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Crystallography, Geometry and Physics in Higher Dimensions. XIII. Tri-Incommensurate Crystal Phases

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Abstract

This paper and the following one [paper XIV; Weigel & Veysseyre (1994). *Acta Cryst.* A50, 444–450] are the fourth and fifth of a series devoted to incommensurate structures; they deal with the tri-incommensurate crystal phases. Owing to physical considerations for the vectors of modulation, the tri-incommensurate point-symmetry operations are defined and listed as well as the tri-incommensurate point-symmetry groups and the tri-incommensurate crystal families of Euclidean space E^6. The first of these two papers mainly consists of the study of the tri-incommensurate point-symmetry operations; therefore, some properties of the point-symmetry operations of Euclidean space E^6 are given. The second paper is devoted to the mono-, di- and tri-incommensurate point-symmetry groups and crystal families. Finally, a comparison between mono-, di- and tri-incommensurate structures is established.

Introduction

A crystal lattice is considered *incommensurate* if the vectors describing the main and satellite reflections may be labelled with $(3 + d)$ Miller indices as follows:

$$\mathbf{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + \sum_{i=1}^{d} m_i\mathbf{q}_i^*, \qquad (1)$$

where h, k, l and m_i are integers and

$$\mathbf{q}_i^* = \alpha_i\mathbf{a}^* + \beta_i\mathbf{b}^* + \gamma_i\mathbf{c}^*. \qquad (2)$$

One, at least, of the three entries α_i, β_i and γ_i is irrational for each value of the index i.

If $d = 1$, the structure is *mono-incommensurate* (MI) (de Wolff, 1974; Weigel & Bertaut, 1986; Veysseyre & Weigel, 1989; Phan, Veysseyre, Weigel & Grébille, 1989).

If $d = 2$, the structure is *di-incommensurate* (DI) (Janner, Janssen & de Wolff, 1983; Phan, 1989; Phan, Veysseyre & Weigel, 1991).

If $d = 3$, the structure is *tri-incommensurate* (TI).

Incommensurate structures have been studied by different scientists, mainly Janner *et al.* (1983), from the crystal structure in physical space. As in our previous paper (Phan *et al.*, 1991), we have adopted a different approach, which consists of describing a reciprocal lattice in a $(3 + d)$-dimensional space as follows:

$$\mathbf{b}_1 = \mathbf{a}^*, \quad \mathbf{b}_2 = \mathbf{b}^*, \quad \mathbf{b}_3 = \mathbf{c}^*,$$
$$\mathbf{b}_{3+i} = \mathbf{q}_i^* + d_i. \qquad (3)$$

The d vectors $\mathbf{d}_i$ are unit orthogonal vectors, orthogonal to the physical space generated by the vectors ($\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$). Moreover, the projection of the reciprocal superlattice is the experimentally observed diffraction pattern, *i.e.* the vector $\mathbf{H}$. As a consequence, the basis vectors of the direct lattice are

$$\mathbf{a}_1 = \mathbf{a} - \sum_{i=1}^{d} \alpha_i\mathbf{d}_i, \quad \mathbf{a}_2 = \mathbf{b} - \sum_{i=1}^{d} \beta_i\mathbf{d}_i,$$
$$\mathbf{a}_3 = \mathbf{c} - \sum_{i=1}^{d} \gamma_i\mathbf{d}_i, \quad \mathbf{a}_{3+i} = \mathbf{d}_i. \qquad (4)$$

They define the dual basis of the basis ($\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$, $\mathbf{b}_{3+i}$).

In this paper and in the following one, we study the tri-incommensurate (TI) structures. Then, as a conclusion, we compare the mono-, di- and tri-incommensurate structures. We begin with the study of the tri-incommensurate point-symmetry operations (TIPSOs); then, we study the tri-incommensurate point-symmetry groups (TIPSGs); finally, we study the tri-incommensurate crystal families of space E^6.

I. Different types of tri-incommensurate point-symmetry operation

A *tri-incommensurate point symmetry operation* is a point-symmetry operation (PSO) that leaves a tri-incommensurate phase invariant, this phase being a crystal in space E^6.

Table 1. *Irrational entries of the vectors* $\mathbf{q}_1^*$, $\mathbf{q}_2^*$ *and* $\mathbf{q}_3^*$

The first column gives the number of the different kinds. For instance, the first kind is the one where all the nine entries α_i, β_i and γ_i are irrational, whereas the last kind (number 23[c]) is the one with three irrational entries only. Columns 2, 3 and 4 list the irrational entries of each vector $\mathbf{q}_i^*$; zero means that the value of the corresponding entry is either zero or rational. Column 5 gives the basis in which the PSO is described. The matrices are listed in the last column. ε_i means $+1$ or -1; I is the identity matrix of space E^6. The different matrices A, B, ..., where M_2 and M_3 are the matrices of crystallographic PSOs of space E^2 and space E^3, respectively, are

$$A=\begin{bmatrix}\varepsilon_1&0&0&0&0&0\\0&\varepsilon_1&0&0&0&0\\0&0&\varepsilon_1&0&0&0\\0&0&0&\varepsilon_1&0&0\\0&0&0&0&\varepsilon_1&0\\0&0&0&0&0&\varepsilon_2\end{bmatrix},\quad B=\begin{bmatrix}\varepsilon_1&0&0&0&0&0\\0&\varepsilon_1&0&0&0&0\\0&0&\varepsilon_1&0&0&0\\0&0&0&\varepsilon_1&0&0\\0&0&0&0&\varepsilon_2&0\\0&0&0&0&0&\varepsilon_2\end{bmatrix},\quad C=\begin{bmatrix}\;&M_2&0&0&0&0\\ \;& &0&0&0&0\\0&0& M_2 & &0&0\\0&0& & &0&0\\0&0&0&0&\varepsilon&0\\0&0&0&0&0&\varepsilon\end{bmatrix},\quad D=\begin{bmatrix}\varepsilon_1&0&0&0&0&0\\0&\varepsilon_1&0&0&0&0\\0&0&\varepsilon_1&0&0&0\\0&0&0&\varepsilon_2&0&0\\0&0&0&0&\varepsilon_2&0\\0&0&0&0&0&\varepsilon_2\end{bmatrix},$$

$$E=\begin{bmatrix}\varepsilon_1&0&0&0&0&0\\0&\varepsilon_1&0&0&0&0\\0&0&\varepsilon_1&0&0&0\\0&0&0&\varepsilon_2&0&0\\0&0&0&0&\varepsilon_2&0\\0&0&0&0&0&\varepsilon_3\end{bmatrix},\quad F=\begin{bmatrix}\varepsilon&0&0&0&0&0\\0&\varepsilon&0&0&0&0\\0&0&\varepsilon&0&0&0\\0&0&0&\varepsilon&0&0\\0&0&0&0& M_2 & \\0&0&0&0& & \end{bmatrix},\quad G=\begin{bmatrix}\varepsilon_1&0&0&0&0&0\\0&\varepsilon_1&0&0&0&0\\0&0&\varepsilon_2&0&0&0\\0&0&0&\varepsilon_2&0&0\\0&0&0&0&\varepsilon_3&0\\0&0&0&0&0&\varepsilon_3\end{bmatrix},\quad H=\begin{bmatrix} & & &0&0&0\\ &M_3& &0&0&0\\ & & &0&0&0\\0&0&0& & & \\0&0&0& &M_3& \\0&0&0& & & \end{bmatrix}.$$

No.	$\mathbf{q}_1(\alpha_1\beta_1\gamma_1)$	$\mathbf{q}_2(\alpha_2\beta_2\gamma_2)$	$\mathbf{q}_3(\alpha_3\beta_3\gamma_3)$	Bases	Matrices
1	$\alpha_1\ \beta_1\ \gamma_1$	$\alpha_2\ \beta_2\ \gamma_2$	$\alpha_3\ \beta_3\ \gamma_3$	$a_1\ a_2\ a_3\ a_4\ a_5\ a_6$	εI
2	$\alpha_1\ \beta_1\ \gamma_1$	$\alpha_2\ \beta_2\ \gamma_2$	$\alpha_3\ \beta_3\ 0$	$a_1\ a_2\ a_3\ a_4\ a_5\ a_6$	εI
3	$\alpha_1\ \beta_1\ \gamma_1$	$\alpha_2\ \beta_2\ 0$	$\alpha_3\ \beta_3\ 0$	$a_1\ a_2\ a_3\ a_4\ a_5\ a_6$	εI
4	$\alpha_1\ \beta_1\ \gamma_1$	$\alpha_2\ 0\ \gamma_2$	$\alpha_3\ \beta_3\ 0$	$a_1\ a_2\ a_3\ a_4\ a_5\ a_6$	εI
5	$\alpha_1\ \beta_1\ \gamma_1$	$\alpha_2\ \beta_2\ \gamma_2$	$\alpha_3\ 0\ 0$	$a_1\ a_2\ a_3\ a_4\ a_5\ a_6$	εI
6	$\alpha_1\ \beta_1\ \gamma_1$	$\alpha_2\ \beta_2\ 0$	$\alpha_3\ 0\ 0$	$a_1\ a_2\ a_3\ a_4\ a_5\ a_6$	εI
7	$\alpha_1\ \beta_1\ \gamma_1$	$0\ \beta_2\ \gamma_2$	$\alpha_3\ 0\ 0$	$a_1\ a_2\ a_3\ a_4\ a_5\ a_6$	εI
8	$\alpha_1\ \beta_1\ 0$	$\alpha_2\ \beta_2\ 0$	$\alpha_3\ \beta_3\ 0$	$a_1\ a_2\ a_4\ a_5\ a_6\ a_3$	A
9	$\alpha_1\ \beta_1\ 0$	$\alpha_2\ \beta_2\ 0$	$\alpha_3\ 0\ \gamma_3$	$a_1\ a_2\ a_3\ a_4\ a_5\ a_6$	εI
10	$\alpha_1\ \beta_1\ 0$	$\alpha_2\ 0\ \gamma_2$	$0\ \beta_3\ \gamma_3$	$a_1\ a_2\ a_3\ a_4\ a_5\ a_6$	εI
11	$\alpha_1\ \beta_1\ 0$	$\alpha_2\ \beta_2\ 0$	$\alpha_3\ 0\ 0$	$a_1\ a_2\ a_4\ a_5\ a_6\ a_3$	A
12	$\alpha_1\ \beta_1\ 0$	$\alpha_2\ 0\ \gamma_2$	$\alpha_3\ 0\ 0$	$a_1\ a_2\ a_3\ a_4\ a_5\ a_6$	εI
13[a]	$\alpha_1\ \beta_1\ 0$	$\alpha_2\ \beta_2\ 0$	$0\ 0\ \gamma_3$	$a_1\ a_2\ a_4\ a_5\ a_3\ a_6$	B
13[b]	$k\ k\ 0$	$k\ k\ 0$	$0\ 0\ \gamma_3$	$a_1\ a_2\ a_4\ a_5\ a_3\ a_6$	C
14	$\alpha_1\ \beta_1\ 0$	$\alpha_2\ 0\ \gamma_2$	$0\ 0\ \gamma_3$	$a_1\ a_2\ a_3\ a_4\ a_5\ a_6$	εI
15	$\alpha_1\ \beta_1\ \gamma_1$	$\alpha_2\ 0\ 0$	$0\ \beta_3\ 0$	$a_1\ a_2\ a_3\ a_4\ a_5\ a_6$	εI
16	$\alpha_1\ \beta_1\ \gamma_1$	$\alpha_2\ 0\ 0$	$\alpha_3\ 0\ 0$	$a_1\ a_2\ a_3\ a_4\ a_5\ a_6$	εI
17	$\alpha_1\ \beta_1\ 0$	$\alpha_2\ 0\ 0$	$\alpha_3\ 0\ 0$	$a_1\ a_2\ a_4\ a_5\ a_6\ a_3$	A
18	$\alpha_1\ \beta_1\ 0$	$\alpha_2\ 0\ 0$	$0\ \beta_3\ 0$	$a_1\ a_2\ a_4\ a_5\ a_6\ a_3$	A
19	$\alpha_1\ \beta_1\ 0$	$0\ 0\ \gamma_2$	$0\ 0\ \gamma_3$	$a_1\ a_2\ a_4\ a_3\ a_5\ a_6$	D
20	$\alpha_1\ \beta_1\ 0$	$0\ \beta_2\ 0$	$0\ 0\ \gamma_3$	$a_1\ a_2\ a_4\ a_5\ a_3\ a_6$	B
21	$\alpha_1\ 0\ 0$	$\alpha_2\ 0\ 0$	$0\ \beta_3\ 0$	$a_1\ a_4\ a_5\ a_2\ a_6\ a_3$	E
22	$\alpha_1\ 0\ 0$	$\alpha_2\ 0\ 0$	$\alpha_3\ 0\ 0$	$a_1\ a_4\ a_5\ a_6\ a_2\ a_3$	F
23[a]	$\alpha_1\ 0\ 0$	$0\ \beta_2\ 0$	$0\ 0\ \gamma_3$	$a_1\ a_4\ a_2\ a_5\ a_3\ a_6$	G
23[b]	$k\ 0\ 0$	$0\ k\ 0$	$0\ 0\ \gamma_3$	$a_1\ a_2\ a_4\ a_5\ a_3\ a_6$	C
23[c]	$k\ 0\ 0$	$0\ k\ 0$	$0\ 0\ k$	$a_1\ a_2\ a_3\ a_4\ a_5\ a_6$	H

The different types of TIPSO result from a study of all possible distributions of irrational entries occurring in (2), *i.e.* in the three vectors $\mathbf{q}_i^*$:

$$\mathbf{q}_i^* = \alpha_i\mathbf{a}^* + \beta_i\mathbf{b}^* + \gamma_i\mathbf{c}^* \quad (i = 1, 2, 3).$$

The vectors describing the crystal cell of a TI structure, in space E^6, are

$$\mathbf{a}_1 = \mathbf{a} - \alpha_1\mathbf{d}_1 - \alpha_2\mathbf{d}_2 - \alpha_3\mathbf{d}_3, \quad \mathbf{a}_4 = \mathbf{d}_1,$$

$$\mathbf{a}_2 = \mathbf{b} - \beta_1\mathbf{d}_1 - \beta_2\mathbf{d}_2 - \beta_3\mathbf{d}_3, \quad \mathbf{a}_5 = \mathbf{d}_2,$$

$$\mathbf{a}_3 = \mathbf{c} - \gamma_1\mathbf{d}_1 - \gamma_2\mathbf{d}_2 - \gamma_3\mathbf{d}_3, \quad \mathbf{a}_6 = \mathbf{d}_3.$$

The study of all possible distributions of irrational entries α_i, β_i and γ_i results in the 23 kinds listed in Table 1 or, in fact, 26 kinds, if we take the particular cases into account. In this table, we have only written the irrational entries of each vector $\mathbf{q}_i^*$; zero means that the value of the corresponding entry is either zero or rational.

We explain the method through three examples.

(1) Kind 8 corresponds to

$$\mathbf{q}_i^* = \alpha_i\mathbf{a}^* + \beta_i\mathbf{b}^* \quad (i = 1, 2, 3),$$

i.e. six irrational entries ($\gamma_1 = \gamma_2 = \gamma_3 = 0$). Therefore, the basis vectors of the direct lattice are

$$\begin{aligned} \mathbf{a}_1 &= \mathbf{a} - \alpha_1\mathbf{d}_1 - \alpha_2\mathbf{d}_2 - \alpha_3\mathbf{d}_3, & \mathbf{a}_4 &= \mathbf{d}_1, \\ \mathbf{a}_2 &= \mathbf{b} - \beta_1\mathbf{d}_1 - \beta_2\mathbf{d}_2 - \beta_3\mathbf{d}_3, & \mathbf{a}_5 &= \mathbf{d}_2, \\ \mathbf{a}_3 &= \mathbf{c}, & \mathbf{a}_6 &= \mathbf{d}_3. \end{aligned}$$

Vector $\mathbf{a}_3$ is the only one that does not depend on the modulation vectors $\mathbf{d}_i$; consequently, the corresponding TIPSO can be regarded as the commutative product of two PSOs:

(i) the first one maps each element of the set ($\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_4$, $\mathbf{a}_5$, $\mathbf{a}_6$) onto itself or onto its opposite and leaves $\mathbf{a}_3$ unchanged;

(ii) the second one acts on $\mathbf{a}_3$; therefore, it maps $\mathbf{a}_3$ onto $\mathbf{a}_3$ or onto its opposite and leaves the set ($\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_4$, $\mathbf{a}_5$, $\mathbf{a}_6$) unchanged.

With respect to the basis ($\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_4$, $\mathbf{a}_5$, $\mathbf{a}_6$, $\mathbf{a}_3$), the matrices of these PSOs are

$$\begin{bmatrix} \varepsilon_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \varepsilon_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \varepsilon_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \varepsilon_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & \varepsilon_2 \end{bmatrix} = \begin{bmatrix} \varepsilon_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \varepsilon_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \varepsilon_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon_1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \varepsilon_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & \varepsilon_2 \end{bmatrix},$$

where ε_i equals $+1$ or -1; ε_1 and ε_2 are independent.

The types of these PSOs are 1 or identity, $\overline{1}_5$ or total *homothetie* of ratio (-1) in the hyperplane ($\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_4$, $\mathbf{a}_5$, $\mathbf{a}_6$), m (reflection through the same hyperplane), $\overline{1}_6$ or total *homothetie* of ratio (-1) in space E^6.

(2) Kind 21 corresponds to

$$\mathbf{q}_1^* = \alpha_1\mathbf{a}^*, \quad \mathbf{q}_2^* = \alpha_2\mathbf{a}^*, \quad \mathbf{q}_3^* = \beta_3\mathbf{b}^*,$$

i.e. three irrational entries. The basis vectors of the direct lattice are

$$\begin{aligned} \mathbf{a}_1 &= \mathbf{a} - \alpha_1\mathbf{d}_1 - \alpha_2\mathbf{d}_2, & \mathbf{a}_4 &= \mathbf{d}_1, \\ \mathbf{a}_2 &= \mathbf{b} - \beta_3\mathbf{d}_3, & \mathbf{a}_5 &= \mathbf{d}_2, \\ \mathbf{a}_3 &= \mathbf{c}, & \mathbf{a}_6 &= \mathbf{d}_3. \end{aligned}$$

$\mathbf{a}_3$ is the only vector that does not depend on the modulation vectors $\mathbf{d}_i$. $\mathbf{a}_2$ depends on the modulation vector $\mathbf{d}_3$ whereas $\mathbf{a}_1$ depends on $\mathbf{d}_1$ and $\mathbf{d}_2$. Therefore, with respect to the basis ($\mathbf{a}_1$, $\mathbf{a}_4$, $\mathbf{a}_5$, $\mathbf{a}_2$, $\mathbf{a}_6$, $\mathbf{a}_3$), the matrix of the corresponding TIPSO is

$$\begin{bmatrix} \varepsilon_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \varepsilon_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \varepsilon_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon_2 & 0 & 0 \\ 0 & 0 & 0 & 0 & \varepsilon_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & \varepsilon_3 \end{bmatrix},$$

where, as previously, ε_i equals $+1$ or -1 and ε_1, ε_2 and ε_3 are independent. The different types of TIPSO corresponding to this kind are

$$1, \quad \overline{1}_3, \quad \overline{1}_4, \quad \overline{1}_5, \quad \overline{1}_6, \quad 2, \quad m.$$

We recall that the PSO denoted 2 is the simple rotation through the angle π in the plane defined by the vectors $\mathbf{a}_2$ and $\mathbf{a}_6$; $\overline{1}_3$ is generally written $\overline{1}$.

(3) Finally, we study kind 22, which corresponds to

$$\mathbf{q}_1^* = \alpha_1\mathbf{a}^*, \quad \mathbf{q}_2^* = \alpha_2\mathbf{a}^*, \quad \mathbf{q}_3^* = \alpha_3\mathbf{a}^*.$$

The basis vectors of the direct lattice are

$$\begin{aligned} \mathbf{a}_1 &= \mathbf{a} - \alpha_1\mathbf{d}_1 - \alpha_2\mathbf{d}_2 - \alpha_3\mathbf{d}_3, & \mathbf{a}_4 &= \mathbf{d}_1, \\ \mathbf{a}_2 &= \mathbf{b}, & \mathbf{a}_5 &= \mathbf{d}_2, \\ \mathbf{a}_3 &= \mathbf{c}, & \mathbf{a}_6 &= \mathbf{d}_6. \end{aligned}$$

As vectors $\mathbf{a}_2$ and $\mathbf{a}_3$ do not depend on the modulation vectors, a TIPSO can act without restriction on $\mathbf{a}_2$ and $\mathbf{a}_3$. With respect to the basis ($\mathbf{a}_1$, $\mathbf{a}_4$, $\mathbf{a}_5$, $\mathbf{a}_6$, $\mathbf{a}_2$, $\mathbf{a}_3$), the matrices of the corresponding PSOs are of the form

$$\begin{bmatrix} \varepsilon & 0 & 0 & 0 & 0 & 0 \\ 0 & \varepsilon & 0 & 0 & 0 & 0 \\ 0 & 0 & \varepsilon & 0 & 0 & 0 \\ 0 & 0 & 0 & \varepsilon & 0 & 0 \\ 0 & 0 & 0 & 0 & \multicolumn{2}{c}{\multirow{2}{*}{M_2}} \\ 0 & 0 & 0 & 0 & & \end{bmatrix},$$

where M_2 is the matrix of a general PSO of space E^2.

Table 2. *The nine types of TIPSO*

The number of different types is in the first column, the matrix in the second one, the type of the corresponding PSO is in the third one and the corresponding kinds previously found are in the last column.

No.	Matrices	PSOs	Previous numbers
I	εI	$1, \bar{1}_6$	1, 2, 3, 4, 5, 6, 7, 9, 10, 12, 14, 15, 16
II	A	$1, \bar{1}_5, \bar{1}_6$ m	8, 11, 17, 18
III	B	$1, \bar{1}_4, \bar{1}_6$ 2	13^a, 20
IV	D	$1, \bar{1}_3, \bar{1}_6$	19
V	E	$1, \bar{1}_3, \bar{1}_4, \bar{1}_5, \bar{1}_6$ $2, m$	21
VI	G	$1, \bar{1}_4, \bar{1}_6$ 2	23^a
VII	F	$1, \bar{1}_4, \bar{1}_5, \bar{1}_6$ 2, 3, 4, 6 m $\bar{1}_4 3, \bar{1}_4 4, \bar{1}_4 6$	22
VIII	C	$1, \bar{1}_4, \bar{1}_6$ 2 33, 44, 66 332, 442, 662	13^b, 23^b
IX	H	$1, \bar{1}_4, \bar{1}_6$ 2 33, 44, 66 332, 442, 662	23^c

Table 3. *The four general types of TIPSO*

The first column gives the name of the type, *i.e.* *a*, *b*, *c* or *d*, the second one, the corresponding matrices, the third one the WPV symbols and the last one the previous numbering.

Type	Matrices	PSOs	Previous numbers
a	F	1 2, 3, 4, 6 m $\bar{1}_4, \bar{1}_5, \bar{1}_6$ $\bar{1}_4 3, \bar{1}_4 4, \bar{1}_4 6$	I, III, VII
b	E	1 $m, 2, \bar{1}, \bar{1}_4, \bar{1}_5, \bar{1}_6$	II, IV, V
c	H	1 $2, \bar{1}_4, \bar{1}_6$ 33, 44, 66 332, 442, 662	VIII, IX
d	G	1 $2, \bar{1}_4, \bar{1}_6$	VI

As a result, the types of the corresponding TIPSOs are

$$1,\ \bar{1}_4,\ m,\ 2,\ 3,\ 4,\ 6,$$
$$\bar{1}_5,\ \bar{1}_6,\ \bar{1}_4 3,\ \bar{1}_4 4,\ \bar{1}_4 6.$$

We explain some of these symbols of point-symmetry operations of space E^6:

(i) PSO $\bar{1}_4 3$, is the product of the total *homothetie* of ratio (-1) in the four-dimensional space ($\mathbf{a}_1$, $\mathbf{a}_4$, $\mathbf{a}_5$, $\mathbf{a}_6$) and of the simple rotation 3 through the angle $2\pi/3$ or $4\pi/3$ in the plane ($\mathbf{a}_2$, $\mathbf{a}_3$).

(ii) PSOs $\bar{1}_4 4$ and $\bar{1}_4 6$ are similarly defined.

These symbols (WPV symbols) are explained by Weigel, Phan & Veysseyre (1987).

Table 4. *The irrational entries of the vectors corresponding to each of the four types of TIPSO*

Type	q_1^* ($\alpha_1\ \beta_1\ \gamma_1$)	q_2^* ($\alpha_2\ \beta_2\ \gamma_2$)	q_3^* ($\alpha_3\ \beta_3\ \gamma_3$)
d	(α_1 0 0)	(0 β_2 0)	(0 0 γ_3)
c	(k k 0)	(k k 0)	(0 0 γ_3)
	(k 0 0)	(0 k 0)	(0 0 γ_3)
	(k 0 0)	(0 k 0)	(0 0 k)
b	(α_1 β_1 0)	(α_2 β_2 0)	(α_3 β_3 0)
	(α_1 β_1 0)	(α_2 β_2 0)	(α_3 0 0)
	(α_1 β_1 0)	(α_2 0 0)	(α_3 0 0)
	(α_1 β_1 0)	(α_2 0 0)	(0 β_3 0)
	(α_1 β_1 0)	(0 0 γ_2)	(0 0 γ_3)
	(α_1 0 0)	(α_2 0 0)	(0 β_3 0)
a		All the other possibilities	

Table 5. *The* 19 *types of TIPSO*

Among the 78 types of crystallographic PSOs of space E^6, only 19 types are TIPSOs

1
m
2, 3, 4, 6
$1, \bar{1}_4, \bar{1}_5, \bar{1}_6$
33, 44, 66
332, 442, 662
$\bar{1}_4 3, \bar{1}_4 4, \bar{1}_4 6$

Table 6. *The* 57 *tri-incommensurate PSGs*

The first column gives the WPV symbol of the group, the second one the types of the PSOs that generate the groups and the last one the number of PSGs belonging to the corresponding type. The underlined symbols are the holohedries of TI crystal families. The last two lines of type *c* are abridged symbols of the 'monoclinic di cubic' family. Its cell includes two equal cubes belonging to two nonorthogonal spaces. This was used for describing a TI cubic wüstite (Weigel, Veysseyre & Carel, 1987). For instance, as we will explain in a next paper, the whole symbol of the holohedry is 44/2, 662, $\bar{1}_4/2$ and we abridge it into 2, 662, 2 as m, $\bar{3}$, m is the abbreviation of $4/m$, $\bar{3}$, $2/m$.

PSGs	Types of PSO	Number of PSGs
$1;\ \underline{\bar{1}_6};\ \bar{1}_4;\ 2;\ \underline{\bar{1}_4 \perp 2}$	*a*, *b*, *c*, *d*	5
$\underline{1_5};\ m;\ \underline{\bar{1}_5 \perp m}$	*a*, *b*	3
$m \perp m;\ \bar{1}_4 \perp m;\ 2, \bar{1}_5, \bar{1}_5;\ \underline{\bar{1}_4 \perp m \perp m};$		
$4;\ \bar{1}_4 4;\ \bar{1}_4 \perp 4;\ 4\ m\ m;\ \bar{1}_4 4\ m;$		
$4, \bar{1}_5 \bar{1}_5;\ \underline{\bar{1}_4 \perp 4\ m\ m};$	*a*	23
$3;\ 6;\ 3, m;\ 6\ m\ m;\ \bar{1}_4 \perp 3;\ \bar{1}_4 \perp 6;$		
$\bar{1}_4 \perp 3\ m;\ \bar{1}_4 6;\ 3, \bar{1}_5;\ 6, \bar{1}_5, \bar{1}_5; \bar{1}_4 6, \bar{1}_5, m;\ \underline{\bar{1}_4 \perp 6\ m\ m}$		
$\bar{1};\ \underline{\bar{1} \perp \bar{1}};$	*b*	6
$\bar{1} \perp 2;\ \bar{1} \perp m;\ 2 \perp m;\ \underline{\bar{1} \perp 2 \perp m}$		
$44^*;\ \underline{44^* \perp 2};$		
$33^*;\ 66^*;\ 33^* \perp 2;\ \underline{66^* \perp 2};$		
$2, 44^*;\ 2, 44^*, 2 \perp 2;$	*c*	17
$2, 66^*, 2;\ 33^*, 2;\ 33^*, 2 \perp 2;\ \underline{2, 66^*, 2 \perp 2}$		
$\bar{1}_4, 33;\ \bar{1}_4, 662;\ 44, 33, \bar{1}_4;$		
$442, 33, 2;\ \underline{2, 662, 2}$		
$2 \perp 2;\ \bar{1}_4, \bar{1}_4;\ \underline{2 \perp 2 \perp 2}$	*d*	3

All 23 kinds have been studied in the same way. Several kinds can be put together in one type and, at a first stage, the result is the nine types of TIPSO listed in Table 2.

Table 7. *Tri-incommensurate crystal families of space E^6*

The names of the TI crystal families are given in the first column, the WPV symbols of their holohedries are to be found in the second column and the order of these holohedries in the third one. The subgroups of each holohedry are listed in the fourth column and their order in the fifth one. In the last column are the numbers of TIPSGs belonging to each TI crystal family. The 57 PSGs are classified family by family.

Name of the family	WPV symbols of the holohedry	Order	WPV symbols of the TIPSGs	Order	Number of TIPSGs
15-Clinic	$\bar{1}_6$	2	1	1	2
Decaclinic-al	$\bar{1}_5 \perp m$	4	$\bar{1}_5$; m	2	3
Hexaclinic oblic	$\bar{1}_4 \perp 2$	4	$\bar{1}_4$; 2	2	3
Di-Triclinic	$\bar{1} \perp \bar{1}$	4	$\bar{1}$	2	2
Hexaclinic rectangle	$\bar{1}_4 \perp m \perp m$	8	$\bar{1}_4 \perp m$; $m \perp m$; 2, $\bar{1}_5$, $\bar{1}_5$	4	4
Hexaclinic square	$\bar{1}_4 \perp 4\,m\,m$	16	4; $\bar{1}_4 4$	4	
			$\bar{1}_4 \perp 4$; $4\,m\,m$; 4, $\bar{1}_5$, $\bar{1}_5$; $\bar{1}_4 4$, $\bar{1}_5$, m	8	7
			3	3	
Hexaclinic hexagon	$\bar{1}_4 \perp$ 6 m m	24	$\bar{1}_4 3$; 6; $\bar{1}_4 6$; $3\,m$; $3\,\bar{1}_5$	6	12
			$\bar{1}_4 \perp 3\,m$; $\bar{1}_4 \perp 6$; $6\,m\,m$; 6, $\bar{1}_5$, $\bar{1}_5$; $\bar{1}_4 6$, $\bar{1}_5$, m	12	
Triclinic oblic-al	$\bar{1} \perp 2 \perp m$	8	$\bar{1} \perp 2$; $\bar{1} \perp m$; $2 \perp m$	4	4
Tri oblic	$2 \perp 2 \perp 2$	8	$2 \perp 2$; $\bar{1}_4$, $\bar{1}_4$, $\bar{1}_4$	4	3
Diclinic di square oblic	$44^* \perp 2$	8	44^*	4	2
Diclinic di hexagon oblic	$66^* \perp 2$	12	33^*	3	
			66^*; $33^* \perp 2$	6	4
Monoclinic di square oblic	2, $44^* \perp 2$	16	2, 44^*, 2	8	2
Monoclinic di hexagon oblic	2, 66^*, $2 \perp 2$	24	33^*, 2	6	
			2,66^*, 2; 33^*, $2 \perp 2$	12	4
Monoclinic di cubic	2, 662, 2	48	$\bar{1}_4$, 33	12	
			2, 33; 44, 33, $\bar{1}_4$; 442, 33, 2	24	5

Table 8. *Separation of physical and additional space*

In this table, we separate physical space and additional space. For each TI crystal family, columns 1, 2 and 3, respectively, give the basis (in space E^6), the name of the family and the WPV symbol of the holohedry; then, the following two columns give the name and symbol of the physical part of the TI crystal family; the last column gives the symbol of the additional part of the TI crystal family according to the nomenclature of Janner *et al.* (1983).

E^6			Physical space E^3		
Bases	Families	Holohedries	Families	Holohedries	Additional space
(x, y, z, t, u, v)	15-clinic	$\bar{1}_6$	Triclinic	$\bar{1}$	$\bar{1}$
(x, y, t, u, v, z)	Decaclinic-al	$\bar{1}_5 \perp m$	Monoclinic	$2/m$	$\bar{1}$ 1
(x, y, t, u, z, v)	Hexaclinic oblic	$\bar{1}_4 \perp 2$	Monoclinic	$2/m$	$2/m$
(x, y, t, z, u, v)	Di triclinic	$\bar{1} \perp \bar{1}$	Monoclinic	$2/m$	$m/2$
(x, t, u, y, v, z)	Triclinic oblic-al	$\bar{1} \perp 2 \perp m$	Orthorhombic	mmm	$\bar{1}\ 2\ m$
(x, t, y, u, z, v)	Tri oblic	$2 \perp 2 \perp 2$	Orthorhombic	mmm	mmm
(x, t, u, v, y, z)	Hexaclinic oblic	$\bar{1}_4 \perp 2$	Monoclinic	$2/m$	1 $\bar{1}$
	Hexaclinic-rectangle	$\bar{1}_4 \perp m \perp m$	Orthorhombic	mmm	$\bar{1}$ 1 1
	Hexaclinic square	$\bar{1}_4 \perp 4mm$	Tetragonal	$4/mmm$	1 $\bar{1}$ 1 1
	Hexaclinic-hexagon	$\bar{1}_4 \perp 6mm$	Hexagonal	$6/mmm$	1 $\bar{1}$ 1 1
(x, y, t, u, z, v)	Diclinic di square oblic	$44^* \perp 2$	Tetragonal	$4/m$	$4/m$
	Diclinic di hexagon oblic	$66^* \perp 2$	Hexagonal	$6/m$	$6/m$
		$3^* \perp 2$	Hexagonal	6	6
	Monoclinic-di square oblic	44^*, $2 \perp 2$	Tetragonal	$4/mmm$	$4/mmm$
	Monoclinic-di hexagon oblic	66^*, $2 \perp 2$	Hexagonal	$6/mmm$	$6/mmm$
(x, y, z, t, u, v)	Monoclinic di cubic	2,662,2	Cubic	$m\,\bar{3}\,m$	$m\,\bar{3}\,m$

However, it is possible to put together these nine types in only four general kinds, numbered a, b, c and d, which are listed in Table 3, the values of the irrational entries being given in Table 4.

In conclusion, among the 78 types of crystallographic PSOs of space E^6 (Veysseyre, Veysseyre & Weigel, 1990), only 19 types of TIPSO appear (Table 5).

In Tables 3, 4, and 5, we use WPV symbols for PSOs of space E^4 or E^6. For instance, we recall that 33 is the symbol of a PSO in space E^4: a double rotation through the angle $2\pi/3$ in a plane and through the angle $2\pi/3$ in the orthogonal plane. Similarly, 662 is the symbol of PSO in space E^6: a triple rotation in three planes orthogonal two by two and through the angles $2\pi/6$, $2\pi/6$ and $2\pi/2$, respectively.

II. Tri-incommensurate point-symmetry groups of E^6

(1) A point-symmetry group of E^6 is considered *tri-incommensurate* if it is composed of PSOs belonging to only one type of TIPSO listed in Table 2.

For instance, let us consider the group $\bar{1} \perp 2 \perp m$. This is a group of order 8, holohedry of the crystal family of space E^6, called 'triclinic oblic-al'. The cell of this family is a right hyperprism whose basis is the rectangular product of the triclinic cell, in a space E^3, and of the parallelogram (oblic) cell in the space E^2 orthogonal to the space E^3. We suggest the abbreviation 'al' for the long expression 'right hyperprism based on ...' and the name 'oblic' instead of parallelogram. So 'oblic-al' means right prism based on a parallelogram; it is generally called 'monoclinic'. Moreover, the names 'orthogonal or rectangular product' are omitted. Some examples will be given in paper XIV.

With respect to the basis ($\mathbf{a}_1$, $\mathbf{a}_4$, $\mathbf{a}_5$, $\mathbf{a}_2$, $\mathbf{a}_6$, $\mathbf{a}_3$) or (x, t, u, y, v, z), the eight PSOs of this group are

$$1,\quad \overline{1}_{xtu},\quad 2_{yv},\quad m_z,\quad \overline{1}_{xytuv},\quad \overline{1}_{xztu},\quad \overline{1}_{yzv},\quad \overline{1}_6.$$

All these PSOs are of kind 21, *i.e.* type V. Therefore, the point group $\overline{1}\perp 2\perp m$ is a TIPSG.

(2) The 57 different TIPSGs of space E^6, generated by all the TIPSOs of this space, are listed in Table 6. Thus, we can notice that:

five PSGs belong to the four types;
three PSGs belong to types *a* and *b*;
23 PSGs belong to type *a*;
six PSGs belong to type *b*;
17 PSGs belong to type *c*;
three PSGs belong to type *d*.

III. Tri-incommensurate crystal families of E^6

A crystal family of space E^6 is a *tri-incommensurate crystal family* if and only if it is composed of TIPSGs.

Owing to our geometrical method of constructing the crystal families of an n-dimensional space (Veysseyre, Weigel & Phan, 1993) and owing to the list of TIPSOs of space E^6 (see Table 6), we easily obtain the TI crystal families of this space. They are listed in Table 7. The result is the existence of 14 TI crystal families.

This method enables us to find all TI crystal families of space E^6 as well as the TI PSGs, *i.e.* the holohedries of these families and their subgroups. These subgroups will be studied in the second part of this series.

Moreover, it is possible to separate the physical structure from the additional incommensurate dimensions. The method is explained through the following three examples:

(1) The first example is that of the '15-clinic family'; its holohedry is the group $\overline{1}_6$ of order 2. In space E^6, the two PSOs of this group are

(i) the identity

(ii) the total *homothetie* of ratio (-1) and of dimension 6; this PSO is $\overline{1}_{xyztuv}$.

In physical space E^3, the corresponding PSOs are 1 (identity) and $\overline{1}_{xyz}$, which generate a group of order 2, *i.e.* the holohedry of the 'triclinic family'.

Table 9. *Incommensurate PSOs*

The first column gives the list of the MIPSOs, the second the list of the DIPSOs, and the third the TIPSOs. The symbols of these PSOs are the Hermann–Mauguin symbols (1, m, 2, 3, 4, 6, ...) or the WPV symbols (23, 233, ...). For instance, $\overline{1_2} = 2$ matrix:

$$\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix},$$

$\overline{1_3}3 = \overline{1_5}6 = \overline{\overline{6}}$; $\overline{1_3}4 = \overline{1_5}4 = \overline{\overline{4}}$; $\overline{1_3}6 = \overline{1_5}3 = \overline{\overline{3}}$,
$m\,3\,3 = \overline{1_5}\,6\,6 = \overline{\overline{66}}$.
The last line gives the number of incommensurate PSOs of each type.

	MIPSOs (four-dimensional)	DIPSOs (five-dimensional)	TIPSOs (six-dimensional)
	1	1	1
	$\overline{1}$; $\overline{1_4}$	$\overline{1}$; $\overline{1_4}$; $\overline{1_5}$	$\overline{1}$; $\overline{1_4}$; $\overline{1_5}$; $\overline{1_6}$
	m	m	m
	2; 3; 4; 6	2; 3; 4; 6	2; 3; 4; 6
	23; 24; 26	$\overline{\overline{3}}$; $\overline{\overline{4}}$; $\overline{\overline{6}}$	$\overline{1_4}\,3$; $\overline{1_4}\,4$; $\overline{1_4}\,6$
		33; 44; 66	33; 44; 66
		$\overline{\overline{33}}$; $\overline{\overline{44}}$; $\overline{\overline{66}}$	233; 244; 266
Sum	11	18	19

In additional space E^3, the two PSOs are 1 and $\overline{1}_{tuv}$. Therefore, we can conclude that the holohedry $\overline{1}_6$ in space E^6 corresponds to the holohedry $\overline{1}$ (triclinic family) in space E^3 and to $\overline{1}$ in the additional space E^3.

(2) The second example is that of the 'decaclinic-al family'. In space E^6, its holohedry is the group $\overline{1}_5\perp m$ of order 4. With respect to the basis ($\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_4$, $\mathbf{a}_5$, $\mathbf{a}_6$, $\mathbf{a}_3$), the PSOs are

$$1,\quad m_z,\quad \overline{1}_{xytuv},\quad \overline{1_6}.$$

They correspond to type *a* or *b* (kind 2).

Therefore, in space E^3, the corresponding PSOs are 2_{xy}, m_z, $\overline{1}$ and 1. They generate the PSG $2/m$, which is the holohedry of the monoclinic family. In additional space E^3, the symbol of the additional PSOs is $\overline{1}$, 1, according to the nomenclature of Janner, Janssen & de Wolff (1983). As previously, we can conclude that the holohedry $\overline{1_5}\perp m$ in space E^6 corresponds to the holohedry $2/m$ in physical space E^3 and $\overline{1}$, 1 in additional space E^3.

(3) The last example is that of 'hexaclinic oblic family'. The symbol of the holohedry is $\overline{1}_4\perp 2$; this group is of order 4. The PSOs are 1, 2, $\overline{1}_4$, $\overline{1_6}$. They belong to types *a*, *b*, *c*, *d* or more exactly to kind 3. With respect of the basis ($\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_4$, $\mathbf{a}_5$, $\mathbf{a}_3$, $\mathbf{a}_6$), the PSOs are

space E^6	1,	$\overline{1}_{xytu}$,	2_{zv},	$\overline{1}_6$,
physical space E^3	1,	2_{xy},	m_z,	$\overline{1}_{xyz}$,
additional space E^3	1,	2_{tu},	m_v,	$\overline{1}_{tuv}$.

Therefore, we can write that the TIPSG $\overline{1}_4\perp 2$ in space E^6 corresponds to the group $2/m$ in the physical space E^3 and to the group $2/m$ in the additional space E^3.

All the different TIPSGs (holohedries of the TI crystal families) have been studied with the same method and the results are listed in Table 8. Therefore, it is possible to establish a correspondance between our approach for defining the TI crystal families and their holohedries (see the left side of Table 8) in space E^6 and the approach of Janner *et al.* (1983) (see the right side of Table 8).

Concluding remarks

As a conclusion of this first paper concerning the TI crystals structures, we compare and list the numbers and types of PSOs that describe the mono-, di- or tri-incommensurate structures (Table 9). In the next paper, we compare the MI, DI and TI PSGs and crystal families; we explain all the symbols of the PSGs given in Table 6.

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Crystallography, Geometry and Physics in Higher Dimensions. XIV. 'Filiation' from One-, Two- and Three-Dimensional Crystal Families and Point Groups to the Mono-, Di- and Tri-Incommensurate Crystal Families in Four-, Five- and Six-Dimensional Spaces

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Abstract

The previous paper in this series [Phan & Veysseyre (1994). *Acta Cryst.* **A50**, 438–444] mainly compared the mono-, di- and tri-incommensurate point-symmetry operations, their number and their symbols. In this paper, the filiation from the g*Z*-irreducible crystal families of the one-, two- and three-dimensional spaces to the mono-, di- and tri-incommensurate families of the four-, five- and six-dimensional spaces is established. The holohedries and the different point groups of these crystal families are compared. The paper begins with a list of the incommensurate families; then a series of nine further tables establishes the connection between the different families and their point groups. It is proved that there are 30 mono-incommensurate (MI) point groups, 47 di-incommensurate (DI) point groups and 57 tri-incommensurate (TI) point groups belonging to the six MI crystal families of four-dimensional space, to the 11 DI crystal families of five-dimensional space and to the 14 TI crystal families of the six-dimensional space.

Introduction

In previous papers, we have studied the mono-incommensurate (MI) crystal families (Veysseyre & Weigel, 1989), the di-incommensurate (DI) crystal families (Phan, Veysseyre & Weigel, 1991), the tri-incommensurate (TI) crystal families (Phan & Veysseyre, 1994) and the incommensurate point operations – mainly their number and their symbols. We recall that the mono-, di- and tri-incommensurate phases of physical space are not crystals in this space. However, they can be considered as sections of crystals of four-, five- or six-dimensional spaces through physical space. Therefore, in this paper, we call a MI family a crystal family in the four-dimensional (4D) space, a DI family a crystal family in five-dimensional (5D) space and a TI family a crystal

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