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Crystallographic point groups of five-dimensional space. 1. Their elements and their subgroups

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The purpose of this work is to introduce a method with a view to obtaining the crystallographic point groups of five-dimensional space, *i.e.* the subgroups of the holohedries of these space crystal families. This paper is specifically devoted to numerical analysis, whereas the following ones deal with some applications to crystallography. These results have been obtained through a collaboration between two teams: H. Veysseyre (Institut Supérieur des Matériaux) for the numerical analysis, R. Veysseyre, D. Weigel and Th. Phan (Ecole Centrale Paris) for the crystallographic part.

1. Introduction

This paper deals with numerical analysis and computer science with a view to determining both groups generated by p elements and its subgroups. In order to apply these results to five-dimensional space crystallography, the number p has been limited to five because it is sufficient for generating all point groups of this space as we shall explain in §3 (Remark 1).

To begin with, some results on the number of crystallographic point-symmetry operations (PSOs, for short) of five-dimensional space (or 5D space) are to be recalled. These are important for the determination of the point groups and for Hermann–Mauguin symbols (HM symbols) or for Weigel–Phan–Veysseyre symbols (WPV symbols) (Weigel *et al.*, 1987). Some of these results are published in the Report of a Subcommittee on the Nomenclature of n-Dimensional Crystallography (Janssen *et al.*, 1999).

Therefore, the first step consists of the list of the 38 PSOs of 5D space, *i.e.* 19 positive PSOs (PSO^+ or proper rotations) and 19 negative PSOs (PSO^- or improper rotations). There are different ways to describe the PSOs. Two of them are taken into consideration. First, we use a matrix representation connected with the crystal family cells, *i.e.* a list of matrices 5×5 with integer entries. Then, these PSOs can be defined by the characteristic polynomials of the associated operators in a Euclidean space (Veysseyre *et al.*, 1990, 1994). The characteristic polynomials are numbered from 1 to 19 for the PSO^+s and from 20 to 38 for the PSO^-s. Here are two examples:

polynomial No. 8 for PSO $4\underline{2}$ $(\lambda - 1)(\lambda + 1)^2(\lambda^2 + 1)$;
polynomial No. 27 for PSO $4\bar{1}$ $(\lambda + 1)^3(\lambda^2 + 1)$.

The characteristic polynomial representation permits one to compare two or several crystallographic point groups isomorphic to the same abstract group as explained in §4.

Symbols of some PSOs are the classical HM symbols such as 2 for a twofold rotation, 3 for a threefold rotation. As far as the other PSOs are concerned, we have already suggested WPV symbols, which are similar to the HM symbols and connected with the PSO geometrical definition (Weigel *et al.*, 1987).

Then, we define the 32 crystal families of 5D space, their classification, their names and their holohedry symbols. We have already suggested a method to construct the crystal cells of 5D space through the cells of crystal families of 2D, 3D and 4D spaces (Veysseyre *et al.*, 1991). Obviously, we have found the same number as the one given by Plesken (1981). Actually, there are:

(i) four crystal families in 2D space: oblique, rectangle, square, hexagon;

(ii) six crystal families in 3D space: triclinic, monoclinic, orthorhombic, tetragonal, hexagonal, cubic;

(iii) 23 crystal families in 4D space: hexaclinic, triclinical, di obliques, oblique rectangle, orthotopic 4d, square oblique, hexagon oblique, diclinic di squares, diclinic di hexagons, square rectangle, hexagon rectangle, monoclinic di squares, monoclinic di hexagons, di squares, hexagon square, di hexagons, cubic-al, monoclinic di iso squares or octodic, decadic, monoclinic di iso hexagons or dodecadic, di iso hexagons, rhombotopic ($-1/4$), hypercubic 4d;

(iv) 32 crystal families in 5D space. They are listed in Table 1.

The construction of some lattice cells should be recalled. For instance:

(1) The 4D hexaclinic lattice cell is based on four unequal vectors; the angles between these vectors have any value.

(2) The 5D decaclinic lattice cell is based on five unequal vectors; the angles between these vectors have any value.

Table 1
Number of point groups of crystal families of five-dimensional space.

First column: No. of the crystal families. Second column: names of the crystal families. Third column: WPV symbols of the crystal family holohedries. Fourth column: order of the holohedries. Fifth column: No. of point groups belonging to each family.

No.	Family names	WPV holohedry symbols	Holohedry order	No. of subgroups
I	Decaclinic	$\bar{1}_5$	2	2
II	Hexaclinic-al	$\bar{1}_4 \perp \mathrm{m}$	4	3
III	Triclinic oblique	$\bar{1} \perp 2$	4	3
IV	Triclinic rectangle	$\bar{1} \perp mm$	8	4
V	(Di obliques)-al	$2 \perp 2 \perp m$	8	4
VI	Triclinic square	$\bar{1} \perp 4mm$	16	7
VII	Triclinic hexagon	$\bar{1} \perp 6mm$	24	12
VIII	Oblique orthorhombic	$2 \perp mmm$	16	8
IX	Orthotopic 5d	$mmmmm$	32	8
X	(Square oblique)-al	$4mm \perp 2 \perp \mathrm{m}$	32	24
XI	(Hexagon oblique)-al	$6mm \perp 2 \perp m$	48	35
XII	(Diclinic di squares)-al	$44 \perp m$	8	3
XIII	(Diclinic di hexagons)-al	$66 \perp m$	12	5
XIV	Square orthorhombic	$4mm \perp mmm$	64	33
XV	Hexagon orthorhombic	$6mm \perp mmm$	96	45
XVI	(Monoclinic di squares)-al	$(44.2) \perp m$	16	4
XVII	(Monoclinic di hexagons)-al	$(66.2) \perp m$	24	7
XVIII	Cubic oblique	$m\bar{3}m \perp 2$	96	16
XIX	(Di squares)-al	$4mm \perp 4mm \perp m$	128	59
XX	(Hexagon square)-al	$6mm \perp 4mm \perp m$	192	119
XXI	(Di hexagons)-al	$6mm \perp 6mm \perp m$	288	116
XXII	Cubic rectangle	$m\bar{3}m \perp mm$	192	31
XXIII	Octodic-al (monoclinic di iso squares-al)	$([8].2) \perp m$	32	7
XXIV	Decadic-al	$([10].2) \perp m$	40	12
XXV	Dodecadic-al (monoclinic di iso hexagons-al)	$([12].2) \perp m$	48	7
XXVI	Cubic square	$m\bar{3}m \perp 4mm$	384	31
XXVII	Cubic hexagon	$m\bar{3}m \perp 6mm$	576	59
XXVIII	(Hypercubic 4 d)-al	$([8].m\bar{3}m) \perp m$	768	90
XXVIIIa	(Hypercubic 4d Z centred)-al	$\{([12].2)m\bar{3}m\} \perp m$	2304	51
XXIX	(Di iso hexagons)-al	$([12].2.6mm) \perp m$	576	104
XXX	{Rhombotopic (−1/4)}-al	$([10].\bar{4}3m) \perp m$	480	23
XXXI	Hypercubic 5d	$([8].m\bar{3}m).[\bar{5}]$	3840	13
XXXII	Rhombotopic (−1/5)	$([10].\bar{4}3m).36$	1440	10
Number of point groups of five-dimensional space: 955				

(3) The 4D di obliques cell is constructed from two different parallelograms belonging to two orthogonal planes (xy) and (zt).

(4) The 5D triclinic square cell is built up from a triclinic cell and a square belonging to two orthogonal subspaces (xyz) and (tu).

(5) The triclinic rectangle, triclinic hexagon, square orthorhombic and hexagon orthorhombic cells follow a similar process.

The definition of the geometrically Z reducible and geometrically Z irreducible crystal families is developed in Weigel & Veysseyre (1991, 1993) and Veysseyre *et al.* (1993). This definition is connected to the geometry and the splitting up of the metric tensor of a crystal cell and to the bases of the irreducible representations of the crystal family holohedry.

Let $x, y, z, t, u, \ldots$ be the n vectors defining a basis of a primitive cell of a crystal family of nD space. This family is said to be 'geometrically Z irreducible' (gZ-irr) if all these operators belong to the same irreducible representation with integer entries of its holohedry character table. If this property is not verified, the family is said to be 'geometrically Z reducible' (gZ-red); in this case, the metric tensor can be split into two or more parts or, in other words, the crystal family cell is the orthogonal product of two or more cells belonging to two or more orthogonal subspaces of nD space.

Out of the 32 crystal families of 5D space, three are gZ-irr. These are the following ones: decaclinic, rhombotopic (−1/5) and hypercubic 5d families. 29 are gZ-red. The cell of each one is the orthogonal product of two, three, four or five elementary cells belonging to spaces of dimension lower than five. For instance, 11 of them are 'right hyperprism based on one irreducible crystal cell' of 4D space. Hence, the suffix 'al' in their names. Six of them are the direct product of the two irreducible crystal cells of 3D space and of the three irreducible crystal cells of 2D space and so on.

The name selected for the crystal families should be both simple and precise. Hence, the suffix 'al' as explained previously. Besides, the adjective 'orthogonal' has been cancelled when situated between two names, for instance the cell of the crystal family named 'cubic oblique' is the orthogonal product of a cubic and an oblique (parallelogram) cell. Moreover, the order adopted for writing the cell names is the decreasing order of the space dimensions on which they are based. Finally, if the elementary cells belong to the same dimensional space, the most symmetrical cell is mentioned first (Weigel & Veysseyre, 1993).

In the case of reducible crystal families, the holohedry symbols can be easily found. Actually, the holohedries of these families are the direct product of the holohedries of the elementary crystal families. Here is an example. The cell of the crystal family numbered III is the Cartesian product of the triclinic cell and of the oblique cell; these two cells belong to two orthogonal spaces. Hence, the abridged name of this crystal family is ' triclinic oblique'. The family holohedry is the direct product of two groups, $\bar{1}$ for the triclinic holohedry and 2 for the oblique holohedry. It is possible to write the holohedry symbol of this family $\bar{1} \times 2$, but owing to the geometrical construction of this cell symbol $\bar{1} \perp 2$ is better. Therefore, the symbol $\perp$ has mathematical and geometrical meanings.

2. Determination of finite group elements

This section begins with the determination of all the elements of a finite group defined by p generators. With a view to applying these results to crystallography, we assume that the group generators are defined by means of invertible square matrices, *i.e.* matrices whose determinant is not null. The studied groups are the holohedries of the 32 crystal families of 5D space. This is the reason why these families, their holohedries together with the order of these groups are listed in Table 1 (the first four columns).

The identity element is denoted I; in nD space, element I is represented by the identity matrix of order n.

(1) The first stage consists in determining a finite group generated by one element, *i.e.* a cyclic group. Let A be this element of order a. Hence, the cyclic group generated by the element A has for elements: $I, A, A^2, \ldots, A^{a-1}$.

If the order of the group is an even number, except for number two, the elements of this cyclic group can be as follows: I, B, A, BA, A^2, BA^2, $\ldots$, $A^{a'-1}$, $BA^{a'-1}$, in which $a = 2a'$ and $B = A^{a'}$, hence $B^2 = I$.

If element B equals $-I$, the cyclic group elements are as follows: $\pm I, \pm A, \pm A^2, \ldots, \pm A^{a'-1}$. In this case, we can stop after finding the following property: $A^{a'} = B = -I$.

(2) The study of a group generated by two elements does not allow an easy generalization to the group generated by any number of elements. Consequently, the groups generated by three elements are thoroughly studied. Then, this process can be and has been generalized to the groups generated by p elements.

Let A, B, C be these three elements and a, b, c their respective orders.

Consequently: $A^a = B^b = C^c = I$. Then, each element of the group can be written for instance as:

$$A^\alpha B^\beta C^\gamma A^{\alpha'} B^{\beta'} C^{\gamma'} A^{\alpha''} B^{\beta''}, \ldots,$$

in which $\alpha, \alpha', \alpha'' \in [0, a-1]$; $\beta, \beta', \beta'' \in [0, b-1]$; $\gamma, \gamma', \gamma'' \in [0, c-1]$. The length of the sequence is always finite for the studied point group.

The different products of type $(A^\alpha B^\beta C^\gamma A^{\alpha'} B^{\beta'} C^{\gamma'} A^{''} B^{\beta''} \ldots)$ obtained by giving to α, β, γ, α', β', γ', α'', β'', $\ldots$ all the possible integers successively generate all group elements. This sequence of products is finished if, in the sequence α, β, γ, α', β', γ', α'', β'', $\ldots$, the different integer values given to two consecutive elements does not give a new result.

In some cases, it is possible to reduce the number of products. If one of the integers a, b or c is even, for instance if $a = 2a'$ and $A^{a'} = -I$, each element of the group can be written:

$$\pm A^\alpha B^\beta C^\gamma E^\varepsilon A^{\alpha'} B^{\beta'} C^{\gamma'} A^{\alpha''} B^{\beta''} \ldots,$$

in which $\alpha, \alpha', \alpha'' \in [0, a'-1]$; $\beta, \beta', \beta'' \in [0, -1]$; $\gamma, \gamma', \gamma'' \in [0, -1]$, with $\tilde{b} = b/2$, if b is even and $B^{b/2} = -I$, and $\tilde{b} = b$ in the other cases. $\tilde{c} = c/2$, if c is even and $C^{c/2} = -I$, and $\tilde{c} = c$ in the other cases.

(3) For a group generated by q elements, the method is similar because each element of the group can be written:

$$A^\alpha B^\beta C^\gamma D^\delta E^\varepsilon A^{\alpha'} B^{\beta'} C^{\gamma'} D^{\delta'} E^{\varepsilon'} A^{\alpha''} B^{\beta''} C^{\gamma''} D^{\delta''} E^{\varepsilon''} \ldots$$

and $(q-1)$ consecutive integers in the sequence α, β, γ, δ, ε, α', β', γ', δ', ε', α'', β'', γ'', δ'', ε'', $\ldots$ cannot be null.

3. Determination of the subgroups of a point group *D*

All the elements of the group being defined by means of matrices, it is possible to determine all the subgroups of this group.

(1) To begin with, it is necessary to determine set G_1 of the distinct groups $g_{1,i}$ in which $i \in [1, \alpha_1]$, generated by one element of group D. These α_1 groups $g_{1,i}$ are classified in set G_1 through a chosen criterion and they are called the G-generators of the group. Generally, the number of G-generators is much lower than the order N of the group.

(2) Then, set G_p is determined through set G_{p-1} as follows: every group $g_{p,j}$ is generated by p G-generators such that $(p-1)$ of them are the generators of a group $g_{p-1,i}$ in which $i \in [1, \alpha_{p-1}]$ and the pth is different. These groups are classified in a set G_p if they are new groups, *i.e.*

$$g_{p,j} = \left[\bigcup_{i=1}^{p-1} G_i\right] \cup \left[\bigcup_{k=1}^{j-1} g_{p,k}\right].$$

(3) If the integer α_p equals 0 (*i.e.* if set G_p is empty), at the end of sequence 2, we pass onto sequence 4.

If not, we come back to sequence 2 with the next value of p.

Remark 1. For the point groups of 5D space, number α_6 equals 0. All point groups of 5D space have been generated by at most five generators and for point groups of 6D space by at most six generators.

(4) When all the sets G_p are obtained, all the groups:

$$g_{p,j} \in G_p \quad \forall j \in [1, \alpha_p] \quad \text{and} \quad \forall p \in [0, 5]$$

are taken into consideration.

Then, each element of every subgroup $g_{p,j}$ is replaced by its characteristic polynomial number. Thus, we obtain $\gamma_{p,j}$ that we put together in a set Γ. We notice that several γs may be identical whereas groups g are different.

$$\gamma_{p,j} \in \Gamma \quad \forall j \in [1, \alpha''_p] \quad \forall p \in [0, 5] \quad \alpha'_p \ll \alpha_p.$$

Hence, Γ is the set of the point-symmetry groups of the studied space.

4. Determination of the point groups

After completing the previous study, a computer program was set up with a view to discovering the subgroups of each holohedry.

Each crystal family of nD space can be defined by its cell metric tensor, *i.e.* a symmetric $n \times n$ matrix, the entries are all the scalar products of the n vectors of the cell. Owing to the possible symmetries of this system of vectors, the independent entry number, *i.e.* the parameter number defining the cell metric tensor, is lower than $n(n+1)/2$ except for one family. The crystal families are classified in decreasing order of this parameter number. For example, in 5D space, family No. I is the decaclinic crystal family [$n(n+1)/2 = 15$ parameters for defining its metric tensor], family No. II is the hexaclinic-al crystal family (11 parameters for defining its metric tensor), ..., family No. XXXII is the rhombotopic $(-1/5)$ crystal family (1 parameter for defining its metric tensor).

All point groups of 5D space are the different subgroups of the 32 holohedries. Our program gradually cancelled the groups that had been found in the crystal families already studied. The holohedry symbols are obtained as the direct product of holohedries of subfamilies for the gZ-red. crystal families and from the study of the point operations defining the gZ-irred. crystal families; for instance, $4mm\perp mmm$ (square orthorhombic family), $[10].\bar{4}3m.36$ (rhombotopic $-1/5$ family).

Yet another difficulty appears owing to the difference between an abstract group and a crystallographic group. For instance, there is one and only one abstract group of order 2 generated by element a such as $a^2 = I$ (identity element). But, if we consider the point groups of order 2, they can be generated by one of the following elements: 2, $\bar{1}_4$, m, $\bar{1}$ and $\bar{1}_5$, which are defined by five different characteristic polynomials. Consequently, there are five different point groups of order 2 in 5D space isomorphic to the same abstract group. This shows the difference between an abstract group and a point group.

This emphasizes the existence of 955 point groups in 5D space belonging to 32 crystal families.

After determining the 5D space subgroups, it seems interesting to draw a diagram between these groups, *i.e.* to point out the connection between the 32 holohedries (Fig. 1), or to point out the relation 'group–subgroup'. Then, considering only 32 families proved unsatisfactory for this purpose.

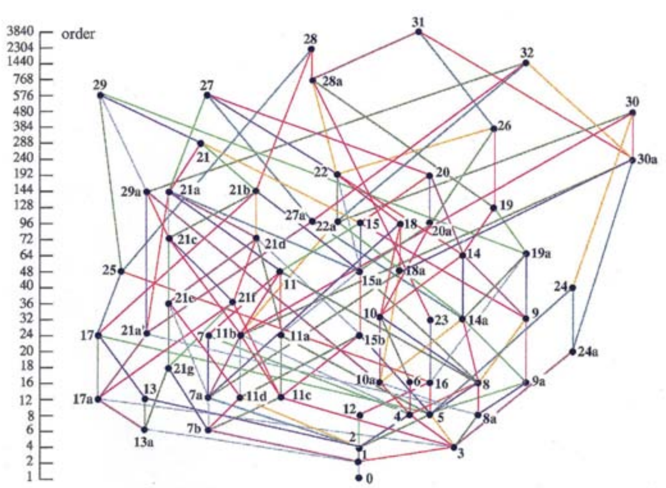

Figure 1
Diagram showing links between the point-symmetry groups of five-dimensional space. Left scale: holohedry order. Nodes of the diagram: No. of the crystal family or subfamily.

Table 2
Number of point groups of crystal subfamilies of five-dimensional space.

First column: names of the crystal families. Second column: No. of the crystal families and of the subfamilies. Third column: holohedry order. Fourth column: No. of point groups belonging to each subfamily.

Family names	Subfamilies	Holohedry order	No. of subgroups
Triclinic hexagon	VIIb	6	2
	VIIa	12	3
	VII	24	7
Oblique orthorhombic	VIIIa	8	3
	VIII	16	5
Orthotopic 5d	IXa	16	4
	IX	32	4
(Square oblique)-al	Xa	16	8
	X	32	16
(Hexagon oblique)-al	XId	12	3
	XIc	12	3
	XIb	24	5
	XIa	24	8
	XI	48	16
(Diclinic di hexagons)-al	XIIIa	6	2
	XIII	12	3
Square orthorhombic	XIVa	32	15
	XIV	64	18
Hexagon orthorhombic	XVb	24	4
	XVa	48	15
	XV	96	26
(Monoclinic di hexagons)-al	XVIIa	12	3
	XVII	24	4
Cubic oblique	XVIIIa	48	5
	XVIII	96	11
(Di squares)-al	XIXa	64	25
	XIX	128	34
(Hexagon square)-al	XXa	96	31
	XX	192	88
(Di hexagons)-al	XXIh	24	7
	XXIg	18	2
	XXIf	36	3
	XXIe	36	3
	XXId	72	8
	XXIc	72	4
	XXIb	144	23
	XXIa	144	23
	XXI	288	43
Decadic-al	XXIVa	20	7
	XXIV	40	5
Cubic hexagon	XXVIIa	96	12
	XXVII	576	47
(Hypercubic 4d)-al	XXVIII	768	90
(Hypercubic 4d Z centred)-al	XXVIIIa	2304	51
(Di iso hexagons)-al	XXIXa	144	15
	XXIX	576	89
{Rhombotopic (−1/4)}-al	XXXa	240	8
	XXX	480	15

Table 3
Number of point symmetry groups (classified order by order) of five-dimensional space.

Order: order of the group. No: number of groups of given order.

Order	1	2	3	4	5	6	8	9	10	12	16	18	20
No.	1	5	2	16	1	18	43	1	5	58	67	13	7
Order	24	32	36	40	48	60	64	72	80	96	120	128	144
No.	121	61	50	5	122	2	33	80	2	58	10	11	63
Order	160	192	240	256	288	320	360	384	480	576	640	720	768
No.	3	26	8	1	24	3	1	9	1	7	1	3	1
Order	960	1152	1440	1920	2304	3840							
No.	1	5	1	3	1	1							

For example, the crystal family XXVI (cubic square) holohedry of order 384 contains subgroups belonging to crystal family XX {(hexagon square)-al} without containing its holohedry of order 192. Consequently, there is a group–subgroup relation between these two crystal families but not between their holohedries. More precisely, crystal family XXVI contains the highest subgroup of crystal family XX. Therefore, this subgroup of order 96 should appear on the diagram connected to crystal family XXVI holohedry. This subgroup is the holohedry of a centred subfamily of crystal family XX and this subfamily is denoted XXa.

18 of the 32 crystal families of 5D space contain one or several centred subfamilies whose holohedries are nodes of the diagram. These are the families:

VII, VIII, IX, X, XI, XIII, XIV, XV, XVII, XVIII, XIX,
XX, XXI, XXIV, XXVII, XXVIII, XXIX, XXX

Thus, we have found 64 nodes on the diagram.

In Table 1, each family is given their number of subgroups (last column) whereas the number of subgroups of each subfamily is given in Table 2

On the other hand, the diagram of Fig. 1 shows that all these holohedries are subgroups of six crystal family holohedries. They are as follows:

Family XXVII cubic hexagon
Family XXVIII (hypercubic 4d Z centred)-al
Family XXIX (di iso hexagons)-al
Family XXX {rhombotopic $(-1/4)$}-al
Family XXXI hypercubic 5d
Family XXXII rhombotopic $(-1/5)$

In order to compare 2D, 3D, 4D and 5D spaces with each other, it should be noted that:

- in 2D space, all the holohedries are subgroups of two crystal family holohedries:

square family   hexagon family

- in 3D space, all the holohedries are subgroups of two crystal family holohedries:

cubic family   hexagonal family

- in 4D space, all the holohedries are subgroups of four crystal family holohedries:

hypercubic 4d Z centred family   rhombotopic $(-1/4)$ family
di iso hexagons family   hexagon square family

A strong analogy between these results is to be noticed.

5. Conclusions

The classification of all subgroups of the 32 holohedries, family by family, results in the conclusions shown Table 1. In Table 3, these subgroups are classified order by order. Finally, some statistical results can be obtained about the subgroup classification, order by order, for the different crystal families and subfamilies. The results of this study are not reported in this paper but they are at the disposal of the reader upon request.

All through this study, the analysis of the different types of centring has appeared as a main and useful fact. Actually, out of the 32 crystal families, 18 are split into two or several centred subfamilies. The study of all these types of centring will be given in a further paper. As for the point-group symbols of some families, they are explained in paper 2 (Veysseyre *et al.*, 2002).

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