

velocities of the pure longitudinal modes along a and b are 4.9 and 5.25 km s⁻¹, respectively.

The group velocities compiled in Tables 1 and 2 give information only for nonsymmetry propagation directions. For both of the listed phonon groups, which belong to different wave vectors, a striking variation of c_g was obtained. Whereas the first group (c_g^{high}) shows an expected angular dependence with the tendency to reach low group velocities around the [110] direction, the second one (c_g^{low}), obtained from edges around 0k0 reflections, presents a surprising high change of c_g for the small angular changes. The behaviour is not understood so far and one may speculate about the effect of phonon focusing in elastically anisotropic crystals in which thermal-phonon group velocities tend to aggregate more around some directions than others. It depends on the curvature of the inverse phase velocity surface and is a common feature in many crystals (Every, 1980). On the other hand, the effect could originate from a violation of the validity condition of the theory owing to greater q values. This conjecture is supported by the calculated wave vectors of the second group, which are by far higher than those of the first group.

Along the b axis, scans were measured at RT as well as some degrees above and below the ferroelectric PT. Except for a slightly reduced intensity in the TDS

patterns of the scans at low temperatures, no characteristic changes (*e.g.* owing to the piezoelectricity in the polar phase) were found within the limits of the given experimental resolution.

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Crystallography, Geometry and Physics in Higher Dimensions. XV. Reducible Crystal Families of Six-Dimensional Space

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Abstract

This paper and the following one of the series deal with the counting and the construction of the crystal families of Euclidean space E^6 ; this paper deals with the geometrically Z -reducible (gZ-red.) crystal families and paper XVI deals with the geometrically Z -irreducible (gZ-irr.) crystal families. The method explained in previous papers for the construction of crystal families of Euclidean space E^5 has been adopted; for the reader's convenience, the main lines of this method are recalled. The method depends on two basic elements, namely, all the splittings of space E^6 into two-by-two orthogonal subspaces and the list of the gZ-irr. crystal families of one- to five-dimensional spaces. Besides the counting of the crystal families, this new geometrical method gives

the names of these families and both the symbols and orders of their holohedries. The name of the crystal family directly introduces its 'conventional'-cell geometrical description and the various parameters (lengths and angles) defining the cell.

Introduction

In two previous papers (Veysseyre, Weigel & Phan, 1993; Weigel & Veysseyre, 1993), we introduced a general method for constructing the crystal families of Euclidean space E^n and emphasized the results for the crystal families of Euclidean spaces E^1 to E^5 . This method is based on: (1) the consideration of every possible partition of space E^n into subspaces E^p , two-by-

Table 1. Geometrically Z-irreducible crystal families of spaces $E^1 \dots E^5$

The second, third, fourth, fifth and sixth columns give the gZ-irr. crystal families of types 1, 2, 3, 4 and 5, respectively, and their symbols and the names of the families belonging to the different considered spaces. The last column gives the numbers of gZ-irr. crystal families belonging to each different considered space.

	Type 1 ($\overline{1, 1, \dots, 1}$)	Type 2 (2, 3, ..., n)	Type 3 ($\overline{2, 2, 2, 2, 3, 3}$)	Type 4 ($\overline{2, 2', 2, 2, 2', 3, 3'}$)	Type 5 ($2', 3', 4', \dots, n'$)	
E^1	Segment					1
E^2	Oblic	Square Hexagon				3
E^3	Triclinic	Cubic				2
E^4	Hexaclinic	Di iso hexagon Rhombotopic (-1/4) Hypercubic 4	Monoclinic di square Monoclinic di hexagon	Diclinic di square Diclinic di hexagon	Monoclinic di iso hexagon Decadic Monoclinic di iso square	11
E^5	Decaclinic	Rhombotopic (-1/5) Hypercubic 5				3

two orthogonal, of dimension p less than n ; (2) the existence of the gZ-irr. crystal families of space E^p for all the values of integer p less than or equal to n . The definition and the properties of the gZ-irr. crystal families and of the gZ-red. crystal families are given by Weigel & Veysseyre (1993) and recalled in the Appendix of Weigel & Veysseyre (1994).

To make this paper easier to read, the gZ-irr. crystal families of one- to five-dimensional spaces are listed in Table 1, and an example of this construction for a gZ-red. crystal family of space E^4 follows.

The different partitions of number 4 are as follows:

$$4; \quad 3 + 1; \quad 2 + 2; \quad 2 + 1 + 1; \quad 1 + 1 + 1 + 1.$$

For instance, the partition $2 + 2$ of number 4 gives the splitting for space E^4

$$E^4 = E^2 \oplus E^2.$$

In space E^2 , three gZ-crystal families can be found:

- the oblic family with a parallelogram cell;
- the square family with a square cell;
- the hexagon family with a hexagon cell.

The rectangular product of two cells, identical or not, gives six cells generating the following six crystal families:

- the di oblic family;
- the di square family;
- the di hexagon family;
- the square oblic family;
- the hexagon oblic family;
- the hexagon square family.

The adjective 'orthogonal' between the names of the two cells has been omitted in order to shorten the name of the crystal family.

A number of precise rules for choosing the crystal family names, which were given by Weigel & Veysseyre (1993), are repeated below. In this paper, we consider the gZ-reducible crystal families, i.e. the families whose cells are the orthogonal products of two or more subcells.

(1) If the subcells are all different from each other, the name of each crystal family thus obtained is the succession of the names of the subcells without the adjective 'orthogonal' between two names.

(2) If some subcells are identical, we shorten the name by using the prefixes *di* for two identical cells, *tri* for three identical cells etc.

(3) When the cell is a right hyperprism based on a polytope of space E^{n-1} , we shorten the name into *polytope-al*. A polytope is a generalized polyhedron, i.e. a polyhedron of space E^n (Phan, Veysseyre & Weigel, 1988). For instance, the crystal family of space E^3 whose cell is a right prism based on a hexagon (polygon of space E^2) is described as *hexagonal*.

(4) A rectangular product being a commutative operation, the order of the subfamilies has no importance. Nevertheless, we propose to start with the name of the family whose holohedry is of the highest order. This is why we have written *hexagon square* instead of *square hexagon*. In the same way, the suffix *al* comes last in the name of a right hyperprism based on a polytope.

(5) Some suggestions have been given for the families constructed from the *segment*, i.e. the unique crystal family of space E^1 . For instance, the rectangular product of two segments is the cell of the *rectangle* family (space E^2) and the rectangular product of three segments is the cell of the *orthorhombic* family (space E^3). As regards space E^n , with $n > 3$, we suggest the general name *orthotopic n*, *orthotope* being the name of the generalized right parallelepiped of space E^n (Phan et al., 1988).

On the other hand, the WPV (Weigel, Phan & Veysseyre) symbols of the holohedries follow the same rules and easily give the order of these groups (Weigel, Phan & Veysseyre, 1987). Here are two examples:

(1) the WPV symbol of the holohedry of the square oblic family is $4mm \perp 2$, $4mm$ being the symbol of the holohedry of the square family and 2 being the symbol of the oblic family;

(2) the WPV symbol of the holohedry of the orthotopic 4 family is $m \perp m \perp m \perp m$.

These symbols enable us to find the order of the holohedry immediately. For instance: the order of the holohedry $4mm \perp 2$ is $8 \times 2 = 16$; the order of the holohedry $m \perp m \perp m \perp m$ is: $2 \times 2 \times 2 \times 2 = 16$.

I. Partition of space E^6

The ten existing partitions of the number 6 into a sum of integers less than 6 are

$$\begin{aligned} &5 + 1; \quad 4 + 2; \quad 3 + 3; \quad 4 + 1 + 1; \quad 3 + 2 + 1; \\ &2 + 2 + 2; \quad 3 + 1 + 1 + 1; \quad 2 + 2 + 1 + 1; \\ &2 + 1 + 1 + 1 + 1; \quad 1 + 1 + 1 + 1 + 1 + 1. \end{aligned}$$

To these, we must add the trivial partition corresponding to the number 6 itself.

A decomposition of space E^6 into two-by-two orthogonal subspaces is associated with each of the ten partitions of the number 6. These splittings of space E^6 generate the gZ-red. crystal families. On the other hand, the nonsplitting of space E^6 , which corresponds to the trivial partition of the number 6, generates the gZ-irr. crystal families (these families will be studied in paper XVI).

In §II, we study in detail some of these decompositions and summarize all the results in Table 2. This table lists the gZ-red. crystal families as well as their reducibility types. However, in order to construct the gZ-red. crystal families of space E^6 , we need the list of all the gZ-irr. crystal families of space E^p for all the values of the integer $p < 6$. This is why we listed these gZ-irr. crystal families in Table 1. In fact, this table summarizes the results obtained by Veysseyre *et al.* (1993) and Weigel & Veysseyre (1993).

II. The gZ-reducible crystal families of space E^6

Let us consider the decomposition $6 = 5 + 1$, which results in the splitting of space E^6 into two two-by-two orthogonal subspaces:

$$E^6 = E^5 \oplus E^1.$$

First, we consider the gZ-irr. crystal families of space E^5 ; there are three (see Table 1):

- the decaclinic crystal family;
- the hypercubic 5 crystal family;
- the rhombotopic $(-1/5)$ crystal family.

Second, we consider the unique crystal family of space E^1 : the segment crystal family (see Table 1). The rectangular product of any gZ-irr. crystal family of space E^5 and of the segment crystal family gives a crystal family whose cell is a right hyperprism based on the cell of the crystal family of space E^5 . Therefore, we obtain the following three crystal families:

- the decaclinic-al crystal family;

- the hypercubic 5-al crystal family;
- the rhombotopic $(-1/5)$ -al crystal family.

Now we must find their reducibility types. To this purpose, we have to consider the irreducibility types of the three crystal families of space E^5 . The type of the first one is $\bar{1}, \bar{1}, \bar{1}, \bar{1}, \bar{1}$, whereas the type of the other two is 5 [Weigel & Veysseyre (1993), Table 1]. Therefore, the irreducibility type of the decaclinic-al family is $\bar{1}, \bar{1}, \bar{1}, \bar{1}, \bar{1} + 1$, and the type of the other two is $5 + 1$. Moreover, this construction enables us to give a symbol to the family holohedry. As previously, we call this the WPV symbol (Weigel *et al.*, 1987). The cell of a gZ-red. family is the rectangular product of two cells; therefore, the holohedry is the direct product of the two holohedries. We have used the symbol \perp to express this property. The WPV symbols of the holohedries of the three families that we have just described are

$$\bar{1}_5 \perp m; \quad (\bar{4}_m \bar{3}_m^2, 88)\bar{55} \perp m, \quad (\bar{4}3m, 10_2)\bar{36} \perp m.$$

The order of these holohedries is the product of the order of the two holohedries of the subfamilies, *i.e.*

$$\begin{aligned} 2 \times 2 &= 4 && \text{for the first one,} \\ 3840 \times 2 &= 7680 && \text{for the second one} \\ 1440 \times 2 &= 2880 && \text{for the third one.} \end{aligned}$$

All these results are easily obtained from our construction. This is why we have adopted this method. These properties are summarized in Table 2(a).

We also give the minimal number of parameters required to describe the crystal cell and we distinguish the parameters of length (the first number) from the angular parameters (the second number). For instance, the cell of the decaclinic-al crystal family depends on:

- six length parameters, five for the decaclinic cell and one for the segment;

Ten angular parameters for the decaclinic cell, all the other angles being equal to $\pi/2$.

The cell of the hypercubic 5-al crystal family depends on:

- two length parameters, one for the hypercubic 5 crystal family and one for the segment;
- no angular parameter, all the angles being equal to $\pi/2$.

The rhombotopic $(-1/5)$ -al crystal family has the same characteristic parameters.

Finally, the last column of Table 2 gives the number of the family in Plesken's classification (Plesken & Hanrath, 1984).

Let us study another example corresponding to the partition $6 = 2 + 2 + 2$. This corresponds to the splitting

$$E^6 = E^2 \oplus E^2 \oplus E^2.$$

In Table 1, we have listed three gZ-irr. crystal families in space E^2 , which are:

Table 2. Names of the geometrically Z-reducible crystal families

The columns give the types of gZ-reducibility, names of crystal families, WPV symbols of holohedries, orders of holohedries, numbers of parameters (length parameters+ angular parameters) and Plesken classification numbers, respectively.

(a) $E^6 = E^5 \oplus E^1$

$\bar{1}, 1, 1, \bar{1}, 1 + 1$	Decaclinic - al	$\bar{1}_5 \perp m$	4	6 + 10	II
5 + 1	Hypercubic 5 - al	$(\frac{4}{m}\bar{3}\frac{2}{m}, 88)\bar{55} \perp m$	7680	2 + 0	LXXXV
5 + 1	Rhombotopic (-1/5) - al	$(\bar{4}3m, 10_2)\bar{36} \perp m$	2880	2 + 0	LXXXVI

(b) $E^6 = E^4 \oplus E^2$

$\bar{1}, 1, 1, \bar{1} + \bar{1}, 1$	Hexaclinic oblic	$\bar{1}_4 \perp 2$	4	6 + 7	III
$\bar{1}, 1, 1, \bar{1} + 2$	Hexaclinic square	$\bar{1}_4 \perp 4mm$	16	5 + 6	VI
$\bar{1}, 1, 1, \bar{1} + 2$	Hexaclinic hexagon	$\bar{1}_4 \perp 6mm$	24	5 + 6	VII
$\bar{2}, \bar{2}' + \bar{1}, \bar{1}$	(Diclinic di square) oblic	$44^* \perp 2$	8	4 + 3	XIX
$\bar{2}, \bar{2}' + \bar{1}, \bar{1}$	(Diclinic di hexagon) oblic	$66^* \perp 2$	12	4 + 3	XX
$\bar{2}, \bar{2} + \bar{1}, \bar{1}$	(Monoclinic di square) oblic	$2, 44^*, 2 \perp 2$	16	4 + 2	XXVII
$\bar{2}, \bar{2} + \bar{1}, \bar{1}$	(Monoclinic di hexagon) oblic	$2, 66^*, 2 \perp 2$	24	4 + 2	XXVIII
$\bar{2}, \bar{2}' + 2$	(Diclinic di square) square	$44^* \perp 4mm$	32	3 + 2	XXXVIII
$\bar{2}, \bar{2}' + 2$	(Diclinic di hexagon) hexagon	$66^* \perp 6mm$	72	3 + 2	XXXIX
$\bar{2}, \bar{2}' + 2$	(Diclinic di square) hexagon	$44^* \perp 6mm$	48	3 + 2	XL
$\bar{2}, \bar{2}' + 2$	(Diclinic di hexagon) square	$66^* \perp 4mm$	24	3 + 2	XLI
$\bar{2}, \bar{2} + 2$	(Monoclinic di square) square	$2, 44^*, 2 \perp 4mm$	64	3 + 1	IL
$\bar{2}, \bar{2} + 2$	(Monoclinic di hexagon) hexagon	$2, 66^*, 2 \perp 6mm$	144	3 + 1	L
$\bar{2}, \bar{2} + 2$	(Monoclinic di square) hexagon	$2, 44^*, 2 \perp 6mm$	96	3 + 1	LI
$\bar{2}, \bar{2} + 2$	(Monoclinic di hexagon) square	$2, 66^*, 2 \perp 4mm$	96	3 + 1	LII
$\bar{2}, \bar{2} + 2$	(Monoclinic di iso square) square	$88, 2 \perp 4mm$	128	2 + 1	LXVII
$\bar{2}, \bar{2} + 2$	(Monoclinic di iso hexagon) square	$12_2, 2 \perp 4mm$	192	2 + 1	LXVIII
$\bar{2}, \bar{2} + 2$	(Monoclinic di iso square) hexagon	$88, 2 \perp 6mm$	192	2 + 1	LXX
$\bar{2}, \bar{2} + 2$	(Monoclinic di iso hexagon) hexagon	$12_2, 2 \perp 6mm$	288	2 + 1	LXXI
4 + $\bar{1}, \bar{1}$	(Hypercubic 4) oblic	$\frac{4}{m}\bar{3}\frac{2}{m}, 88 \perp 2$	764	3 + 1	LVII
4 + $\bar{1}, \bar{1}$	(Di iso hexagon) oblic	$6mm \perp 6mm, 12_2 \perp 2$	576	3 + 1	LVIII
4 + $\bar{1}, \bar{1}$	Rhombotopic (-1/4) oblic	$\bar{4}3m, 10_2 \perp 2$	480	3 + 1	LIX
4' + 2	(Monoclinic di iso square) oblic	$88, 2 \perp 2$	32	3 + 2	XLIII
4' + 2	(Monoclinic di iso hexagon) oblic	$12_2, 2 \perp 2$	48	3 + 2	XLIV
4' + 2	Decadic oblic	$10_2, 2 \perp 2$	40	3 + 2	XLV
4' + 2	Decadic square	$10_2, 2 \perp 4mm$	160	2 + 1	LXIX
4' + 2	Decadic hexagon	$10_2, 2 \perp 6mm$	240	2 + 1	LXXXII
4 + 2	(Hypercubic 4) square	$\frac{4}{m}\bar{3}\frac{2}{m}, 88 \perp 4mm$	3072	2 + 0	LXXXIX
4 + 2	(Di iso hexagon) square	$6mm \perp 6mm, 12_2 \perp 4mm$	2304	2 + 0	LXXX
4 + 2	Rhombotopic (-1/4) square	$\bar{4}3m, 10_2 \perp 4mm$	1920	2 + 0	LXXXI
4 + 2	(Hypercubic 4) hexagon	$\frac{4}{m}\bar{3}\frac{2}{m}, 88 \perp 6mm$	4608	2 + 0	LXXXII
4 + 2	(Di iso hexagon) hexagon	$6mm \perp 6mm, 12_2 \perp 6mm$	1728	2 + 0	LXXXIII
4 + 2	Rhombotopic (-1/4) hexagon	$\bar{4}3m, 10_2 \perp 6mm$	2880	2 + 0	LXXXIV

(c) $E^6 = E^3 \oplus E^3$

$\bar{1}, 1, 1 + \bar{1}, 1, 1$	Di triclinic	$\bar{1} \perp \bar{1}$	4	6 + 6	IV
3 + $\bar{1}, 1, 1$	Cubic triclinic	$\frac{4}{m}\bar{3}\frac{2}{m} \perp \bar{1}$	96	4 + 3	XXI
3 + 3	Di cubic	$\frac{4}{m}\bar{3}\frac{2}{m} \perp \frac{4}{m}\bar{3}\frac{2}{m}$	2304	2 + 0	LXXVIII

(d) $E^6 = E^4 \oplus E^1 \oplus E^1$

$\bar{1}, 1, \bar{1}, \bar{1} + 1 + 1$	Hexaclinic rectangle	$\bar{1}_4 \perp m \perp m$	8	6 + 6	V
$\bar{2}, \bar{2}' + 1 + 1$	(Diclinic di square) rectangle	$44^* \perp m \perp m$	16	4 + 2	XXV
$\bar{2}, \bar{2}' + 1 + 1$	(Diclinic di hexagon) rectangle	$66^* \perp m \perp m$	24	4 + 2	XXVI
$\bar{2}, \bar{2} + 1 + 1$	(Monoclinic di square) rectangle	$2, 44^*, 2 \perp m \perp m$	32	4 + 1	XXXIII
$\bar{2}, \bar{2} + 1 + 1$	(Monoclinic di hexagon) rectangle	$2, 66^*, 2 \perp m \perp m$	48	4 + 1	XXXIV
4' + 1 + 1	(Monoclinic di iso square) rectangle	$88, 2 \perp m \perp m$	64	3 + 1	LIV
4' + 1 + 1	(Monoclinic di iso hexagon) rectangle	$12_2, 2 \perp m \perp m$	96	3 + 1	LV
4' + 1 + 1	Decadic rectangle	$10_2, 2 \perp m \perp m$	80	3 + 1	LVI
4 + 1 + 1	(Hypercubic 4) rectangle	$\frac{4}{m}\bar{3}\frac{2}{m}, 88 \perp m \perp m$	1536	3 + 0	LXIII
4 + 1 + 1	(Di iso hexagon) rectangle	$6mm \perp 6mm, 12_2 \perp m \perp m$	1152	3 + 0	LXXIV
4 + 1 + 1	Rhombotopic(-1/4) rectangle	$\bar{4}3m, 10_2 \perp m \perp m$	960	3	LXXV

(e) $E^6 = E^3 \oplus E^2 \oplus E^1$

$\bar{1}, \bar{1}, \bar{1} + \bar{1}, \bar{1} + 1$	Triclinic oblic-al	$\bar{1} \perp 2 \perp m$	8	6 + 4	VIII
$\bar{1}, \bar{1}, \bar{1} + 2 + 1$	Triclinic square-al	$\bar{1} \perp 4mm \perp m$	32	5 + 3	XIV
$\bar{1}, \bar{1}, \bar{1} + 2 + 1$	Triclinic hexagon-al	$\bar{1} \perp 6mm \perp m$	48	5 + 3	XV
3 + $\bar{1}, \bar{1} + 1$	Cubic oblic-al	$\frac{4}{m}\bar{3}\frac{2}{m} \perp 2 \perp m$	192	4 + 1	XLII
3 + 2 + 1	Cubic square-al	$\frac{4}{m}\bar{3}\frac{2}{m} \perp 4mm \perp m$	768	3 + 0	LXIV
3 + 2 + 1	Cubic hexagon-al	$\frac{4}{m}\bar{3}\frac{2}{m} \perp 6mm \perp m$	1152	3 + 0	LXV

Table 2 (cont.)

$(f) E^6 = E^2 \oplus E^2 \oplus E^2$					
$\overline{1}, \overline{1}, \overline{1}, \overline{1}, \overline{1}, \overline{1}$	Tri oblic	$2 \perp 2 \perp 2$	8	6 + 3	IX
$2 + \overline{1}, \overline{1} + \overline{1}, \overline{1}$	Square di oblic	$4mm \perp 2 \perp 2$	32	5 + 2	XVII
$2 + \overline{1}, \overline{1} + \overline{1}, \overline{1}$	Hexagon di oblic	$6mm \perp 2 \perp 2$	48	5 + 2	XVIII
$2 + 2 + \overline{1}, \overline{1}$	(Di square) oblic	$4mm \perp 4mm \perp 2$	128	4 + 1	XXXV
$2 + 2 + \overline{1}, \overline{1}$	(Di hexagon) oblic	$6mm \perp 6mm \perp 2$	288	4 + 1	XXXVI
$2 + 2 + \overline{1}, \overline{1}$	Hexagon square oblic	$6mm \perp 4mm \perp 2$	192	4 + 1	XXXVII
$2 + 2 + 2$	Tri square	$4mm \perp 4mm \perp 4mm$	512	3 + 0	LX
$2 + 2 + 2$	Tri hexagon	$6mm \perp 6mm \perp 6mm$	1728	3 + 0	LXI
$2 + 2 + 2$	Hexagon (di square)	$6mm \perp 4mm \perp 4mm$	768	3 + 0	LXII
$2 + 2 + 2$	(Di hexagon) square	$6mm \perp 6mm \perp 4mm$	1152	3 + 0	LXIII
$(g) E^6 = E^3 \oplus E^1 \oplus E^1 \oplus E^1$					
$\overline{1}, \overline{1}, \overline{1} + 1 + 1 + 1$	Triclinic orthorhombic	$\overline{1} \perp m \perp m \perp m$	16	6 + 3	X
$3 + 1 + 1 + 1$	Cubic orthorhombic	$\frac{a}{m} \frac{a}{3} \frac{a}{m} \perp m \perp m \perp m$	384	3 + 1	LIII
$(h) E^6 = E^2 \oplus E^2 \oplus E^1 \oplus E^1$					
$\overline{1}, \overline{1} + \overline{1}, \overline{1} + 1 + 1$	Di oblic rectangle	$2 \perp 2 \perp m \perp m$	16	6 + 2	XIII
$2 + \overline{1}, \overline{1} + 1 + 1$	Square oblic rectangle	$4mm \perp 2 \perp m \perp m$	64	5 + 1	XXIII
$2 + \overline{1}, \overline{1} + 1 + 1$	Hexagon oblic rectangle	$6mm \perp 2 \perp m \perp m$	96	5 + 1	XXIV
$2 + 2 + 1 + 1$	Di square rectangle	$4mm \perp 4mm \perp m \perp m$	256	4	XLVI
$2 + 2 + 1 + 1$	Di hexagon rectangle	$6mm \perp 6mm \perp m \perp m$	576	4	XLVII
$2 + 2 + 1 + 1$	Hexagon square rectangle	$6mm \perp 4mm \perp m \perp m$	384	4	XLVIII
$(i) E^6 = E^2 \oplus E^1 \oplus E^1 \oplus E^1 \oplus E^1$					
$\overline{1}, \overline{1} + 1 + 1 + 1 + 1$	Oblic (orthotopic 4)	$2 \perp m \perp m \perp m \perp m$	32	6 + 1	XVI
$2 + 1 + 1 + 1 + 1$	Square (orthotopic 4)	$4mm \perp m \perp m \perp m \perp m$	128	5	XXXI
$2 + 1 + 1 + 1 + 1$	Hexagon (orthotopic 4)	$6mm \perp m \perp m \perp m \perp m$	192	5	XXXII
$(j) E^6 = E^1 \oplus E^1 \oplus E^1 \oplus E^1 \oplus E^1 \oplus E^1$					
$1 + 1 + 1 + 1 + 1 + 1$	Orthotopic 6	$m \perp m \perp m \perp m \perp m \perp m$	64	6	XXII

the oblic crystal family;
the square crystal family;
the hexagon crystal family.

We must make the orthogonal product of three cells, identical or not, selected among the previous three, for example the tri oblic crystal family and the hexagon di square crystal family.

All the rules mentioned in the *Introduction* have obviously been respected:

(i) the suffix di or tri if two or three subcells are the same;

(ii) the cell order, for instance the hexagon, is written before the square, its point-group order being twelve, higher than that of the square which is eight;

(iii) the adjective *orthogonal* is not given between the names of two cells.

These crystal families as well as their characteristics are listed in Table 2(*f*). It is not very difficult to find the number of crystal families constructed from these three subcells: it is equal to ten, in fact, it is the number of combinations with repetitions of three elements taken three at a time, *i.e.*

$$\binom{3 + 3 - 1}{3} = \binom{5}{3} = 10.$$

All the other cases of splittings of space E^6 have been similarly studied, the results are listed in Table 2. We

only explain how the number of crystal families corresponding to each splitting of this space can be obtained.

Splitting $E^6 = E^5 \oplus E^1$. There are three gZ-irr. crystal families in space E^5 which generate three gZ-red. crystal families in space E^6 , as we explained in §2 [see Table 2(*a*)].

Splitting $E^6 = E^4 \oplus E^2$. There are eleven gZ-irr. crystal families in space E^4 and three in space E^2 (Table 1), which generate $11 \times 3 = 33$ gZ-red. crystal families in space E^6 [see Table 2(*b*)].

Splitting $E^6 = E^3 \oplus E^3$. There are two gZ-irr. crystal families in space E^3 (Table 1), which generate three gZ-red. crystal families in space E^6 , three being the number of combinations with repetitions of three elements taken two at a time [see Table 2(*c*)].

Splitting $E^6 = E^4 \oplus E^1 \oplus E^1$. There are eleven gZ-irr. crystal families in space E^4 and one in space E^1 (Table 1), which generate eleven gZ-red. crystal families in space E^6 because the splitting $E^1 \oplus E^1$ only generates the rectangle family [see Table 2(*d*)].

Splitting $E^6 = E^3 \oplus E^2 \oplus E^1$. There are two gZ-irr. crystal families in space E^3 , three in space E^2 and one in space E^1 , which generate $2 \times 3 \times 1 = 6$ gZ-red. crystal families in space E^6 [see Table 2(*e*)].

Splitting $E^6 = E^2 \oplus E^2 \oplus E^2$. There are three gZ-irr. crystal families in space E^2 , which generate ten gZ-red.

crystal families in space E^0 , as explained in §II [see Table 2(f)].

Splitting $E^6 = E^3 \oplus E^1 \oplus E^1 \oplus E^1$. There are two gZ-irr. crystal families in space E^3 and one in space E^1 , which generate two gZ-red. crystal families in space E^6 because the splitting $E^1 \oplus E^1 \oplus E^1$ only generates the orthorhombic crystal family [see Table 2(g)].

Splitting $E^6 = E^2 \oplus E^2 \oplus E^1 \oplus E^1$. There are three gZ-irr. crystal families in space E^2 and one in space E^1 which generate six gZ-red. crystal families in space E^6 . Indeed, the splitting $E^2 \oplus E^2$ generates six crystal families, six being the number of combinations with repetitions of three elements taken two at a time, whereas the splitting $E^1 \oplus E^1$ only generates the rectangular crystal family [see Table 2(h)].

Splitting $E^6 = E^2 \oplus E^1 \oplus E^1 \oplus E^1 \oplus E^1$. There are three gZ-irr. crystal families in space E^2 and one in space E^1 . The splitting $E^1 \oplus E^1 \oplus E^1 \oplus E^1$ only generates the orthotopic 4 crystal family; therefore, we obtain three gZ-red. crystal families in space E^6 [see Table 2(i)].

Splitting $E^6 = E^1 \oplus E^1 \oplus E^1 \oplus E^1 \oplus E^1 \oplus E^1$. This splitting generates the orthotopic 6 crystal family of space E^6 [see Table 2(j)].

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Heights and Widths of *Umweganregung* Profiles in Comparison with Bragg Reflection Profiles

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Abstract

The excellent agreement between experimental *Umweganregung* patterns and those calculated with *UMWEG90* [Rossmannith (1992). *Acta Cryst.* **A48**, 596–610] has been demonstrated by Rossmannith, Adiwidjaja, Eck, Kumpat & Ulrich [*J. Appl. Cryst.* (1994), **27**, 510–516]. It has also been shown that, by fitting calculated to experimental ψ scans, consistent and physically significant parameters for the mosaic-structure parameters of the sample – mosaic spread and mosaic-block size – and for the divergence parameter of the X-ray beam can be obtained. In this paper, it is shown that, furthermore, the relative intensities of ψ scans of different forbidden reflections of a particular sample are predicted satisfactorily with *UMWEG90* using the parameters obtained in the previously mentioned paper. To make an appraisal of the possible maximum gain due

to *Umweganregung*, ω - 2θ - ψ scans of 14 forbidden reflections of a particular zinc sample were analysed. By comparison of the ω - 2θ intensity profiles and integrated intensities of the multiple diffraction events with those of the rocking curves of 15 Bragg reflections with neighbouring Bragg angles, the statements given in standard textbooks, that the profiles of *Umweganregung* events are much sharper and the intensities much smaller than those of possible Bragg reflections, are disproved.

Introduction

For the determination of distortions of atomic charge densities from spherical symmetry due to anharmonic motion and chemical bonding, very weak 'almost forbidden' as well as weak high-order Bragg reflections have to be measured. These weak intensities may be

Concluding remarks

The geometrical method that introduced by Veysseyre *et al.* (1993) and Weigel & Veysseyre (1993) is a convenient and powerful means to construct all the gZ-red. crystal families of space E^n ; this method enables us to describe the cell of the crystal family and to give a name to this family as well as a symbol to its holohedry. Moreover, we can summarize the previous results by mentioning the number of crystal families belonging to each type of splitting of space E^6 . This enables us to prove the results given in Table 3 of Weigel & Veysseyre (1993).

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