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Crystallography in Spaces E^2, E^3, E^4, E^5 ⋯ N°I Isomorphism Classes: Properties and Applications to the Study of Incommensurate Phase Structures, Molecular Symmetry Groups and Crystal Families of Space E^5

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Abstract

This paper mainly consists of the classification of all crystallographic point groups of n-dimensional space with n ≤ 6 into different isomorphism classes. An isomorphism class is defined by a type of finite mathematic group; for instance, the different types of mathematic groups have been well defined and studied by Coxeter. This classification may be used in the investigation of several domains of crystallography such as the study of the incommensurate phases, the quasi crystals … Indeed, each mathematic substitution group characterizes an isomorphism class of crystallographic point groups (spaces E^2 or E^3), of point groups of super crystals (spaces E^4 or E^5), and of molecular symmetry groups (spaces E^2 or E^3). This mathematic group gives interesting information about: 1) the incommensurate phase structures and their phase transitions according to the Landau's theory in their super spaces E^4, E^5, E^6, ⋯; 2) the molecular symmetry group of chemisorbed molecules in space E^2 (paragraph 2) or of the molecular crystal or solution in view of studying the molecule structure or its rotations or vibrationsin space E^3; 3) the geometric polyhedron symmetry groups as the regular rhombohedron in space E^3, the rhombotope $\cos\alpha = -1/4$ in space E^4 or the rhombotope $\cos\alpha = -1/5$ in space E^5. Then, thanks to the isomorphism classes, we shall give properties of some crystal families that we have not published up to now. This formalism may be used to study crystal families in n-dimensional space with n > 6.

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Keywords

Crystallographic Point Groups, Isomorphism Classes, Incommensurate Phase Structures, WPV (Weigel Phan Veysseyre) Symbols of Point Groups

1. Introduction: Mathematics, Crystallography and Chemistry, Cayley's Theorem

The crystallographers use Hermann-Mauguin's symbols for the crystallographic point groups while the spectroscopists and the chemists use Schöenflies's symbols in order to characterize the symmetry groups of the molecules which are crystallographic point groups too. For instance, the symbols 3 m (crystallographers) and C3v (chemists) are different symbols for isomorphic groups; it is the same property for the symbols 6 mm (crystallographers) and C6v (chemists).

From now, we use cr for crystallographic.

The point symmetries of a crystal are the cr point operations which are compatible with the translational symmetries of this crystal in a given space (E^2 or E^3). They are mainly described by means of group study based on the properties of finite mathematic groups together with a geometric approach. This process was used by Hermann and Mauguin, almost a century ago, when they established the cr symbols of point groups of two- and three-dimensional spaces [1]. We recalled that Hermann and Mauguin were different scientists, one of them was rather crystallographer and the other one rather mathematician. Before explaining the properties of the WPV symbols and the isomorphism classes (Paragraphs 2-1 and 2-2), we give a first example of this mathematic approach. We select the finite mathematic dihedral group D_4 of order 8 and the cr point group of the square 4 mm of order 8 in the space E^2; the eight symmetry operations of group 4 mm are the following ones: two rotations of order 4 *i.e.* of angles $2\pi/4$ and $3 \times 2\pi/4$, one rotation of order 2 *i.e.* of angle $2\pi/2$, then 4 reflections denoted m and the identity. We write the set of these elements on the form 2(4) 5(2) 1(1), *i.e.* 2 elements of order 4, 5 elements of order 2 and the identity. Mathematic group D_4 has elements of the same type. Hence, among the ten cr point groups of space E^2, the group 4 mm is a realization of the group D_4 in space E^2. The two groups, D_4 and 4 mm, were isomorphic as Hermann and Mauguin said. All the cr point groups isomorphic to mathematic group D_4 are listed in **Table 2** (Paragraph 5-1). Among the infinite set of symmetry groups of all the possible molecules of space E^3, the symmetry group of the molecule BrF_5 is a realization of this group D_4. The chemists and the spectroscopists use the Schöenflies's symbol C4v, the same point group as the group 4 mm with the same list of elements. Let's note that the groups, C4v (BrF5 molecule), C3v (ammonia molecule) and C2v (molecule water) are polar groups.

As a second example, we consider the holohedry of the tetragonal family, *i.e.* the cr point group 4 mm $\perp$ m of order $8 \times 2 = 16$, in space E^3; the mark $\perp$ means that the group 4 mm $\perp$ m is the direct product of the two subgroups 4 mm and m. Moreover, these two subgroups act in two orthogonal subspaces of space E^3: group 4 mm acts in a two-dimensional space, and group m acts in a one-dimensional space orthogonal to the first one. Group 4 mm $\perp$ m has four elements of order 4, and seven elements of order 2 (five elements m, 2, $\bar{1}$). This group is isomorphic to the mathematic group $D_4 \times C_2$, direct product of the two groups D_4 and C_2 (**Table 5**, Paragraph 5-2).

These two examples translate the Cayley's theorem: any group G is isomorphic to a subgroup of the symmetric group S(G) of the permutations of this group. Especially, if the group G is a finite group of order n, it is isomorphic to a subgroup of the symmetric group Sn. The demonstration is summarized in the Annex.

The spectroscopists and the chemists add to the mathematical symbol a letter. For instance, the letter h in group C3h means that a horizontal plane of symmetry is added to the axis of rotation of group C_3, and the letter v in group C3v means that three vertical planes of symmetry are added to the axis of rotation of group C_3. So, for each cr point group and for each symmetry group of a molecule of spaces E^3, E^4 and E^5, we give the mathematic symbol, *i.e.* the one of its isomorphism class and the Hermann-Mauguin's symbol (spaces E^2 and E^3), or the WPV (Weigel Phan Veysseyre)'s symbol (spaces E^4, E^5, $\cdots$).

By the way, the real structure of the (mono, di and tri) incommensurate phases takes place in their superspace (E^4, E^5 and E^6) where they become crystals, therefore for crystallographers these super spaces are real physical spaces. Hence, it is essential to use point and space groups in spaces E^4, E^5 and E^6. Then, the section of this "physical" superstructure by the physical space, *i.e.* the three-dimensional space, gives the description of the structure. It is one of the main reasons which support our work. In this paper, we give an example of phase transition, between a mono incommensurate (inc) modulated phase and its basic structure (Paragraph 5-4).

When the physicists of the condensed matter will study the phase transitions of the inc phases in the super spaces systematically, these super spaces will be considered as real physical spaces. The space E^3 is the crystal physical space while the spaces E^4, E^5 and E^6 are the real crystal physical super spaces of the inc phases.

Thanks to the study of the isomorphism classes, we complete the description of the crystal families of space E^5 that we have published previously. Five families are studied in the following paper (number II), *i.e*. the (monoclinic di iso squares)-al, decadic-al, (monoclinic di iso hexagons)-al, (rhombotopic $\cos\alpha = -1/4$)-al and rhombotopic $\cos\alpha = -1/5$ crystal families. Three more families, (di iso hexagons)-al, hypercube 4 dim.)-al and hyper- cube 5 dim., will be studied in a next paper. So, all the crystal families of space E^5 will be studied.

2. Properties of WPV (Weigel Phan Veysseyre) Geometric Symbols. Definition and Properties of the Isomorphism Classes. Example of the Class C_6

2.1. WPV (Weigel Phan Veysseyre) Symbols. Definition and Properties

In order to study each crystal family of space E^5, we used the geometric nature of the cell and the results given by the Scientific Software established by Veysseyre in [2], we design this software by the expression SS E^5.

This SS E^5 gives for each of 32 crystal families of space E^5:

- The list of the cr point symmetry operations of order 2, 3, 4, $\cdots$ with their number for any subgroup of the holohedries.
- The list of the subgroups of each subgroup of the holohedries.

The geometric approach allows us to give a name to the 32 crystal families of space E^5.

The list of all the subgroups of each holohedry gives 955 cr point groups in the space E^5. This list of the 955 cr point groups of space E^5 contains the 10 cr point groups of space E^2, the (32-10) cr point groups of space E^3, the (227-32) crpoint groups of space E^4. Moreover, thanks to the list of the cr point symmetry operations of order 2, of order 4, of order 5, $\cdots$, with their number, it is possible to assign to each cr point group a symbol as well as a mathematic symbol. These symbols are named "WPV symbols", from the initials of this study's authors (Weigel, Phan and Veysseyre [3]).

The assigned WPV symbols to the cr point groups of space E^5 are in agreement with the Hermann-Mauguin's symbols of spaces E^2 and E^3 and they respect the International Sub-Commission Nomenclature recommendations in [4]. However, others rules must be given. Indeed, in spaces E^4 and E^5, several regular polytopes appear with symmetry operations compatible with the fourth and the fifth dimensions. In addition, for the study of the mono cubic families in [5], we had to define and to study a new kind of symmetry operations that we called "iso cubic" operations.

The 955 cr point groups of space E^5 are isomorphic to some mathematic groups. Most of these mathematic groups are the direct product of two or more cyclic groups. After the work of Fedorov and Schöenflies (1891) for the space groups in the three-dimensional space and the work of Brown in [6] for the cr point and space groups in four-dimensional space, we can cite the publications of Plesken in [7]-[9] which give a classification of the cr point and space groups respectively in 5 and 6 dimensions from a set of algorithms. The Cayley's theorem (1854) specifies that all finite groups are isomorphic to a product of permutation groups. Thanks to the two lists named previously, *i.e*. the symmetry point operation and the subgroup lists, we are in position to give a complete classification of the cr point groups of five-dimensional space. So all the cr point groups isomorphic to a same mathematic group belong to an isomorphism class, these cr point groups are the cr realizations of the same mathematic group.

The WPV symbol contains more geometric information than the mathematic symbol and gives the geometric nature of the cell, the symmetry operations together with the supports of the group generators. A WPV symbol defines one and only one cr point group while the mathematic symbol is the same for all the groups of an isomorphism class.

2.2. Isomorphism Class, Definition and Properties

An isomorphism class is the infinite set of all point groups isomorphic to a mathematic group, either cr point groups or molecule symmetry groups or symmetry groups of polygons, polyhedrons, polytopes; these groups are the realizations of a mathematic group whatever the dimension of space is. The authors of the book [6] have given a mathematic type for all the 227 cr point groups of space E^4; these types are characterized either by a mathematic symbol such as C_n $(n = 2,3,4,\cdots)$ or $D_n\cdots$ or by a number, for instance 128-1, and Plesken in [8] [9] gave the isomorphic types of all the holohedries of the crystal families of spaces E^5 and E^6.

Indeed, any cr point group of a given space can be considered as the realization of one finite mathematic group; therefore, it is possible to gather all the cr point groups in different isomorphism classes. Of course, all the cr point groups of an isomorphism class have the same order and the same number of elements of each order *i.e.* the same arrangement of its elements. We recall that the order of an element g of a finite group is the smaller integer n such as the element g^n equals the identity.

To sum up, an isomorphism class is characterized by:

1) A mathematic symbol for instance, C_n cyclic group, D_n dihedral group, S_n symmetric group, An alternate group, $D_n \times C_n$ direct product of the two groups D_n and C_n, Dicn or Qndicyclic group, or by a more complicate symbol defined in [10]. Some mathematicsymbols are explained in Annex.

2) A list of elements which is the same for all the cr point group of the class; this list gives the different symmetry elements classified order by order with their number.

Let's give the cyclic group C_6 as a simple example. The cyclic group C_6 is isomorphic to the direct product of two cyclic groups C_3 and C_2, *i.e.* $C_6 = C_3 \times C_2$ because 3 and 2 are coprime. Each group of the class C_6 has two elements of order 6, two elements of order 3, one element of order 2 and the identity. We write this list under the form 2(6) 2(3) 1(2). From now on, we omit the identity in the list of elements of a group. All the cr point groups which have two symmetry elements of order 6, two symmetry elements of order 3 and one symmetry element of order 2 belong to the isomorphism class C_6. **Table 1** listed all the groups isomorphic to group C_6 which belong to four crystal families of space E^5, *i.e.* the Hexagon triclinic, (Hexagon oblique)-al, (Diclinic de hexagons)-al and (D_i hexagons)-al families; these groups belong to spaces E^2, E^3, E^4, E^5. This table lists the symbol of the holohedry and its order for each family. The name of the different families explains the construction of the cell, for instance (Hexagon oblique)-al, the cell is a right hyper prism (suffix al) and its base is the Cartesian product of a hexagon and a parallelogram.

Let be denoted (x, y, z, t, u), the five axes of space E^5. The group $\overline{\overline{33}}$ is the cyclic group generated by the symmetry operation $3^1_{xy}3^1_{zt}\bar{1}_5$ or by the equivalent operation $6^1_{xy}6^1_{zt}m_u$ the six elements of the group $\overline{\overline{33}}$ are thefollowing ones:

$$6^1_{xy}6^1_{zt}m_u,\ 3^1_{xy}3^1_{zt},\ \bar{1}_5\ 3^{-1}_{xy}3^{-1}_{zt},\ 6^{-1}_{xy}6^{-1}_{zt}m_u,\ 1$$

$\bar{1}_5$ is the total homotethie of space E^5. The group $\overline{\overline{36}}$ is the cyclic group generated by the symmetry operation $3^1_{xy}6^1_{zt}\bar{1}_5$ or by the equivalent operation $6^1_{xy}3^1_{zt}m_u$; the six elements of this group are the following ones

$$6^1_{xy}3^1_{zt}m_u,\ 3^1_{xy}3^{-1}_{zt},\ \bar{1}_{ztu},\ 3^{-1}_{xy}3^1_{zt},\ 6^{-1}_{xy}3^{-1}_{zt}m_u,\ 1$$

Remark

The cr point groups of an isomorphism class often belong to several crystal families.

Table 1. Crystallographic point groups of crystal families of space E^5 isomorphicto mathematical group C_6.

Family names	WPV symbol and order of the holohedries		WPV symbol of point groups of class C_6			
			space E^2	space E^3	space E^4	space E^5
Hexagon triclinic	$6mm \perp \bar{1}$	(24)	6			$3 \perp \bar{1}$, $\overline{\overline{3}}$
(Hexagon oblique)-al	$6mm \perp 2 \perp m$	(48)		$3 \perp m$, $\bar{3}$	62	$3 \perp 2$
(Diclinic di hexagons)-al	$66 \perp m$	(12)			66	$33 \perp m$, $\overline{\overline{33}}$
(Di hexagons)-al	$6mm \perp 6mm \perp m$	(288)			63	$\overline{\overline{36}}$

Table caption: First column: Family names. Second column: WPV symbol and order of the holohedries. Point groups isomorphic to group C_6: of space E^2. Third column: of space E^3. Fourth column: of space E^4. Fifth column: of space E^5 sixth column. SS E^5 gives this information.

3. From Mathematic Groups to Crystallographic and Molecular Symmetry Point Groups. Realizations of Isomorphism Classes D_3 and $D_3 \times C_2$ in Spaces E^2, E^3, E^4, E^5 as cr Point Groups or Molecular Symmetry Groups

Let's give the example of the isomorphism class D_3 (dihedral group of order 6) with the list of elements 2(3) 3(2) and the one of the class $D_3 \times C_2$ (of order 12) with the list of element 2(6) 2(3) 7(2). The realizations of these cr point groups belong to spaces E^2, E^3, E^4, E^5 in crystallography and to spaces E^2, E^3 in chemistry and spectroscopy.

Before start with these examples, it is useful to compare the arrangements of the two mathematic groups G and G × C_2 where G is a finite group and C_2 is the cyclic group of order 2. Let be denoted $n(z)$ the number of elements of order z in the group G and $\mathrm{N}(z)$ this number in the group G × C_2. The relations between the numbers $n(z)$ and $\mathrm{N}(z)$ are the following ones:

$$\mathrm{N}(12)=2n(12) \quad \mathrm{N}(10)=n(5) \quad \mathrm{N}(5)=n(5) \quad \mathrm{N}(6)=n(3)+2n(6)$$

$$\mathrm{N}(3)=n(3) \quad \mathrm{N}(2)=2n(2)+1 \quad \mathrm{N}(4)=n(4)$$

3.1. Isomorphism Class D_3, in Space E^3

The hexagonal crystal family (holohedry 6 mm ⊥ m, order 24) has two point groups isomorphic to group D3, *i.e.* the cr point groups 3 m and (3 2) (Hermann-Mauguin's symbols).

The Schöenflies's symbol of these groups, used by the chemists, is C3v. As example, we can cite the crystal Fe2P (cr point group (3 2), space group P 321).

3.2. Isomorphism Class D_3, in Space E^4

Three crystal families of space E^4 have cr point groups which belong to this isomorphism class. They are:

- The hexagon rectangle crystal family (holohedry 6 mm ⊥ mm, order 48) with the cr point group (3 2).
- The hexagon oblique crystal family (holohedry 6 mm ⊥ 2, order 24) with two cr point groups, 3 m and $\left(3\ \bar{1}\right)$.
- The (monoclinic di hexagons) crystal family (holohedry (66 2 2), order 12), with the cr point (33 2).

3.3. Isomorphism Class D_3, in Space E^5

Three crystal families of space E^5 have cr point groups which belong to this isomorphism class. They are:

- The hexagon triclinic crystal family (holohedry 6 mm ⊥ 1 of order 24) with two cr point groups 3 m and $\left(3\ \bar{1}_4\right)$.
- The (hexagon oblique)-al crystal family (holohedry 6 mm ⊥ 2 ⊥ m of order 48) with two cr point groups, (3 2) and $\left(3\ \bar{1}\right)$.
- The (monoclinic di hexagons)-al crystal family (holohedry (66 2 2) ⊥ m of order 24) with two cr point groups (33 2) and $\left(33\ \bar{1}\right)$.

3.4. Example of the Molecule BF_3 (Trifluoride Boron)

The set of the point groups of the equilateral triangle is isomorphic to mathematic group D_3 (order 6) in space E^2 and to group $D_3 \times C_2$ (order 12) in space E^3. The Schöenflies and H.M. symbols of each BF_3 molecule are:

- D_3 or 3 m for the chemisorbed (mono layer) BF_3 molecules on a very clean divided solid; indeed in this case, the plane of the molecule is not a reflection mirror, because from one side there are strong chemical bonds between the chemisorbed molecule and the solid while on the other side, there are weak chemical bonds between the chemisorbed molecule and the polylayerphysisorbed BF_3 ones. So, here the chemisorbed molecules are strictly in space E^2. Let us note that the three π rotations through three BH axes in a BF_3 chemisorbed molecule are not possible just as the vibrations of this chemisorbed molecule orthogonal to the plane BF_3 (one axis BH is the line which links the center B of the equilateral triangle of the molecule to one of its vertices).
- D3h or 3 m ⊥ m for the physisorbed BF_3 molecules in their multilayer state (just the contact between the mono layer) as well as in the tri fluoride boron liquid or molecular crystal where the molecules are in space E^3.

4. Realizations of Mathematic Classes A_5, Order 60 and S_5 ($A_5 \times C_2$) Order 120 as Symmetry Groups in E^3 (I, Ih) and as cr Point Groups of Super Crystals in E^4 and E^5, of Polyhedrons or Molecules in Spaces E^3 or as cr Point Groups in Spaces E^4 and E^5

The list of the elements of the group A_5 is the following one 24(5) 20(3) 15(2) and the one of the group $S_5 = A_5 \times C_2$ is 24(10) 24(5) 20(6) 20(3) 31(2), the relation between these two lists is explained in paragraph 3.

The mathematic substitution group A5 is the rotation group of the regular dodecahedron and of the regular icosahedron in space E^3 and the group S5 is the point symmetry group of these polyhedrons. The regular dodecahedron has 20 vertices, 30 sides and 12 faces which are regular pentagons, three to each vertex. The Euler's theorem is verified by these three numbers, indeed 20 − 30 + 12 = 2. The regular icosahedron has 12 vertices, 30 sides and 20 faces which are equilateral triangles, three to each vertex. The Euler's theorem is verified by these three numbers 12 − 30 + 20 = 2. These two regular Platonic polyhedrons are dual to each other and their realizations as cr point groups in spaces E^4 and E^5 also.

These two polyhedrons are two geometric realizations of groups A_5 and S_5 in space E^3. The group S_5 has other realizations such as for instance the symmetry group of the two molecules C_{60} and $C_{20}H_{20}$. The group A_5 has other realizations such as the rotation group of the two molecules C_{60} and $C_{20}H_{20}$. The Schoënflies symbol of this symmetry group is Ih.

So, the two molecules of space E^3, the buckminsterfullerene C_{60} and the dodecahedrane $C_{20}H_{20}$ have the same rotation group of order 60, Schoenflies's symbol I and the same symmetry group of order 120, Schoenflies's symbol Ih. The groups I and Ih are two "molecular" realizations in space E^3 of the mathematic groups A_5 and S_5.

More details about groups A_5 and S_5 are given in the paper number II with the study of the two crystal families (rhombotopic $\cos\alpha = -1/4$)-al and rhombotopic $\cos\alpha = -1/5$ (space E^5).

5. Isomorphism Classes D_4 Order 8, $D_4 \times C_2$ Order 16 and $D4 \times C_2 \times C_2$ Order 32 in Spaces E^2, E^3, E^4, E^5. Application to the Study of the Mono Incommensurate NbTe4 Phase Transition in Its Super Space

5.1. Isomorphism Class D_4, One of the Five Types of Mathematic Groups of Order Eight

Sixteen cr point groups of space E^n $(n \le 5)$ are isomorphic to mathematic group D_4. They are listed **Table 2** together with their symmetry operations and with the crystal families and two examples in spaces E^6 and E^7 are given in **Table 3**.

The symmetry elements of group D_4 are the following ones: 2(4) 5(2), *i.e.* this group has two symmetry operations of order 4 and five symmetry operations of order 2 besides the identity.

The inversion has for symbol m in space E^1, 2 in space E^2, $\bar{1}$ in space E^3, $\bar{1}_4$ in space E^4 and so on; $\bar{1}$ is the short symbol for the inversion $\bar{1}_3$ in space E^3.

5.1.1. Remarks about Table 2

- The WPV symbols are very similar to the Hermann-Mauguin's symbols 4 mm, 422. It is easy to verify that all these groups have the same distribution of elements, 2(4) 5(2) and the identity. These results are in agreement with the SS E5 lists.
- These sixteen cr point groups belong to one crystal family of space E^2, the square family, to one crystal family of space E^3, the tetragonal family, to three crystal families of space E^4, the square oblique, the square rectangle and the monoclinic di squares families and to four crystal families of space E^5, the triclinic square, the (square oblique)-al, the square orthorhombic and the (monoclinic di squares)-al families.
- As for every isomorphism class, the number of cr point groups of class D_4 depends on the dimension of the studied space. For instance, one group acts in space E^2 strictly, two in E^3, five in E^4 and eight in E^5.
- Thanks to the geometric approach which has been rarely used in the crystallography in the super space and to the WPV symbols which in fact generalize Hermann-Mauguin's symbols, it is possible to predict the existence of cr point groups and crystal families in space E^n with $n \ge 6$ from the results obtained in space E^n with $n \le 5$. Some results are given in **Table 3**. This list is not exhaustive.

5.1.2. Remark about Table 3

- The geometrical supports of cr point groups of spaces E^6, E^7 can be obtained from those of space E^5:

Table 2. Crystallographic point groups isomorphic to mathematic group D_4 in spaces E^2, E^3, E^4 and E^5.

Groups and the symmetry operations	Crystal families
4 mm $(1, 4_{xy}^{\pm1}, 2_{xy}, m_x, m_y, m_{x\pm y})$	square, tetragonal, square oblique, square triclinic
422 $(1, 4_{xy}^{\pm1}, 2_{xy}, 2_{xz}, 2_{yz}, 2_{x\pm y z})$	tetragonal, square rectangle, (square oblique)-al
$4\ \bar{1}\ \bar{1}$ $(1, 4_{xy}^{\pm1}, 2_{xy}, \bar{1}_{xzt}, \bar{1}_{yzt}, \bar{1}_{x\pm y zt})$	square oblique, (square oblique-)al
$\bar{4}2$ m $(1, 4_{xy}^{\pm1} m_z, 2_{xy}, 2_{x\pm y z}, m_x, m_y)$	tetragonal, square rectangle, (square oblique)-al
$\bar{4}\ 2\ \bar{1}$ $(1, 4_{xy}^{\pm1} m_z, 2_{xy}, 2_{x\pm y t}, \bar{1}_{xzt}, \bar{1}_{yzt})$	square rectangle, square orthorhombic
42 m $\bar{1}$ $(1, 4_{xy}^{\pm1} 2_{zt}, 2_{xy}, m_x, m_y, \bar{1}_{x\pm y zt})$	square oblique, (square oblique)-al
42 2 2 $(1, 4_{xy}^{\pm1} 2_{zt}, 2_{xy}, 2_{xz}, 2_{yz}, 2_{x\pm y t})$	square rectangle, square orthorhombic
44 2 2 $(1, 4_{xy}^{\pm1} 4_{zt}^{\pm1}, 2_{xz}, 2_{yt}, 2_{x+y z+t}, 2_{x-y z-t}, \bar{1}_{xyzt})$	monoclinic di squares, (monoclinic di squares)-al
$4\ \bar{1}_4\ \bar{1}_4$ $(1, 4_{tu}^{\pm1}, 2_{tu}, \bar{1}_{xyzt}, \bar{1}_{xyzu}, \bar{1}_{xyz t\pm u})$	triclinic square
$\bar{\bar{4}}\ \bar{1}_4$ m $(1, 4_{tu}^{\pm1} \bar{1}_{xyz}, 2_{tu}, \bar{1}_{xyz t\pm u}, m_t, m_u)$	triclinic square
$\bar{\bar{4}}\ 2\ \bar{1}$ $(1, 4_{xy}^{\pm1} \bar{1}_{ztu}, 2_{xy}, 2_{xu}, 2_{yu}, \bar{1}_{x\pm y ztu})$	(square oblique)-al
42 2 $\bar{1}_4$ $(1, 4_{xy}^{\pm1} 2_{zt}, 2_{xy}, 2_{xu}, 2_{yu}, \bar{1}_{x\pm y ztu})$	(square oblique)-al
$\bar{4}\ \bar{1}_4\ \bar{1}$ $(1, 4_{x-y z-t}^{\pm1} m_{x+y-z-t}, 2_{x-y z-t}, \bar{1}_{x+y ztu}, \bar{1}_{xyu z\pm t}, \bar{1}_{x+z y+t u}, \bar{1}_{x+t y+z u})$	(square oblique)-al
42 $\bar{1}\ \bar{1}$ $(1, 4_{xy}^{\pm1} 2_{zt}, 2_{xy}, \bar{1}_{xzu}, \bar{1}_{yzu} \bar{1}_{x\pm y tu})$	square orthorhombic
44 $\bar{1}\ \bar{1}$ $(1, 4_{xy}^{\pm1} 4_{zt}^{\pm1}, \bar{1}_{xyzt}, \bar{1}_{xzu}, \bar{1}_{ytu}, \bar{1}_{x+y z+t u}, \bar{1}_{x-y z-t u})$	(monoclinic di squares)-al
$\overline{\overline{44}}\ 2\ \bar{1}$ $(1, 4_{xy}^{\pm1} 4_{zt}^{\pm1} m_u, 2_{xz}, 2_{yt}, \bar{1}_{xyzt}, \bar{1}_{x+y z+t u}, \bar{1}_{x-y z-t u})$	(monoclinic di squares)-al

Table caption: First column: WPV symbol and geometric supports of the symmetry operations. ($x\ y\ z\ t\ u$) is a basis of space E^5. The axes x and y on the one hand and z and t on the other hand are orthogonal, the axis u is orthogonal to space E^4. Second column: Names of the crystal families. SS E^5 gives this information.

Table 3. Crystallographic point groups of isomorphism class D_4 in spaces E^2, $\cdots$, E^7.

Spaces	WPV symbol point groups	Crystal families	WPV symbol holohedries	Orders
E^2	4 mm	square	4 mm	8
E^3	422	tetragonal	$4mm \perp m$	16
E^4	$4\ \bar{1}\ \bar{1}$	square oblique	$4mm \perp 2$	16
E^5	$4\ \bar{1}_4\ \bar{1}_4$	square triclinic	$4mm \perp \bar{1}$	16
E^6	$4\ \bar{1}_5\ \bar{1}_5$	square hexaclinic	$4mm \perp \bar{1}_4$	16
E^7	$4\ \bar{1}_6\ \bar{1}_6$	square decaclinic	$4mm \perp \bar{1}_5$	16

Table caption: First column: Spaces. Second column: WPV symbol point groups. Third column: Names of the crystal families. Fourth column: WPV symbol of the holohedries. Fifth column: Order of the holohedries.

Space E^6	$4\ \bar{1}_5\ \bar{1}_5$	$1,\ 2_{xy},\ 2_{x\pm yt},\ \bar{1}_{xztuv},\ \bar{1}_{yztuv},\ \bar{1}_{x+yztuv},\ \bar{1}_{x-yztuv}$
Space E^7	$4\ \bar{1}_6\ \bar{1}_6$	$1,\ 2_{xy},\ 2_{x\pm yt},\ \bar{1}_{xztuvw},\ \bar{1}_{yztuvw},\ \bar{1}_{x+yztuvw},\ \bar{1}_{x-yztuvw}$

5.1.3. Complement about the Family Numbered I

C_2 is the only mathematic group of order 2. In space E^n, it contains the two elements 1 and $\bar{1}$. The cyclic group generated by this inversion has for WPV symbol $\bar{1}_n$ in space E^n. **Table 4** lists some families which have group $\bar{1}_n$ for holohedry and numbered I in all spaces.

5.2. Isomorphism Class $D_4 \times C_2$

The symmetry elements of group $D_4 \times C_2$ of order 16 are the following ones 4(4) 11(2), this group has four symmetry operations of order 4 and eleven symmetry operations of order 2, besides the identity. **Table 5** lists the cr point group of this class. As previously, SS E^5 gives this information.

5.3. Isomorphism Class $D_4 \times C_2 \times C_2$

The symmetry elements of group $D_4 \times C_2 \times C_2$ of order 32 are the following ones: 8(4) 23(2), *i.e.* 8 symmetry operations of order 8 and 23 symmetry operations of order 2 besides the identity. Among the 227 cr point groups of space E^4, only one group belongs to this isomorphism class, it is the holohedry of the crystal family square rectangle, the group $4\text{ mm} \perp \text{mm}$. Other groups of this isomorphism class belong to spaces E^n with $n \geq 5$.

5.4. Study in the Super Space E^4 of a Mono Incommensurate Modulated Phase $NbTe_4$ and of Its Phase Transitions, between Itself (50 K < T < 793 K), Its Basic Structure and Its Lock-in Phase (L.IN) T < 50 K

The diffraction experiments prove that the inc phase $NbTe_4$ is a mono inc phase so the super space of this structure is the four-dimensional space E^4.

Table 4. Crystal families numbered I.

Spaces	Geometric names of the family	Crystal cell names	Length parameters	Angular parameters
E^2	oblique	parallelogramm	2	1
E^3	triclinic	oblique parallelepipede	3	3
E^4	hexaclinic	«maxiclinic» parallelotope	4	6
E^5	decaclinic		5	10
E^6	pentadiclinic		6	15

Table caption: Firstcolumn: Spaces. Second column: Geometric names of the family. Third column: Names of the crystal cells. Fourth column: Number of length parameters. Fifth column: Number of angular parameters.

Table 5. Crystallographic point groups isomorphic to mathematical group $D_4 \times C_2$.

Family names and spaces	WPV point group symbols
Tetragonal (E^3)	$4\text{mm} \perp \text{m}(4/\text{mm})$
Square oblique (E^4)	$4\text{mm} \perp 2$
Square rectangle (E^4)	$\bar{4}2\text{m} \perp \text{m},\ \bar{4}2\text{m} \times \bar{1}_4,\ 422 \times \bar{1}_4,\ 422 \perp \text{m},\ 4\text{m} \perp \text{m}$
Square triclinic (E^5)	$4\text{mm} \perp \bar{1}$
(Square oblique)-al (E^5)	
Centred family	$\bar{4}2\text{m} \times \bar{1}_5$
Primitive family	$422 \perp 2,\ 4\text{mm} \perp \text{m},\ (42\text{m}\ \bar{1}) \perp \text{m},\ 4\text{mm} \perp 2,\ \bar{4}2\text{m} \perp 2,\ (4\ \bar{1}\ \bar{1}) \perp \text{m},\ 422 \times \bar{1}_5$
Square orthorhombic (E^5)	
Centred family	$\bar{4}2\text{m} \times \bar{1}_4,\ (42\ 2\ 2) \times \bar{1}_4,\ \bar{4}2\text{m} \perp \text{m},\ (42\ 2\ 2) \times \bar{1}_5,\ (\bar{4}\ \bar{1}\ \bar{1}) \perp \text{m},\ (42\text{m}\ \bar{1}) \times \bar{1}_4,\ 422 \times \bar{1}_5$
Primitive family	$422 \times \bar{1}_4,\ (\bar{4}\ \bar{1}\ \bar{1}) \times 2,\ (42\ 2\ 2) \perp \text{m},\ 422 \perp \text{m},\ (4\ \bar{1}\ \bar{1}) \times 2$
(Monoclinic di squares)-al (E^5)	$(44\ 2\ 2) \perp \text{m}$
Di squares-al (E^5)	
Centred family	$(44\ 2\ 2) \times 2,\ (44\ 2\ 2) \times \bar{1},\ (44\ \bar{1}\ \bar{1}) \times 2,\ (\bar{\bar{44}}\ 2\ \bar{1}) \times \bar{1}$

Table caption: First column: Family names and spaces. Second column: WPV symbol of the point groups isomorphic to the mathematic group $D_4 \times C_2$. SS E^5 gives this information.

As early as 1984, Van Smaalen in [11] determined the structure of this inc. phase in its super space E^4. They proved that the cr point group of this structure is the group $4mm \perp 2$ of order 16, the holohedry of the crystal square oblique family. The basic structure, (BS), can be considered:

- As a crystal in the usual three-dimensional space (x, y, z). Its cr point group is the group $4mm \perp m$, holohedry of the tetragonal family with the space group P4/mcc, *i.e.* P 4cc $\perp$ m [12].
- As well as a crystal in the four-dimensional space (x, y, z, t) because, if the temperature of the inc phase increases, the modulation so the polarization of this phase is cancelled by the superimposition of two out of phase modulated inc states.

So, we have to consider two "out of phase operators". A linear operator which does not bring any new information, *i.e.* the element identity of the binary group m_t. One antilinear operator which "reverses the phase of the inc phase", *i.e.* the element m_t, reflection in the super space E^4 (x, y, z, t) through the physical space E^3 (x, y, z). To sum up, if we consider the BS of $NbTe_4$ in space E^4, its cr point group is $(4mm \perp 2)m$, the product of the cr point group of the inc phase in space E^4 with the binary group m (preservation and out of phase change). The order of this group is 32, the geometrical supports of the generators are the following ones: space (x, y) for the group 4mm, space (z, t) for the symmetry 2 and the axe *t* for the reflexion m. This cr point group belongs to the isomorphism class $D_4 \times C_2 \times C_2$, which has for arrangement 8(4) 23(2). Of course, the point group $4mm \perp 2$ belongs to the isomorphism class $D_4 \times C_2$ (Paragraph 5-2 and **Table 5**).

Now, we prove that the point group of the BS of $NbTe_4$ in space E^4 is the cr point group $4mm \perp m \perp m$, thanks to the Landau's theory of a second order transition. Indeed, the one group of the isomorphism class $D_4 \times C_2 \times C_2$ which has $4mm \perp 2$ as subgroup of index 2 is the cr point group $4mm \perp mm$ which is the holohedry of the crystal square rectangle family. So, if we consider the BS in the super space E4, we also prove that the WPV symbol of its cr point group is $(4mm \perp 2)m = 4mm \perp mm$

To sum up, the group subgroup relation between the cr point group of the BS and the cr point group of the inc phase in their common super space E^4 is the following one $4mm \perp 2$; it is an index 2 subgroup of the group $4mm \perp mm$.

If we are not afraid to work in the super space E^4, the Landau's theory of second order phase transition is verified.

6. Conclusions

As early as 1854, Arthur Cayley proved that any finite group *G* is isomorphic to a subgroup of the permutation group of *G*.

In this paper, we show that the geometric, physical, chemical and crystallographic isometry point groups which are isomorphic to the same mathematic group of permutations can be gathered together in one isomorphism class. As the cr point groups of an isomorphism class have the same mathematic structure, their Hermann-Mauguin's symbols or Weigel Phan Veysseyre's symbols are very similar and they have the same list of elements (arrangements). For instance, the symmetry group Ih of order 120 of the dodecahedron molecule C20H10 is isomorphic to the cr point group [5] $\times \bar{4}3m$ is the hemihedry of the (rhombotopic $\cos\alpha = -1/4$) crystal family of space E^4. These two groups are two realizations of the same mathematic group S5: the first one, Ih, among the infinite set of the molecule symmetry groups in space E^3, and the second one [5] $\times \bar{4}3$ m in the finite set of the 227cr point groups of space E^4.

Actually, these isomorphic cr point groups are either the symmetry groups of polytopes in geometry (spaces E^2, E^3, E^4, E^5, $\cdots$) or the cr point groups (spaces E^2, E^3, E^4, E^5, $\cdots$) or the chemistry molecular symmetry groups (spaces E^2 and E^3) or the magnetic point groups (space E^4, $\cdots$) or the inc phase point groups (in their super spaces, E^4 for the mono, E^5 for the di, and E^6 for the tri inc phases).

For instance, a mathematic group, such as D_6, characterizes an isomorphism class in physics, chemistry, $\cdots$; the groups of this class are either molecular symmetry groups such as C6v for the chemisorbed molecule C6H6 in the space E^2 or cr point groups such as 6 mm in space E^2 (identical to C6v) or geometric point groups of the Platon's polyhedrons such as 6 mm for the regular hexagon of the space E^2.

Yet, it is no sense to speak about an isomorphism class without specifying the spaces where these groups act. Indeed, if we do not limit the dimension of the space, an isomorphism class can contain an infinite number of groups.

Schöenflies [13] and Fedorov [14] proved that there were ten cr point groups in space E^2 and thirty-two in space

E^3. Carl Hermann and Victor Mauguin gave the mathematic and crystallographic structures through the symbols called Hermann-Mauguin symbols. These thirty-two cr point groups of space E^3 are the realizations of twenty mathematic permutation finite groups only. To sum up, they belong to the following isomorphic classes:

C_1, C_2, $C_2 \times C_2$, $C_2 \times C_2 \times C_2$ in the triclinic, monoclinic and orthorhombic crystal families;

C_4, $C_4 \times C_2$, D_4, $D_4 \times C_2$ in the tetragonal crystal family;

C_3, $C_3 \times C_2$, D_3, $D_3 \times C_2$, C_6, $C_6 \times C_2$, D_6, $D_6 \times C_2$ in the hexagonal crystal family;

A_4, $A_4 \times C_2$, S_4, $S_4 \times C_2$ in the cubic crystal family.

Therefore, the thirty-two cr point groups of space E^3 are built from a set of twenty generators (the generators are the subgroups which allow to building the group) and there are only twenty types of Hermann-Mauguin symbols, *i.e.* twenty mathematical structures for the thirty-two cr point groups of space E^3.

Then, the spectroscopists and the theorist chemists used the molecular symmetry groups with the Schöenflies's molecular symbols and they simplified the theoretical approach of the bonds, of the rotations and of the vibrations of the molecules.

Of course, some of them, the cr point group Oh of SF6 in space E^3, are identical to a cr point group, e.g. Cu in space E^3, while the others are not identical to any cr point group of space E^3 but they are identical to one cr point group of the 227 cr point groups of space E^4. The group Ih of the molecule C60 in space E^3 is identical to the group [5] $\times \bar{4}3$ m hemihedry of the (rhombotopic $\cos\alpha = -1/4$) family of space E^4.

After that, when Shubnikov [15] and Bertaut [16] [17] studied the magnetic crystals in their super space E^4, they used the primed symmetry operators or antisymmetry operators or time reversal operators along the fourth dimension; the time's inversion in space E^4 was actually the reflection through the mirror physical space (x, y, z).

Let us give an example. A finite mathematic group such as $C_2 \times C_2 \times C_2$ of order 8 can realize itself in the magnetic point group of space E^4 22.1', (1' is the binary group with the conservation of the time 1 and the inversion of the time 1') in the set of the 122 magnetic point groups of space E^4.

We see that a ferromagnetic mono inc. phase will be a super crystal in space E^5 where the time's inversion will be a reflection through the super space E^4 (x, y, z, t).

The first structure determinations of inc phases which were super crystals in their super spaces were made by De Wolf in [18], Janner and Janssen [19], and Grébille, Weigel, Veysseyre and Phan [20].

Now, the super crystallographers find the mono, di and triinc phase structures in the superspaces E^4, E^5 and E^6 and soon they will study their physical properties and their transitions of phases in these same super spaces.

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Annex

Abstract Mathematic Groups

We summarize the main properties of some types of abstract groups. The used notations are those of Coxeter for the greatest part.

E is the unit element of the group, and the mark × is used for a direct product.

Cyclic Group C_n

A cyclic group C_n is a group of order n generated by only one element *g* such as $g^n = \mathrm{E}$. It contains all the successive powers of the generator.

Dihedral Group D_n

The dihedral group D_n is a group of order 2*n*; it is the group of the *n* rotations and of the *n* symmetries of a plane which preserve a regular polygon to *n* vertices. This group is generated by two elements *T* and *R* such as:

$$T^n = R^2 = (TR)^2 = \mathrm{E}$$

Particular cases of dihedral groups

- If $n = 2m$ and if m is an odd number, $D_{2m} = D_m \times C_2$, its order equals 4 m. For instance $D_6 = D_3 \times C_2$, it is of order 12.
- $D_2 = D_1 \times C_2 = C_2 \times C_2$.

Symmetric Group S_n

The symmetric group S_n is the permutation group of the *n* vertices of a regular simplex in the (*n*-1)-dimensional space; it is of order *n*!

Alternating Group A_n

The alternating group A_n is the group of the even permutation of *n* objects; it is of order *n*!/2.

Dicyclic Group

The dicyclic group $\langle 2, 2, \mathrm{m} \rangle$ of order 4 m is defining by two generators *S* and *T* such as:

$$T^2 = S^m, \ T^{-1}ST = S^{-1} \ \text{ or } \ S^m = T^2 = (ST)^2$$

Of course, the symbol $\langle 2, 2, \mathrm{m} \rangle$ can be written $\langle 2, \mathrm{m}, 2 \rangle$ or $\langle \mathrm{m}, 2, 2 \rangle$

Quaternion Group

The smallest dicyclic group is the group $\langle 2, 2, 2 \rangle$, it is called "quaternion group", its order is 8 and it is defined by the relations:

$$T^2 = S^2 = (ST)^2 \ \text{ or } \ R^2 = T^2 = S^2 = RST$$

Cayley's Theorem

"Any group *G* is isomorphic to a subgroup of the symmetric group $S(G)$" (group of the permutations of *G*)

If the group *G* is a finite group of order *n*, this group *G* is isomorphic to a subgroup of S_n

Demonstration

Let be g an element of the group *G*. We consider the application f_g of *G* in *G*:

$x \to gx$. This application is a left translation.

This application is bijective, indeed:
$\forall y \in G, \exists x \in G$ such as $y = gx$, $\left(x = g^{-1}y\right) \Rightarrow$ surjective application
$gx = gx' \Rightarrow g^{-1}gx = g^{-1}gx'$ therefore $x = x' \Rightarrow$ injective application
As the law of the group *G* is associative, it is possible to write:

$$\forall g, \forall h, f_{gh} = f_g o f_h$$

Therefore, this application is a permutation and the application φ of *G* in $S(G)$ as follows:

$$\forall g \in G : \varphi(g) = f_g$$

is a morphism of group, then the picture of φ, *i.e.* $\mathrm{Im}(\varphi)$ is a subgroup of *G*.
As the application of *G* in $\mathrm{Im}(\varphi)$ is injective and surjective, it is an isomorphism.
If the order of *G* is finite, the picture of *G* is a subgroup of S_n (*n* order of *G*)