

## Crystallographic point groups of five-dimensional space. 2. Their geometrical symbols

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Our previous paper emphasized a method for obtaining the crystallographic point groups of five-dimensional space, *i.e.* the subgroups of the crystal family holohedries. Moreover, it recalled the names of the crystal families and the symbols of their holohedries. These results being obtained, this paper gives a geometrical symbol to each of these point groups described as Weigel–Phan–Veysseyre symbols (WPV symbols). In most cases, these symbols make it possible to reconstitute all the elements of the groups. The point symmetry operation symbols, which are the basis of the Hermann–Mauguin symbols (HM symbols) as well as of the WPV symbols, that have been defined from the cyclic groups generated by the five-dimensional point symmetry operations are recalled. The basic principles of the WPV system of crystallographic point-group symbols are explained and a list of 196 symbols of five-dimensional space out of 955 is given. All the information given by the WPV symbol of a point group is detailed and analysed through some examples and the study of the (hexagon oblique)-al crystal family. Finally, the polar point groups of five-dimensional space are specified.

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### 1. Introduction

The elements that have been used are to be found in Brown *et al.* (1978), and in some of our papers published either in *Acta Crystallographica* (Weigel *et al.*, 1987, 1990; Veysseyre *et al.*, 1991; Phan *et al.*, 1991; Weigel & Veysseyre, 1993) or in *Compte Rendus de l'Académie des Sciences* (Veysseyre *et al.*, 1990) or in theses (Veysseyre, 1987; Phan, 1989).

The first step consists of listing the crystal families and the symbols of the 227 crystallographic point groups of four-dimensional space (or 4D space for short). In the previous paper (Veysseyre, & Veysseyre, 2002), we explained how the crystal families of 5D space and their names had been found. Owing to some geometrical properties of the unit cells, each crystal family holohedry and all their subgroups (or point groups) have been given a geometrical symbol, as shown in Table 1, for the symbols of three crystal families of 4D space which are different from the symbols published in the Report of a Subcommittee on the Nomenclature of *n*-Dimensional Crystallography (Janssen *et al.*, 1999). These symbols have already been published in Weigel *et al.* (1987); however, according to the Report of the Subcommittee and in order to apply these results to the point groups of 5D space, some of these symbols have been changed. The classification order given by Janssen *et al.* (1999) has been kept.

The second step consists of listing the 38 cyclic groups generated by the 38 crystallographic point symmetry opera-

tions (PSOs) of 5D space. All these symbols are summarized in Table 2. Each of these point groups is to be given a symbol connected with the generator element. We intend to explain some of them:

- $\bar{1}$  is the symbol of the cyclic group generated by the total inversion (homothetic  $\bar{1}$ ) in 3D space, its order is two. In the same way, symbol  $\bar{1}_5$  or  $\bar{1}$  is given to the cyclic group of order two generated by total inversion (homothetic  $\bar{1}_5$ ) in 5D space.

- $\bar{4}$  is the symbol of the cyclic group generated by the  $\text{PSO}^- 4.\bar{1}$ , *i.e.* a simple rotation–inversion, whereas  $\bar{4}$  is the symbol of the cyclic group generated by the  $\text{PSO}^- 4.\bar{1}$ , *i.e.* a double rotation–inversion.

- $44$  is the symbol of a cyclic group of order four generated by the double rotation  $44$  whereas  $\bar{44}$  is the symbol of the cyclic group generated by the  $\text{PSO}^- 44.\bar{1}$ , *i.e.* a double rotation–inversion, or by the point operation  $44m$ , *i.e.* a double rotation–reflection.

- $[10]$  is the cyclic group of order ten, generated by the double crystallographic rotation  $10_{xy}^1 10_{zt}^3$ , *i.e.* a rotation through angle  $2\pi/10$  in the plane ( $xy$ ) and a rotation through angle  $6\pi/10$  in the orthogonal plane ( $zt$ ), whereas  $\bar{[10]}$  is the symbol of a cyclic group of order ten generated by the  $\text{PSO}^- 10_{xy}^1 10_{zt}^3.\bar{1}$  (see Table 2). In the same way,  $[5]$ ,  $[8]$  and  $\bar{[12]}$  are the symbols of cyclic groups of order ten, eight and twelve, respectively.

**Table 1**

Alternative WPV point-group symbols in 4D space, complementing the Subcommittee Report.

The symbols of the Report (Janssen *et al.*, 1999, Table 1) are in brackets.

Hexagon square family		
18-1	Order 24	3.(422) [3m1(1m4)]
	Order 48	6.(422) [6m1(1m4)]; 6. $\bar{4}2m$ [6m1(14m)]; $\bar{3}m.4$ [6m1(m14)]
Cubic-al family		
19-1	Order 24	$\bar{4}.3.\bar{1}$ [432(m1m)]
19-2	Order 24	42.3.2 [ $\bar{4}3m(m1m)$ ]
	Order 48	$m\bar{3}\perp m$ [ $m\bar{4}3m(m1m)$ ]; 42.3.2.m [ $m\bar{3}m(11m)$ ]
Di hexagons family		
20-2	Order 18	(32).3 [3m1(1m3)]
	Order 36	$\bar{3}\times 3m$ [6m1(613)]; $\bar{3}.\bar{3}$ [6m1(m63)]; {(32).3} $\times\bar{1}_4$ [6m1(6m3)]; $\bar{3}m.3$ [6m1(m13)]
	Order 72	Holohedry: $(3m\perp 3m)\times\bar{1}_4$ [6m11(613m)]
20-3	Order 36	6. $\bar{3}$ [6m1(163)]; (622).3 [6m1(1m3)]
	Order 72	(622).6 [6m1(1m6)]; $\bar{3}m.6$ [6m11(163m)]

So, a single bar above a symbol means ‘product with the homothetic  $\bar{1}$ ’ in a 3D space, and a double bar means ‘product with the homothetic  $\bar{1}(\bar{1}_5)$ ’ in a 5D space.

*Remark 1.* Whatever the dimension of the space, any reflection always acts along a straight line (orthogonal to the mirror), any simple rotation acts in a plane, any inversion  $\bar{1}$  acts in a 3D space, any double rotation acts in a 4D space, any inversion  $\bar{1}$  acts in a 5D space.

In the previous paper, we explained how the number of crystallographic point groups belonging to each family had been found and their elements have been listed.

The basic principles of our system of point-group symbols (WPV symbols) are developed in §2 and the properties of these symbols in §3; some point-group symbols of 4D space which have not been listed in Table 1 of Janssen *et al.* (1999) are explained in §4. A specific family, *i.e.* the (hexagon oblique)-al family, is thoroughly studied in §5. The subgroups of 15 families are listed in Table 3. Polar groups of 5D space are all the crystallographic point groups of 4D space, as shown in §6. Obviously, these 227 point groups have the same WPV symbol in 4D space as in 5D space.

## 2. Basic principles of the WPV system of crystallographic point-group symbols

The point-group symbols of 1D, 2D and 3D spaces are the well known HM symbols; they are tabulated in Volume A of *International Tables for Crystallography* (1996).

The five basic principles for the WPV system of point-group symbols in the *n*D spaces are given in the following lines:

*Principle 1.* Any symbol is the product of either a cyclic point-group symbol (see Table 2) or a HM symbol of a point group; some examples are given after the second principle.

**Table 2**

The WPV symbols of the 38 crystallographic cyclic point groups in 5D space.

These are the symbols of their only generator except for those that are listed in the table footnotes.

19 rotation groups (or GP <sup>+</sup> )		19 non-rotation groups (or GP <sup>-</sup> )		
1	33	$m$	$33\perp m$	(66)
2	43	$\bar{1}$	$\bar{6}4$	(64)
3	63	$\bar{3}$	$\bar{6}3$	(63)
4	44	$\bar{4}$	$\bar{4}4$	(44)
6	64	$3\perp m$	$\bar{4}3$	(43)
$\bar{1}_4$	[5]	$\bar{1}_5$	$\bar{3}5$	(33)
$3\perp 2$	(32)	$3\perp\bar{1}$	( $\bar{3}2$ )	( $\bar{5}$ )
42	[8]	$3\times\bar{1}_5$	(62)	( $\bar{8}$ )
62	[12]	$\bar{4}$	(42)	( $\bar{10}$ )
	[10]		$\bar{1}2$	( $\bar{1}2$ )

About the choice of some symbols:

For some groups, we suggest the following symbols because the definition of the operations that generate these groups clearly appears. Moreover, the double bar is suppressed whenever possible:

$$3\perp m = \bar{6} \quad \bar{1}_5 = \bar{1} \quad 3\perp\bar{1} = \bar{6} \quad 3\times\bar{1}_5 = \bar{3} \quad 33\perp m = \bar{6}\bar{6}.$$

$3\perp 2$  is the symbol of the cyclic group generated by a threefold rotation through a plane  $P_1$  and by a twofold rotation through a plane  $P_2$  orthogonal to plane  $P_1$ . The order of group  $3\perp 2$  equals  $3 \times 2 = 6$ . Another possible symbol for this group should be 32 because this group can also be considered as generated by the double rotation denoted 32. However, the symbol  $3\perp 2$  is correct because 3 is prime relative to 2 and it has a geometrical meaning. *Moreover, we prefer to avoid the symbol 32 for this group because it is the HM symbol of another crystallographic group.*

In 3D space (hence in 4D, 5D, ..., *n*D space), there are two groups whose HM symbols 32 and 23 may be mistaken for each other. However, we have decided to keep them. The point group denoted 32 is isomorphic to the abstract dihedral group  $D_6$ ; its order is six and its elements are as follows: the identity, the rotations through a ternary axis and three binary axes. The point group denoted 23 is the rotation group of group  $43m$ , *i.e.* of the regular tetrahedron; its order is 12 and its elements are as follows: the identity and the rotations through four ternary axes and three binary axes.

This cyclic group or the group defined by one HM symbol which appears in a WPV symbol is called a ‘point-group factor’.

Whenever possible, the use of the HM symbols absolutely retains priority for the choice of the factors of the WPV symbols except for groups  $\bar{6}$  and  $\bar{6}2m$  denoted respectively as  $3\perp m$  and  $3m\perp m$ .

*Principle 2.* The different kinds of group products are characterized by three different symbols. For a direct product of groups, we use either the mark  $\times$  (mathematical meaning) or the mark  $\perp$  if the spaces in which the two groups act are orthogonal. For a product of groups (not a direct product), a dot . is used. Moreover, *the mark permits one to precisely know the dimension in which the point group (PG) acts* (see §3).

The choice of mark has the following priority:  $\perp$  (if convenient), then  $\times$  (if  $\perp$  is not convenient), and last . (if  $\times$  and  $\perp$  are not convenient). Here are some examples:

- Group  $4\perp(222)$  acts in 5D space because rotation 4 acts in 2D space and group 222 acts in 3D space.

- Group  $\bar{4}\times(222)$  acts in 5D space because PSO  $\bar{4}_{xy}$  acts in 5D space ( $xyztu$ ) (see Table 2) while group 222 acts in 3D space ( $ztu$ ).

- However,  $\bar{4}\perp(222)$  is the WPV symbol of a point group which acts in 8D space because 4 acts in 5D space and 222 acts in 3D space.

**Table 3**

Five-dimensional point groups of the first 15 families.

For each family, the first column gives its indicating number, its name and its point-group numbers. Then, the number of subgroups of given order is indicated and the WPV symbols of these groups are listed. The family holohedry together with its order is listed in the right part of the table. The subfamilies of a given family are denoted by lowercase letters. For instance, XVb, XVa are two subfamilies (*i.e.* centred families) of family XV 'Hexagon orthorhombic family'. Some generators are written at the bottom of this table.

Family name	Order	Point-group symbols	Order	Holohedry symbol
I Dicaclinic (2 PGs)	1	1	2	$\bar{1}_5$
II Hexaclinic-al (3 PGs)	2	$\bar{1}_4; m$	4	$\bar{1}_4 \perp m$
III Triclinic oblique (3 PGs)	2	$2; \bar{1}$	4	$\bar{1} \perp 2$
IV Triclinic rectangle (4 PGs)	4	$\bar{1}_4 \times 2; mm; \bar{1} \perp m$	8	$\bar{1} \perp mm$
V (Di obliques)-al (4 PGs)	4	$2 \perp 2; 2 \perp m; \bar{1}_4 \times \bar{1}$	8	$2 \perp 2 \perp m$
VI Triclinic square (7 PGs)	4	$4; \bar{4}$	16	$\bar{1} \perp 4mm$
	8	$\bar{1}_4 \times 4; 4mm; \bar{1} \perp 4; \bar{4}.m$		
VII Triclinic hexagon				
VIIb (2 PGs)	3	3	6	$3 \times \bar{1}_5$
VIIa (3 PGs)	6	$\bar{1}_4.3; 3m$	12	$3m \times \bar{1}_5$
VII (7 PGs)	6	$6; \bar{1} \perp 3$		
	12	$\bar{1}_4.6; 6mm; \bar{1} \perp 6; \bar{1} \perp 3m$	24	$\bar{1} \perp 6mm$
VIII Oblique orthorhombic				
VIIIa (3 PGs)	4	$222; 2 \times \bar{1}$	8	$(222) \times \bar{1}_5$
VIII (5 PGs)	8	$2 \perp (222); mmm; 2 \perp mm; (2 \times \bar{1}) \perp m$	16	$2 \perp mmm$
IX Orthotopic 5d				
IXa (4 PGs)	8	$(222) \times \bar{1}_4; (222) \perp m; (2 \times \bar{1}) \times \bar{1}_4$	16	$(222) \perp m \times \bar{1}_5$
IX (4 PGs)	16	$22222; mmmm; (222) \perp mm$	32	$mmmmm$
X (Square oblique)-al				
Xa (8 PGs)	4	$42; \bar{4}$		
	8	$42.\bar{1}_4; \bar{4}2m; \bar{4}.\bar{1}_4; 42.m; \bar{4} \times \bar{1}_5$	16	$(\bar{4}2m) \times \bar{1}_5$
X (16 PGs)	8	$422; \bar{4}.\bar{1}; 4 \perp 2; \bar{4} \perp 2; 4 \perp m; 4.\bar{1}; 42 \perp m$		
	16	$(422) \perp 2; 4mm \perp m; (422) \times \bar{1}_5; (\bar{4}2m) \perp 2; (42.m) \perp m; 4mm \perp 2; 4 \perp 2 \perp m; (4.\bar{1}) \perp m$	32	$4mm \perp 2 \perp m$
XI (Hexagon oblique)-al				
XIId (3 PGs)	6	$62; 3 \perp m$	12	$62 \times \bar{1}_5$
XIc (3 PGs)	6	$32; 3.\bar{1}$	12	$(32) \times \bar{1}_5$
XIb (5 PGs)	12	$62.\bar{1}_4; 3m \perp m; (3 \perp m).\bar{1}_4; 3m.\bar{1}_4$	24	$(3m \perp m) \times \bar{1}_5$
XIa (8 PGs)	6	$3 \perp 2;$		
	12	$(32) \perp 2; \bar{3}m; 3m \perp 2; \bar{3} \perp 2; \bar{3}.\bar{1}_4$	24	$(\bar{3}m) \times \bar{1}_5$
XI (16 PGs)	12	$622; (32).\bar{1}; 6 \perp 2; 6 \perp m; 6.\bar{1}; 3 \perp 2 \perp m; \bar{3} \times \bar{1}_4$		
	24	$(622) \perp 2; 6mm \perp m; (622) \times \bar{1}_5; 3m \perp 2 \perp m; (\bar{3}m) \times \bar{1}_5; 6mm \perp 2; 6 \perp 2 \perp m; (6.\bar{1}) \perp m$	48	$6mm \perp 2 \perp m$
XII (Diclinic di squares)-al (3 PGs)	4	$44; \bar{4}\bar{4}$	8	$44 \perp m$
XIII (Diclinic di hexagons)-al				
XIIIa (2 PGs)	3	33	6	$33 \times \bar{1}_5$
XIII (3 PGs)	6	$66; 33 \perp m$	12	$66 \perp m$
XIV Square orthorhombic				
XIVa (15 PGs)	8	$42.2; \bar{4}.\bar{1}; 42 \times \bar{1}_4; \bar{4} \times \bar{1}_4; \bar{4} \perp m; 42.\bar{1}$		
	16	$(42.2) \times \bar{1}_4; (\bar{4}2m) \times \bar{1}_4; (\bar{4}2m) \perp m; (42.2) \times \bar{1}_5; (\bar{4}.\bar{1}) \times \bar{1}_4; (\bar{4}.\bar{1}) \perp m; (42.\bar{1}) \times \bar{1}_4; (\bar{4} \times \bar{1}_4) \perp m$	32	$(\bar{4}2m \perp m) \times \bar{1}_5$
XIV (18 PGs)	16	$(422) \times \bar{1}_4; (\bar{4}.\bar{1}) \times 2; (422) \perp m; (42.2) \perp m; 4 \perp (222); \bar{4} \times (222); 4 \perp mmm; (4.\bar{1}) \times 2; \bar{4} \perp mmm$		
	32	$(422) \times (222); 4mm \perp mmm; \{(422) \times \bar{1}_4\} \perp m; (42m) \times (222); (\bar{4}2m) \perp mmm; (422) \perp mmm; 4mm \perp (222); 4 \perp mmmm$	64	$4mm \perp mmmm$
XV Hexagon orthorhombic				
XVb (4 PGs)	12	$62.2; (32) \perp m; 62.\bar{1}$	24	
XVa (15 PGs)	12	$(32) \times 2; \bar{3}.\bar{1}; 62 \times \bar{1}_4; 3 \perp mmm; (3.\bar{1}) \times 2; \bar{3} \perp m$		
	24	$(62.2) \times \bar{1}_4; 3m \perp mmm; \{(32) \times 2\} \times \bar{1}_5; \bar{3}m \perp m; (32) \perp mmm; (\bar{3}.\bar{1}) \perp m; (62.\bar{1}) \times \bar{1}_4; \bar{3} \perp mmm$	48	$\{(32) \perp m\} \times \bar{1}_5$ $\bar{3}m \perp mmm$
XV (26 PGs)	12	$3 \perp (222); \bar{3} \times 2$		
	24	$(622) \times \bar{1}_4; (32) \times (222); (622) \perp m; \bar{3}m \times 2; \{(32) \times 2\} \perp m; (\bar{3}.\bar{1}) \times \bar{1}_4; 6 \perp (622); (\bar{3}.\bar{1}_4) \times 2; 3m \perp (222); 3 \perp mmmm; \{3 \perp (222)\} \times \bar{1}_5; 6 \perp mmm; (6.\bar{1}) \times \bar{1}_4; (\bar{3} \times 2) \perp m$		

Table 3 (continued)

Family name	Order	Point-group symbols	Order	Holohedry symbol
	48	$(622) \times (222)$ ; $6mm \perp mm$ ; $\{(622) \times \bar{1}_4\} \perp m$ ; $3m \perp mmm$ ; $\bar{3}m \times (222)$ ; $(\bar{3}m \perp m) \times \bar{1}_4$ ; $(622) \perp mm$ ; $6mm \perp (222)$ ; $6 \perp mmm$	96	$6mm \perp mmm$

Generators of some point groups

The following abridged notations are used:  $mm$  instead of  $m \perp m$ ,  $mmm$  instead of  $m \perp m \perp m$ , ... and PG for point group.

$(222) \cdot (2\bar{1}_4)$ :	$(222)_{(xzu)}$ , $2_{xy}$ , $\bar{1}_{4(xyzt)}$	$62\bar{1}$ :	$6_{xy}2_{zt}$ , $\bar{1}_{ztu}$	$(6\bar{1}) \times \bar{1}_4$ :	$6_{xy}$ , $\bar{1}_{xzt}$ , $\bar{1}_{4(xyzt)}$	$42\bar{1}_4$ :	$4_{xy}2_{zt}$ , $\bar{1}_{4(x+yzt)}$ id for $62\bar{1}_4$
$42m$ :	$4_{xy}2_{zt}$ , $m_z$ , $\bar{1}_{xzu}$	$4\bar{1}$ :	$4_{xyz}$ , $\bar{1}_{xzt}$ id for $\bar{3}\bar{1}$	$4\bar{1} \times \bar{1}_4$ :	$\bar{1}_{4(xyzt)}$ id for $\bar{3}\bar{1} \times \bar{1}_4$	$4\bar{1} \times 2$ :	$2_{tu}$
$\bar{3}\bar{1}_4$ :	$\bar{3}_{xyz}$ , $\bar{1}_{4(xztu)}$	$\bar{3}\bar{1}_4 \times 2$ :	$2_{zt}$	$\bar{3} \times 2$ :	$\bar{3}_{xyz}$ , $2_{zt}$	$\bar{3}m \times 2$ :	$\bar{3}m_{(xyz)}$ , $2_{zt}$
$4\bar{1}$ :	$4_{xy}$ , $\bar{1}_{xzt}$	$4m$ :	$4_{xy}$ , $m_x$				

**Principle 3.** The point-group order is the product of the factor point-group orders of the WPV symbol.

For instance, the order of group  $4 \times (222)$  is  $16 = 4 \times 4$ , the same as  $4 \perp (222)$  order.

The order of group  $(622) \times (222)$  is  $48 = 12 \times 4$  and this point group acts in 5D space.

**Principle 4.** The WPV symbol defines the group itself in a one-to-one way among the same order group; if it is necessary, two (or three) characteristic generators are given at the bottom of Table 3.

**Principle 5.** The symbols of the geometrically Z-reducible crystal family holohedries in the nD space are always as follows:

$$H_n = H_p \perp H_q \perp \dots \perp H_r,$$

where  $p + q + \dots + r = n$  and  $H_p, H_q, \dots, H_r$  are crystal family holohedries of  $p$ -,  $q$ -, ...  $r$ -dimensional spaces, indices  $p, q, \dots, r$  are classified in decreasing order. If two indices are equal, the point-group factor of the highest order always appears at the beginning of the WPV symbol (see Table 3).

**Example:**  $\bar{1}$  is the holohedry of the triclinic family in 3D space and  $4mm$  is the holohedry of the square family in 2D space; so  $\bar{1} \perp 4mm$  is the holohedry of the triclinic square family in 5D space.

Some examples have been given in the Abstracts from the European Crystallographic Meeting in Prague in 1998 (Weigel *et al.*, 1998).

### 3. The meaning of the point-group WPV symbols

The WPV symbol of a point group immediately gives the following three sets of data:

(1) *The dimension n of the space in which it acts.*

**Examples:** groups  $4mm$  (or  $4m$ );  $422$  (or  $4_2$ );  $4\bar{1}$ ;  $4\bar{1}_4$ .

First, it should be recalled that  $m, 2, \bar{1}, \bar{1}_4$  are the total inversions in the 1D, 2D, 3D, 4D spaces. Rotation 4 acts in the 2D space ( $xy$ ). Then, group  $4mm$  acts in plane ( $xy$ ). Actually, none of the  $m$  inversions can act along axis  $z$  because, if they could, the WPV symbol of the corresponding point group would be  $4 \perp m$  (Principle 2, §2). The latter is the WPV symbol

of a point group in 3D, 4D, 5D, ... spaces. As a result, the four reflections of group  $4mm$  only act along four directions of plane ( $xy$ ), *i.e.*  $m_x, m_y, m_{x+y}, m_{x-y}$ .

In the same way, group 422 acts in space ( $xyz$ ), while group  $4\bar{1}$  acts in the 4D space ( $xyzt$ ), because PSO  $\bar{1}$  does not act in the space ( $xyz$ ). Indeed, if PSO  $\bar{1}$  acts in space ( $xyz$ ), the WPV symbol of the point group would be  $4 \perp m$  (as previously defined). So, the supports of the four inversions  $\bar{1}$  of group  $4\bar{1}$  are necessarily in spaces ( $xzt$ ), ( $yzt$ ), ( $x+yzt$ ), ( $x-yzt$ ).

Group  $4\bar{1}_4$  acts in the 5D space ( $xyztu$ ) where the supports of the four inversions  $\bar{1}_4$  are the spaces ( $xztu$ ), ( $yztu$ ), ( $x+yztu$ ), ( $x-yztu$ ).

(2) *The name and the holohedry WPV symbol of the crystal family it belongs to, in the spaces of n, n+1, n+2, ... dimensions (n is the smallest dimension of the space in which the point group acts).*

**Example 1:** group  $4mm$  belongs to the following crystal families: square crystal family (2D space, holohedry  $4mm$ ), tetragonal (or square-al) crystal family (3D space, holohedry  $4mm \perp m$ ), square oblique crystal family (4D space, holohedry  $4mm \perp 2$ ) and square triclinic crystal family (5D space, holohedry  $4mm \perp \bar{1}$ ). Indeed, the holohedry orders of these crystal families are the lowest order among the crystal families containing the square symmetry.

**Example 2:** group  $4\bar{1}$  belongs to square oblique crystal family (4D space, holohedry  $4mm \perp 2$ ), and to (square oblique)-al crystal family (5D space, holohedry  $4mm \perp 2 \perp m$ ).

**Example 3:** group  $\bar{1} \perp 4$  belongs to triclinic square crystal family because its holohedry,  $\bar{1} \perp 4mm$ , is the lowest order among the crystal families containing the square symmetry (it should be noted that any cell remains unchanged by the total inversion in its space).

(3) *The elements of the point-group factors together with the subspaces in which they act, which enable one to list all the elements and the geometrical supports of the point group (see Principle 1, the definition of the group factor).* As can be seen in Table 3, it is necessary to know the geometrical supports of the generators in very few cases.

**Example:** group  $(622) \times (222)$ , of order 48, belongs to the hexagon orthorhombic crystal family of the 5D space and its elements are as follows:

- The rotations of subgroup 6 of group 622, *i.e.*  $6_{xy}$ , in plane  $(xy)$  and the twofold rotations of group 222 acting in orthogonal supplementary space  $(ztu)$ ; consequently, we obtain the supports of the six elements of cyclic group 6, and the ones of the three rotations 2.

- There are three hexagonal subcells in three 3D subspaces (in which three subgroups 622 act), *i.e.* spaces  $(xyz)$ ,  $(xyt)$ ,  $(xyu)$ . Hence, the supports of the 18 corresponding rotations 2.

- The products of  $6_{xy}^{\pm 1}$  and  $3_{zt}^{\pm 1}$  by the three rotations  $2_{zt}$ ,  $2_{zu}$  and  $2_{uu}$  enable one to obtain the six rotations 62 and the six rotations 32 whose supports are  $(xy,zt)$ ,  $(xy,zu)$  and  $(xy,tu)$ .

- Finally, the products of all the single twofold rotations give either one twofold other rotation or one of the nine  $\bar{1}_4$  inversions whose supports are spaces  $(xyzt)$ ,  $(xyzu)$ ,  $(xytu)$ ,  $(xztu)$ ,  $(yztu)$ ,  $(x+y,ztu)$ ,  $(x-y,ztu)$ ,  $(x-2y,ztu)$ ,  $(2x-y,ztu)$ .

Therefore, the geometrical supports of the 48 elements of group  $(622) \times (222)$  can easily be obtained. Moreover, it should be noted that all the elements of this group are pure rotations. Then, group  $(622) \times (222)$  is the rotation group of the hexagon orthorhombic crystal family holohedry, *i.e.* group  $6mm \perp mmm$  (order  $96 = 12 \times 8$ ).

However, group  $(622) \perp (222)$  is a point group acting in a 6D space because group 622 acts in space  $(xyz)$  and group 222 in space  $(tuv)$ ; its order is also 48.

Therefore, for any point group, it is possible to find the order, the dimension  $n$  of the space in which it acts, the name of its crystal family, the WPV symbol holohedry, together with its elements and their geometrical supports. A particular family, (hexagon oblique)-al crystal family will be studied in §5.

#### 4. Crystallographic WPV point-group symbols in 4D and 5D spaces

Most of the WPV symbols of 4D space have been adopted in Table 3 of the Subcommittee Report (Janssen *et al.*, 1999), either as principal or alternative ones for the first 20 crystal families of this space. But some symbols are missing in families 18, 19 and 20. These symbols are listed in Table 1 when they are different of the symbols of the Report. Through three examples, we verify that each WPV symbol unambiguously defines one and only one group, together with its elements and their geometrical supports.

- Group  $\bar{3}m.4$  belongs to the hexagon square crystal family; it is a group of order  $12 \times 4 = 48$ . Rotation 4 acts in plane  $(zt)$  while two subgroups  $\bar{3}m$  (of order 12) act in spaces  $(xyz)$  and  $(xyt)$ , respectively.

- Group 423.2 belongs to the cubic-al crystal family. The three types of double rotations 42 act in spaces  $(xyzt)$ ,  $(yztx)$  and  $(xztu)$  while rotations 3 and 2 are the rotations of the cubic family in 3D space  $(xyz)$ .

- Group  $\bar{3}m.3$  belongs to the di hexagons crystal family; it is a group of order  $6 \times 6 = 36$ . It is possible to obtain these 36 PSOs from one PSO  $\bar{3}$  ( $m_{x-y} 6_{zt}^{\pm 1}$ ), one PSO  $m$  ( $m_z$ ) of group  $\bar{3}m$  and one rotation 3 ( $3_{xy}^{\pm 1}$ ) of group 3. The elements of this group are the following ones: 1 or identity; two threefold rotations,

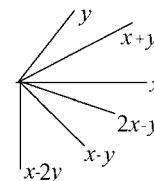
$3_{xy}^{\pm 1}$ ,  $3_{zt}^{\pm 1}$  (hence four elements); one double rotation  $3_{xy}^{\pm 1} 3_{zt}^{\pm 1}$  (hence four elements); six elements  $\bar{3}$ ; six elements  $3m$  (or 6); nine twofold rotations 2; three elements  $m$ ; three elements 1.

### 5. Study of a particular family

Table 2 lists the WPV symbols of the 38 cyclic point groups and Table 3 the WPV symbols of 15 crystal families of 5D space. Here, we give a detailed study of the (hexagon oblique)-al crystal family.

#### 5.1. Crystal cell of the (hexagon oblique)-al family

The crystal cell of the (hexagon oblique)-al family is the orthogonal product of the following three subcells: one hexagon in plane  $(xy)$ , one parallelogram (oblique cell) in plane  $(zt)$ , and one segment in a 1D space defined by axis  $u$ . Obviously, the three subspaces  $(xy)$ ,  $(zt)$  and  $(u)$  are mutually orthogonal and the choice of the axes  $x$  and  $y$  is as follows:



#### 5.2. (Hexagon oblique)-al family holohedry

The holohedry symbol of this family is easily obtained, *i.e.*  $6mm \perp 2 \perp m$ . Actually, this holohedry is the direct product of the holohedry of the three subcells generating the studied family cell. Point-group order equals  $12 \times 2 \times 2 = 48$ , *i.e.* the product of the three holohedry orders.

#### 5.3. Symbols of the 48 point operations of the (hexagon oblique)-al family holohedry

The direct product of the 12 PSOs of group  $6mm$  by the two PSOs of group 2 and then by the two PSOs of group  $m$  give the 48 PSOs of the studied family holohedry. In this group, there are 24  $PSO^+$ s and 24  $PSO^-$ s.

The 24  $PSOs^+$  are the following ones:

Identity	1
8 PSOs 2	$2_{xy} 2_{xu} 2_{yu} 2_{x+yu} 2_{2x-yu} 2_{x-2yu} 2_{zt}$
7 PSOs $\bar{1}_4$	$\bar{1}_{xyzt} \bar{1}_{xztu} \bar{1}_{yztu} \bar{1}_{x\pm y,ztu} \bar{1}_{2x-y,ztu} \bar{1}_{x-2y,ztu}$
2 PSOs 3	$3_{xy}^{\pm 1}$
2 PSOs 6	$6_{xy}^{\pm 1}$
2 PSOs 32	$3_{xy}^{\pm 1} 2_{zt}$
2 PSOs 62	$6_{xy}^{\pm 1} 2_{zt}$

The 24  $PSOs^-$  are the following ones:

Total homothetic	$\bar{1}_5$ or $\bar{1}$
8 PSOs $\bar{1}$	$\bar{1}_{xyu} \bar{1}_{xzt} \bar{1}_{yzt} \bar{1}_{ztu} \bar{1}_{x\pm yzt} \bar{1}_{2x-yzt} \bar{1}_{x-2yzt}$
7 PSOs $m$	$m_x m_y m_{x\pm y} m_{2x-y} m_{x-2y} m_u$
2 PSOs $\bar{6}$	$3_{xy}^{\pm 1} m_u$
2 PSOs $\bar{3}$	$6_{xy}^{\pm 1} m_u$
2 PSOs $\bar{6}$	$3_{xy}^{\pm 1} \bar{1}_{ztu}$
2 PSOs $\bar{3}$	$6_{xy}^{\pm 1} \bar{1}_{ztu}$

#### 5.4. Different crystallographic subgroups of the (hexagon oblique)-al family

Point group  $6mm\perp 2\perp m$  has 71 subgroups. Of these 71 subgroups, 36 belong to the families numbered I to X (see Table 3) which are overlooked here. However, some of these groups can be recalled as examples:

the subgroups of order 2:  $m$ ,  $2$ ,  $\bar{1}$ ,  $\bar{1}_4$ ,  $\bar{1}_5$  (or  $\bar{1}$ );

the subgroup of order 3:  $3$ ;

the following ten subgroups of order 4:  $222$ ,  $2\perp 2$ ,  $mm$ ,  $2\perp m$  (or  $2/m$ ),  $2.\bar{1}$ ,  $\bar{1}\perp 2$ ,  $\bar{1}\perp m$ ,  $\bar{1}_4\perp m$ ,  $\bar{1}_4.\bar{1}$ ,  $2.\bar{1}_4$ .

For instance,  $m$  belongs to the hexaclinic-al family,  $2$  to the triclinic oblique family (see Table 3).

Now, the new 35 point groups of this crystal family are studied through the list of their point operations. Consequently, a WPV symbol is suggested for each of these groups. These point groups are as follows:

(i) Six subgroups of order 6. The elements of these subgroups are listed in brackets.

$$\begin{aligned}
 32 & (1, 2_{x-yz}, 2_{2x-yz}, 2_{x-2yz}, 3_{xy}^{\pm 1}) \\
 3\perp 2 & (1, 2_u, 3_{xy}^{\pm 1}, 3_{xy}^{\pm 1} 2_u) \\
 62 & (1, 3_{xy}^{\pm 1}, 6_{xy}^{\pm 1} 2_{z+tu}, \bar{1}_{xyzt+tu}) \\
 3\perp m & (1, m_u, 3_{xy}^{\pm 1}, 3_{xy}^{\pm 1} m_u) \\
 3.\bar{1} & (1, 3_{xy}^{\pm 1}, \bar{1}_{xtu}, \bar{1}_{ytu}, \bar{1}_{x+ytu}) \\
 \bar{3} & (1, 3_{xy}^{\pm 1}, 6_{xy}^{\pm 1} m_u, \bar{1}_{xyu}).
 \end{aligned}$$

(ii) Eighteen subgroups of order 12.

$$\begin{aligned}
 62 \times \bar{1}_5 & (32) \times \bar{1}_5 \quad 62.\bar{1}_4 \quad 3m\perp m \quad (3\perp m).\bar{1}_4 \quad 3m \times \bar{1}_4 \\
 (32)\perp 2 & \quad \bar{3}m \quad 3m\perp 2 \quad \bar{3}\perp 2 \quad \bar{3}.\bar{1}_4 \quad 622 \\
 (32).\bar{1} & \quad 6\perp 2 \quad 6\perp m \quad 6.\bar{1} \quad 3\perp 2\perp m \quad \bar{3} \times \bar{1}_4.
 \end{aligned}$$

(iii) Ten subgroups of order 24.

$$\begin{aligned}
 (3m\perp m) \times \bar{1}_5 & \quad \bar{3}m \times \bar{1}_5 \quad (622)\perp 2 \quad 6mm\perp m \quad (622) \times \bar{1}_5 \\
 3m\perp 2\perp m & \quad (\bar{3}m).\bar{1}_4 \quad 6mm\perp 2 \quad 6\perp 2\perp m \quad (6.\bar{1})\perp m.
 \end{aligned}$$

(iv) One subgroup of order 48, i.e. holohedry  $6mm\perp 2\perp m$ .

#### 6. Polar crystallographic point symmetry groups of five-dimensional space

A general definition of a polar crystallographic point symmetry group in  $nD$  space has been given in Veysseyre &

Weigel (1989): 'A crystallographic point symmetry group of  $nD$  space is polar if all its elements (i.e. its PSOs) leave unchanged, point by point, a subspace of dimension  $p$  less than  $n$ .'

Consequently, any point group acting in an  $n$ -dimensional space is a polar (or ferroelectric) point group in  $n+1$ -,  $n+2$ -, ... dimensional spaces.

Therefore, the number of polar crystallographic point groups of  $n$ -dimensional space is equal to the number of crystallographic point groups of  $n-1$ -dimensional space.

Indeed, the ten point groups of 3D space acting in 2D space ( $1$ ;  $m$ ;  $2$ ;  $3$ ;  $4$ ;  $6$ ;  $mm$ ;  $3m$ ;  $4mm$ ;  $6mm$ ) are the ferroelectric (or polar) point groups of the physical space. These are all the point groups of 2D space. Two of them ( $1$  and  $m$ ) are the point groups of 1D space, so they keep all the vectors of the physical space parallel to a plane unchanged; the other eight keep all the vectors of the physical space parallel to an axis,  $z$  for example, unchanged.

For instance, among the above-listed 35 groups of the (hexagon oblique)-al crystal family:

- Groups  $32$ ;  $3\perp m$ ;  $\bar{3}$ ;  $\bar{3}m$ ;  $622$ ;  $3m\perp m$ ;  $6\perp m$ ;  $6mm\perp m$  are polar groups in 5D space. Actually, these groups act in a 3D space, as shown by their geometrical supports which contain only three vectors (see §5.4). Moreover, these groups have the same symbol as in 3D space. So they keep all the vectors of the 5D space parallel to a plane unchanged.

- Groups  $3\perp 2$ ;  $3.\bar{1}$ ;  $6.\bar{1}$ ;  $3m \times \bar{1}_4$ ;  $6\perp 2$ ;  $3m\perp 2$ ;  $6mm\perp 2$  are polar groups in 5D space. Actually, these groups act in a 4D space, as shown by their geometrical supports which contain only four vectors (see §5.4). So they keep all the vectors of the 5D space parallel to an axis unchanged. Moreover, these point groups have the same symbol in 4D space.

Consequently, every point group of 1D, 2D, 3D or 4D spaces is a polar group of 5D space.

#### 7. Conclusions

In this paper, the WPV symbols of the 196 crystallographic point groups belonging to the 'first' 15 crystal families of the 5D space have been given (Table 3).

As shown through some examples, this partial list of the point groups of 5D space allows one, thanks to their symbol, to find the order of the point group, the crystal family that it belongs to (and its cell), as well as its holohedry symbol, the dimension  $n \leq 5$  of the space in which it acts, the elements and their geometrical supports in the point group.

It is obvious that only 75 point groups of 4D space among the 227 ones are the bases of the 196 point groups of 5D space which are being studied here. But the WPV symbols of the other 152 point groups of 4D space are published in the Abstracts of the European Crystallographic Meeting in 1998 (Weigel *et al.*, 1998).

Among the 227 point groups of 4D space, 32 of them act in 1D, 2D and 3D spaces, the other 195 (227-32) acting in 4D space. If  $G$  is the symbol of one group among these 195,  $G\perp m$  is the symbol of one group acting in 5D space because PSO  $m$

acts in space defined by axis  $u$ , a straight line orthogonal to 4D space ( $xyzt$ ). Then, it is possible to know the WPV symbols together with their detailed description of 500 point symmetry groups of 5D space:

227 PGs of type  $G$  (polar groups of 5D space);

195 PGs of type  $G\perp m$ ;

78 PGs among the 196 PGs listed Table 3, which are neither  $G$  type nor  $G\perp m$  type.

Finally, WPV symbols are very useful for the tabulation and the description of the space groups in the  $nD$  spaces in the same way as the HM symbols do in the physical space.

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