Acta Cryst. (1984). A**40**, 331–337

Crystallography, Geometry and Physics in Higher Dimensions. II. Point Symmetry of Holohedries of the Two Hypercubic Crystal Systems in Four-Dimensional Space

By R. Veysseyre, D. Weigel, T. Phan and J. M. Effantin*

Laboratoire de Chimie-Physique du Solide (Equipe de Recherche Associée au CNRS) and Laboratoire de Mathématiques de la Physique, Ecole Centrale des Arts et Manufactures, 92290 *Châtenay-Malabry, France*

(*Received* 25 *April* 1983; *accepted* 3 *January* 1984)

Abstract

The interpretation of physical properties of incommensurate modulated crystals leads to the use of their point groups and their total character tables in their superspaces. Examples are chosen of point groups of holohedries of the two hypercubic crystal systems – primitive and body-centred – in four-dimensional space. A geometrical presentation is given of the point group – including its character table – of the primitive hypercubic crystal system, as it is useful for the prediction and simplification of tensorial physical properties of the corresponding crystals. Through geometrical considerations, the exceptional splitting of the hypercubic family of $\mathbb{E}^4$ into two crystal systems is easily proved. Finally, the two different relations – according to the parity of n – existing between the point group of the primitive hypercube of $\mathbb{E}^n$ and its subgroup of rotations are explained.

Introduction

Incommensurate modulated crystals do not show lattice periodicity in three-dimensional space. Accordingly, their macroscopic physical properties such as morphology, thermal expansion, *etc.* are no longer explained only by the symmetry of the basic 'crystal':

On modulated single crystals of Rb_2ZnBr_4 and Rb_2ZnCl_4, satellite faces have been observed which can be interpreted by the classical morphological theory which has been extended by including superspace-group symmetry (Janner, Rasing, Bennema & Linden, 1980; Rasing, 1982);

The continuous variation of incommensurate wavelength as a function of the temperature added to the thermal expansion of the basic structure gives the complete thermal expansion of the crystal which is a tensorial physical property – of rank 2 – of the superspace (four, five or six dimensions).

To simplify the understanding of physical properties with the aid of symmetry, it is necessary to use the point-symmetry groups (PSGs) and their character tables in superspace as we do in three-dimensional space.

In this paper, we choose the example of PSGs of the hypercube of $\mathbb{E}^4$ since most of the 227 crystallographic PSGs of four-dimensional space are subgroups of it. This example is also interesting because the hypercubic crystal family of $\mathbb{E}^4$ is particular: it splits into two crystal systems – primitive and body-centred (Neubüser, Wondratschek & Bülow, 1971; Bülow, Neubüser & Wondratschek, 1971; Wondratschek, Bülow & Neubüser, 1971) – in contrast to the square, cubic and hypercubic crystal families of $\mathbb{E}^2$, $\mathbb{E}^3$ and higher-dimensional spaces $\mathbb{E}^5$, $\mathbb{E}^6$, *etc.* each of them giving only one crystal system. With the aid of geometry, we easily explain this anomaly in § IV.

The hypercube, one of the six regular polytopes of the four-dimensional Euclidean space has been described geometrically by some authors such as Coxeter (1973). The list of symmetry operations of this polytope has been given by several authors, every type of element being characterized either by letters (Hurley, 1951) or by four symbols (Hermann, 1949). Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978) have established the character table of the group of order 384 isomorphic to the symmetry group of the hypercube: it is the group (32/21) of the family XXII. Because of the properties of the hyperstereographic projection, Whittaker (1973, 1976) has described geometrically some of its elements and has in particular listed some planes about which the elementary rotations take place, *i.e.* the geometric supports of these operations.

In this paper, we describe symmetry elements of the hypercube geometrically; we give all the twofold, threefold, fourfold, sixfold and eightfold rotation planes, *i.e.* the planes about which these rotations take place and all the hyperplanes of reflection for the negative symmetry operations; this point of view led us naturally to describe in a concrete way, through the geometry, the different classes of conjugate elements for the symmetry group of the hypercube and for its rotation subgroup. We also give concrete illustrations of notions of geometrical supports of

*Present address: DRF–DN–CENG, 38041 Grenoble Cedex, France.

0108-7673/84/040331-07$01.50 © 1984 International Union of Crystallography

point-symmetry operations (PSOs) in superspaces defined in the previous paper (Weigel, Veysseyre, Phan, Effantin & Billiet, 1984; referred to as paper I).

I. Geometric description of the hypercube

The hypercube of the four-dimensional Euclidean space may be obtained by translating a cube situated in three-dimensional space along the line orthogonal to $\mathbb{E}^3$ by a length equal to its side. It follows that it has 16 vertices or corners, 32 sides or edges, 24 faces, like any parallelotope of $\mathbb{E}^4$ (Weigel, Veysseyre & Charon, 1980).

In order to describe it analytically, we can choose a direct orthonormal basis $(0, \mathbf{i}, \mathbf{j}, \mathbf{k}, \mathbf{l})$ such that the origin 0 is the centre of the hypercube, the 16 corners having coordinates $(\pm 1, \pm 1, \pm 1, \pm 1)$. This hypercube, whose side length is 2, is limited by eight equal cubes, each pair of them belonging to hyperplanes $(\mathbf{i}, \mathbf{j}, \mathbf{k})$, $(\mathbf{i}, \mathbf{j}, \mathbf{l})$ and so on. The centres of these 'elementary' cubes are the points 0_i whose three coordinates are 0, the fourth being $+1$ or -1, for instance the point $(0, -1, 0. 0)$.

Order of the symmetry group of the hypercube

We record (Weigel *et al.*, 1980), if $a_1, \ldots, a_n$ are n points of a polytope in an n-dimensional Euclidean space defining with an invariant point 0 of this polytope a true basis, the order of the symmetry group of this polytope is given by the formula

$$N = N(a_1)N_{a_2}(a_1) \ldots N_{a_n}(a_1a_2a_3 \ldots a_{n-1}),$$

where $N_{a_i}(a_1a_2 \ldots a_{i-1})$ is the number of mappings of the vertex a_i when the points $a_1a_2 \ldots a_{i-1}$ are fixed, *i.e.* the number of vertices of the polytope situated at the same distance from a_1 as a_i, from a_2 as a_i, from a_3 as a_i, *etc.*

Before considering the hypercube, we take simple examples in order to explain this formula:

In $\mathbb{E}^2$ the square: we choose $(0a_1a_2)$ as basis (see Fig. 1) and we find $N(a_1) = 4$; $N_{a_2}(a_1) = 2$, the vertices a_2a_4 are at the same distance from the point a_1; hence: $N = 4 \times 2 = 8$.

In $\mathbb{E}^3$ the cube or the octahedron: we can visualize the octahedron as the figure formed by six points equidistant from the point 0, the three axes a_1a_4, a_2a_5, a_3a_6, being orthogonal two by two (see Fig. 2). We choose $(0a_1a_2a_3)$ as a basis and we find: $N(a_1) = 6$; $N_{a_2}(a_1) = 4$; the vertices $a_2a_3a_5a_6$ are equidistant from the point a_1; $N_{a_3}(a_1a_2) = 2$, the vertices $a_3a_2a_5a_6$ are equidistant from the point a_1, the vertices $a_3a_1a_4a_6$ are equidistant from the point a_2, thus a_3 and a_6 are equidistant from a_1 and a_2; hence $N = 6 \times 4 \times 2 = 48$.

In $\mathbb{E}^4$ we now consider the hypercube; let the points $0\ A_1A_2A_3A_9$ be chosen as basis (see Fig. 3): $N(A_1) = 16$, the 16 vertices are equidistant from the centre 0; $N_{A_2}(A_1) = 4$, the vertices $A_2A_4A_5A_9$ are equidistant from A_1; $N_{A_3}(A_1A_2) = 3$; the vertices $A_3A_6A_8A_{10}A_{12}A_{13}$ are equidistant from A_1, the vertices $A_1A_3A_6A_{10}$ are equidistant from A_2, therefore $A_3A_6A_{10}$ are equidistant from A_1 on one hand and from A_2 on the other; $N_{A_9}(A_1A_2A_3) = 2$ because $A_2A_4A_5A_9$ are equidistant from A_1, $A_4A_5A_7A_9A_{11}A_{14}$ are equidistant from A_2, $A_5A_9A_{14}A_{16}$ are equidistant from A_3, thus A_5 and A_9 are equidistant from A_1A_2 and A_3; and finally: $N = 16 \times 4 \times 3 \times 2 = 384$.

Therefore, we find by using a simple geometric method that the point-symmetry group of the hypercube of $\mathbb{E}^4$ contains 384 point-symmetry operations.*

Table 1 summarizes all these results.

Subgroup of rotations (PSO^+) *subset of* (PSO^-)

Among the symmetry operations, there appear rotations or PSO$^+$ and also PSO$^-$. Indeed, the reflection through a hyperplane orthogonal to an axis M_x^1 for instance is really an element of symmetry of this

* There exists a formula which gives the order of the symmetry group of the hypercube: $2^n n!$ (Coxeter, 1973), where n denotes the dimension of the space. We find again for the hypercube: $2^4 \times 4! = 384$. But our proof is very easy and our formula is good for any polytope of any space.

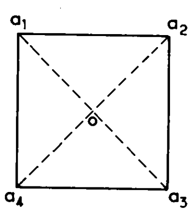

Fig. 1. Square in $\mathbb{E}^2$.

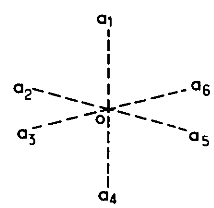

Fig. 2. Regular octahedron in $\mathbb{E}^3$.

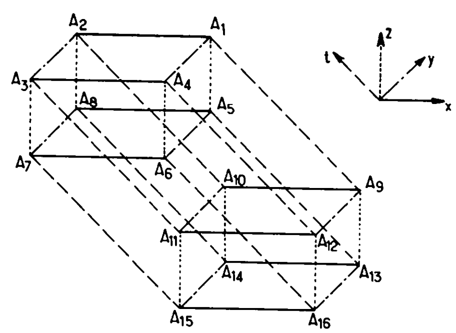

Fig. 3. Hypercube in $\mathbb{E}^4$.

Table 1. *Order of point group of regular polytopes with the symmetry of square, cube, hypercube, etc.*

Polytopes	Square	Regular octahedron	Cube	Regular Hyper-octahedron	Hypercube	Hypercube with 8 cubic hyperpyramids	Regular Hyper-octahedron	Hypercube
Dimension of Euclidean space	2	3	3	4	4	4	5	5
N_1	4	6	8	8	16	24	10	32
$N_2(a_1)$	2	4	3	6	4	8	8	5
$N_3(a_1 a_2)$		2	2	4	3	3	6	4
$N_4(a_1 a_2 a_3)$				2	2	2	4	3
$N_5(a_1 a_2 a_3 a_4)$							2	2
Order	8	48	48	384	384	1152	3840	3840
Bravais type of cells	Square p	Cubic P, F and I		Hypercubic P		Hypercubic Z-centred	Hypercubic	
Holohedric point group of crystal systems	$4mm$	$4/m\,\bar{3}\,2/m$ or O_h						

hypercube: A_1 has for mapping A_2, A_3 has for mapping A_4, and so on.

Considering that there exists at least one PSO^-, we easily show that the set of PSO^+ is an invariant subgroup of index 2. So there are 192 PSO^+ and also 192 PSO^-.

II. Symmetry elements of the hypercube

In order to simplify the presentation of this paper we first consider the 48 elements of the cube of $\mathbb{E}^3$ and we then generalize them to the space $\mathbb{E}^4$.

PSO^+ or rotations of the hypercube

Rotation identity 1^1

Rotation or (*total*) *homothetie* (-1). We recall in four-dimensional space that the total *homothetie* -1 is an entirely degenerate rotation $2^1 2^1$, the support of which is therefore not defined.

Elementary threefold rotation. Consider the ternary axes of any 'elementary' cube, *i.e.* its four diagonals. To each axis corresponds, for the hypercube, a plane about which the rotation takes place or the geometric support* of this rotation: this plane is defined by one diagonal, A_1A_7 for instance, written $x+y+z$ (instead of $\mathbf{i}+\mathbf{j}+\mathbf{k}$ for simplicity) and by the axis $\mathbf{l}$ orthogonal to the hyperplane where the cube is situated and written t for the same reason.

For each of these planes, there exists only one orthogonal plane (which intersects the first only at the point 0): it is the plane of rotation,† *i.e.* the plane in which the rotation through angle $2\pi/3$ takes place.

The plane orthogonal to the plane $(x+y+z,\ t)$ may be described by $(x-y,\ x-z)$, a simplified way of writing $(\mathbf{i}-\mathbf{j},\ \mathbf{i}-\mathbf{k})$.

* Being an elementary PSO (a single rotation) these planes are actually the geometric supports of these symmetry operations (see paper 1).

† We recall that the rotation plane always means the plane in which the rotation takes place.

Now, let the number of these elements be counted; for each one of the four types of 'elementary' cubes we can define four planes and then two angles of rotation, *i.e.* $4\times4\times2=32$ elements, hence:

32 ELEMENTARY PSO^+ written briefly $3^{1\text{ or }2}_{x\pm y,x\pm z}$.

We find two choices for the angle 3^1 or 3^2, four for the letters which do not appear in the writing of the rotation‡ and four choices for all possible combinations of signs $(++)\,(+-)\,(-+)\,(--)$, *i.e.* $2\times4\times4=32$.

Elementary twofold and fourfold rotations. In the same way, from the three fourfold axes of an 'elementary' cube, for instance x, y, z, for the cube $A_1A_2A_3A_4A_5A_6A_7A_8$, we define three planes about which rotations through angles $\pm2\pi/4$ take place. For the hypercube these planes are the planes xt, yt, zt; they are geometric supports of the corresponding PSO; thus the three planes of rotations are the planes yz, xz, xy, orthogonal to the previous planes. For the whole of the hypercube, we shall obtain $(3\times4)/2=6$ planes (each plane is counted twice). These planes of rotation are parallel to the faces of the hypercube. As there are two possible angles of rotation, we find: $6\times2=12$ elements. Hence:

12 ELEMENTARY PSO^+ $4^{1\text{ or }3}_{xy}$.

This formula gives $\binom{4}{2}=6$ choices for the pair (xy) and two choices for the angle.

In the same way, we find six planes of rotation $2\pi/2$, *i.e.*

6 ELEMENTARY PSO^+ 2^1_{xy}.

We recall that 2^1_{xy} is the rotation through the angle $2\pi/2$ in the plane (xy), *i.e.* the plane $(\mathbf{ij})$.

From the six binary axes of an elementary cube, the lines joining the middles of opposite edges, we define for the hypercube six planes of rotation $(2\pi/2)$ associated with this cube, *i.e.* $6\times4=24$ planes for the

‡ For instance, the letter t for the rotations $3^{1\text{ or }2}_{x\pm y,x\pm z}$ which generalize the eight rotations $3^{1\text{ or }2}_{x\pm y\pm z}$ of the cube in $\mathbb{E}^3$.

whole. For instance, let the axis joining the middles of A_1A_2 and A_7A_8 be considered; a vector of this axis is the vector $\mathbf{j}+\mathbf{k}$ written $y+z$; the rotation takes place about the plane $\mathbf{j}+\mathbf{k}$, $\mathbf{l}$ or $y+z$, t; the plane of rotation, orthogonal to this plane, is defined by the vectors $\mathbf{j}-\mathbf{k}$ and $\mathbf{i}$, for instance, which are written $(y-z)$ and x. Then, one of these rotations through the angle π is denoted $2^1_{y-z;x}$ and we define

24 ELEMENTARY PSO$^+$ $2^1_{x\pm y;z}$.

We may choose the pair (x, y) in $\binom{4}{2}=6$ ways; then we have two choices for the sign + or − and again two choices for the last letter z or t, *i.e.* $6\times2\times2=24$ elements.

Finally, the products of previous elements give

12 ELEMENTARY PSO$^+$ $2^1_{x\pm y,z\pm t}$,

For the planes (xy, zt) there are three different combinations: (xy, zt) $(xz, yt)(xt, yz)$ and four for the signs $(++)$ $(+-)$ $(-+)$ $(--)$.

Non-elementary fourfold rotations of type $2^14^{1\text{ or }3}$. The product of elements 2^1 and $4^{1\text{ or }3}$ gives

12 NON-ELEMENTARY PSO$^+$ $2^1_{xy}4^{1\text{ or }3}_{zt}$.

This is the product of a rotation through an angle π about the plane (xy) by a rotation through an angle $2\pi/4$ about the plane (zt) orthogonal to the previous plane.

We really obtain 12 elements as there are $\binom{4}{2}=6$ choices for a plane (xy), the other (zt) being well defined and two choices for the angle 4^1 or 4^3.

Non-elementary fourfold rotations of types 4^14^3 *or* 4^34^1. The products of previous elements give

6 NON-ELEMENTARY PSO$^+$ $4^1_{xy}4^3_{zt}$ and $4^3_{xy}4^1_{zt}$.

We have already shown that there are three different manners of choosing the pairs of planes of rotation and then two choices for the angles.

Non-elementary and degenerate rotations of type 4^14^1 *or* 4^34^3. We have seen (paper I) that a double rotation through the same angle about two orthogonal planes is degenerate and that the supports of elementary rotations, namely the two orthogonal planes, are not defined in a unique manner. This is the reason why we write these elements $4^1_{XY}4^1_{ZT}$, for instance:

$$X=\lambda x-\mu z \qquad Z=\mu x+\lambda z \qquad \lambda^2+\mu^2=1$$
$$Y=\lambda y+\mu t \qquad T=-\mu y+\lambda t \qquad \lambda,\mu\in\mathbb{R}.$$

Hence:

6 NON-ELEMENTARY AND DEGENERATE PSO$^+$ $4^1_{XY}4^1_{ZT}$ and $4^3_{XY}4^3_{ZT}$.

These last two sets of six rotations form exactly one class of conjugate elements for the symmetry group of the hypercube but form two different classes of conjugate elements for the subgroup of the rotations.

Non-elementary sixfold rotations of type $2^16^{1\text{ or }5}$. Since the *homothetie* -1 may be considered as a product of two rotations through the angle $2\pi/2$ about two orthogonal planes chosen arbitrarily, we obtain $3^1_{\alpha\beta}\times\text{hom}(-1)=6^5_{\alpha\beta}2^1_{\gamma\delta}$, where $(\alpha\beta)$ and $(\gamma\delta)$ are two orthogonal planes. Hence:

32 NON-ELEMENTARY PSO$^+$ $2^1_{x\pm y\pm z,t}6^{1\text{ or }5}_{x\pm y,x\pm z}$

are generated very simply from the elementary threefold rotations. In fact, to every $3^{1\text{ or }2}$, we associated only one element 2^1; thus $3^2_{y-z,y+t}$ gives $2^1_{y+z-t,x}6^1_{y-z,y+t}$.

Non-elementary eightfold rotations of type 88. These elements belong to two classes of conjugate elements.

The rotations of types $8^1_{\alpha\beta}8^{-3}_{\gamma\delta}$ *or* $8^{-3}_{\alpha\beta}8^1_{\gamma\delta}$. For these elements, the rotation planes are defined as

$$\alpha=(x+y)+\sqrt{2}\,t \qquad \gamma=(x+y)-\sqrt{2}\,t$$
$$\beta=(x-y)-\sqrt{2}\,z \qquad \delta=(x-y)+\sqrt{2}\,z$$

with all the possible permutations of the letter x, y, z, t. As soon as α is chosen, so are β, γ, δ. Now, to determine α, we have six choices for (xy) as we have already seen and then two choices for the last letter z or t, *i.e.* $6\times2=12$ families of orthogonal planes. We have two possible choices for the first angle $\pi/4$ (8^1) or $5\pi/4$ (8^{-3}). Hence:

24 NON-ELEMENTARY PSO$^+$ $8^1_{\alpha\beta}8^{-3}_{\gamma\delta}$ or $8^{-3}_{\alpha\beta}8^1_{\gamma\delta}$,

α, β, γ, δ being defined as previously.

In the same way, we determine

24 NON-ELEMENTARY PSO$^+$ $8^1_{\alpha\beta}8^3_{\gamma\delta}$ or $8^3_{\alpha\beta}8^1_{\gamma\delta}$,

the rotation planes being those which have just been defined.

We see that in the first case the angles of rotation differ from π and in the second case from $\pi/2$.

Same comment as for case 44. One class of conjugate elements for the symmetry group of the hypercube gives two classes for the rotation group.

Table 2 gives the list of the 192 rotations of the hypercube.

PSO$^-$ or improper rotations of the hypercube

8 PSO$^-$ are easy to illustrate.

4 ELEMENTARY PSO$^-$ $\bar{1}^1_{xyz}$

These are *homotheties* of dimension 3 about a hyperplane orthogonal to an axis.

4 ELEMENTARY PSO$^-$ M^1_x

Reflexions about a (mirror) hyperplane orthogonal to an axis or partial *homothetie* of dimension 1.

Table 2. *The 192 PSO^+s of the hypercube of* $\mathbb{E}^4$

They belong to 11 classes of conjugate elements for the group of the hypercube but to 13 for its subgroup of rotations.

PSO^+ (rotations)		Hermann–Mauguin generalized notation	Schoenflies generalized notation	‡
1 PSO^+	$e+d$	1	E	$C1$
1 PSO^+	$e+d$*	$\bar{1}^1_4$	j	$C6$
6 PSO^+	e	2^1_{xy}	$6C_2$	$C5$
12 PSO^+	e	$2^1_{x\pm y,z\pm t}$	$12C_2$	C_2
24 PSO^+	e	$2^1_{x\pm y,z}$	$24C_2$	$C8$
12 PSO^+	e	$4^{1\text{ or }3}_{xy}$	$12C_4$	$C11$
12 PSO^+	ne	$2^1_{xy}4^{1\text{ or }3}_{zt}$	$12C_2C_4$	$C15$
12 PSO^+	{6 ne / 6 $ne+d$	$4^1_{xy}4^3_{zt}$ / $4^1_{XY}4^1_{ZT}$ †	$12C_4C_4$	$C13$
48 PSO^+	{24 ne / 24 ne	$8^1_{\alpha\beta}8^{-3}_{\gamma\delta}$ or $8^{-3}_{\alpha\beta}8^1_{\gamma\delta}$ / $8^1_{\alpha\beta}8^3_{\gamma\delta}$ or $8^3_{\alpha\beta}8^1_{\gamma\delta}$	$48C_8C_8$	$C16$
32 PSO^+	e	$3^{1\text{ or }2}_{x\pm y,x\pm z}$	$32C_3$	$C17$
32 PSO^+	ne	$2^1_{x\pm y\pm z}6^{1\text{ or }5}_{x\pm y,x\pm z}$	$32C_2C_6$	$C18$

Notes:
e: elementary PSO; *ne*: non-elementary PSO; *d*: degenerate PSO.
Notation:

$$\bar{1}^1_{1D}=M^1_x=\sigma;\ \bar{1}^1_{2D}=2^1_{xy}=C_2;\ \bar{1}^1_{3D}=\bar{1}_{xyz}=i;\ \bar{1}^1_{4D}=\bar{1}^1_4=j.$$

* We recall that in $\mathbb{E}^4$, the *homothetie* -1, called $\bar{1}^1_4$ or j, is a rotation which may be written 2^12^1 but whose support is not defined (PSO entirely degenerate).

† This is a degenerate PSO, so we recall that (XY), (ZT) are not unique but verify the relations given in § II.

‡ This column gives the number of classes of conjugate elements used in Brown *et al.* (1978).

All the other PSO^- of the hypercube are obtained by finding the products of elementary rotations of the cube with a reflexion about a correctly chosen hyperplane which is equivalent to the product of the following matrices (in a correct basis):

$$\begin{pmatrix} 1 & & \\ & 1 & \\ & & \Delta\theta \end{pmatrix}\begin{pmatrix} \bar{1} & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}=\begin{pmatrix} \bar{1} & & \\ & 1 & \\ & & \Delta\theta \end{pmatrix}.$$

So we obtain:

12 ELEMENTARY PSO^- $\bar{1}^1_{x\pm y,z,t}$.

There are six manners of choosing the pair (x, y), then two choices for the sign. We can also write these 12 PSO^-: $2^1_{x\pm y,z}M^1_t$ but this notation is improper because it gives priority to one of the axes of the space $\mathbb{E}^3$ in which the PSO^- *homothetie* -1 is totally degenerate.

12 ELEMENTARY PSO^- $M^1_{x\pm y}$

32 NON-ELEMENTARY PSO^- $M^1_t3^{1\text{ or }2}_{x\pm y,x\pm z}$.

We had found 32 elements $3^{1\text{ or }2}_{x\pm y,x\pm z}$ which are multiplied by M^1_t, t being the missing letter.

32 NON-ELEMENTARY PSO^- $M^1_{x+y+z}6^{1\text{ or }5}_{x\pm y,x\pm z}$

24 NON-ELEMENTARY PSO^- $M^1_{z\pm t}4^{1\text{ or }3}_{xy}$.

Table 3. *The 192 PSO^-s of the hypercube of* $\mathbb{E}^4$

They belong to nine classes of conjugate elements.

PSO^-		Hermann–Mauguin generalized notation	Schoenflies generalized notation	†
4 PSO^-	e	$\bar{1}^1_{xyz}$	$4i$	$C7$
12 PSO^-	e	$\bar{1}^1_{x\pm y,z,t}$	$12i$	$C4$
4 PSO^-	e	M^1_x	4σ	$C9$
12 PSO^-	e	$M^1_{x\pm y}$	12σ	$C3$
32 PSO^-	ne	$M^1_t3^{1\text{ or }2}_{x\pm y,x\pm z}$	$32\sigma C_3$	$C19$
32 PSO^-	ne	$M^1_{x+y+z}6^{1\text{ or }5}_{x\pm y,x\pm z}$	$32\sigma C_6$	$C20$
24 PSO^-	ne	$M^1_z4^{1\text{ or }3}_{xy}$	$24\sigma C_4$	$C10$
48 PSO^-	ne	$M^1_{D_i}4^{1\text{ or }3}_{\alpha_i\beta_i}$	$48\sigma C_4$	$C12$
24 PSO^-	ne	$M^1_{z\pm t}4^{1\text{ or }3}_{xy}$	$24\sigma C_4$	$C14$

Notes:
e: elementary PSO; *ne*: non-elementary PSO; *d*: degenerate PSO.
Notation:

$$\bar{1}^1_{1D}=M^1_x=\sigma;\ \bar{1}^1_{2D}=2^1_{xy}=C_2;\ \bar{1}^1_{3D}=\bar{1}_{xyz}=i;\ \bar{1}^1_{4D}=\bar{1}^1_4=j.$$

† See footnote to Table 2.

There are 12 elements $4^{1\text{ or }3}_{xy}$ and one of the reflections M^1_{z+t} or M^1_{z-t} is associated with each of these.

24 NON-ELEMENTARY PSO^- $M^1_z4^{1\text{ or }3}_{xy}$.

One of the reflections M^1_z or M^1_t is associated with each of the 12 rotations $4^{1\text{ or }3}_{xy}$.

48 NON-ELEMENTARY PSO^- $M^1_{D_i}4^{1\text{ or }3}_{\alpha_i\beta_i}$.

The writing of these elements is a little complicated. Indeed, if D_i is one of the eight diagonals of the hypercube, the vectors directed along D_i $(i=1,\ldots,8)$ are: $x+y+z+t$; $x+y+z-t$; $x+y-z+t$; $x-y+z+t$; $x+y-z-t$; $x-y+z-t$; $x-y-z+t$; $x-y-z-t$.

(a_i, β_i) is a plane orthogonal to D_i and to one of the other three diagonals orthogonal to D_i. Consider, for instance, the diagonal D_1 $(x+y+z+t)$. It is orthogonal to D_2 $(x+y-z-t)$, to D_3 $(x-y-z+t)$, to D_4 $(x-y+z-t)$. One of the planes $(\alpha_i\beta_i)$ is defined by the vectors $(x-y, z-t)$ orthogonal to the plane (D_1D_2); another is defined by the vectors $(x-z, y-t)$ orthogonal to the plane (D_1D_4). When the axis D_i is chosen, there are therefore three possibilities for the plane (α, β) and two again for the angle 4^1 or 4^3. Hence, $8\times3\times2=48$ elements.

Let us write some of these:

$$M_{x+y-z-t}4^{1\text{ or }3}_{x+y,x+t};\qquad M_{x-y+z+t}4^{1\text{ or }3}_{x-t,y+z};$$

We sum up the 192 PSO^- of the hypercube in Table 3.

III. Character table of the hypercube

Our research of the point-symmetry operations of the hypercube has shown the different classes of conjugate elements, but not all the classes of the rotation subgroup.

The character table of the mathematical group isomorphic with the point group of the hypercube

Table 4. *Character table of the hypercube group in* $\mathbb{E}^4$

	$C1$	$C2$	$C3$	$C4$	$C5$	$C6$	$C7$	$C8$	$C9$	$C10$	$C11$	$C12$	$C13$	$C14$	$C15$	$C16$	$C17$	$C18$	$C19$	$C20$
	E	$12C_2$	12σ	$12i$	$6C_2$	j	$4i$	$24C_2$	4σ	$24\sigma C_4$	$12C_4$	$48\sigma C_4$	$12C_4C_4$	$24\sigma C_4$	$12C_2C_4$	$48C_8C_8$	$32C_3$	$32C_2C_6$	$32\sigma C_3$	$32\sigma C_6$
R_1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
R_2	1	1	−1	−1	1	1	1	−1	1	−1	−1	−1	1	1	−1	−1	1	1	1	1
R_3	1	1	1	1	1	1	−1	−1	−1	1	−1	1	1	−1	−1	−1	1	1	−1	−1
R_4	1	1	−1	−1	1	1	−1	1	−1	−1	1	−1	1	−1	1	1	1	1	−1	−1
R_5	2	2	0	0	2	2	2	0	2	0	0	0	2	2	0	0	−1	−1	−1	−1
R_6	2	2	0	0	2	2	−2	0	−2	0	0	0	2	−2	0	0	−1	−1	1	1
R_7	3	−1	1	1	3	3	3	1	3	1	1	−1	−1	−1	1	−1	0	0	0	0
R_8	3	−1	−1	−1	3	3	3	−1	3	−1	−1	1	−1	−1	−1	1	0	0	0	0
R_9	3	−1	1	1	3	3	−3	−1	−3	1	−1	−1	−1	1	−1	1	0	0	0	0
R_{10}	3	−1	−1	−1	3	3	−3	1	−3	−1	1	1	−1	1	1	−1	0	0	0	0
R_{11}	4	0	2	−2	0	−4	−2	0	2	0	−2	0	0	0	2	0	1	−1	−1	1
R_{12}	4	0	−2	2	0	−4	−2	0	2	0	2	0	0	0	−2	0	1	−1	−1	1
R_{13}	4	0	2	−2	0	4	2	0	−2	0	2	0	0	0	−2	0	1	−1	1	−1
R_{14}	4	0	−2	2	0	−4	2	0	−2	0	−2	0	0	0	2	0	1	−1	1	−1
R_{15}	6	−2	0	0	−2	6	0	−2	0	0	2	0	2	0	2	0	0	0	0	0
R_{16}	6	−2	0	0	−2	6	0	2	0	0	−2	0	2	0	−2	0	0	0	0	0
R_{17}	6	2	−2	−2	−2	6	0	0	0	2	0	0	−2	0	0	0	0	0	0	0
R_{18}	6	2	2	2	−2	6	0	0	0	−2	0	0	−2	0	0	0	0	0	0	0
R_{19}	8	0	0	0	0	−8	−4	0	4	0	0	0	0	0	0	0	−1	1	1	−1
R_{20}	8	0	0	0	0	−8	4	0	−4	0	0	0	0	0	0	0	−1	1	−1	1
R'_{10}	10	2	4	4	2	10	4	2	4	0	2	0	−2	0	2	0	1	1	1	1
R'_{20}	20	0	6	−6	0	−20	−6	0	6	0	−2	0	0	0	2	0	2	−2	0	0

Invariants of the first, second and third order of a symmetrical tensor

x, y, z, t belong to the representation R_{11}.

The ten components of a symmetrical tensor of second order span a space of dimension ten. We can define a representation of dimension ten for the group of the hypercube called R'_{10}; its characters are given above. This representation is reducible: $R'_{10} = R_1 \oplus R_7 \oplus R_{18}$. Possible bases are: $x^2+y^2+z^2+t^2$ for R_1; (x^2-y^2), (x^2-z^2), (x^2-t^2) for R_7; xy, xz, xt, yz, yt, zt for R_{18}.

The 20 components of a symmetrical tensor of third order span a space of dimension 20. In the same way, we define a representation of dimension 20 for the group of the hypercube called R'_{20}; its characters are given above. This representation is reducible: $R'_{20} = R_{19} \oplus R_{13} \oplus 2R_{11}$. Possible bases are: $3x(y^2-z^2)$, $3y(z^2-t^2)$, $3z(t^2-x^2)$, $3t(x^2-y^2)$, $3x(z^2-t^2)$, $3y(t^2-x^2)$, $3z(x^2-y^2)$, $3t(y^2-z^2)$ for R_{19} (8D); x^3, y^3, z^3, t^3 for one of the representations R_{11}; $x(y^2+z^2+t^2)$, $y(x^2+z^2+t^2)$, $z(y^2+t^2+x^2)$, $t(x^2+y^2+z^2)$ for the other representation R_{11}; xyz, xyt, xzt, yzt, for the representation R_{13}.

has been given by Brown *et al.* (1978). We give this table with the clear geometric meaning of the classes of conjugate elements. Further, using the theory of the projectors, we have found the invariants of the first, second and third order of a symmetrical tensor and so we obtain the whole character table: Table 4 and its caption, where are indicated the components of the tensorial physical properties.

Application

The crystals are never ferroelectric and the molecules are non-polar (Weigel & Veysseyre, 1982) because none of the four coordinates of the vector 'spontaneous polarization' or dipolar moment belong to the identity or trivial representation.

The ten components of a symmetrical tensor of second order are reduced to only one; actually only $x^2+y^2+z^2+t^2$ belongs to the irreducible trivial representation and the hyperellipsoid associated with such a tensor of $\mathbb{E}^4$ is reduced to a sphere. We deduce from this that the thermal expansion of such a crystal is isotropic or that the polarizability tensor of such a molecule is reduced to a scalar.

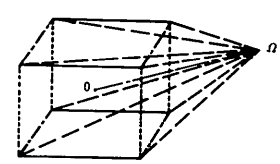

Fig. 4. Right hyperpyramid with a cubic basis in $\mathbb{E}^4$. **0Ω** is orthogonal to the hyperplane $\mathbb{E}^3$ which contains the cube whose 0 is the center. 0Ω is equal to the side length of the cube.

The 20 components of a symmetrical tensor of third order are all zero for these two groups; actually, each of the components of a tensor of odd order belongs to a representation u (*ungerade*) having the character (-1) for the degenerate rotation '*homothetie* -1'; they cannot therefore belong to the irreducible identity representation. Thus, such crystals cannot be piezoelectric in $\mathbb{E}^4$.

We must use the same method for the prediction of physical properties of any incommensurate crystal from its point group into its superspace.*

IV. Point-symmetry group of holohedry for the second hypercubic crystal system of $\mathbb{E}^4$

The regular polytope of $\mathbb{E}^4$ – called '24 cells' (Coxeter, 1973) – can be obtained by considering the 16 corners of a central hypercubic cell and the eight centres of the eight adjacent cells of a hypercubic Z (centred) lattice. This polytope contains eight cubic hyperpyramids added to the central hypercube – see Fig. 4; it is regular because the half diagonal of the

* For instance, the molecule $\Omega\pi_8$ obtained by putting eight atoms π at the same distance from the atom Ω on four lines orthogonal, two by two. It is inscribed into the hypercube of $\mathbb{E}^4$, the eight atoms occupying the eight centres of the eight cubes limiting the hypercube.

hypercube of $\mathbb{E}^4$ equals the length of its side: $4(a/2)^2 = a^2$. Accordingly, its 96 ($32+8\times 8$) edges are equal and its 24 corners are equidistant from its centre. Consequently, all corners are equivalent. From our general formula – see § I – one very quickly finds the order of its symmetry group:

$$n = 24\times 8\times 3\times 2 = 1152 = 384\times 3 \text{ (Table 1).}$$

Indeed, there are three ways of considering the eight tops of hyperpyramids among the 24 corners. So there are three sets of six fourfold planes of elementary rotations $\alpha\beta,\ldots$ and there are 36 rotations $4_{\alpha\beta}^{1\text{ or }3}$ instead of 12 for the symmetry group of the hypercube – see § II – and so on.*

This distinctive feature – the half diagonal being equal to the side of the hypercube – only occurs in four-dimensional space because $n(a/2)^2 = a^2$ if and only if $n=4$. It explains the exceptional splitting of the hypercubic family of $\mathbb{E}^4$ into two crystal systems.

Conclusion

The previous results can be generalized in an obvious manner for n-dimensional space and we can express the following theorem:

In the space of dimension n with n odd, the symmetry group of the hypercube is the direct product of the rotation subgroup and of the binary group $\bar{1}$ constituted by the identity and the total *homothetie* -1 which is here called 'inversion', *i.e.* the product of two scalar matrices. Thus, the PSO$^+$ fall into the same classes of conjugate elements for the two groups (see for instance character tables of $4/m\ \bar{3}\ 2/m$ and 432 of $\mathbb{E}^3$: PSG and rotation group of the cube).

The same result is found in $\mathbb{E}^5$ where the hypercube is bounded by ten hypercubes of $\mathbb{E}^4$, the length of a side being a and the centres being situated at a distance $a/2$ from the centre of the first hypercube on both sides of five lines orthogonal two by two.

This result is not true for the spaces $\mathbb{E}^n$ with n even as the *homothetie* -1 is in this case a rotation. It is easy to verify this property for the Abelian group of the rotations of the square in $\mathbb{E}^2$ where the four elements each belong to a class of conjugate elements, whereas they form only three classes in the PSG of the square in $\mathbb{E}^2$, $4mm$, the three classes being E, $2C_4$, C_2. In this paper we have also verified this property for the PSG of the hypercube of $\mathbb{E}^4$ and for its rotation group.

DW warmly thanks Professor A. Janner of the University of Nijmegen for fruitful discussions on these subjects.

* There are also rotations such as $12^1 12^5$ which do not belong to the symmetry group of the hypercube.

References

Brown, H., Bülow, R. Neubüser, J., Wontradschek, H. & Zassenhaus, H. (1978). *Crystallographic Groups of Four-Dimensional Space.* New York: John Wiley.
Bülow, R., Neubüser, J. & Wondratschek, H. (1971). *Acta Cryst.* **A27**, 520–523.
Coxeter, H. S. M. (1973). *Regular Polytopes.* York: Dover Publications.
Hermann, C. (1949) *Acta Cryst.* **2**, 139–145.
Hurley, A.C. (1951) *Proc. Cambridge Philos. Soc.* **47**, 650–661.
Janner, A., Rasing, T., Bennema, P. & Linden, W. H. (1980). *Phys. Rev. Lett.* **45**, 21, 37–39.
Neubüser, J., Wontratschek, H. & Bülow, R. (1971). *Acta Cryst.* **A27**, 517–520.
Rasing, T. (1982). Thesis, Nijmegen, The Netherlands.
Weigel, D. & Veysseyre, R. (1982). *C.R. Acad. Sci. Paris* Ser. II, **295**, 317–322.
Weigel, D., Veysseyre, R. & Charon, J. L. (1980). *C.R. Acad. Sci. Paris Ser. B*, **291** 287–290.
Weigel, D., Veysseyre, R., Phan, T., Effantin, J. M. & Billiet, Y. (1984). *Acta Cryst.* A **40**, 323–330.
Whittaker, E. J. W. (1973). *Acta Cryst.* **A29** 673–678, 678–684.
Whittaker, E. J. W. (1976). *Acta Cryst.* **A32**, 477–482.
Wondratschek, H., Bülow, R. & Neubüser, J. (1971). *Acta Cryst.* **A27**, 523–535.