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Crystallography, Geometry and Physics in Higher Dimensions. IX. Counting and Geometry of the 32 Crystal Families of Five-Dimensional Space

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Abstract

This paper mainly consists in counting the crystal families of five-dimensional space and then in giving a geometrical name to each of them. All crystal cells of E^5 are obtained as orthogonal products of cells belonging to spaces of dimension less than five. Thanks to this geometrical approach, many general results can easily be found as WPV symbols of the holohedries (Weigel, Phan, Veysseyre symbols), the quadratic form associated with each lattice, the subgroups of these holohedries. The number of crystal families counted here is obviously the same as the number given by Plesken [*Match* (1981), No. 10, pp. 97-119] by a quite different method.

I. Introduction

To study the crystal families of five-dimensional space, various methods are possible.

One of these consists in writing all quadratic forms of the space E^5 systematically and in finding the point symmetry group (PSG) which leaves each of these quadratic forms invariant. Plesken (1981) proposed this method.

Another one consists in splitting the space E^5 into two orthogonal supplementary spaces such as $E^2 \oplus E^3$ or $E^1 \oplus E^4$ (Phan, 1989) or, more exactly, into two, three, four or five orthogonal subspaces. Then, a cell of E^5 will be considered as the orthogonal product of a cell of E^2 and of E^3, or as a right hyperprism based on a polytope of E^4.

This systematic approach, based on the geometry, seems to be well adapted to the study of the crystal lattices of E^5 and has enabled us to know their exact number and their most important properties. The names of the crystal families are easily accessible as well as the WPV symbols (Weigel, Phan, Veysseyre symbols) (Weigel, Phan & Veysseyre, 1987) of the holohedries of these families; from these it is possible to find some subgroups. Then, the quadratic form associated with each lattice can be quickly written.

We intend to illustrate this approach through an example. Let us consider the triclinic family of the space E^3 and the square family of the space E^2. The orthogonal product of the two cells, triclinic and square, gives a polytope which is the cell of a lattice of E^5; the crystal family so defined is called

orthogonal triclinic (XYZ) square (TU)

if the basic five-dimensional lattice has ($XYZTU$) as basic cell vectors. With respect to this basis, the matrix of the quadratic form associated with the lattice is matrix no. 1.

$$\left(\begin{array}{ccc|cc} a & d & e & 0 & 0 \\ d & b & f & 0 & 0 \\ e & f & c & 0 & 0 \\ \hline 0 & 0 & 0 & g & 0 \\ 0 & 0 & 0 & 0 & g \end{array}\right)$$

Matrix no. 1. Associated with the family orthogonal triclinic (XYZ) square (TU), $a=\|X\|^2$, $b=\|Y\|^2$, $c=\|Z\|^2$, $g=\|T\|^2=\|U\|^2$, $d=X.Y$, $e=X.Z$, $f=Y.Z$. The dot means scalar product.

The WPV symbol of the holohedry of this crystal family is obviously

$$\bar{1}\perp 4, m, m,$$

where $\bar{1}$ is the Hermann-Mauguin symbol of the holohedry of the triclinic family in E^3 and $4mm$ the symbol of the square family in E^2. Consequently, the order of this PSG equals

$$2\times 8=16.$$

For writing the name of a crystal family of E^5, we shall adopt a precise rule:

The first written polytope is the least symmetrical, *i.e.* the order of its PSG is the smallest.

Before studying all the crystal families of the space E^5, we shall recall some properties of crystal cells of spaces E^1, E^2, E^3 and of their orthogonal products.

II. Decompositions of the space E^5

All possible decompositions of the space E^5 into orthogonal supplementary subspaces are the

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following ones:

$$E^1 \oplus E^1 \oplus E^1 \oplus E^1 \oplus E^1$$
$$E^1 \oplus E^1 \oplus E^1 \oplus E^2$$
$$E^1 \oplus E^1 \oplus E^3$$
$$E^1 \oplus E^4$$
$$E^2 \oplus E^3$$

and obviously E^5.

First, we consider the direct sum: $E^1 \oplus E^1$ and the orthogonal product of two segments of each space. The crystal cell so obtained in the space E^2 is the rectangle or orthotope (Coxeter, 1973). Its well known Hermann-Mauguin symbol is $2mm$ but the best one should be $m \perp m$. Indeed, if we choose an orthogonal basis (xy), the two reflections m_x and m_y generate the PSG of the rectangular cell which has elements

$$m_x,\ m_y,\ 2_{xy},\ 1.$$

In the same way, to the direct sum $E^1 \oplus E^1 \oplus E^1 = E^3$ corresponds the orthorhombic cell of the space E^3, or orthotope. With respect to an orthogonal basis (xyz), the matrix of the quadratic form associated with this cell is matrix no. 2.

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

Matrix no. 2. Associated with the orthorhombic lattice, $a = \|X\|^2$, $b = \|Y\|^2$, $c = \|Z\|^2$.

The Hermann-Mauguin symbol of this cell is $2/m\ 2/m\ 2/m$ or $2/mmm$ for short.

As previously, the WPV symbol $m \perp m \perp m$ is better. The PSOs of this PSG are the three reflections m_x, m_y, m_z and all their products: 2_{xy}, 2_{xz}, 2_{yz}, $\bar{1}_{xyz}$, 1.

The generalization is obvious and the WPV symbol of the orthotope of the space E^n is

$$\underbrace{m \perp m \perp m \perp \ldots \perp m}_{n \text{ symbols } m.}$$

This recalls the construction of the orthotope cell: n vectors mutually perpendicular.

As a matter of fact, the system 6 of the crystal family V of the space E^4 called di orthogonal rectangles in a previous paper (Weigel *et al.*, 1987) must be called

orthotope of E^4

so that the WPV symbol of the holohedry is

$$m \perp m \perp m \perp m.$$

We shall use it in future instead of

$$m,\ m,\ 2 \perp 2,\ m,\ m.$$

Table 1. *The three irreducible crystal cells of* E^2

Name of the crystal cell	Hermann-Mauguin symbol of the holohedry	Order of the PSG
Parallelogram	2	2
Square	$4mm$	8
Hexagon	$6mm$	12

Table 2. *The two irreducible crystal cells of* E^3

Name of the crystal cell	Hermann-Mauguin symbol of the holohedry	Order of the PSG
Triclinic	$\bar{1}$	2
Cube	$4/m\,\bar{3}\,2/m$	48

Table 3. *The* 11 *irreducible geometrical cells of* E^4

Names of the crystal cell	WPV symbol of the holohedry	Order of the PSG
Hexaclinic	$\bar{1}_4$	2
Di diclinic squares	44^*	4
Di diclinic hexagons	66^*	6
Di monoclinic squares	$44^*, 2$	8
Di monoclinic hexagons	$2, 66^*, 2$	12
Di monoclinic isosquares	$88 \wedge 2$	16
Di monoclinic isohexagons	$1212 \wedge 2$	24
Decagonal	$1010 \wedge 2$	20
Di orthogonal isohexagons	$(m, m, 6 \perp 6, m, m)1212$	288
Icosahedral*	$(\bar{4}, 3, m)1010$	240
Hypercube	$(4/m\,\bar{3}\,2m)88$	384

* Particular rhombotope $\cos\alpha = -1/4$.

Indeed, this PSG has four rotations 2 and the symbol $m, m, 2 \perp 2, m, m$ seems to devote a peculiar role to two of them, which is not the case.

Now, we consider all irreducible crystal cells of the space E^2 (irreducible from a geometrical point of view). They are listed in Table 1.

A family is said to be irreducible if the n translation operators $x, y, z, t, u, \ldots$ corresponding to a basis of the n-dimensional space E^n belong to the same irreducible representation (IR) of the holohedry of this family. In the opposite case, the family is said to be reducible (Weigel & Veysseyre, 1990). For instance, the square family of E^2 is irreducible because (x, y) belong to the two-dimensional IR E of the character table of $4mm$ (C_{4v}) which is the holohedry of this family. The tetragonal family of E^3 is reducible because (x, y) belong to the two-dimensional IR E_u of $4/mmm$ (D_{4h}) and z to the one-dimensional IR A_{2u}.

Then, we consider the two irreducible crystal cells of the space E^3; they are listed in Table 2.

Lastly, we consider the crystal cells of the space E^4 which are not products of polygons or polyhedra of the spaces E^2 or E^3, namely the irreducible crystal cells of E^4; there are 11 among the 23 cells of the crystal families of E^4 which are listed in Table 3.

III. Names of the crystal families of the space E^5

(1) $E^5 = E^1 \oplus E^1 \oplus E^1 \oplus E^1 \oplus E^1$

Only one cell corresponds to this decomposition. It is the orthotope. It is defined by five parameters of length; the WPV symbol of its PSG is

$$m \perp m \perp m \perp m \perp m$$

as we have already explained and its order is $2^5 = 32$.

(2) $E^5 = E^1 \oplus E^1 \oplus E^1 \oplus E^2$

We obtain three different cells and, therefore, three crystal families called respectively

orthogonal parallelogram orthorhombic
orthogonal orthorhombic square
orthogonal orthorhombic hexagon.

We respected the rule previously given, *i.e.* the first name is for the least-symmetrical polytope and we also kept the well known term of orthorhombic instead of orthotope.

(3) $E^5 = E^1 \oplus E^1 \oplus E^3$

We obtain two crystal families only which are

orthogonal triclinic rectangle (holohedry $\bar{1} \perp 2mm$ or $\bar{1} \perp m \perp m$)
orthogonal rectangle cube (holohedry $2mm \perp 4/m\ \bar{3}\ 2/m$ or $m \perp m \perp 4/m\ \bar{3}\ 2/m$).

(4) $E^5 = E^1 \oplus E^2 \oplus E^2$

All corresponding crystal cells are right hyperprism based on the rectangular product of two polygons listed in Table 1. So we find six crystal families which are

right hyperprism based on di orthogonal parallelograms
right hyperprism based on di orthogonal squares
right hyperprism based on di orthogonal hexagons
right hyperprism based on orthogonal parallelogram square
right hyperprism based on orthogonal parallelogram hexagon
right hyperprism based on orthogonal square hexagon.

(5) $E^5 = E^1 \oplus E^4$

This decomposition leads to 11 right hyperprisms based on the polytopes of E^4 given in Table 3. Let us mention some of them:

right hyperprism based on hexaclinic
right hyperprism based on di monoclinic iso-squares

and so on.

All these crystal families are listed in the general Table 4.

(6) $E^5 = E^2 \oplus E^3$

Six crystal families correspond to the orthogonal product of one of the three cells of Table 1 and one of the two cells of Table 2.

orthogonal triclinic parallelogram
orthogonal triclinic square
orthogonal triclinic hexagon
orthogonal parallelogram cube
orthogonal square cube
orthogonal hexagon cube.

(7) The three types of geometrically irreducible cells

(i) *Decaclinic cell.* It depends on 15 parameters: five parameters of length and ten parameters of angle; hence the name of the corresponding crystal family.

The WPV symbol of the holohedry is $\bar{1}$ (Weigel, Veysseyre & Phan, 1990). Indeed, its two elements are 1 (identity) and $\bar{1}_5 = \bar{1}$ or inversion.

(ii) *Hypercubic cell.* It depends on one parameter of length only. The hypercubic lattice is generated by five mutually orthogonal vectors of the same length. The matrix of the associated quadratic form is the diagonal matrix no. 3, with respect to the basis lattice.

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

Matrix no. 3. Associated with the hypercubic lattice, $a = \|X\|^2 = \|Y\|^2 = \|Z\|^2 = \|T\|^2 = \|U\|^2$.

It is a peculiar case of the orthotope cell. In a previous paper (Veysseyre, Weigel, Phan & Effantin, 1984), we described the hypercube of the space E^4. In a similar way, we can describe the hypercube of the space E^5 and all its elements of symmetry. It has $2^5 = 32$ vertices for instance and it is bounded by 5×2 = hypercubes which belong to the five subspaces of dimension 4 defined by four vectors chosen among the five vectors of the lattice.

The Hermann-Mauguin symbol of the PSG of the cube is $4/m\ \bar{3}\ 2/m$.

The WPV symbol of the PSG of the hypercube of E^4 (Weigel *et al.*, 1987) is

$$(4/m\ \bar{3}\ 2/m)88,$$

where 88 is the symbol of a cyclic group generated by the double rotation $8^1 8^3$. Then, the WPV symbol of the hypercube of E^5 is

$$[(4/m\ \bar{3}\ 2/m)88]\overline{\overline{55}},$$

where $\overline{\overline{55}}$ is the symbol of a cyclic group generated by the double rotation-inversion $\overline{55}$ (Weigel & Veysseyre, 1990; Weigel, Veysseyre & Phan, 1990).

The order of the PSG of the hypercube of E^5 is equal to $2^5 5! = 3840$ (Veysseyre, 1987).

Its elements, determined by computer, are listed in Table 5. There are 1920 PSO$^+$s, *i.e.* 1920 rotations or double rotations and 1920 PSO$^-$s or improper rotations (inversion-rotations or reflection-rotations). The notations used here are explained in a previous paper (Weigel, Veysseyre & Phan, 1990).

Table 4. *Names of the crystal families of the space* E^5

The first column gives the number of the family in the Plesken classification; the second column gives the number of length parameters and the third the number of angle parameters. For each family, the fourth column gives its geometrical name, the fifth gives the WPV symbol of the corresponding holohedry and the order of this PSG is indicated in the last column.

Family	Parameters		Name	WPV symbol of the holohedry	Order of the PSG
I	5	10	Decaclinic	$\bar{\bar{1}}$	2
II	5	6	Right hyperprism based on hexaclinic (*YZTU*)	$m\perp\bar{1}_4$	$2\times2=4$
III	5	4	Orthogonal triclinic (*XYZ*) parallelogram (*TU*)	$\bar{1}\perp2$	$2\times2=4$
IV	5	3	Orthogonal triclinic (*XYZ*) rectangle (*TU*)	$\bar{1}\perp2, m, m$	$2\times4=8$
V	5	2	Right hyperprism based on di orthogonal parallelograms (*YZ*)(*TU*)	$m\perp2\perp2$	$2\times2\times2=8$
VI	4	3	Orthogonal triclinic (*XYZ*) square (*TU*)	$\bar{1}\perp4, m, m$	$2\times8=16$
VII	4	3	Orthogonal triclinic (*XYZ*) hexagon (*TU*)	$\bar{1}\perp6, m, m$	$2\times12=24$
VIII	5	1	Orthogonal parallelogram (*XY*) orthorhombic (*ZTU*)	$2\perp\frac{2}{m}, \frac{2}{m}, \frac{2}{m}$	$2\times8=16$
IX	5	0	Orthotope	$m\perp m\perp m\perp m\perp m$	$2^5=32$
X	4	1	Right hyperprism based on orthogonal parallelogram (*YZ*) square (*TU*)	$m\perp2\perp4, m, m$	$2\times2\times8=32$
XI	4	1	Right hyperprism based on orthogonal parallelogram (*YZ*) hexagon (*TU*)	$m\perp2\perp6, m, m$	$2\times2\times12=48$
XII	3	2	Right hyperprism based on di diclinic squares (*YZ*)(*TU*)	$m\perp44^*$	$2\times4=8$
XIII	3	2	Right hyperprism based on di diclinic hexagons (*YZ*)(*TU*)	$m\perp66^*$	$2\times6=12$
XIV	4	0	Orthogonal orthorhombic (*XYZ*) square (*TU*)	$\frac{2}{m}, \frac{2}{m}, \frac{2}{m}\perp4, m, m$	$8\times8=64$
XV	4	0	Orthogonal orthorhombic (*XYZ*) hexagon (*TU*)	$\frac{2}{m}, \frac{2}{m}, \frac{2}{m}\perp6, m, m$	$8\times12=96$
XVI	3	1	Right hyperprism based on di monoclinic squares (*YZ*)(*TU*)	$m\perp44^*, 2$	$2\times8=16$
XVII	3	1	Right hyperprism based on di monoclinic hexagons (*YZ*)(*TU*)	$m\perp2, 66^*, 2$	$2\times12=24$
XVIII	3	1	Orthogonal parallelogram (*XY*) cube (*ZTU*)	$2\perp\frac{4}{m}, \bar{3}, \frac{2}{m}$	$2\times48=96$
XIX	3	0	Right hyperprism based on di orthogonal squares (*YZ*)(*TU*)	$m\perp m, m, 4\perp4, m, m$	$2\times8\times8=128$
XX	3	0	Right hyperprism based on orthogonal square (*YZ*) hexagon (*TU*)	$m\perp m, m, 4\perp6, m, m$	$2\times8\times12=192$
XXI	3	0	Right hyperprism based on di orthogonal hexagons (*YZ*)(*TU*)	$m\perp m, m, 6\perp6, m, m$	$2\times12\times12=288$
XXII	3	0	Orthogonal rectangle (*XY*) cube (*ZTU*)	$m, m, 2\perp\frac{4}{m}, \bar{3}, \frac{2}{m}$	$4\times48=192$
XXIII	2	1	Right hyperprism based on di monoclinic iso squares (*YZ*)(*TU*)	$m\perp(88\wedge2)$	$2\times16=32$
XXIV	2	1	Right hyperprism based on di monoclinic iso hexagons (*YZ*)(*TU*)	$m\perp(1212\wedge2)$	$2\times24=48$
XXV	2	1	Right hyperprism based on 'decagonal' (*YZTU*)*	$m\perp(1010\wedge2)$	$2\times20=40$
XXVI	2	0	Orthogonal square (*XY*) cube (*ZTU*)	$m, m, 4\perp\frac{4}{m}, \bar{3}, \frac{2}{m}$	$8\times48=384$
XXVII	2	0	Orthogonal hexagon (*XY*) cube (*ZTU*)	$m, m, 6\perp\frac{4}{m}, \bar{3}, \frac{2}{m}$	$12\times48=576$
XXVIII	2	0	Right hyperprism based on hypercube (*YZTU*)	$m\perp\left(\frac{4}{m}, \bar{3}, \frac{2}{m}\right)88$	$2\times384=768$
XXIX	2	0	Right hyperprism based on di orthogonal iso hexagons (*YZ*)(*TU*)	$m\perp[(m, m, 6\perp6, m, m)1212]$	$2\times288=576$
XXX	2	0	Right hyperprism based on icosahedral (*YZTU*)	$m\perp(\bar{4}, 3, m)1010$	$2\times240=480$
XXXI	1	0	Hypercube	$\left[\left(\frac{4}{m}, \bar{3}, \frac{2}{m}\right)88\right]\overline{\overline{55}}$	$2^5\times5!=3840$
XXXII	1	0	Particular rhombotope $\cos\alpha=-1/5$	$[(\bar{4}, 3, m)1010]\overline{\overline{36}}$	$6!\times2=1440$

* Or right hyperprism based on the particular rhombotope $\cos\alpha=-1/4$.

(iii) *The particular rhombotope* $\cos\alpha=-1/5$. Some properties of this polytope were given by Veysseyre (1987).

A rhombus is a parallelogram in which all edges are equal. A rhombohedron is a parallelepiped in which all faces are equal rhombuses; and in the space E^n a rhombotope is a peculiar parallelotope in which all faces are equal rhombuses. In the space E^5, let us consider the lattice defined by five vectors $\mathbf{e}_i$ ($i=1, 2, 3, 4, 5$) of the same length and such that

$$\cos(\mathbf{e}_i, \mathbf{e}_j)=-1/5\forall i\ \forall j\neq i.$$

The parallelotope built on these vectors is a rhombotope, all its faces being equal rhombuses. In addition, as the cosine of the obtuse angle has value $-1/5$, it is possible to inscribe in it a regular simplex or hexatope (Phan, Veysseyre & Weigel, 1988; Veysseyre, 1987). The matrix of the quadratic form associated with this lattice is matrix no. 4 with respect to the basis vectors $\mathbf{e}_i$.

$$\begin{pmatrix} a & -a/5 & -a/5 & -a/5 & -a/5 \\ -a/5 & a & -a/5 & -a/5 & -a/5 \\ -a/5 & -a/5 & a & -a/5 & -a/5 \\ -a/5 & -a/5 & -a/5 & a & -a/5 \\ -a/5 & -a/5 & -a/5 & -a/5 & a \end{pmatrix}$$

Matrix no. 4. Associated with the particular rhombotope $\cos\alpha=-1/5$ $a=\|\mathbf{e}_i\|^2$, $-a/5=\mathbf{e}_i\cdot\mathbf{e}_j$.

We recall that a simplex is the generalization of a triangle. Any set of $n+1$ points which do not lie in

Table 5. *The* 3840 *PSOs of the hypercube of* E^5

The PSO^-s in the second column are the commutative products of the PSO^+s of the first column and of the total homothetic of ratio (-1): $\bar{1}_5 = \bar{\bar{1}}$. For instance,

$3 \times \bar{1}_5 = m26$

$5^15^3 \times \bar{1}_5 = m10^{-3}10^1$, which is the generator of the cyclic group $\overline{\overline{55}}$ (Weigel, Veysseyre & Phan, 1990).

The multiplication by $\bar{1}_5$ does not change the number of PSOs. So the number of PSO^+s equals the number of PSO^-s and this number is given in the third column.

Type of PSO^+s	Type of PSO^-s	Number
1	$\bar{1}_5$	1
2	$\bar{1}_3$	130
3	$m26$	80
4	$m24$	20
$\bar{1}_4$	m	25
23	$m6$	80
24	$m4$	420
26	$m3$	320
43	$m46$	160
44	$m44$	60
5^15^3	$m10^{-3}10^1$	384
8^18^3	$m8^58^{-1}$	240

an $(n-1)$-dimensional space are the vertices of an n-dimensional simplex (Coxeter, 1973). A regular simplex has all its edges equal, all its faces equal and so on. An equilateral triangle is bounded by three segments, a regular tetrahedron by four equilateral triangles, a regular pentatope by five regular tetrahedra, a regular hexatope by six regular pentatopes. Thanks to these geometrical remarks, we can write the WPV symbol of the holohedry of the crystal family defined by this particular rhombotope. The order of the PSG of the simplex is $(n+1)!$

Indeed, the Hermann–Mauguin symbols of the PSG of the simplexes are the following ones:

m for the segment (in the space E^1)
$3m$ for the equilateral triangle (in the space E^2)
$\bar{4}3m$ for the regular tetrahedron (in the space E^3).

The WPV symbol of the regular pentatope is

$$(\bar{4}, 3, m)55$$

and the symbol of the regular hexatope is

$$[(\bar{4}, 3, m)55]\overline{\overline{36}},$$

where $\overline{\overline{36}}$ is the symbol of the cyclic group generated by the PSO $\overline{\overline{36}} = 63\bar{1}_5$ (Weigel, Veysseyre & Phan, 1990). Then, we deduce the WPV symbol of this crystal family:

$$[(\bar{4}, 3, m)1010]\overline{\overline{36}}.$$

The cell of the lattice includes two centrosymmetric regular simplexes and the order of its PSG is

$$6! \times 2 = 1440$$

(6! being the order of the regular simplex built in the space E^5) and this property explains the symbol $[(\bar{4}, 3, m)1010]\overline{\overline{36}}$.

IV. Subgroups of some crystal families

Let us consider one example: the crystal family IV of Table 4:

orthogonal triclinic (XYZ) rectangle (TU), where $(XYZTU)$ is the lattice basis.

The WPV symbol of the holohedry is

$$\bar{1}\perp 2, m, m.$$

$\bar{1}$ is a subgroup (generator $\bar{1}_{xyz}$); $2, m, m$ is another subgroup generated by the PSOs m_t and m_u. It has two subgroups: 2 (generator 2_{tu}) and m (generator m_t for instance).

The products of two (or more) PSOs generate other subgroups:

$\bar{1}\perp m$ (generators $\bar{1}_{xyz}$ and m_u) of order 4
$\bar{1}_4$ (generator $\bar{1}_{xyz}m_t = \bar{1}_{xyzt}$) of order 2
$\bar{\bar{1}}$ (generator $\bar{1}_{xyz}m_tm_u = \bar{1}_{xyztu}$) of order 2
$\bar{1}_4\perp m$ (generators $\bar{1}_{xyzt}$ and m_u) of order 4
$\bar{1}\perp 2$ (generators $\bar{1}_{xyz}$ and 2_{tu}) of order 4
$2, \bar{1}_4, \bar{1}_4$ (generators $\bar{1}_{xyzt}$ and 2_{tu}) of order 4.

Therefore, this holohedry has ten proper subgroups; seven of them have been encountered previously:

$\bar{\bar{1}}$ in the family I whose holohedry is $\bar{\bar{1}}$;
$m, \bar{1}_4$ and $m\perp\bar{1}_4$ in the family II whose holohedry is $m\perp\bar{1}_4$;
$\bar{1}$, 2 and $\bar{1}\perp 2$ in the family III whose holohedry is $\bar{1}\perp 2$.

Thus, there remain three subgroups, *i.e.* three crystallographic GPSs which are $2, m, m$; $\bar{1}\perp m$; $2, \bar{1}_4, \bar{1}_4$ and finally the holohedry $\bar{1}\perp 2mm$ for the crystal family IV orthogonal triclinic rectangle.

The WPV symbols that we chose for all the holohedries enables us to determine all the subgroups, *i.e.* the crystallographic PSGs, in a very easy manner. But when the order of this PSG becomes higher, a computer is required.

Concluding remarks

All the crystal families of the space E^5 have been counted through an original method. The names of these families are connected to the geometry as well as to the WPV symbols of their holohedries. They are listed in the general Table 4. For this enumeration, we have adopted the order and the numbers given by Plesken (1981). The crystal families are classified according to the number of parameters necessary for describing each of them.

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Frequency-Restrained Structure-Factor Refinement. II. Comparison of Methods

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Abstract

The frequency distribution of electron-density-function values encountered in a protein crystal has a characteristic shape and may be predicted for a protein with unknown spatial structure. It is shown that various methods of refinement of structure-factor phases (frequency-restrained refinement, histogram matching, density modification) may be regarded as various approaches to the same problem of obtaining the electron-density distribution which agrees with the X-ray experimental data and has a prescribed histogram. Test computations illustrate the relative efficiency of the methods analyzed.

0. Introduction

The method of isomorphous replacement, which is used to solve the phase problem in protein crystallography, fails sometimes to give the desired quality of electron-density-distribution maps. Additional ways of improving maps are needed. One of them is using, or rather trying to use, the knowledge of the mathematical properties of the electron-density-distribution function, in addition to the data from X-ray experiments. In previous papers (Lunin, 1986, 1988; Lunin, Urzhumtsev & Skovoroda, 1990; Lunin & Skovoroda, 1991), we showed that a valuable source of information on a protein can be a histogram corresponding to a finite-resolution image of its distribution function. Analogous approaches were suggested by Luzzati, Mariani & Delacroix (1988), Harrison (1988) and Zhang & Main (1990).

Let us recall the main point. Let $\rho(\mathbf{r})$ be a function defined for points $\mathbf{r}$ of a unit cell V and

$$F(\mathbf{s}) \exp[i\varphi(\mathbf{s})] = \int_V \rho(\mathbf{r}) \exp[2\pi i(\mathbf{s}, \mathbf{r})]\, \mathrm{d}V_r$$

be its structure factors.

By the image of $\rho(\mathbf{r})$ at a resolution d we mean the function

$$\rho_d(\mathbf{r}) = (1/|V|) \sum_{|\mathbf{s}| \le 1/d} F(\mathbf{s}) \exp[i\varphi(\mathbf{s})] \times \exp[-2\pi i(\mathbf{s}, \mathbf{r})]. \quad (1)$$

We define the cumulative function for the image $\rho_d(\mathbf{r})$,

$$N(t) = (1/|V|) \operatorname{mes}\{\mathbf{r}: \rho_d(\mathbf{r}) \le t\},$$

and its density,

$$\nu(t) = \frac{\mathrm{d}}{\mathrm{d}t} N(t) = \frac{1}{|V|} \frac{\mathrm{d}}{\mathrm{d}t} \operatorname{mes}\{\mathbf{r}: \rho_d(\mathbf{r}) \le t\}. \quad (2)$$

Here $|V|$ is the total volume of the unit cell and $\operatorname{mes}\{\mathbf{r}: A\}$ is the volume of the part of the cell occupied by points $\mathbf{r}$ satisfying condition A. The value $\nu(t)\Delta t$ is the probability that the value $\rho_d(\mathbf{r})$ will belong to the interval $(t, t+\Delta t)$ for a random choice of point $\mathbf{r}$ in the cell. It was shown earlier (Podjarny & Yonath, 1977; Lunin, 1986; Zhang & Main, 1990) that, if $\rho(\mathbf{r})$ is the function of electron-density distribution in a protein, the graph of the function $\nu(t)$ has a characteristic shape. An approach to calculating the function $\nu(t)$ for proteins with unknown space structure has been suggested (Lunin & Skovoroda, 1991). [As before, it is called here the histogram of the image $\rho_d(\mathbf{r})$.] We denote this *a priori* defined histogram as $\nu^a(t)$ and refer to it as a 'standard' (for a given object and a given resolution).

In practice, the values of phases $\varphi(\mathbf{s})$ and of moduli $F(\mathbf{s})$ used to calculate the image (1) often contain errors. Moreover, part of the phases, and of moduli as well, may be dropped out of calculation. It results in a distorted image $\rho_d(\mathbf{r})$.

In this paper we shall show how the *a priori* knowledge of the histogram $\nu^a(t)$ [or, which is equivalent, of the cumulative function $N^a(t)$] can be used for a more exact determination of the phases and moduli

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