(2) The FF X-ray tubes are recommended for the diffractometers with monochromator geometry H/PA (or V/PE), as, in this case, the homogeneity of the monochromated beam is not influenced by the width of the X-ray tube focus.

(3) All the graphite-monochromated X-ray beams, including the Cu $K\alpha$ one, have a bell-shaped profile along \mathbf{v}_{\perp}^{i} and a plateau along \mathbf{v}_{\parallel} .

The quality of the primary beam should be taken into consideration when preparing a sample crystal for data collection (Tanaka, 1978). For Mo $K\alpha$ FF tube and H/PE geometry the 90% region of the beam is less than 0.25 mm and drops steeply outside this range, which introduces the possibility of serious systematic errors. Large and irregular-shaped crystals are especially objectionable as the volume of such a crystal contained within the high-intensity region changes significantly when the crystal is reoriented for different diffractometer settings. Unfortunately, large platelets or needle-shaped samples, longer than 0.5 or even 0.7 mm, are occasionally used when Mo $K\alpha$ FF X-ray tubes and H/PE monochromator geometry are applied.

The intensity data measured for large irregularshaped crystals are often corrected for absorption



Fig. 7. A platelet sample crystal positioned for a Ψ scan on a diffractometer with H/PE geometry.

and often Furnas's method based on reflection intensity measurements at different Ψ settings is applied (North, Phillips & Mathews, 1968). It can be seen from Fig. 7 that the rotation of the crystal about the Ψ axis will cause systematic errors due to inhomogeneities of the beam (besides those of absorption) which, when this 'correction' is applied, will add new systematic errors to all the data already affected by the inhomogeneity effect during the data collection. It should be ensured that the sample crystal is small enough to avoid this kind of errors. There are no such errors in Ψ -scanned reflection intensities for H/PA (or V/PE) geometry, as the beam is homogeneous along z for this geometry.

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Crystallography, Geometry and Physics in Higher Dimensions. IV. Crystallographic Cells and Polytopes or 'Molecules' of Four-Dimensional Space \mathbb{E}^4

BY T. PHAN, R. VEYSSEYRE AND D. WEIGEL

Laboratoire de Chimie-Physique du Solide (Unité associée au CNRS no. 453) et Laboratoire de Mathématiques de la Physique, Ecole Centrale des Arts et Manufactures, Grande Voie des Vignes, 92295 Châtenay-Malabry CEDEX, France

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Abstract

In a recent paper [Weigel, Phan & Veysseyre (1987). Acta Cryst. A43, 294–304] the 'WPV' notation was proposed for the crystallographic point symmetry groups (PSGs) in four-dimensional space \mathbb{E}^4 . The geometry of crystal families, systems and cells of \mathbb{E}^4 is illustrated with a few geometrical examples of crystallographic point symmetry operations (PSOs). The cells of the 33 crystal systems in \mathbb{E}^4 are described and various polytopes are analysed. Some examples of geometry in higher dimensions are explained.

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Table 1. Crystallographic types of cells in \mathbb{E}^2

Crystal family	Bravais type of cells	Holohedry
Parallelogram	Parallelogram p	2
Rectangle	$\begin{cases} \text{Rectangle } p \\ \text{Rectangle } c^* \end{cases}$	2 <i>m m</i>
Square	Square p	4 <i>m m</i>
Hexagon	Hexagon p	6 <i>m m</i>
n: primitive: c: centred.		

* The primitive cell is a rhombus.

Introduction

Symmetry groups in higher dimensions may be used in the investigation of several domains of crystallography, such as incommensurate phase studies, quasicrystals, etc. For example, it is always possible to associate an incommensurate phase with a periodic structure in a (3+d)-dimensional superspace, the actual crystal solid being a three-dimensional section of this space. So a thorough introduction to the geometry of four or more dimensions is required.

The purpose of this paper is the study of families, systems and cells of \mathbb{E}^4 from a geometrical point of view and the retrieval of the cells of such families among polytopes of \mathbb{E}^4 , be they regular or not. We shall also put emphasis on some families of \mathbb{E}^5 and \mathbb{E}^6 .

Tables 1 and 2 briefly summarize the set of families, systems and Bravais types of cells in two- and threedimensional spaces. We recall that there are six crystal families and seven crystal systems in threedimensional space.

Any cell is a parallelotope, *i.e.* a generalized parallelepiped. A parallelotope may be constructed by successive translations. Indeed, a point moving along a line traces out a segment. Then a segment translated in a direction different from its own line describes a parallelogram. The same process is easily generalized. An n-dimensional parallelotope is



Fig. 1. The centred rectangular cell and primitive rhombic cell of \mathbb{F}^2 .



Fig. 2. Hexagonal R and rhombohedral P lattices of \mathbb{E}^3 .

Table 2. Crystallographic types of cells in \mathbb{E}^3

Crystal family	Bravais type of cells	Holohedry		
Triclinic	Triclinic P	1		
Monoclinic	Monoclinic P or A	2/m		
Orthorhombic	Orthorhombic P, C, I or F	2/m 2/m 2/m		
Tetragonal	Tetragonal P or I	4/m 2/m 2/m		
Hexagonal	Hexagonal <i>P</i> Hexagonal description of <i>R</i>	6/m 2/m 2/m 32/m		
Cubic	Cubic P, I or F	4/m 3 2/m		

P: primitive; A, B or C: one-centred face; I: body-centred; F: all the faces centred; R: rhombohedron.

generated by translating an (n-1)-dimensional parallelotope in a direction which does not belong to the superspace \mathbb{E}^{n-1} . Bravais types of cells have the maximum number of possible right angles compatible with the geometric supports of the point symmetry operations (PSO for short) of the holohedry (orientation symmetry of the lattice). However, these cells are not always of primitive nature. Other primitive cells can describe the same lattice but they do not have the maximum number of possible right angles. We recall two well known examples: (1) the centred rectangular cell and primitive rhombic cell of \mathbb{E}^2 (Fig. 1), where (x, y) is the conventional nonprimitive basis, (x', y') is the primitive basis of the rhombic lattice; and (2) hexagonal R and rhombohedral P lattices of \mathbb{E}^3 (Fig. 2), where (x, y, z) is the basis of the hexagonal R lattice, and (x', y', z') is the primitive basis of the rhombohedral lattice, i.e. a parallelepiped of which all the faces are equal rhombs.

The crystal systems are characterized by the point symmetry group or PSG of the lattice (holohedry). Let us consider a geometrical representation of PSOs with respect to an orthonormal basis (x, y, z, t) of the vector space \mathbb{E}^4 and the matrices associated with these PSOs. (1) Homothetie around the point O: $\overline{1}_4$ (Fig. 3). Its matrix is the matrix number 1. (2) Inversion around the axis x'x: $\overline{1}_{yzt}$ (Fig. 4). Its matrix is number 2. (3) Rotation in the plane xy around the plane zt: 3_{xy}^{1} (Fig. 5). Its matrix is number 3. (4) Reflection on the hyperplane yzt: m_x (Fig. 6), with matrix number 4. (5) Double rotation $5_{xy}^1 5_{zt}^2$ (Fig. 7), with matrix



Fig. 3. Homothetie around the point $O: \overline{1}_4$.



Fig. 4. Inversion around the axis x'x: $\overline{1}_{vz_1}$.

$$\begin{pmatrix} \bar{1} & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & \bar{1} \end{pmatrix}$$
Matrix number 1. Homothetie $\bar{1}_4$.

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} & 0 \\ 0 & 0 & 0 & \bar{1} \end{pmatrix}$$
Matrix number 2. Inversion $\bar{1}_{yzt}$.

$$\begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 & 0 \\ \sqrt{3}/2 & -1/2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$
Matrix number 3. Rotation 3^1_{xy} .

$$\begin{pmatrix} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$
Matrix number 4. Reflection m_x .

$$\begin{pmatrix} \cos 2\pi/5 & -\sin 2\pi/5 & 0 & 0 \\ \sin 2\pi/5 & \cos 2\pi/5 & 0 & 0 \\ 0 & 0 & \sin 4\pi/5 & \cos 4\pi/5 \end{pmatrix}$$
Matrix number 5. Double rotation $5^1_{xy}5^2_{zt}$.

$$\begin{pmatrix} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \sin 4\pi/5 & \cos 4\pi/5 \end{pmatrix}$$
Matrix number 5. Rotation reflection $m_x 4^1_{zt}$.

number 5. (6) Rotation reflection or rotation inversion: $m_x 4_{zt}^1$ (Fig. 8), with matrix number 6.

In §§ III and IV, we shall study the geometry of the cells of all the crystal systems of \mathbb{E}^4 , but before



Fig. 5. Rotation in the plane xy around the plane zt: 3_{xy}^1 .



Fig. 6. Reflection on the hyperplane yzt: m_x .

that some simple examples of cells and polytopes are described (§ I) and a general formula which gives the order of the PSG of a polytope is proved (§ II). Finally, right hyperprisms and hyperpyramids in \mathbb{E}^4 are described in § V.

I. Some examples of crystal cells and polytopes or molecules in \mathbb{E}^4

1. Crystal cells

(a) Right hyperprism based on parallelepiped: family II (Fig. 9). The notation of its holohedry is $\overline{1} \perp m$ (Weigel, Phan & Veysseyre, 1987) and the order of this PSG is 4. This order can be immediately calculated by computing the product 2×2 where the first term represents the order of the PSG of the parallelepiped in \mathbb{E}^3 and the second one corresponds to the right hyperprism (see § II).



Fig. 7. Double rotation: $5_{xy}^1 5_{zt}^2$.



Fig. 8. Rotation reflection: $m_x 4_{zt}^1$.



Fig. 9. Right hyperprism based on parallelepiped.

(b) Orthogonal square hexagon: family XV (Fig. 10). Let (x, y, z, t) be four vectors of \mathbb{E}^4 such that x and y are perpendicular and of equal length a; z and t are of equal length b; the angle is $2\pi/3$ and the plane xy is orthogonal to the plane zt. The whole polytope is generated by translating the regular hexagon (zt) along the two sides and one diagonal of the square (xy). We count 24 vertices. The notation of the holohedry of this family is m, m, $4 \perp 6$, m, m (Weigel et al., 1987). The order of the PSG of this polytope is equal to 96, *i.e.* 8×12 where 8 is the order of the PSG of the square and 12 that of the hexagon in \mathbb{E}^2 (see § II), yet the cell or parallelotope built on (x, y, z, t) is three times smaller. The cell is drawn with dotted lines in Fig. 10.

2. Polytopes or molecules

(a) Simplex: regular pentatope or molecule, $\Omega \Pi_5$ (Fig. 11). A simplex is the generalization of a triangle. Any (n+1) points which do not lie in an (n-1)dimensional space are the vertices of an *n*dimensional simplex (Coxeter, 1973). A pentatope is the four-dimensional simplex and a regular pentatope has all edges equal, all faces equal and so on. The notation of the PSG of the regular pentatope is $(\bar{4}, 3, m)55$. Its order is 120 = 5! (Weigel, Veysseyre & Charon, 1980).

(b) Right hyperpyramid based on cube, $\Omega \Pi_8$ (Fig. 12). Let Ω be the vertex of the right hyperpyramid and O the centre of the cube; the vector $\overrightarrow{O\Omega}$ is orthogonal to the space \mathbb{E}^3 containing the cube. The notation of the PSG is 4/m, $\overline{3}$, 2/m, and its order is 48, the same as the order of the PSG of the cube in \mathbb{E}^3 .

II. Order of the point symmetry group of a convex polytope

The group of all the isometries of a polytope leaves at least one point invariant - the isobarycentre (centre



Fig. 10. Orthogonal square hexagon.



Fig. 11. Molecule $\Omega\Pi_5$.

of gravity) of the vertices of the polytope. Other points may also be left invariant, as the axis of a right hyperprism, for instance. We recall that an isometry is a one-to-one mapping which preserves lengths or distances. The isobarycentre Ω and *n* vertices a_1, \ldots, a_n define the polytope perfectly if $(\Omega a_1, \ldots, a_n)$ is a basis R of \mathbb{E}^n . We show the following result: The order of the PSG of a polytope is equal to the number of distinct transforms of the basis R by all the isometries of this PSG and this number does not depend on the choice of the basis.

Two transforms of a basis are said to be distinct or different if they differ by one point at least.

Proof. It is easy to show that: the transform of a basis is a basis (indeed, because an isometry is a one-to-one mapping, the image of \mathbb{E}^n cannot be a space of dimension p < n); the transform of a basis R by every isometry except the identity is a basis distinct from R because an isometry of \mathbb{E}^n cannot have (n+1) invariant points if it is not the identity; and two different isometries do not give the same image of R.

We shall explain how to count these images; but first we give some definitions.

Two vertices a'_1 and a''_1 of the polytope are said to be 'equivalent' if an isometry leaving the polytope invariant is such that the transform of a'_1 is a''_1 ; therefore these points are equidistant from Ω . This relation is a relation of equivalence among the vertices, the equivalence classes being the different orbits. Let Na_1 be the number of vertices equivalent to a_1 , *i.e.* the number of points located at the same distance from Ω as a_1 .

In the same way, two vertices a'_2 and a''_2 are equivalent when the vertex a_1 is fixed, if there exists an isometry leaving the polytope and the point a_1 invariant and permuting a'_2 and a''_2 . We denote by $Na_2(a_1)$ the number of vertices equivalent to a_2 when a_1 is fixed, *i.e.* the number of vertices equivalent to a_2 located at the same distance from a_1 as a_2 ; they satisfy the relations (where d means 'distance')

$$d(\Omega a_2) = d(\Omega a'_2) = d(\Omega a''_2) = \dots$$

$$d(a_1 a_2) = d(a_1 a'_2) = d(a_1 a''_2) = \dots$$

The number $Na_2(a_1)$ does not depend on the choice of a_1 among the points equivalent to a_1 .

Then we define $Na_3(a_1a_2)$, $Na_4(a_1a_2a_3)$ and so on. The number of transforms of the basis R and consequently the order of the PSG of the polytope is



Fig. 12. Right hyperpyramid based on a cube.

given by the formula

$$N = Na_1 \times Na_2(a_1) \times Na_3(a_1a_2) \times \ldots$$
$$\times Na_n(a_1 \ldots a_{n-1}).$$

Indeed, there are Na_1 choices for the first vertex a_1 , then $Na_2(a_1)$ choices for a_2 when a_1 is chosen, then $Na_3(a_1a_2)$ choices for a_3 when a_1 , a_2 are chosen.

In order to illustrate this method, we now give some examples.

First, we choose a simple example of a polygon: the square (Fig. 13). The centre Ω is an invariant point. A possible basis tied to the square is $(\Omega a_1 a_2)$.

$$Na_1 = 4$$
: all the vertices are equivalent.

 $Na_2(a_1) = 2$: when a_1 is chosen, the vertices a_2 and a_4 are equivalent.

Hence $N = 4 \times 2 = 8$.

Secondly we choose as an example of a polyhedron of E' the regular tetrahedron (Fig. 14). Only the centre Ω is an invariant point and all the four vertices are equivalent. A possible basis tied to this polyhedron is $(\Omega a_1 a_2 a_3)$.

> $Na_1 = 4$: we have already shown that all the vertices are equivalent.

 $Na_2(a_1) = 3$: the vertices a_2 , a_3 , a_4 are equidistant from a_1 .

 $Na_3(a_1a_2) = 2$: $a_3a_2a_4$ are equidistant from $a_1, a_3a_1a_4$ are equidistant from a_2 ;

therefore a_3 and a_4 are equidistant from a_1 on the one hand and from a_2 on the other hand.

So $N = 4 \times 3 \times 2 = 24 = 4!$

This result is general. The order of the PSG of the regular simplex of the *n*-dimensional space is equal to (n+1)! (Weigel *et al.*, 1980.)

The previous formula can be simplified when the polytope is an orthogonal product of two polytopes, as, for instance, the hypercube of \mathbb{E}^4 is the orthogonal product of two equal squares. More generally, let it be supposed that a polytope P_n is the orthogonal product of the polytopes P_i , P_j , the order of the PSG of P_n being g_n , that of P_i being g_i and that of P_j being g_j. Then

$$g_n = g_i \times g_j$$

if the decomposition is unique, and





Fig. 13. Square.

where $\binom{n}{i}$ is the number of ways to realize the decomposition.

Let us take the example of the hypercube of \mathbb{E}^4 . It may be considered as: (a) the orthogonal product of four equal segments, therefore $g_n = 2 \times 2 \times 2 \times 2 \times 4! =$ 384, where 2 is the order of the PSG of a segment and 4! the number of ways to consider this decomposition; or (b) the orthogonal product of two equal squares, therefore $g_n = 8 \times 8 \times 6$, where 8 is the order of the PSG of the square and

$$\binom{4}{2} = 6$$

is the number of ways to realize this decomposition; or (c) the orthogonal product of a cube and of a segment equal to the side of the cube, therefore $g_n =$ $48 \times 2 \times 4$ where 48 is the order of the PSG of the cube, 2 that of the segment and

$$\binom{4}{3} = \binom{4}{1} = 4$$

. .

is the number of ways to realize this decomposition.

This formula also gives the order of the PSG of a molecule, or rather of the polytope defined by the nuclei in their equilibrium positions, provided that we specify the notion of equivalent points: two points are said to be equivalent if they belong to the same chemical species, the following being unchanged.

As an example, we can consider the molecule SF_6 (Fig. 15). The invariant point is S, the centre of the octahedron. A possible basis is $(S, F_1F_2F_3)$.

 $NF_1 = 6$: the six nuclei are equivalent.

 $NF_2(F_1) = 4$: the nuclei $F_2F_3F_4F_5$ are equidistant from F_1 ;

the nuclei $F_3F_5F_1F_6$ are equidistant from F_2 . So F_3 and F_5 are equidistant from F_1

and F_2 .

So $N = 6 \times 4 \times 2 = 48$.



Fig. 14. Regular tetrahedron.



Fig. 15. Molecule SF₆.

III. Crystal families of \mathbb{E}^4 , their cell types and their holohedries

With the aim of giving a geometrical name to each primitive system of the 23 crystal families of \mathbb{E}^4 we have studied the quadratic form associated with the corresponding lattice. Each crystal lattice is described by four vectors (x, y, z, t) which define a lattice basis. The matrix of the quadratic form associated with these vectors is matrix number 7. This symmetric

$$\begin{pmatrix} \|x\|^2 & x.y & x.z & x.t \\ x.y & \|y\|^2 & y.z & y.t \\ x.z & y.z & \|z\|^2 & z.t \\ x.t & y.t & z.t & \|t\|^2 \end{pmatrix}$$

Matrix number 7. A general quadratic form. x. y denotes the scalar product of the two vectors x and y; $||x||^2 = x \cdot x$ and ||x|| is the norm of the vector x.

matrix is determined by four parameters of length and six parameters of angle; Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978) list it for each lattice.

From this quadratic form we have looked for a polytope describing the associated lattice and we have tried to respect conventional crystallographic axes. For instance, the matrix of the quadratic form of the system 13 is matrix number 8. We can easily see that

$$\begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & c & 0 \\ 0 & 0 & 0 & c \end{pmatrix}$$

Matrix number 8. Associated with system 13. $||x||^2 = a$, $||y||^2 = b$,
 $||z||^2 = ||t||^2 = c$.

the planes xy and zt are orthogonal and ||z|| = ||t||, z. t = 0, x. y = 0. So we denote it by

orthogonal rectangle (xy) square (zt).

Frequently the form of the matrix suggests the possibility of choosing two polygons in the two planes xy and zt or xz and yt. The two planes xy and zt are orthogonal or monoclinic or diclinic. The angles between these two planes depend on four parameters, the scalar products x . z, x . t, y . z and y . t. If these angles depend only on two parameters (one parameter) we say that the two planes, and furthermore the polygons located at these planes, are diclinic (monoclinic). For example, the matrix of the quadratic form of system 11 is matrix number 9. In each plane xy and zt we recognize a rhombus and the four angles between these two planes depend on two

$$\begin{pmatrix} a & a/2 & m & m-n \\ a/2 & a & n & m \\ m & n & c & c/2 \\ m-n & m & c/2 & c \end{pmatrix}$$

Matrix number 9. Associated with system 11. $x \cdot z = y \cdot t = m$;
 $y \cdot z = n$; $x \cdot t = m - n$.

parameters, m and n. We call this family

di diclinic hexagons (xy), (zt).

In two cases the cell is described by a hyperprism. We return to these in § V.

Three systems are of particular interest: system 32 has been described in an earlier publication (Veysseyre, Weigel, Phan & Effantin, 1984). It is the hypercubic system. Systems 27 and 31 are the only ones in which rotations 55 and 1010 appear. System 31 is a particular case of the system 27; we study it here. The matrix of the quadratic form of system 31 is number 10. The four vectors of the lattice basis

$$\begin{pmatrix} a & -a/4 & -a/4 & -a/4 \\ -a/4 & a & -a/4 & -a/4 \\ -a/4 & -a/4 & a & -a/4 \\ -a/4 & -a/4 & -a/4 & a \end{pmatrix}$$

Matrix number 10. Associated with system 31. $||x||^2 = ||y||^2 = ||z||^2 = ||z||^2 = a; \cos(x, y) = \cos(x, z) = \dots = \cos(z, t) = -\frac{1}{4}.$

have the same norm a and the angle between any two vectors has a cosine equal to $-\frac{1}{4}$. With this quadratic form we can associate a regular simplex of \mathbb{E}^4 or a regular pentatope, which is not a crystal cell.

Let us recall briefly some geometrical properties of regular simplexes of \mathbb{E}^2 , \mathbb{E}^3 and \mathbb{E}^4 . In \mathbb{E}^2 the regular simplex is the equilateral triangle (Fig. 16). If A_1 , A_2 , A_3 are the vertices and Ω_2 the barycentre, then

$$\overrightarrow{\Omega_2 A_1} + \overrightarrow{\Omega_2 A_2} + \overrightarrow{\Omega_2 A_3} = 0.$$

Therefore

$$\cos\left(\overline{\Omega_2 A_i}, \overline{\Omega_2 A_j}\right) = -\frac{1}{2} \quad \forall (i, j) \quad i \neq j.$$

In \mathbb{E}^3 the regular simplex is the regular tetrahedron (Fig. 17). If A_1, \ldots, A_4 are the vertices and Ω_3 the barycentre, then

$$\overline{\Omega_3 A_1} + \overline{\Omega_3 A_2} + \overline{\Omega_3 A_3} + \overline{\Omega_3 A_4} = 0,$$

$$\cos\left(\overline{\Omega_3 A_i}, \overline{\Omega_3 A_j}\right) = -\frac{1}{3} \quad \forall (i, j) \quad i \neq j.$$

In \mathbb{E}^4 the regular simplex is the regular pentatope (Fig. 18). If A_1, \ldots, A_5 are the vertices and Ω_4 the



Fig. 16. Equilateral triangle.



Fig. 17. Regular tetrahedron.

barycentre, then

$$\overrightarrow{\Omega_4 A_1} + \ldots + \overrightarrow{\Omega_4 A_5} = 0$$

 $\cos\left(\overline{\Omega_4 A_i}, \overline{\Omega_4 A_j}\right) = -\frac{1}{4} \quad \forall (i, j) \quad i \neq j \text{ as stated above.}$

Let us explain how a regular simplex can be inscribed in a particular parallelotope which defines a crystal system.

 \mathbb{E}^2 : Construction of an equilateral triangle in a rhombus. Let (x, y) be a lattice basis of the rhombus (Fig. 19):

$$||x|| = ||y||$$
 and $\cos(x, y) = -\frac{1}{2}$.

We denote by S_0 the origin of the cell and by A_1 , A_2 and A_3 the other vertices:

$$S_O A_1 = x$$
, $S_O A_2 = y$, $S_O A_3 = x + y$.

If Ω_1 and Ω_2 are the mid-points of S_0A_1 and S_0A_2 , then Ω_1 , Ω_2 and A_3 are the vertices of an equilateral triangle.

 \mathbb{E}^3 : Construction of a regular tetrahedron in a particular rhombohedron. Let (x, y, z) be a lattice basis of the particular rhombohedron $(\cos \alpha = -\frac{1}{3})$ (Fig. 20).

||x|| = ||y|| = ||z||

and

$$\cos(x, y) = \cos(x, z) = \cos(y, z) = -\frac{1}{3}$$

We denote by S_O the origin of the cell and by A_1 , A_2, \ldots, A_7 the other vertices:

$$S_OA_1 = x \quad S_OA_2 = y \quad S_OA_3 = z$$

$$S_OA_4 = x + y \quad S_OA_5 = x + z \quad S_OA_6 = y + z$$

$$S_OA_7 = x + y + z.$$

All the faces of this parallelotope are equal rhombs, so it is a rhombotope.

 S_0A_7 is the diagonal of smallest length:

$$\|S_O A_7\|^2 = \|x\|^2$$
$$\|A_1 A_6\|^2 = \|A_2 A_5\|^2 = \|A_3 A_4\|^2 = (11/3)\|x\|^2.$$



Fig. 18. Regular pentatope.



Fig. 19. Equilateral triangle inscribed in a rhombus.

Three faces have a common vertex in S_0 . If I_1 , I_2 and I_3 are the centres of these faces and Ω the barycentre of the parallelotope we can easily show the relations

$$\Omega I_3 = -\frac{1}{2}z \quad \Omega I_2 = -\frac{1}{2}y \quad \Omega I_1 = -\frac{1}{2}x.$$

So

$$\|\Omega I_1\| = \|\Omega I_2\| = \|\Omega I_3\|$$

and the angles between any two vectors have a cosine equal to $-\frac{1}{3}$. I_1 , I_2 and I_3 are three vertices of a regular tetrahedron, the fourth being A_7 , and

$$\Omega A_7 = \frac{1}{2}(x+y+z).$$

 \mathbb{E}^4 : Construction of a regular pentatope in a particular rhombotope such that $\cos \alpha = -\frac{1}{4}$. Let (x, y, z, t) be a lattice basis of the rhombotope (Fig. 21).

$$\|x\| = \|y\| = \|z\| = \|t\|$$

$$\cos (x, y) = \cos (x, z) = \cos (x, t) = \cos (y, z)$$

$$= \cos (y, t) = \cos (z, t) = -\frac{1}{4}.$$

As previously we denote by S_0 the origin of the cell and by A_1, A_2, \ldots, A_{15} the vertices:

$$S_O A_1 = x$$
 $S_O A_2 = y$... $S_O A_6 = x + z$...
 $S_O A_{15} = x + y + z + t.$



Fig. 20. Regular tetrahedron in a particular rhombohedron: $\cos \alpha = -\frac{1}{3}$.



Fig. 21. Regular pentatope in a particular rhombotope: $\cos \alpha = -\frac{1}{4}$.

Table 3. Geometric names and WPV notation for primitive Bravais cells of \mathbb{E}^4

This list of primitive systems of \mathbb{E}^4 includes: in the first column the family, indicated by a roman numeral, and the system, indicated by an arabic numeral; in the second column, the geometric name of each system; in the third column, the parameters required for the quadratic form associated with the lattice.

If (x, y, z, t) denotes the lattice basis, the following notation is used:

α:

$$a = ||x||^2 \quad b = ||y||^2 \quad c = ||z||^2 \quad d = ||t||^2$$

the angle between y and z $\quad \delta$: the angle between x and t

 β : the angle between x and z ϵ : the angle between y and t

 γ : the angle between x and y η : the angle between z and t;

the angles are chosen between 0 and π .

The fourth column gives the relations between parameters when they are required for the complete definition of the cell; the fifth column gives the order of the PSG of the holohedry of the system; the sixth column gives the holohedries in WPV notation (Weigel *et al.*, 1987); and the seventh column gives the PSG^+ in the same notation.

Family;		_	Additional		PSG of the	Rotation group
system	Bravais type of cells (primitive)	Parameters	relations	Order	holohedry	of the holohedry
1 01	Hexaclinic	a, b, c, d		2	14	
		α, β, γ, δ, ε, η				_
II 02	Right hyperprism based on	a, b, c, d		4	ī⊥m	$\overline{1}_4$
	parallelepiped (xyz)	α, β, γ				
111 03	Di orthogonal parallelograms (xy), (zt)	a, b, c, d		4	212	
		γ, η				
IV 04	Orthogonal parallelogram (xy)	a, b, c, d		8	2⊥2, m, m	212
	rectangle (zt)	. γ				
V 06	Di orthogonal rectangles (xy) , (zt)	a, b, c, d		16	$m, m, 2 \perp 2, m, m$	$(2, 2, 2) \otimes I_4$
VI 07	Orthogonal parallelogram (xy)	a, b, c		16	214, m, m	214
1/11 00	square (zi)	Ŷ		24	2.6	214
VII 09	Orthogonal parallelogram (xy)	a, b, c		24	$2 \pm 6, m, m$	210
VIII 10	$\frac{1}{2} \frac{1}{2} \frac{1}$	Ŷ	o R	4	11*	
VIII IU	Di dicimic squares (xy), (21)	и, с в 8	$\varepsilon = \rho$	4	44	
18 11	Di diclinic heragons (ru) (zt)	ρ, σ	a = n = b	6	66*	
	Di dicinine nexagons (xy), (21)	μ, c β δ	$cos \alpha = cos \beta - cos \delta$	U	00	
X 13	Orthogonal rectangle (xy) square (zt)	a b c	000 u 000 p 000 v	32	m. m. 214. m. m	214.2.2
XI 15	Orthogonal rectangle (xy) becagon (zt)	a, b, c		48	$m, m, 2 \perp 6, m, m$	$2\pm 6, 2, 2$
XII 16	Di monoclinic squares (xy) , (zt)	a. c	$\alpha = \delta = \pi/2$	8	44*, 2	, , –
		β	$\varepsilon = \beta$,	
XIII 17	Di monoclinic hexagons (xy) , (zt)	a, c	$\varepsilon = \beta$	12	2,66*,2	
	0	β	$\cos \alpha = \cos \delta = \frac{1}{2} \cos \beta$			
XIV 19	Di orthogonal squares (xy), (zt)	a, c		64	m, m, 4⊥4, m, m	(4⊥4) ∧ 2
XV 20	Orthogonal square (xy) hexagon (zt)	а, с		96	<i>m</i> , <i>m</i> , 4⊥6, <i>m</i> , <i>m</i>	2, 2, 4⊥6
XVI 23	Di orthogonal hexagons (xy), (zt)	а, с		144	m, m, <u>6</u> ⊥6, m, m	$(6 \perp 6) \land 2$
XVII 25	Right hyperprism based on cube (xyz)	a, d		96	$(4/m, 3, 2/m) \perp m$	$(4, 3, 2) \otimes 1_4$
XVIII 26	Di monoclinic isosquares (xz), (yt)	а	$\alpha = \eta = \gamma$	16	88 ^ 2	
		γ	$\delta = \pi - \gamma$			
XIX 27	Di particular monoclinic	а	$\alpha = \eta = \gamma$	20	1010 ^ 2	
	isorhombs (xy), (zt)	γ	$\beta = \delta = \varepsilon$			
	— • • • • • • • • • • • • • • • • • • •		$\cos\beta + \cos\gamma = -\frac{1}{2}$			
XX 28	Di monoclinic isohexagons (xz) , (yt)	a	$\gamma = \eta = \pi/2$	24	1212 ^ 2	
XXI 20		ð	$\alpha = \pi - \delta$	200	(1010 616 1010
XXI 30	DI OTINOGONAL ISONEXAGONS (Xy) , (zl)	a		288	$(m, m, 0 \pm 0, m, m)$ 1212 $(\overline{A}, 2, m)$ 1010	(2, 2) 1010
XXII 31	Particular rnombolope $\cos \alpha = -\frac{1}{4}$	a	$\alpha = \beta = \gamma = o = \varepsilon = \eta$	240	(4, 3, m) 1010	(2, 3) 1010 (4, 3, 3) 88
AAIII 32	пурегсионс	a		304	(4/m, 5, 2/m) 88	(4, 3, 2) 00

This parallelotope contains eight parallelepipeds and four of them have a vertex in S_0 . The centres I_1 , I_2 , I_3 and I_4 of these parallelepipeds are four vertices of a regular pentatope, the centre of which is Ω , the fifth vertex being A_{15} , and

$$\Omega A_{15} = \frac{1}{2}(x+y+z+t).$$

We can now summarize the construction of the pentatope: the five vertices of the regular pentatope inscribed in a particular rhombotope of \mathbb{E}^4 (cos $\alpha = -\frac{1}{4}$) are the centres of the four parallelepipeds having a vertex in S_O (the origin of the cell) and the point S opposite to S_O .

Table 3 lists the geometric names and the WPV notations (Weigel *et al.*, 1987) for primitive Bravais cells of \mathbb{E}^4 .

IV. Non-primitive crystal systems of E⁴, their cell types and holohedries

Ten systems are not primitive. For each non-primitive system, the matrix of the quadratic form is given by Brown *et al.* (1978). With respect to a well chosen basis this matrix is identical to the matrix of the primitive system of the same family.

Table 4. Geometric names and WPV notation for non-primitive Bravais cells of \mathbb{E}^4

This table is similar to Table 3 except on three points. The second column indicates the primitive type of cells. The fifth column indicates the Bravais type of cells which are centred. The sixth column gives the multiplicity order of the cell (number of centring points).

Family; system	Primitive cell (non-Bravais cell)	Parameters	Additional relations	Bravais type of cells (non-primitive)	N	Order	PSG of the holohedry	Rotation group of the holohedry
V 05	Di diclinic	а	$\alpha = \delta$	Di orthogonal				
	isorhombs (xy), (zt)	γ, β, δ	$\varepsilon = \beta$	rectangles (xy), (zt) KU centred	16	8	$(2,2,2)\otimes \overline{1}_4$	
VII 08	Oblique hyperprism	a, b	$\epsilon = \beta$	Orthogonal				
	based on rhombohedron (yzt)	γ, α	$\alpha = \delta = \gamma$	parallelogram (xy) hexagon (zt) R(2, 3, 4) centred	3	12	26, <i>m</i> , 1	26
X 12	Di monoclinic	а	$\varepsilon = \beta$	Orthogonal				
	isorhombs (xy), (zt)	γ, β	$\alpha = \delta = \gamma$	rectangle (xy) square (zt) KG centred	8	16	2⊥ 4 , 2, <i>m</i>	(2, 2, 2)⊗ī₄
XI 14	Right hyperprism	a, b		Orthogonal				
	based on	α		rectangle (xy)	3	24	26/m, 2, 2	26, 2, 2
	rhombohedron (yzt)			hexagon (zt) R(2, 3, 4) centred				
XIV 18	Di orthogonal	а		Di orthogonal				
	isorhombs (xt), (yz)	δ		squares (xy) , (zt) D(1, 4)(2, 3) centred	4	32	m, 44, m	2, 44, 2
XVI 21	Rectangle (xt)	a, d		Di orthogonal				
	hexagon (<i>yz</i>) very particular		*	hexagons (xy) , (zt) G(2, 3) centred	4	24	$(36,2,2)\otimes\overline{1}_4$	
XVI 22	Di monoclinic	а	$\delta = \alpha = \beta = \varepsilon =$	Di orthogonal				
	isohexagons (xz), (yt) γ	$\frac{2\pi/3}{\cos\eta + \cos\gamma = \frac{1}{2}}$	hexagons (xy), (zt) RR ₂ centred	3	72	$(m, 3 \perp 3, m) \otimes \overline{1}_4$	$[(3 \perp 3) \land 2] \otimes \overline{1}_4$
	Di isorhombs (xy)	а	$\beta = \delta = \alpha = \varepsilon$	Right hyperprism				
XVI 24	(zt) particular	γ	$=\eta=\gamma$	based on cube (yzt) KU centred	16	48	$(\overline{4}, 3, m) \otimes \overline{1}_4$	$(2,3)\otimes\overline{1}_4$
	Di isohexagons (xz)	а	$\cos \gamma = \cos \eta = \frac{1}{4}$	Di iso-				
XXI 29	(yt) particular		$\alpha = \delta = 2\pi/3$	hexagons (xy), (zt) orthogonal RR ₂ centred	3	144	$[\bar{4}(m, 3\perp 3, m)\bar{4}]\otimes \bar{1}_4$	$[(36,3\bot3)\land2]\otimes\overline{1}_4$
	Di isosquares (xz)	а	$\gamma = \delta = \alpha = \pi/3$	Hypercubic				
XXIII 33	(yt) particular		$\eta = 2\pi/3$	Z centred	2	1152	$(4/m, \bar{3}, 2/m)1212$	(4, 3, 2)1212

* $b = c = \frac{1}{4}(a+d)$; $\cos \beta = 2 \cos \gamma = \sqrt{a}/(\sqrt{a}+b)$; $\cos \varepsilon = 2 \cos \eta = \sqrt{b}/(\sqrt{a}+b)$; because $\cos \alpha = \frac{1}{2}, \delta = \pi/2$.

For example, the matrix of the quadratic form of system 18 in the basis (x, y, z, t) is matrix number 11. This primitive type of cell is called

di orthogonal isorhombs (xt), (yz).

$$\begin{pmatrix} a & 0 & 0 & m \\ 0 & a & m & 0 \\ 0 & m & a & 0 \\ m & 0 & 0 & a \end{pmatrix}$$

Matrix number 11. Associated with system 18. $||x||^2 = ||y||^2 = ||x||^2 = a; x.t = y.z = m.$

In a new basis (x', y', z', t') defined by

$$x' = x + t \quad z' = -y + z$$
$$y' = y + z \quad t' = -x + t$$

the matrix of the quadratic form is matrix number 12.

We recognize two orthogonal squares. So we denote it

di orthogonal squares (xy), (zt)

$$D(1, 4)(2, 3)$$
-centred.

$$\begin{pmatrix} a' & 0 & 0 & 0 \\ 0 & a' & 0 & 0 \\ 0 & 0 & c' & 0 \\ 0 & 0 & 0 & c' \end{pmatrix}$$

Matrix number 12. Associated with system 18. Basis (x', y', z', t'); x' = x + t; y' = y + z; z' = -y + z; t' = -x + t. $||x'||^2 = ||y'||^2 = a'$; $||z'||^2 = ||t'||^2 = c'$; a' = 2(a + m) and c' = 2(a - m).

The four nodes of the cell are defined by

(0, 0, 0, 0) $(\frac{1}{2}, 0, 0, \frac{1}{2})$ $(0, \frac{1}{2}, \frac{1}{2}, 0)$ $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$.

In Table 4 we give the geometry of the cells related to non-primitive systems. This table differs from Table 3 by three items: in column 2 we have indicated the primitive type of cells; in column 5 we have given the Bravais type of cells which are centred; and we have added a column 6, headed N, for the multiplicity order of the cell (number of centring points).

V. Right hyperprisms and hyperpyramids in \mathbb{E}^4

The right hyperprism generalizes the right prism of \mathbb{E}^3 . It is generated by a line passing through a polytope of \mathbb{E}^{n-1} , which is called the basis, the line being

Table 5. Right hyperpyramids and hyperprisms in \mathbb{E}^4

In this table we have listed right hyperprisms and hyperpyramids based on solids of \mathbb{E}^3 . These solids are given in the first column. We recall that tetragonal, hexagonal, pentagonal, octagonal mean right prisms of \mathbb{E}^3 based on square, regular hexagon, regular pentagon and regular octagon. For each hyperpyramid or each hyperprism we have given its PSG and its PSG⁺ when the PSG is a PSG⁻ (Weigel, Veysseyre, Phan, Effantin & Billiet, 1984). The first part of the table concerns the types of cells which are crystallographic in three-dimensional space; we give the order of each PSG (column 3 and column 6) and we indicate in columns 7 and 9 by an h if the PSG or PSG⁺ is a holohedry. In the second part of the table examples of point symmetry groups which are not crystallographic in three-dimensional space are given.

	Right hyperpyramids			Right hyperprisms				
Basis in E ³	PSG	0	PSG ⁺	PSG	0		 PSG⁺	
Triclinic cell	1	2	1	$\overline{1} \perp m$	4	h	Ī,	h
Monoclinic cell	2/ m	4	2	2⊥2, <i>m</i> , <i>m</i>	8	h	212	ĥ
Orthorhombic cell	2/m, 2/m, 2/m	8	2, 2, 2	$m, m, 2 \perp 2, m, m$	16	h	$(2, 2, \overline{2}) \otimes \overline{1}_{4}$	ĥ
Tetragonal	4/m, 2/m, 2/m	16	4, 2, 2	$m, m, 2 \perp 4, m, m$	32	h	2 4, 2, 2	
Rhombohedral cell	$\bar{3}, 2/m$	12	3.2	26/m, 2, 2	24	h	26 2 2	
Hexagonal	6/m, 2/m, 2/m	24	6.2.2	$m, m, 2 \perp 6, m, m$	48	ĥ	216.2.2	
Cube	$4/m, \bar{3}, 2/m$	48	4, 3, 2	$(4/m, \bar{3}, 2/m) \perp m$	96	h	$(4, 3, 2) \otimes \overline{1}$	
Tetrahedron	$\bar{4}, 3, m$	24	2,3	$(\bar{4}, 3, m) \perp m$	48		24.3.2	
Pyramid based on square	4, <i>m</i> , <i>m</i>	8	4	()-)			_ ,,,,_	
Pyramid based on equilateral triangle	3, m	6	3					
Pyramid based on regular hexagon	6, <i>m</i> , <i>m</i>	12	6					
Right prism based on equilateral triangle	6, m, 2	12	3.2	$m, m, 2 \perp 3, m$	24		213.2	
Molecule of allene*	4 , 2, <i>m</i>	8	2, 2, 2	· · · · · · · · · · · · · · · · · · ·			220,2	
Pentagonal	10, m, 2	20	5,2	$m, m, 2 \perp 5, m$	40		2+5.2	
Octagonal	8/m, 2/m, 2/m	32	8, 2, 2	$m, m, 2 \perp 8, m, m$	64		218.2.2	
Antiprism based on regular pentagon [†]	5, 2, m	10	5,2	, , , , ,				
Regular icosahedron or regular dodecahedron	$\bar{5}, \bar{3}, 2/m$	120	5, 3, 2	$(\overline{5},\overline{3},2/m) \perp m$	240		$(5,3,2)\otimes\overline{1}_4$	

* The molecule of allene (1, 2-propadiene) C_3H_4 (Fig. 22). The four hydrogen atoms are the vertices of a tetrahedron inscribed on a right prism based on a square; the three atoms of carbon are located at the axis of the prism.

[†] For instance the molecule of 'staggered ferrocene' $Fe(C_5H_5)_2$ (Fig. 23). The atoms of carbon are the vertices of two regular pentagons situated in two parallel planes symmetrical about the atom Fe. A rotation through angle $2\pi/5$ transforms one pentagon onto the other one.

orthogonal to the space \mathbb{E}^{n-1} (see, for instance, Fig. 9). In the same way the hyperpyramid generalizes the pyramid of \mathbb{E}^3 . It is generated by a line passing through a point (or vertex) S and a polytope of \mathbb{E}^{n-1} , called the basis. If the orthogonal projection of the vertex falls on the barycentre of the basis, the hyperpyramid is called a right hyperpyramid (see, for instance, Fig. 12).

Let us consider a crystal cell of \mathbb{E}^{n-1} and its PSG G_0 of order q. Thanks to the formula of § II we can state the following properties. (i) The PSG of the right hyperpyramid of \mathbb{E}^n built on this cell is of order q and has the same symbol as G_0 ; it is a polar PSG (Weigel & Veysseyre, 1982; Weigel *et al.*, 1987). (ii) The PSG of the right hyperprism of \mathbb{E}^n built on this cell is of order 2q.

Two examples illustrate these results. The first concerns the square: in \mathbb{E}^2 the order of the PSG, 4mm, of the square is 8; in \mathbb{E}^3 the order of the PSG, 4mm, of the right pyramid built on a square, is 8 (molecule BrF₅) and the order of the PSG, 4/m 2/m 2/m, of the right prism built on a square is 16 (holohedry of



Fig. 22. Molecule of allene (1, 2-propadiene).

the tetragonal system); in \mathbb{E}^4 the order of the PSG, 4, *m*, *m*, of the right hyperpyramid built on the right pyramid based on a square is 8.

The second example concerns the regular pentagon: in \mathbb{E}^2 the order of the PSG of the regular pentagon is 10; in \mathbb{E}^3 the order of the PSG of the right prism based on a regular pentagon (called pentagonal) is 20; and in \mathbb{E}^4 the order of the PSG of the right hyperpyramid based on pentagonal is 20 and that of the PSG of the right hyperprism based on pentagonal is 40.

In Table 5 we have listed right hyperprisms and hyperpyramids based on solids of \mathbb{E}^3 , their PSGs and possibly PSG⁺s. In the second part of the table we give examples of non-crystallographic point symmetry groups of right hyperpyramids and hyperprisms.



Fig. 23. Molecule of 'staggered ferrocene'.

Concluding remarks

All the results obtained for the regular simplexes of \mathbb{E}^4 can be generalized to the space of higher dimensions both from the geometrical point of view and also in the framework of the WPV notation.

In \mathbb{E}^3 the regular tetrahedron has four faces which are equilateral triangles, in \mathbb{E}^4 the regular pentatope is bounded by five regular tetrahedra, in \mathbb{E}^5 the regular hexatope is bounded by six regular pentatopes. More generally, the regular simplex of \mathbb{E}^n will be bounded by (n+1) regular simplexes of \mathbb{E}^{n-1} .

The Hermann-Mauguin notation of the PSG of the regular tetrahedron is $\overline{43}m$, the notation for the equilateral triangle in \mathbb{E}^2 being 3m. In the same way the WPV symbol of the PSG of the regular pentatope is 55 ($\overline{4}$, 3, m) and that for the PSG of the regular hexatope will be 66 [55 ($\overline{4}$, 3, m)], where 66 is the notation of a cyclic group containing PSOs 6_{xy}^1 , $6_{zt}^5m_u$.

The order of the PSG of the regular tetrahedron in \mathbb{E}^3 is 24, *i.e.* the product of 4 (order of the PSG 4) and 6 (order of the PSG 3m). The order of the PSG of the regular pentatope in \mathbb{E}^5 is 120, *i.e.* the product of 5 (order of the PSG 55) and 24 (order of the PSG $\overline{4}, 3, m$). The order of the PSG of the regular hexatope in \mathbb{E}^6 is 720, *i.e.* the product of 6 (order of the PSG 66) and 120. The generalization is obvious.

In § III we explained how we can inscribe a regular simplex in a particular rhombotope ($\cos \alpha = -1/n$) in the spaces \mathbb{E}^2 , \mathbb{E}^3 and \mathbb{E}^4 . The same construction is possible in \mathbb{E}^n . Let (x_1, \ldots, x_n) be a lattice basis such that

$$||x_i|| = ||x_i||$$
 and $\cos(x_i, x_j) = -1/n \quad \forall (i, j) \quad i \neq j.$

The 2^n vertices of the rhombotope cell are S_O (origin) and A_1, A_2, \ldots . This rhombotope P_n contains 2n hypervolumes or rhombotopes P_{n-1} belonging to subspaces of dimension (n-1), n rhombotopes have a vertex in S_O and n others have no vertex in S_O .

The regular simplex has the following vertices: the centres of the *n* rhombotopes P_{n-1} which do not have a vertex in S_O and the point S_O .

A second regular simplex, symmetrical with the previous one about the centre Ω of the cell, can also be inscribed in the rhombotope.

From the 2(n+1) vertices of these two regular simplexes, we can define a convex polytope inscribed in P_n . The order of its PSG is 2(n+1)!

For example, in \mathbb{E}^5 , we obtain the bi centrosymmetrical hexatope or isometric dodecatope. The order of its PSG is 1440; it is the holohedry of the crystal family XXXII (Plesken, 1981).

We can also compare the properties of some crystal of families of \mathbb{E}^3 , \mathbb{E}^4 and \mathbb{E}^5 . In \mathbb{E}^3 the convex polytope built on the 2×4 vertices of the regular tetrahedra is the cube $[2(n+1)=2^n$ only if n=3]. But in spaces of higher dimensions the particular rhombotope, $\cos \alpha = -1/n$ (or the two regular simplexes inscribed), and the hypercube are the holohedries of two different crystal families:

> in \mathbb{E}^4 families XXII and XXIII in \mathbb{E}^5 families XXXII and XXXI.

Besides, two different systems belong to the family XXIII, in \mathbb{E}^4 (Veysseyre *et al.*, 1984):

hypercubic system number 32 hypercubic Z-centred system number 33.

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