N-DIMENSIONAL CRYSTALLOGRAPHY

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ABSTRACT. After a reminder of the basic concepts relevant to the study of group action, we apply them to n-dimensional crystallography. We obtain simple and natural answers to questions which are still controversial on the literature.

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August 1985

The content of this paper was presented at the crystallographic workshop held at IHES in January 1985. A preliminary version was presented at the Niggli Symposium, Zurich, August 1984.

0. INTRODUCTION.

Most of the basic concepts used for classification in crystallography were introduced in the XIXth century without being "formally" defined. Later, when definitions were given they did not always coincide, or they relied on special features of geometry in 2 or 3 dimension. Already in 1900, in his famous list of mathematical problems, Hilbert had asked if the number of crystallographic group types were finite in any dimension n. In 1910, Bieberbach [8a] answered affirmatively for the number of isomorphic classes of crystallographic groups, and two years later, he could extend the affirmative answer for the crystallographic types refered by the crystallographers.

To define all other concepts for any dimension n is felt as a scientific need, although it is not so simple*). This was done in two recent books :

[1] H. Brown, R. Bülow , J. Neubüser, H. Wondratschek, H. Zassenhaus, Crystallographic groups of four dimensional space, John Wiley & sons, New-York, 1978.

[2] R.L.E. Schwarzenberger, N-dimensional crystallography, Pitman Publ. London, 1980.

as well as in the new edition of the first volume of the International Crystallographic Tables (specially ch. 8) [3]. We find that some definitions are not completely explicit and partly unnatural. Most of these concepts appear naturally in the study of group actions; this will be clear in the set of definitions we give here. Some four points are probably original, but most of this paper is expository and self-contained. Section 1 is devoted to group actions. Section 2 to crystallographic concepts. Section 3 answers the question :
Given a crystallographic group, what is its crystal system and its Bravais system ?

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*) In reference [4] two of the authors had each proposed earlier a definition of a crystallographic system, the third author had shown that they failed for n=7.

We conclude by giving other applications of group actions in crystallography.

1. GROUP ACTIONS.

An action of a group G on a mathematical structure M whose automorphism group is $\mathrm{Aut}\, M$, is defined by a group homomorphism $G \xrightarrow{f} \mathrm{Aut}\, M$. The action is effective if $\mathrm{Ker}\, f$, the kernel of f, is trivial. This action defines also naturally an action of G on the subsets or the substructures of M. In a given G action on M, the orbit $G.m$ is the subset of M whose elements are the G transforms of $m \in M$. The elements of G which leave m fixed form a subgroup G_m which is called the isotropy group of m, or, equivalently, the stabilizer of m. For instance, G acts on itself by inner automorphism ; the orbit $G.x$ of $x \in G$ is the conjugation class of x, i.e. the set of elements of the form gxg^{-1}. The isotropy group G_x is called the centralizer of x. In the corresponding action of G on its subgroups the orbit of $H < G$ ($<$ reads "subgroup of") is the class of G-subgroups conjugated to H, it is denoted by $[H]_G$; the stabilizer of H for this G-action is called the normalizer of H in G and it is denoted by $N_G(H)$: it is the largest subgroup of G which contains H as invariant subgroup.

If two elements m,m' are on the same orbit, $\exists g$, $m' = gm$ then $G_{g.m} = gG_m g^{-1}$. The isotropy groups of the orbit G,m form a conjugation class $[G_m]_G$ of subgroups. It is convenient to denote by M^g the set of elements invariant by $g \in G$. Similarly, $M^H = \bigcap_{g \in H} M^g$. Then $M^{G_m} \cap G.m = N_G(G_m).m$, i.e., the subset of elements of the orbit $G.m$ which have G_m as isotropy group is the orbit of m by the normalizer in G of G_m.

There is not a complete agreement in the mathematical literature for defining

the equivalence of actions. However, the most common definition is : Given two isomorphic structures M,M' (which may be the same one) two actions $G \xrightarrow{f}$ Aut $M, G \xrightarrow{f}$ Aut M' are equivalent if there is an isomorphism $M \xrightarrow{\theta} M'$ such that

$$\forall G \in G \qquad f'(g) = \theta f(g) \theta^{-1}$$

One then writes : $(G,f,M) \approx (G,f',M')$.

For instance, when the M's are vector spaces, Aut M = GL(M), the general linear group on M) f and f' define two linear representations of G and (1) is the usual definition of their equivalence.

A prototype of G-orbit with isotropy groups $[H]_G$ is the action by left translation $xH \xrightarrow{g} gxH$ of G on the set $[G:H]$ of left cosets of H . It does transform any coset into other one. Consider another orbit $G.m$ and let $H = G_m$, the isotropy group of m . Then it is easy to show that the map $G.m \xrightarrow{\theta} [G:H]$ defined by $\theta(f(g)m) = gH$ is a bijection commuting with the group action, so it defines the equivalence of the orbits. The type of this orbit is generally denoted $[G:H]$ where H is any subgroup of $[H]_G$.

A group action $G \xrightarrow{f}$ Aut M partitions M into orbits. We denote by $G|M$ the set of orbits, which is called the <u>orbit space</u>. The union of orbits of the same type is called stratum ; an equivalent definition of $S(m)$, the stratum of m : It is the set of all $x \in M$ whose isotropy group G_x belongs to the conjugat class $[G_m]_G$. We will denote by $S_{G,f}(M)$ the set of strata. In most physical applications this set is finite, so the classification into strata is very important. There is a canonical injection :

$$S_{G,f}(M) \xrightarrow{\phi} \{[<G]\} \qquad (2)$$

into the set of conjugation classes of the $< G$ (read "sugbroups of G) . For an arbitrary group G , in general, there is no natural partial ordering on the set $\{[<G]\}$. But for the finite subgroups of an arbitrary group, or for the closed subgroups of a compact Lie group, there is a natural partial ordering by inclusion of subgroups up to a conjugation. In the smooth action of a compact Lie group on a manifold M , when there is a finite number of strata (this is the case if M is compact, or a vector space carrying a linear action) there is a unique minimal element of $\mathrm{Im}\,\phi = \phi(S_{G,1}(m))$ and the corresponding stratum is open dense : We call it the <u>generic stratum</u> (see e.g. the review [5] and the references it contains or [6] for physical applications).

Let us give a general application. Let $Q \xrightarrow{f} \mathrm{Aut}\ A$ an action of the <u>group</u> A ; then one can define the semi direct product $A \overset{f}{\rtimes} Q$. In the applications we consider, A will be Abelian ; we will denote its elements by Greek letters and those of Q by Latin letters ; moreover $f(a)\alpha$ is simply denoted $a.\alpha$; the semi-direct product law is

$$(\alpha, a)\ (\beta, b) = (\alpha + a.\beta, ab) \tag{3}$$

When the action f is trivial (i.e. $a.\beta = \beta$ for all a's , all β's) , one has the direct product $A \times Q$. We denote by V_n the n dimensional vector space on $\mathbf{R}$, the field of real numbers, whose additive topological group is denoted by R . So the additive group of V_n is R^n (the direct product of n copies of R) and by definition

$$GL(n,R) = \mathrm{Aut}\ V_n \equiv \mathrm{Aut}\ R^n \quad . \tag{4}$$

The action of R^n on V_r has only one orbit $[V_n : 0]$, called the affine space A_n . It's automorphism group is

$$\mathrm{Aff}(n) = R^n \rtimes GL(n,R) \ . \tag{5}$$

As we shall see, physicists want also to consider $GL_+(n,R)$ the subgroup of general linear transformations of positive determinant and the corresponding

$$\mathrm{Aff}_+(n) = R^n \times GL_+(n,R) \quad . \tag{5'}$$

We denote by H_n the n-dimensional real Hilbert space i.e., V_r equipped with a definite positive quadratic form. The corresponding affine space E_n is called an Euclidean space and by definition of the orthogonal $O(n)$ and Euclidean $E(n)$ groups

$$O(n) = \mathrm{Aut}\ H_n \ , \quad E(n) = \mathrm{Aut}\ E_n \tag{6}$$

$$E(n) = R^n \rtimes O(n) \tag{6'}$$

$O(n)$ is a $n(n-1)/2$ dimensional compact Lie group and its maximal connected subgroup $O_+(n)$ is also denoted $SO(n)$.

To end this section, we give another, weaker, equivalence $\sim$ of group action, when M and M' are two mathematical objects with the same structure :

<u>Definition</u>. $(G \xrightarrow{f} \mathrm{Aut}\ M) \sim (G' \xrightarrow{f'} \mathrm{Aut}\ M')$, $\exists$ isomorphism $M \xrightarrow{\theta} M'$

$$\theta(\mathrm{Im}\ f) \in [\mathrm{Im} f']_{\mathrm{Aut}\ M'}$$

In words two actions Gf and G'f' (the groups can be different) on M are weakly equivalent if $f(G)$ and $f'(G')$ are conjugated subgroups of Aut M . We have emphasized elsewhere [7] that weaker equivalence of actions is often useful in physics and we shall show here that it is essential for crystallography.

We give here a fundamental example. Let $\alpha \in$ Aut G and consider the two actions (G,f,M) , (G,f',M) where $f' = f \circ \alpha$ and f (and f') are injective homomorphisms.

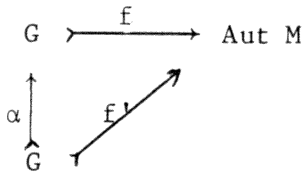


Diagram 1.

The decompositions of M into orbits and strata are the same for the two actions. But when these weakly equivalent actions are not strongly equivalent $\approx$; the orbits and strata have not the same name . Indeed, in the action of Aut G on G , Aut G acts on set $\{[<G]\}$ of conjugated classes of G subgroups ; if two distinct classes $[H]_G$ and $[H']_G$ are on the same orbit of Aut G , $[G:H] \not\sim [G:H']$ and $[G:H] \sim [G:H']$.

Exercise. In diagram 1, $(G,f,M) \sim (G,f\circ\alpha,M)$. When does $\approx$ hold ?

Answer. When $\alpha \in \mathrm{Im}\ \psi$ where ψ is the canonical homomorphism

$$N_{\mathrm{Aut}\ M}(\mathrm{Im}f) \xrightarrow{\psi} \mathrm{Aut}\ G\ .$$

Finally, we recall that if H is the unique element of $[H]_G$, H is an invariant subgroup of G and one writes $H \lhd G$. Similarly, if H is invariant by Aut G , H is called a characteristic subgroup of G and one writes $H \lhd\!\lhd G$.

2. DEFINITIONS OF THE CONCEPTS IN N-DIMENSIONAL CRYSTALLOGRAPHY.

What is a crystal ? With the existence of modulated crystals, incommensurate crystals, quasi-crystals, the answer to this question is not so easy. But, we

consider here only "classical" crystals. The art of approximations is essential in physics. An interesting approximation for studying an actual classical crystal is to neglect its symmetry defects and its surface effects by assuming that it is perfect and extends indefinitely in space. In that case, any function describing a physical property of the crystal is 3-periodic, i.e., it is invariant by a translation lattice T .

Definition. A n-dimensional translation lattice is a closed subgroup of R^n (the translation group of E_n) isomorphic to Z^n . It is generated by a basis $\{t_i\}$, $1 \leq i \leq n$ of H_n . With $n > 3$, n-periodic functions are used for the description of non classical crystals ; this has recently increased the interest of n-dimensional crystallographic.

There is a complete agreement on the concept of n-dimensional crystallographic group ; here is one of the possible equivalent definitions :

Definition. A crystallographic group G is a discrete closed subgroup of $E(n)$ whose intersection $T = G \cap R^n$ with the translations of $E(n)$ is a translation lattice.

In a crystal the interatomic distances depend on the temperature θ , so its symmetry group G is a function of θ . However its symmetry is not considered as different as long as θ does not reach a critical temperature (where a phase transition occurs) ; under such a variation of temperature the crystal changes only by dilations. This corresponds to conjugations of G by $g(\theta)$ a continuous function of θ valued in $Aff_+(n)$. Hence a physical crystallographic class (P.C.C.) is the set of crystallographic subgroups of $E(n)$ which, as subgroups of $Aff(n)$, are conjugated by elements of $Aff_+(n)$. If G is a crystallographic

group, its crystallographic class is

$$P.C.C(G) = [G]_{Aff_+(n)} \cap \{< E(n)\} \tag{8}$$

Similarly, its mathematical crystallographic class is

$$M.C.C(G) = [G]_{Aff(n)} \cap \{< E(n)\} \tag{8'}$$

A M.C.C can split into two P.C.C. which are "enantiomorphic" ; e.g., for $n=3$ there are 230 P.C.C and among them 11 enantiomorphic pairs, so there are 219 M.C.C.

Crystallographic groups, C.G., in n-dimensions have interesting and important properties. Their translation subgroup T is characteristic. Any invariant subgroup is a C.G. in $n' \leq n$ dimensions . Bierberbach proved [8b] that isomorphic C.G.'s are conjugated in $Aff(n)$. Finally, [9,10] every abstract automorphism of a crystallographic group G can be induced by an affine transformation, i.e., the natural homomorphism $N_{Aff(n)}(G) \xrightarrow{\psi} \text{Aut } G$ is surjective. The automorphism group of T is isomorphic to

$$GL(n,Z) = \text{Aut } Z^n \ , \tag{9}$$

the group of matrices with integer elements and with determinant ± 1 (indeed if $u \in GL(n,Z)$, $\det u$ and $\det u^{-1}$ must be integers) . Given a crystallographic group $G < E(n)$ (one often says a space-group , e.g. [3]) , the quotient

$$P = G/T$$

is called the point-group of G . It is in $O(n) \cap \text{Aut } T$, so it is finite (as the intersection of a compact group and a discrete group) and the action on T is defined by the injective homomorphism

$$O(n) > P \xrightarrow{f} \text{Aut } T = \text{Aut } Z^n \qquad (10)$$

From the properties of the crystallographic groups that we have listed a possible abstract definition is :

Definition. A n-dimensional crystallographic group is an extension G of a translation lattice $\mathbb{Z}^n$ by a finite subgroup $P < GL(n,Z)$.

Most crystallographers prefer to use some coordinate systems. Let us do it just once for them. Let $\{e_i\}$ be an orthonormal basis $(e_i,e_j) = \delta_{ij}$ of $\mathcal{H}_n$. If $\{b_j\}$ is a set of generators of the lattice T there is a $X \in GL(n,R)$ whose matrices (in the basis e_i) is X_{ij} and $b_j = \sum_i e_i X_{ij}$. Similarly, any other set of T-generators b'_k is given by $b'_k = \sum_j b_j Y_{jk}$, $Y \in GL(n,R)$. Then Aut $T = X(GL(n,Z))\ X^{-1}$.

We recall that only injective orthogonal (in the $\{e_i\}$ basis) action (10) of the point group on the translation lattice are taken into account in crystallography. They are classed according to weak equivalence, i.e., according to (7), the different action of a point group P correspond to the different conjugation classes $[P]_{\text{Aut } T}$. Jordan [11] proved that for all n , the number of conjugation classes of finite subgroups of $GL(n,Z)$ is finite. In crystallography these classes are called "arithmetic classes" (A.G.) ; there are 73 of them for n=3 and 13 for n=2 . Note for instance that the Coexter groups A_2,B_2,G_2 (i.e., in crystallographic notation C_{kv} = k m m for k = 3,4,6 respectively) have each two strongly inequivalent actions (i.e. representations by integral matrices) but, B_2 and G_2 (who have Z_2 as outer automorphism group) have only one conjugation class in $GL(2,Z)$ (their normalizer in $O(2)$ is isomorphic to their automorphism group, i.e., C_{8v}, $C_{12\,v}$ respectively, but these groups have no 2-dimensional integral representations).

It is well-known that any finite subgroup $P < GL(n,R)$ is conjugated to a subgroup P of $O(n)$. One can prove the stronger result : If finite subgroups of $O(n)$ are conjugated in $GL(n,R)$ they are conjugated in $O(n)$. Equivalently, if two finite $O(n)$ subgroups P_1, P_2 are not conjugated in $O(n)$, they are not conjugated in $GL(n,R)$ and a fortiori in $GL(n,Z)$ if they both have integral representations. So, in crystallography, point groups are classed by their conjugation class in $O(n)$, one says the geometric class (G.G.) and not by their isomorphic class (I.C.P.G.). For $n=3$, there are 32 C.C.'s and 18 I.C.P.G's. Given a point group P and its action $f : P \longrightarrow \mathrm{Aut}\ T$, on T, i.e. its arithmetic class (= conjugation class in $GL(n,Z)$ how many crystallographic groups are there in this arithmetic class ? One of them is the semi-direct product $T \times P$. It is called a symmorphic group in crystallography. The others do not contain P as subgroups ; indeed some of the elements, e.g. $p \in P$ is accompanied by a non primitive translation $\tau(p)$ (i.e. $\tau(p) \notin T$). So in equation (3) applied to $E(n)$, $(\tau(p),1)$, $(0,p)$ $(\tau(p),p)$ are elements of $E(n)$ but only the last one is also an element of the crystallographic subgroup $G < E(n)$. The non primitive translations depends of the choice of origin. One can also give the group law in the form

$$\{\alpha,a\}\ \{\beta,b\} = (\alpha+a\beta+\omega(a,b),a,b\} \tag{11}$$

with $$\omega(a,b) = \tau(a) - \tau(ab) + a\tau(b) \tag{11'}$$

The two variable function defined on P, valued in T independent from the choice of origin. However, it has still some arbitrariness, depending on the choice of the group elements $\{0,a\} \in G$ for all $a \in P$. All possible $\omega(a,b)$ differ by functions valued in T of the type.

$$\varphi(a,b) = \varphi(a) - \varphi(ab) + a\varphi(b) \equiv (\delta\varphi)\ (a,b) \tag{12}$$

Such function is in $B_f^2(G,T)$ the group of 2 coboundaries while the ω's for all crystallographic groups of the arithmetic class $p \xrightarrow{f} \text{Aut } T$ are in $Z_f^2(G,T)$ the group of 2 cocycles. Indeed they satisfy

$$(\delta\omega)(a,b,c) \equiv \omega(a,b) - \omega(ab,c) + \omega(ab,c) - a\omega(b,c) = 0 \qquad (12')$$

The cohomology group $H_f^2(G,T) = Z_f^2(G,T)/B_f^2(G,T)$ is the group of extensions of P by T belonging to the arithmetic class (P,f,Aut T) . The zero represents $T \overset{f}{\rtimes} P$. However two inequivalent extensions may be isomorphic and correspond to the same crystallographic (space-) group. Indeed the normalizer $N_{\text{Aut}}(P)$ acts on P and on T so it acts naturally on the functor $H_f^2(P,T)$: the C.C. (crystallographic classes) of the given arithmetic class $P \xrightarrow{f} \text{Aut } T$ are described by the orbits of $N_{\text{Aut } T}(P)$ on $H_f^2(P,T)$.

3. WHAT IS THE CRYSTALLOGRAPHIC SYSTEM AND THE BRAVAIS CLASS OF A CRYSTALLOGRAPHIC GROUP ?

We must now study the classification of the translation lattices. As we have seen, each basis of V_n defines a T. Their set is $\mathcal{T}$. The general linear group transforms any basis of V_n into another basis of V_n ; $\mathcal{T}$ is <u>one</u> orbit of GL(n,R) and, according to (9) :

$$\mathcal{T} = [GL(n,R) : GL(n,Z)] \qquad (13)$$

In the action of the subgroup O(n) of GL(n,R) on $\mathcal{T}$, the strata correspond to the different <u>crystal systems</u> (C.S.). There are 7 of them in 3-dimensions. Triclinic, Monoclinic, Orthorhomb , Tetragonal, Trigonal, Hexagonal, Cubic. We will use the short bounds : Tri, Mon, Ort, Tet, Trg, Hex, Cub. To each O(n) stratum = crystal system, corresponds a O(n) conjugation class $[P_H]_{O(n)}$ of

isotropy groups P_H called holohedry of the lattice T . The holohedries are distinguished geometric classes. And the set of arithmetic class of the holodedries form the Bravais classes (B.C.) of the lattices. There are 14 of them for n=3 . To label them one simply add different letters for the different conjugation classes of $[P_H]_{GL(n,Z)}$ which are included in the class $[P_H]_{GL(n,R)}$ i.e., the same crystallographic system. For n=3 , the 14 Bravais classes are :

$$\left.\begin{array}{c}\text{Tri P, Mon P, Mon B, Ort P, Ort C, Ort F, Ort I, Tet P, Tet I,} \\ \text{Trg R, Hex P, Cub P, Cub F, Cub I}\end{array}\right\} \quad (14)$$

As conjugation classes of finite subgroups of GL(n,Z) , there is a natural ordering on the set of arithmetic classes and on its subset of Bravais classes.

It is very important to remark that in a crystallographic class (M.C.C. or P.C.C.) the translation lattices of all the space groups of this C.C may have different holohedries and they belong to different Bravais classes. For instance, the unique crystallographic class corresponding to the point group P = I (the identity) contains all T's ! So the crystal system and the Bravais flock of a space group G are determined by considering the whole set G of space groups of the C.C of G (equations (8)). The orthogonal group O(n) acts on the lattices in G . All lattices of the open dense generic stratum belong to the same crystal system and Bravais class : which are naturally those of G .

Unhappily, this simple, natural definition of the crystallographic systems (called the "French crystal systems" in [3]) is not that adopted by [1] , [2] and the International Crystallographic Tables [3]. There is presently a competition for giving mathematically well defined but very unnatural definitions of so called "crystallographic systems". This seems to be based on the a priori

requirement that the natural mapping from the set {A.C.} to {B.C} (arithmetic classes to Bravais classes) factorizes through {C.C} the set of geometric class. This can be done (it is done in the International Crystallographic Tables !) but it is against mathematical nature and simply against Nature as in deeply felt by some crystallographers (e.g. [12]).

In the table, we give in a nut-shell the definition of the different classification sets and the mapping which arise between them.

4. OTHER CRYSTALLOGRAPHIC APPLICATIONS OF GROUP ACTIONS.

In science groups were introduced (before the creation by Galois of the word itself) through their actions. We hope to have shown that group actions form the basic tools for crystallographic classification. We end this paper by other applications.

The classification of m-color crystallographic groups is the classification of the m-element orbits of a crystallographic space group G under weak equivalence (see e.g. [13] for extensive tables for dimension in n=2). The study of the action of a crystallographic space group G on the Euclidean space $E(n)$ is helped by the study of the simpler action of $P = G/T$ on the orbit space $E(n)|T$ (topologically $(S_1)^n$, the n-dimensional torus) [14] . In both action the isotropy groups are isomorphic ; there is an open dense stratum corresponding to the trivial isotropy group. The strata in the action of G on $E(n)$ are called in [3] Wyckoff positions. The maximal conjugation classes of isotropy group correspond to

closed strata : and there is a natural bijection between the different closed strata in the action of G on $E(n)$ and the different connected components of closed strata in the action of P on $E(n)|T$. (The closed strata may have different dimensions. For $n=3$, there is one group $57 \equiv D_{2h}^{11} \equiv$ Pbcm with closed strata of dimensions $0,1,2$) .

The Euclidean $E(n)$ group acts naturally on the orbit $G.x$, G crystallographic group, $x \in E(n)$. The isotropy group $\Gamma_x \equiv E(n)_{G.x}$ is a crystallographic group which contains G . When G is a strict subgroup of Γ_x the orbit $G.x$ is called non characteristic. For $n=3$ a complete classification of the orbits of space groups and of their symmetry groups Γ is given in [15]. The action of $N_{Aff(n)}(G)$ on the G-strata is also studied there.

The unitary representations of G induced from the unitary irreducible representation from G_x , the finite isotropy group of $x \in E(3)$ classify the electron energy bands in crystals (see [14]). The irreducible unitary representations of G are also obtained by induction from those of the isotropy group G_k with $k \in T^*$ (isomorphic to $U(1)^n$) the dual group (or group of characters) of T and called the Brillouin zone in the physics literature (where the group structure of T^* is not enough used !). Since T acts trivially on T^* , $T < G_k$ and the G_k''s are also crystallographic groups. In 3-dimensions to the zero dimensional strata (called set of higher symmetry wave vectors in physics literature) of the 14 actions (one per Bravais class) of the seven holohedries, there correspond nearly four thousand inequivalent irreducible representations of the G_k's . It is remarkable that they have only 37 images ![15], but this is well understood by a geometrical approach of the study of crystallographic groups and their actions.

TABLE CRYSTALLOGRAPHIC CLASSIFICATION IN n- DIMENSIONS

$\rightarrowtail$ injective map , $\twoheadrightarrow$ surjective map , $\longleftrightarrow$ bijective map .

Notation $<$: closed subgroup ; $\{< G\}$ set of closed subgroups of G .

$H < G$, $k < G$, $[H]_K$ = subgroups of G conjugated to H by elements of K

$$Aff(n) = R^n \rtimes GL(n,R) \; ; \; E(n) = R^n \rtimes O(n)$$

T = translation lattice is any $Z^n < R^n < E(n) < Aff(n)$

$\{T\} = \mathcal{T}_n$, the set of T's , is the orbit $[GL(n,R) : GL(n,Z)]$

Definitions. Crystallographic group $G < E(n)$, $G \cap R^n = T$ a translation lattice

Point group of G : $P = (G/T) < O(n)$

PCC : Physical crystallographic class of G : $\{< E(n)\} \cap [G]_{Aff_+(n)}$

MCC : Mathematical crystallographic class of G : $\{< E(n)\} \cap [G]_{Aff(n)}$

AC : Arithmetic class of G : $[P]_{GL(n,Z)}$

GC : Geometric class of G : $[P]_{O(n)} \longleftrightarrow [P]_{GL(n,R)}$

ICPG : Isomorphic class of point group.

Holohedries P_H = isotropy groups in the action of $O(n)$ on $\mathcal{T}_n$

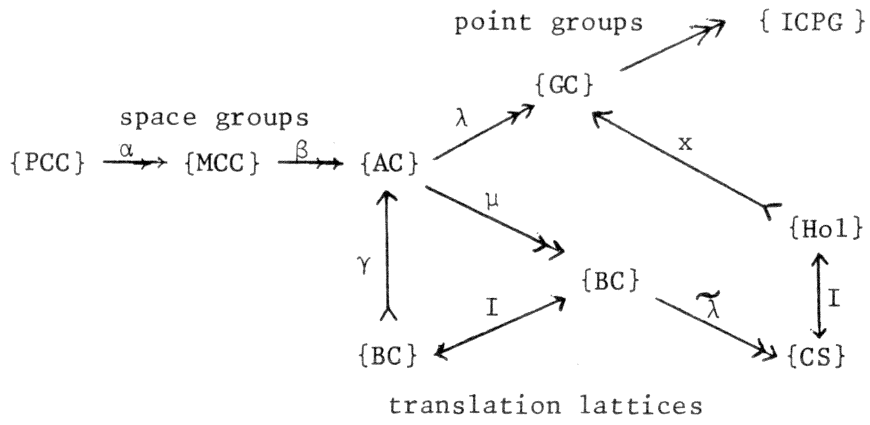
C.S. : Crystallographic Systems = Strata in the action of $O(n)$ on $\mathcal{T}_n$

$\{C.S\} = \{Hol.\}$ the set of conjugation classes $[P_H]_{O(n)} \longleftrightarrow [P_H]_{GL(n,R)}$

B.C. : Bravais class = Arithmetic class of a holohedry.

C.S. and BC classify the lattices $\in \mathcal{T}$. They can also be attributed to G as those of the T's in the generic stratum in the action of O(n) on the T subgroups of the crystallographic groups of $[G]_{Aff(n)} \cap \{< E(n)\} = C.C.(G)$

Commutative diagram of resulting maps.



Remark. There are no map from {GC} to {BC} or {CS} .

REFERENCES

[1] H. Brown, R. Bülow, J. Neubüser, H. Wondratschek, H. Zassenhaus, Crystallographic groups of four dimensional space, John Wiley & sons, New-York, 197

[2] R.L.E. Schwarzenberger, N-dimensional crystallography, Pitman Publ. London 1980.

[3] International Crystallographic Tables, Vol. A, mainly Chapter 8 by H. Wondratschek. Reidel (1983).

[4] J. Neubüser, W. Plesken, H. Wondratschek, Match (Comm. Math. Chem.) 10 (1981) 77.

[5] D. Montgomery p. 43 in "Differential Analysis "Bombay Colloquium (1964) Tata Institute Bombay.

[6] L. Michel, Rev. Mod. Phys. 52 (1980) 617-651.

[7] L. Michel, J. Mozrzymas, Match 10 (1981) 223.

[8] L. Bieberbach, Math. Annalen a) 70 (1911) 297 b) 72(1912) 400.

[9] M. Delaney, H. Zassenhauss, Comm. Algebra 4 (1976) 305.

[10] G. Maxwell, Comm. Algebra 6 (1978) 1489.

[11] C. Jordan, J. Ecole Polytechnique 48 (1880) 112.

[12] J.D.H. Donnay, Acta Cryst. A 33 (1977) 979.

[13] H. Bacry, L. Michel, J. Zak (to be published).

[15] P. Engel, T. Matsumoto, G. Steinmann , H. Wondratschek, "The non characteristic orbits of the space gorups" supp. N° 1 of Zeits. Kristal.(1984).

[16] L. Michel, J. Mozrzymas, "The structure of unitary representations of space groups" in Groups theoretical methods in Physics XI, Lecture Notes in Physics 180 (1983) 292.