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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(*Received* 16 *July* 1993; *accepted* 2 *December* 1993)

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

ISSN 0108-7673 ©1994

family in the six-dimensional (6D) space if these crystal families describe the incommensurate structures.

In Table 1, we list the MI, DI and TI families. By means of the geometrical names that we suggest for these families, the connection between them can easily be seen. The choice of names recalls both these relations and the construction of the crystal cells. For instance, the hexaclinic family of 4D space is a MI family, whereas the hexaclinic-al family of 5D space is a DI family and the hexaclinic oblic family of 6D space is a TI family. As we shall explain here, the cell of the hexaclinic-al family is a right hyperprism based on the hexaclinic cell. The cell of the hexaclinic oblic family is the rectangular product of the hexaclinic cell and of the parallelogram (oblic) cell. We recall that 'oblic' means parallelogram; the crystal family 'oblic-al' is generally called 'monoclinic'. Moreover, 'hexagonal' must only be used in three-dimensional (3D) space; 'hexagon' is used in two-dimensional (2D) space.

Table 1 shows how powerful are the names that we suggest for the crystal families, either the incommensurate or the non-incommensurate ones. Their properties are explained in the following sections. Then, in Tables 2–9, we compare the different point groups that describe the incommensurate crystal structures, classified family by family according to their geometrical construction. Finally, in Table 10, we summarize their number.

Table 1. *Incommensurate crystal families*

'al' means 'right hyperprism based on ...' 'orthogonal' is not written between two names of cells belonging to two orthogonal subspaces.

6 MI families (4D)	11 DI families (5D)	14 TI Families (6D)
		15-clinic
	Decaclinic	Decaclinic-al
Hexaclinic	Hexaclinic-al	Hexaclinic oblic
Triclinic-al	Triclinic oblic	Triclinic oblic-al
		Di triclinic
Di oblic	Di oblic-al	Tri oblic
Oblic rectangle	Triclinic rectangle	Hexaclinic rectangle
Oblic square	Triclinic square	Hexaclinic square
Oblic hexagon	Triclinic hexagon	Hexaclinic hexagon
	Diclinic di square-al	Diclinic di square oblic
	Diclinic di hexagon-al	Diclinic di hexagon oblic
	Monoclinic di square-al	Monoclinic di square oblic
	Monoclinic di hexagon-al	Monoclinic di hexagon oblic
		Monoclinic di cubic

I. Filiation and geometrical isomorphism

We establish and prove a filiation and a geometrical isomorphism between the g*Z*-*irreducible crystal families* of one-dimensional space (1D) (segment), of 2D space (oblic, square, hexagon) and of 3D space (triclinic, cubic) and the g*Z*-*reducible MI, DI and TI crystal families* of the 4, 5 and 6D spaces.

The definition and the properties of the g*Z*-irreducible (g*Z*-irr.) crystal families and of the g*Z*-reducible (g*Z*-red.) crystal families are given by Weigel & Veysseyre (1991) and are recalled in the Appendix.

In a series of eight tables (Tables 2–9), we describe this filiation and this isomorphism, which actually appear in the WPV names of the families as well as in the WPV symbols of the holohedries of these families. The WPV (Weigel, Phan & Veysseyre) symbols are explained in some papers, for instance Weigel, Phan & Veysseyre (1987). The last table (Table 10) summarizes the number of incommensurate crystal families and point groups.

Tables 2, 3 and 4 are, respectively, devoted to the incommensurate crystal families connected to the triclinic, oblic and segment crystal families, which are g*Z*-irr. crystal families. Tables 5 and 6 are devoted to the incommensurate crystal families connected to the g*Z*-irr. square crystal family. Then, Tables 7 and 8 are devoted to the incommensurate crystal families connected to the g*Z*-irr. hexagon crystal family and, lastly, Table 9 is devoted to the incommensurate crystal families connected to the g*Z*-irr. cubic crystal family. As these tables are similar, it will be enough if we explain a series of them, for instance, the crystal families obtained from the square family of 2D space.

Therefore, in Table 5, we start with the square crystal family whose cell is a square; $4mm$ is the symbol of its holohedry of order 8. The following crystal families are constructed out of this family:

The tetragonal family in 3D space: its cell is a right prism based on a square; $4mm \perp m$ or $4/mmm$ is the symbol of its holohedry of order 16 (8×2) and there exist six proper subgroups or point groups in this family, which are: $4mm$; 422; $\bar{4}2m$; $m \perp 4$; 4; $\bar{4}$. This family is a g*Z*-red. crystal family.

The oblic square family in 4D space: its cell is the rectangular product of a parallelogram (oblic) and a square belonging to two orthogonal subspaces; $4mm \perp 2$ is the symbol of its holohedry of order 16 (8×2) and six point groups belong to this family as in the tetragonal family. We can compare the symbols of the point groups of the oblic square family and of the tetragonal family. Some of these are the same as $4mm$ or 4, for instance. Others are different but these differences have a geometrical explanation. For instance, the point-symmetry operation (PSO) m is changed into 2, then $4mm \perp m$ becomes $4mm \perp 2$, $4 \perp m$ becomes $4 \perp 2$. The PSO 2 is changed into $\bar{1}$, thus 422 becomes $4, \bar{1}, \bar{1}$. Actually, m is a PSO of 1D space, and 2 is a PSO of 2D space, whereas $\bar{1}$ is a PSO of 3D space. Another example is the PSO $\bar{4}$,

Table 2. *MI, DI and TI crystal families and point groups from the gZ-irreducible and degenerate triclinic, hexaclinic, decaclinic and 15-clinic crystal families*

In the first column, we give the general name (g*Z*-irr. or incommensurate) of the crystal family as well as the dimension of the space. g*Z*-irr. means 'geometrically *Z*-irreducible' (*Z* is the set of positive and negative integers). The g*Z*-irr. crystal families are underlined. The subsequent columns give the Hermann–Mauguin and WPV symbols of the point groups. The last column gives the number *p* of incommensurate point groups listed in the table. We can write: $\overline{1_5} = \overline{\overline{1}}$.

Order of the point groups		4	2	1		4	2		4	2		2	*p*
g*Z*-irr. CF (3D)	Triclinic		$\overline{1}$	1									
MI CF (4D)	Triclinic-al	$\overline{1}\perp m$	$\overline{1}$	1	Hexaclinic		$\overline{1_4}$						4
DI CF (5D)	Triclinic oblic*	$\overline{1}\perp 2$	$\overline{1}$	1	Hexaclinic-al	$\overline{1_4}\perp m$	$\overline{1_4}$	Decaclinic		$\overline{1_5}$			6
TI CF (6D)	Di triclinic	$\overline{1}\perp\overline{1}$	$\overline{1}$	1	Hexaclinic oblic*	$\overline{1_4}\perp 2$	$\overline{1_4}$	Decaclinic-al	$\overline{1_5}\perp m$	$\overline{1_5}$	15-clinic	$\overline{1_6}$	8

* These two families also appear in Table 3; the other PSGs belonging to these families are listed in Table 3.

Table 3. *MI, DI and TI crystal families and point groups from the gZ-irreducible oblic crystal family of 2D space*

See caption of Table 2.

Order of the point groups		8	4		4	2		8	4	4	4	*p*
g*Z* CF (2D)				Oblic (parallelogram)		2						
CF (3D)				Monoclinic (oblic-al)	$2\perp m$ $(2/m)$	2						
MI CF (4D)				Di oblic	$2\perp 2$	2						2
DI CF (5D)				Triclinic oblic*		2	Di oblic-al	$2\perp 2\perp m$	$2\perp m$	$2\perp 2$	$\overline{1_4}$, $\overline{1},\overline{1}$	6
TI CF (6D)	Triclinic oblic-al	$\overline{1}\perp 2\perp m$	$\overline{1}\perp 2$ $\overline{1}\perp m$ $2\perp m$	Hexaclinic oblic*		2	Tri oblic	$2\perp 2\perp 2$		$2\perp 2$	$\overline{1_4}$, $\overline{1_4}$	9

* These two crystal families also appear in Table 2; in this table, we only list the PSGs 2 that are not listed in Table 2.

Table 4. *MI, DI and TI crystal families and point groups from the gZ-irreducible segment crystal family of 1D space*

See caption of Table 2.

Order of the point groups		8	4	4	4	2	*p*
g*Z*-irr. CF (1D)	Segment					*m*	
CF (2D)	Rectangle		$m\perp m$ (2 *mm*)			*m*	
MI CF (4D)	Oblic rectangle	$2\perp m\perp m$	$m\perp m$	$2\perp m$	$2,\overline{1},\overline{1}$	*m*	5
DI CF (5D)	Triclinic rectangle	$\overline{1}\perp m\perp m$	$m\perp m$	$\overline{1}\perp m$	$2,\overline{1_4},\overline{1_4}$	*m*	5
TI CF (6D)	Hexaclinic rectangle	$\overline{1_4}\perp m\perp m$	$m\perp m$	$\overline{1_4}\perp m$	$2,\overline{1_5},\overline{1_5}$	*m*	5

Table 5. *MI, DI and TI crystal families and point groups from the gZ-irreducible crystal square family of 2D space*

The first line gives the order of the PSGs. The remaining lines give the PSGs belonging to the families, the first PSG being the holohedry in each case. Actually, $\overline{1_2} = 2$, $\overline{1_3} = \overline{1}$, $\overline{1_5} = \overline{\overline{1}}$; it is easy to see that $\overline{\overline{4}} = \overline{1_5}4 = \overline{1_3}4$; indeed, $\overline{1_5} = \overline{1}2$ and $4^12 = 4^3$ (rotation of $3\pi/4$).

Order of the point groups	16	8	8	8	8	4	4	*p*
Square g*Z*-irr. CF (2D)		4*mm*				4		
Tetragonal 3D	$m\perp 4mm$ (4/mm)	4mm	422	$\bar{4}2m$	$m\perp 4$	4	$\bar{4}$	
Oblic square MI family (4D)	$2\perp 4mm$	4*mm*	$4,\overline{1},\overline{1}$	$24,\overline{1},m$	$2\perp 4$	4	24	7
Triclinic square DI family (5D)	$\overline{1}\perp 4mm$	4*mm*	$4,\overline{1_4},\overline{1_4}$	$\overline{1}4,\overline{1_4},m$ $(\overline{\overline{4}},\overline{1_4},m)$	$\overline{1}\perp 4$	4	$\overline{1}4$ $(\overline{\overline{4}})$	7
Hexaclinic square	$\overline{1_4}\perp 4mm$	4*mm*	$4,\overline{1_5},\overline{1_5}$	$\overline{1}4,\overline{1_5},m$	$\overline{1_4}\perp 4$	4	$\overline{1_4}4$	7

Table 6. *DI and TI crystal families and point groups from the gZ-irr. diclinic di square and monoclinic di square crystal families of 4D space*

p = number of incommensurate (I) point groups.

Order	16	8	4	p
Non-incommensurate gZ-irr. CF diclinic di square (4D)			44*	
DI CF diclinic di square-al (5D)		$44^*\perp m$	44*	2
TI CF diclinic di square oblic (6D)		$44^*\perp 2$	44*	2
Non-incommensurate gZ-irr. CF monoclinic di square (4D)		2,44*,2		
DI CF monoclinic di square-al (5D)	$2,44^*,2\perp m$	2,44*,2		2
TI CF monoclinic di square oblic (6D)	$2,44^*,2\perp 2$	2,44*,2		2

which becomes 24. We recall that 24 is the symbol of a double rotation, *i.e.* the commutative product of two rotations that take place in two orthogonal planes, a rotation through the angle $2\pi/2$ and a rotation through the angle $2\pi/4$.

The triclinic square family in 5D space: its cell is the orthogonal product of a triclinic cell (oblic parallelepiped cell) and a square cell belonging to two orthogonal subspaces of three and two dimensions, respectively, $\bar{1}\perp 4mm$ is the symbol of its holohedry of order 16 and six point groups belong to this family, as in the oblic square family. As previously, we can compare these symbols and the symbols of the point group of the previous two families. For instance, the PSO $\bar{1}$ in 3D space is changed into $\bar{1}_4$ in 4D space and $\bar{1}_4$ into $\bar{1}_5$ in 5D space.

The hexaclinic square family in 6D space: its cell is the rectangular product of a hexaclinic cell (oblic parallelotope cell) and a square cell belonging to two orthogonal subspaces of four and two dimensions, respectively; $\bar{1}_4\perp 4mm$ is the symbol of its holohedry of order 16. Six point-symmetry groups (PSGs) belong to this family, they are listed in Table 5.

Then, in Table 6, we start with the gZ-irr. crystal family '*diclinic di square*', which gives the DI diclinic di square-al crystal family and the TI diclinic di square oblic crystal family; the second part of this table is devoted to the DI and TI crystal families out of the monoclinic di square crystal families.

II. Some properties of the incommensurate crystal families connected to the gZ-irreducibility

We are going to explain why the MI, DI and TI crystal families cannot be gZ-irreducible crystal families, except for two families: the gZ-irreducible crystal families of type $(\overline{1, 1, ..., 1})$, *i.e.* degenerate, and the gZ-irreducible crystal family of type $\overline{3,3}$ (monoclinic di cubic crystal family of 6D space E^6). We prove this property for the TI crystal families; the proof can be easily applied to the MI and DI crystal families.

The vectors describing the main and satellite reflections of an incommensurate structure are as follows in reciprocal space (see Phan & Veysseyre, 1994):

$$\mathbf{H} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* + \sum_{i=1}^{3} m_i\mathbf{q}_i^*$$

$$\mathbf{q}_i^* = \alpha_i\mathbf{a}^* + \beta_i\mathbf{b}^* + \gamma_i\mathbf{c}^*,$$

where h, k, l and m_i are integers and at least one of the three entries α_i, β_i and γ_i is irrational for each value of the index i. Then, we consider an additional space generated by three unit orthogonal vectors orthogonal to the physical space. So we study the incommensurate structures in 6D space, E^6:

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

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

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

But all or some entries α_i, β_i, γ_i are irrational. Therefore, only some point operations and consequently some point groups and some crystal families of the space E^6 can describe these structures. Indeed, any vector of the crystal lattice of E^6 cannot have as picture any vector of this lattice. According to the number and the value of the irrational entires, α_i, β_i and γ_i, which are different from 0, according to their position in the vectors $\mathbf{q}_i^*$, the TI crysal families are split up in various ways as 6, 5 + 1, ..., 3 + 3, ... We explain these results through four examples.

(1) At first, we suppose that all the nine entries are irrational and unequal. It is easy to prove that the PSOs compatible with this hypothesis are: (i) the *identity*, which leaves unchanged all the vectors; (ii) the *total homothetie* of ratio (-1), which changes each vector into its opposite. In space E^6, there only exists one crystal family of which the point group has these two PSOs: the '15-clinic' family. Now, in space E^6, we consider the gZ-irr. crystal families of type $(\overline{1,1,1,1,1,1})$, *i.e.* degenerate. The crystal families belonging to this type of irreducibility cannot have only two PSOs, the identity and the total homothetie of ratio (-1). Therefore, they can be used for the description of an incommensurate structure.

(2) We consider the so-called type no. 8 (Phan & Veysseyre, 1994).

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

Six entries are irrational and unequal; only one vector ($\mathbf{a}_3$) of the reciprocal lattice is not associated with these entries. The other five vectors depend on the irrational entries. The only PSOs that can act on these five vectors are the *identity* (all the vectors are unchanged) and the *total homothetie* of ratio (-1)

Table 7. *MI, DI and TI crystal families and point groups from the gZ-irreducible crystal family hexagon of 2D space*

See caption of Table 2.

Order of the point groups	24	12	12	12	12	12	6	6	6	6	6	3	p
Hexagon (2D)		$6mm$					6		$3m$			3	
Hexagonal (3D)	$m\perp 6mm$ ($6/mmm$)	$6mm$	622	$\bar{6}m2$	$\bar{3}m$	$m\perp 6$ ($6/m$)	6	$\bar{6}$ ($m\perp 3$)	$3m$	32	$\bar{3}$	3	
Oblic hexagon MI CF (4D)	$2\perp 6mm$	$6mm$	$6,\bar{1},\bar{1}$	$26,m,\bar{1}$	$2\perp 3m$	$2\perp 6$	6	$2\perp 3$	$3m$	$3,\bar{1}$	26	3	12
Triclinic hexagon DI CF (5D)	$\bar{1}\perp 6mm$	$6mm$	$6,\overline{1_4},\overline{1_4}$	$\bar{\bar{3}},m,\overline{1_4}$	$\bar{1}\perp 3m$	$\bar{1}\perp 6$	6	$\bar{1}\perp 3$	$3m$	$3,\overline{1_4}$	$\bar{\bar{3}}$	3	12
Hexaclinic hexagon TI CF (6D)	$\overline{1_4}\perp 6mm$	$6mm$	$6,\overline{1_5},\overline{1_5}$	$\overline{1_4}6,m,\overline{1_5}$	$\overline{1_4}\perp 3m$	$\overline{1_4}\perp 6$	6	$\overline{1_4}\perp 3$	$3m$	$3,\overline{1_5}$	$\overline{1_4}6$	3	12

Table 8. *DI and TI crystal families and point groups from the gZ-irr. diclinic di hexagon and monoclinic di hexagon crystal families of 4D space*

$66^* = 6_2^*$ = double rotation of angles $2\pi/6$ in the plane $(\alpha\beta)$ and $2\pi/6$ in the plane $(\gamma\delta)\perp(\alpha\beta)$; $33^* = 3_2^*$; p = number of incommensurate (I) point groups.

Order	24	12	12	6	6	3	p
Non-incommensurate (I) gZ-irr. CF diclinic di hexagon (4D)				66^*	33^*		
DI CF diclinic dihexagon-al (5D)		$66^*\perp m$		$33^*\perp m$	66^*	33^*	4
TI CF diclinic dihexagon oblic (6D)		$66^*\perp 2$		$33^*\perp 2$	66^*	33^*	4
Non-incommensurate gZ-irr. CF monoclinic di hexagon (4D)		$2,66^*,2$		$2,33^*,2$			
DI CF monoclinic di hexagon-al (5D)	$2,66^*,2\perp m$	$2,66^*,2$	$2,33^*,2\perp m$	$2,33^*,2$			4
TI CF monoclinic di hexagon oblic (6D)	$2,66^*,2\perp 2$	$2,66^*,2$	$2,33^*,2\perp 2$	$2,33^*,2$			4

(each vector has its opposite for mapping). As in the previously studied case, the 'decaclinic' cell [gZ-irr. crystal family of type $(\overline{1,1,1,1,1})$] is the only crystal family of space E^5 having only these two PSOs. If we add the vector $\mathbf{a}_3$, we find either the crystal family '15-clinic' if the vector $\mathbf{a}_3$ is not orthogonal to the space generated by the other five vectors, or the 'decaclinic-al' crystal family if the vector $\mathbf{a}_3$ is orthogonal to the space generated by the other five vectors. This crystal family is gZ-red. of type 5 + 1.

(3) We consider a third example with three irrational entries as follows:

$$\mathbf{a}_1 = \mathbf{a} - \alpha_1\mathbf{d}_1, \quad \mathbf{a}_4 = \mathbf{d}_1,$$
$$\mathbf{a}_2 = \mathbf{b} - \beta_2\mathbf{d}_2, \quad \mathbf{a}_5 = \mathbf{d}_2,$$
$$\mathbf{a}_3 = \mathbf{c} - \gamma_3\mathbf{d}_3, \quad \mathbf{a}_6 = \mathbf{d}_3.$$

The splitting of the crystal cell in space E^6 into three subcells belonging to three subspaces of dimension two is obvious. If these three subspaces *are not* two-by-two orthogonal, we again find the first case. Therefore, we suppose that they *are* two-by-two orthogonal and we consider one of them, for instance the subspace generated by the vectors $\mathbf{a}_1$ and $\mathbf{a}_4$ or $\mathbf{d}_1$. As the entry α_1 is irrational, the only PSOs are the identity and the homothetie of ratio (-1) and of dimension two. In this space E^2, we find the gZ-irr. crystal family of type $(\overline{1,1})$ *i.e.* the oblic family. In space E^6, we obtain the tri-oblic family, which is gZ-red. of type $\overline{1,1} + \overline{1,1} + \overline{1,1}$.

All the various cases listed by Phan & Veysseyre (1994) should be studied in this way. To finish with, we study the second exception, *i.e.* the gZ-irr. crystal family of type $(\overline{3,3})$ or monoclinic di cubic crystal family of 6D space. Indeed, the cell of this family consists of two equal cubes belonging to two non-orthogonal subspaces (if the subspaces were orthogonal, the crystal family would be the hypercubic family, which cannot describe an incommensurate structure because the point-symmetry operations of a hypercube permute all the sides). In the case of the monoclinic di cubic family, one cube cannot be changed in the other. This case appears when the nine entries are as follows:

$$\alpha_1 = \beta_2 = \gamma_3 = k \quad \text{(irrational value)}$$
$$\alpha_2 = \alpha_3 = \beta_1 = \beta_3 = \gamma_1 = \gamma_2 = 0.$$

As a result, the incommensurate structure is described by the vectors

$$\mathbf{a}_1 = \mathbf{a} - k\mathbf{d}_1, \quad \mathbf{a}_4 = \mathbf{d}_1,$$
$$\mathbf{a}_2 = \mathbf{b} - k\mathbf{d}_2, \quad \mathbf{a}_5 = \mathbf{d}_2,$$
$$\mathbf{a}_3 = \mathbf{c} - k\mathbf{d}_3, \quad \mathbf{a}_6 = \mathbf{d}_3.$$

Space E^6 splits up into two orthogonal 2D subspaces generated by ($\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$) for the first one and by ($\mathbf{d}_1$, $\mathbf{d}_2$, $\mathbf{d}_3$) for the second one. We obtain the monoclinic di cubic family [gZ-red. of type $(\overline{3,3})$ if the vectors ($\mathbf{a}_i$) are unit orthogonal vectors].

Table 9. *TI crystal family out of the gZ-irreducible cubic crystal family of 3D space*

In the first line, we give the order of the different point groups belonging to the two crystal families considered; we start with the holohedry. In the second line, we list the different point groups belonging to the cubic family which is a g*Z*-irr. crystal family; for two point groups, we give two symbols: the abbreviated symbol and, in brackets, the full symbol. In the same way, in the third line we list the different point groups belonging to the monoclinic di cubic family which is a TI crystal family; as for the cubic family, we give two symbols to two point groups: the abbreviated symbol and, in brackets, the full symbol. The symbols of the point groups of these two families are similar: *m* becomes 2, 2 becomes $\overline{1_4}$, a simple rotation of 3D space such as 3 becomes a double rotation 33 of 6D space and so on. The last column gives the number of PSGs belonging to each of the crystal families.

Order of the point groups	48	12	24	24	24	p
g*Z*-irr. CF: cubic (3D)	$m\bar{3}m$ $\left(\frac{4}{m}\bar{3}\frac{2}{m}\right)$	23	$m\bar{3}$ $\left(\frac{2}{m}\bar{3}\right)$	432	$\bar{4}3m$	5
TI CF: monoclinic di cubic (6D)	2,662,2 $\left(\frac{44}{2}, 662, \frac{\overline{1_4}}{2}\right)$	$\overline{1_4}$,33	2,662 $\left(\frac{\overline{1_4}}{2}, 662\right)$	44,33,$\overline{1_4}$	442,33,2	5

Table 10. *Number of MI, DI and TI crystal families and point groups in 4, 5 and 6D spaces*

	Number of crystal families			Number of point groups		
	MI	DI	TI	MI	DI	TI
Table 2	2	3	4	4	7	10
Table 3	1	1	2	4	6	7
Table 4	1	1	1	3	3	4
Table 5	1	1	1	7	7	7
Table 6		2	2		4	4
Table 7	1	1	1	12	12	12
Table 8		2	2		8	8
Table 9			1			5
Sum	6	11	14	30	47	57

So we can see how the WPV names (Weigel *et al.*, 1987) are a powerful tool especially in view of determining the g*Z*-irreducibility of the MI, DI and TI crystal families (CFs) as well as their types of decomposition, *i.e*:

2 + 2 for the oblic hexagon MI CF 4D-(oblic = 2D; hexagon = 2D).

3 + 2 for the triclinc square DI CF 5D-(triclinic = 3D; square = 2D).

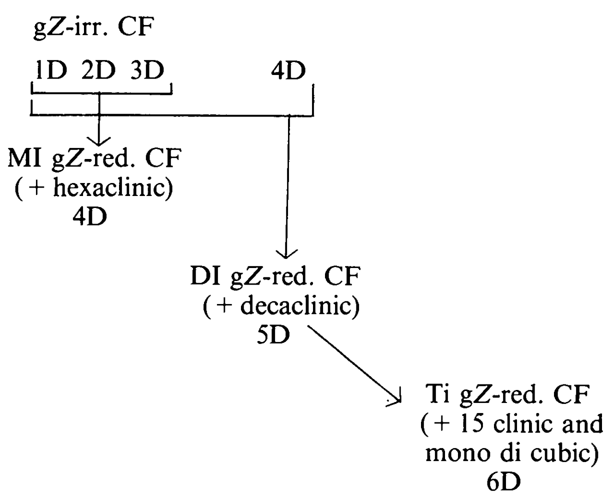
4 + 1 for the diclinic di square-al CF 5D. Actually, the cell is a right hyperprism based on the diclinic di square cell (4D) and al is the contraction of orthogonal plus one dimension.

3 + 2 + 1 for the triclinic oblic-al TI CF 6D-(triclinic = 3D; oblic = parallelogram = 2D; al = 1D).

4 + 2 for the hexaclinic square TI CF 6D (hexaclinic = 4D; square = 2D).

4 + 2 for the diclinic di square oblic TI CF 6D (diclinic di square = 4D; oblic = 2D).

We summarize these results by:



Concluding remarks

This paper proves the filiation from the g*Z*-irreducible crystal families and their point groups in 1, 2, 3 and 4D spaces to the MI, DI and TI g*Z*-reducible crystal families in 4, 5 and 6D spaces with the maxiclinic g*Z*-irr. crystal families and the TI monoclinic di cubic g*Z*-irreducible crystal family of the 6D space and their point groups.

APPENDIX

In two papers, Weigel & Veysseyre (1991) and Veysseyre, Weigel & Phan (1993), we give a definition of the so-called g*Z*-irreducible crystal families and of the g*Z*-reducible crystal families. As we explain in these papers, our concept is slightly different from the definition given by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978).

These authors give a mathematical definition connected to the unimodular $n \times n$ matrices of finite group associated to a Z class.

Our definition is connected to the geometry and the splitting up of the metric tensor of a crystal cell and to the bases of the irreducible representations of the holohedry of the crystal family. For these reasons, the letter 'g' is the abbreviation of 'geometrical'; 'Z' is the group of positive or negative integers.

We suggested this definition:

Let $x, y, z, t, u, v, ...$ be the n translation operators corresponding to a basis of a primitive Bravais cell of a crystal family of the n-dimensional space E^n. This family is said to be 'geometrically Z-irreducible' (gZ-irr.) if all these operators belong to the same *irreducible representation with integer entries of the character table of its holohedry*. If this property is not verified, the crystal family is said to be 'geometrically Z-reducible' (gZ-red.); in this case, the metric tensor can be split into two or more parts or, in other words, the cell of the crystal family is the orthogonal product of two or more cells belonging to two or more orthogonal subspaces of space E^n. Now, we give two simple examples:

The rectangular family of space E^2 is a gZ-reducible family, the WPV symbol of the holohedry is $m \perp m$, the construction of the cell is explained as the rectangular product of two unequal segments. It is easy to see that the two operators x and y belong to two different irreducible representations of the character table of this holohedry.

The oblic family and the square family are gZ-irr. crystal families of space E^2. Indeed, the two operators x and y belong to the same irreducible representation of dimension 1 (which is not the identity representation) for the oblic family and to the same irreducible representation of dimension 2, for the square family. If we consider the metric tensor of these two cells, we notice that it is impossible to split them into two parts.

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The Centrosymmetric–Noncentrosymmetric Ambiguity: Some More Examples

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(*Received* 16 *June* 1992; *accepted* 17 *November* 1993)

Abstract

Four more examples are provided to emphasize the extreme difficulty in deciding, by diffraction methods, whether a crystal structure is centrosymmetric or only approximately so. In these examples, earlier workers described and refined structures in noncentrosymmetric space groups; refinements in the corresponding centrosymmetric space groups, based on the original data, lead to improved results. In one case, apparent violations of systematic absences seem to preclude the centrosymmetric description; however, other evidence – in particular, improved agreement for the very weak reflections (which are the most sensitive to the centrosymmetric–noncentrosymmetric ambiguity) – suggest that the space-group violations might be spurious. In any event, the moral is clear: extreme caution is needed when attempting to derive a noncentrosymmetric description of a closely centrosymmetric structure.

Introduction

For a number of years, I have been interested in the problem of attempting to decide, by means of X-ray diffraction alone, whether a particular crystal structure is centrosymmetric or only approximately so. As has been noted often, perhaps beginning with Ermer & Dunitz (1970), the first small deviation from centrosymmetry cannot be detected by normal diffraction methods since the centrosymmetric model

* Contribution no. 8375.