 97	$O^{1,2,5,8}$
$(O_h,D_2')_{12}$	214= 20+194	O_h^{1-10}
$(O_h,C_{2v}'')_{12}$	107= 10+ 97	
$(O_h,D_3)_8$	214= 20+194	
$(O_h,C_{4v})_6$	214= 20+194	
Total	2801=399+2402	

PT may be continuous. One of them is associated with the color group $O_h^5/D_{4h}^6/D_{2h}^2(O,C_4)_6$ (see Table1) and should be associated with the irreducible representation $D_7^{[k10]}=\varphi^{-1}(\Gamma_4^f)$. Experimentally such rotational PT $O_h^5 \rightarrow D_{4h}^6$ has been observed[14] in K_2SeBr_6.

In the same way all possible symmetry descents from O_h^5, associated with the colour groups and their $D_G^{H'}$ in Table 1, have been investigated (The upper index "s" of $D_{O_h}^j$ means that LSC is violated; the asterisk assigned to the multiplicity of $D^j_{O_h}$ means that for the corresponding triad $(G,H',D^j_{O_h})$ CSC is fulfilled.

The application of colour groups and their permutational representations in the Landau theory of PT gives results analogic to those of Gufan[15], Michel[16] and Stokes,Hatch,Kim[17]. However, the present method shows at least two merits. 1)With every cuple of groups G and $H' \subset G$ not only one but whole set of irreps $D^j_G \in D^{H'}_G$ is associated.This means that irreps that contribute primary as well as secondary order parameters are simultaneously identified.2) The chromomorphic classification of G^P allows more detailed classification of the triads:for example all 1712 triads with the same image $ImD^j_G = \Gamma_4^-$ of O_h (C48ª in Ref.17) are given by 1712 G^P , but they are subdevided in 11 chromomorphic classes $(O_h,A')_n$.The triads in 5 of these classes, containing 749 groups do not satisfy CSC and therefore they are not related to any PT.

Complete tables of colour space groups ,containing all the necessary information for analysis of PT would be given elsewhere.[11]

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