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Crystallography, Geometry and Physics in Higher Dimensions. VII. The Different Types of Symbols of the 371 Mono-Incommensurate Superspace Groups

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Abstract

The 371 four-dimensional superspace symmetry groups for the mono-incommensurate modulated structures have been classified with different but equivalent notations by de Wolff, Janner & Janssen (WJJ) and Weigel, Phan & Veysseyre (WPV). The exact correspondence between the two types of symbols and examples of physical modulated structures are given in this paper.

Introduction

In the last decade, there have been many structural investigations of incommensurate modulated structures; as far as three-dimensional (3D) methods are concerned, a group-theoretical analysis which takes time reversal into account correctly describes the displacements in two examples: γ-Na_2CO_3 and K_2SeO_4 (Bertaut, 1984, 1985). A new formalism has been developed in $(3+n)$-dimensional space, to take into account simultaneously the symmetry of the modulation wave and the basic symmetry of the average structure (de Wolff, Janssen & Janner, 1981; Janner, Janssen & de Wolff, 1983; Yamamoto, Janssen, Janner & de Wolff, 1985; Janssen & Janner, 1987). An important part of these new structures is mono-incommensurate (MI), *i.e.* it has only one direction of incommensurability, and their description leads to the construction of all four-dimensional (4D) superspace symmetry groups, appropriate for MI structures.

In this first analysis, the 4D-mono-incommensurate superspace groups have been derived from the consideration of their 3D average structure, characterized by its own 3D space symmetry group. A more mathematical analysis (Brown, Bülow, Neubüser, Wondratschek & Zassenhaus, 1978) allowed us to derive all the 4D point symmetry groups (4D PSGs) and all the 4D space symmetry groups (4D SSGs), but in such a way that it becomes very difficult to handle and to visualize these groups for a crystallographer. Lately, a more geometrical description has been proposed (Weigel, Phan & Veysseyre, 1987; Phan, Veysseyre, Weigel & Grebille, 1989), in order to generalize the principles of the notations of the 3D SSGs as they are now normalized in *International Tables for Crystallography* (1983), and to take into account the previous mathematical analysis.

These three independent 4D descriptions and notations can be used to classify the mono-incommensurate structures and we shall first illustrate them by a simple physical example, the modulated structure of γ-Na_2CO_3.

This modulated structure has already been analysed in the 4D description (van Aalst, den Hollander, Peterse & de Wolff, 1976; Veysseyre & Weigel, 1989) and the symmetry operators have been derived and listed from the observation of the diffraction pattern. The average structure belongs to the monoclinic system (space group $C2/m$, unique axis b) and the modulation wavevector is $\mathbf{q}=\alpha\mathbf{a}^*+\gamma\mathbf{c}^*$ ($\alpha=0{\cdot}182$ and $\gamma=0{\cdot}318$ at room temperature). The new reciprocal basis vectors are $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ and $\mathbf{q}+\mathbf{d}^*$, where $\mathbf{d}^*$ is a unit vector orthogonal to the reciprocal 3D space, and in the direct space, the new basis vectors are $\mathbf{a}-\alpha\mathbf{d}$, $\mathbf{b}$, $\mathbf{c}-\gamma\mathbf{d}$, $\mathbf{d}$, where $\mathbf{d}$ is a unit vector orthogonal to the physical 3D space ($\mathbf{a},\mathbf{b},\mathbf{c}$). The orthogonality and modulus relations lead either to the *triclinic* system (Brown *et al.*, 1978), to the system *right hyperprism based on parallelepiped* (Weigel *et al.*, 1987) or to the system *planar monoclinic* (de Wolff *et al.*, 1981). The analysis of the extinction conditions of the diffraction pattern and of the basic symmetry leads to the following symmetry operations (in the notations of the Wyckoff positions of the *International Tables for Crystallography*).

In a 3D symmetry where $u(\tau)$, $v(\tau)$ and $w(\tau)$ are the atomic displacement functions from the average atomic positions x, y and z and τ is a phase variable:

$S1$	$x+u(\tau)$	$y+v(\tau)$	$z+w(\tau)$
$S2$	$-x-u(-\tau)$	$-y-v(-\tau)$	$-z-w(-\tau)$
$S3$	$x+u(\tau+1/2)$	$-y-v(\tau+1/2)$	$z+w(\tau+1/2)$
$S4$	$-x-u(-\tau+1/2)$	$y+v(-\tau+1/2)$	$-z-w(-\tau+1/2)$;

in a 4D symmetry, where t is the fourth coordinate:

$S1$	x	y	z	t
$S2$	$-x$	$-y$	$-z$	$-t$
$S3$	x	$-y$	z	$t+1/2$
$S4$	$-x$	y	$-z$	$-t+1/2$.

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One can recognize the following:

(*a*) $S1$ is the identity in $\mathbb{E}^3$ or $\mathbb{E}^4$.

(*b*) S2 is the inversion in $\mathbb{E}^3$ and the '*homothetie* minus 1' (which is the double rotation $\bar{1}_4$) in $\mathbb{E}^4$.

(*c*) $S3$ is a mirror through a plane orthogonal to $\mathbf{b}$ in $\mathbb{E}^3$ and a glide reflection through a hyperplane orthogonal to $\mathbf{b}$ combined with a translation $\mathbf{d}/2$ along the t axis in $\mathbb{E}^4$.

(*d*) $S4$ is a twofold rotation about the b axis in $\mathbb{E}^3$ and an inversion $\bar{1}$ through an axis parallel to $\mathbf{b}$ in $\mathbb{E}^4$ (Veysseyre, Phan & Weigel, 1985).

Moreover, we have to take into account a centring condition, so the corresponding notations of the SSG are respectively II-02/03/02/002, $S(X, Y)\ \bar{1}\perp m_{\mathbf{d}}$ and $P^{C}\,{}^{2/}_{\bar{1}}\,{}^{m}_{s}$ in BBNWZ (Brown *et al.*, 1978), WPV (Phan *et al.*, 1989) and WJJ (de Wolff *et al.*, 1981) notations.

In the present paper, our purpose is to specify the general equivalence between these different descriptions and notations, more particularly for WJJ and WPV notations, since the last ones are derived from those of BBNWZ in a simpler presentation; we shall propose a simple way to derive a symbol of a 4D SSG from either description.

General correspondence between WJJ and WPV symbols

A complete list of the $(3+1)$-dimensional superspace groups has already been established in order to describe the crystal symmetry of the mono-incommensurate modulated structures (de Wolff *et al.*, 1981). A two-line symbol has been proposed, which clearly refers to the diffraction symmetry and to the distinction between main and satellite reflections or between the three physical dimensions of the basic structure and the internal dimension. These symbols can be written under the generic form

$$\begin{array}{cc} & \mathbf{Y} \\ \mathbf{X} & \\ & \mathbf{Z} \end{array}$$

where $\mathbf{X}$ is related to the rational components $\mathbf{q}_r$ of the wavevector $\mathbf{q}$, $\mathbf{Y}$ is the Hermann–Mauguin symbol of the group of the basic structure in the physical space and $\mathbf{Z}$ describes the symmetry operations $\mathbf{g}_I$ in the fourth dimension associated with each generator $\mathbf{g}_E$ of the basic space group $\mathbf{Y}$. 775 WJJ symbols are used to describe the 371 mono-incommensurate crystallographic space groups of $\mathbb{E}^4$ (Phan *et al.*, 1989; de Wolff *et al.*, 1981; Yamamoto *et al.*, 1985).

It is clear that the 371 WPV and the 775 WJJ symbols deal with the same mathematical objects and our purpose in this section is to establish a correspondence between these notations. As explained earlier, WJJ notations are directly related to the three-dimensional physical symmetry of the average structure, which is most of the time the real symmetry of a high-temperature basic structure. Consequently, the WJJ symbols introduce a dichotomy between the external space (the physical space) and the internal space (the modulation space), and so each symmetry operation $\mathbf{g}$ is the product of two symmetry operations $\{\mathbf{g}_E, \mathbf{g}_I\}$; $\mathbf{g}_E$ is present in the $\mathbf{Y}$ symbol while the corresponding operator $\mathbf{g}_I$ is present in the $\mathbf{Z}$ line. In the same way, a centring condition is present partly in the $\mathbf{Y}$ line, as far as it concerns the basic structure, and partly in the $\mathbf{X}$ letter, because a rational component of the modulation vector is equivalent to a centring condition in the fourth dimension. With WPV notations, the four-dimensional space group is treated as a whole, and, consequently, the symbols are more general and not uniquely related to the structural description of mono-incommensurate modulated phases; the symmetry operations and the centring conditions are then defined in the four dimensions of $\mathbb{E}^4$.

(*a*) *Notations of the point symmetry operations* (*PSOs*) *of* $\mathbb{E}^4$

As we are only concerned with mono-incommensurate space groups in our analysis, we must deal with the PSOs occurring in the corresponding crystal families, *i.e.* the families I, II, III, IV, VI and VII (Phan *et al.*, 1989). These PSOs are listed in Table 1. For each of them, we must consider the restriction of the operator to the external and internal spaces to derive the corresponding WJJ symbols. Most of the time, there is no ambiguity because the symmetry conditions for incommensurate structures imply the form of the matrix associated with the symmetry operation:

$$\left(\begin{array}{c|cc} \mathbf{Q} & \multicolumn{2}{c}{\mathbf{0}} \\ \hline \mathbf{0} & \varepsilon & 0 \\ & 0 & \varepsilon \end{array}\right),$$

where $\mathbf{Q}$ is a 2×2 matrix and $\varepsilon = \pm 1$ (de Wolff, 1974). This form imposes a choice concerning the fourth dimension. Nevertheless, the rotation 2 is either in a plane containing the fourth dimension or not, and this leads either to a mirror plane m or to a 2-axis in the physical space. To remove the ambiguity, we characterize the $(\mathrm{MI})^-$ symmetry operations which invert the internal dimension, *i.e.* which transform $\mathbf{q}$ to $-\mathbf{q}$, by the extra symbol $^{\blacktriangledown}$. The WPV–WJJ correspondences are listed in Table 1.

(*b*) *Notations of the point symmetry groups* (*PSGs*) *of* $\mathbb{E}^4$

The correspondences between WPV and WJJ notations are listed in Table 2 for the 31 mono-incommensurate WJJ PSGs, which correspond to 30 crystallographic PSGs among the 227 ones in $\mathbb{E}^4$ (Weigel *et al.*, 1987); indeed, one of them, 2, splits into two, 2 and $2^{\blacktriangledown}$, when we distinguish between the

Table 1. *WPV and WJJ symbols for the elementary PSOs associated with the mono-incommensurate space groups*

Elementary PSO full symbol	WPV symbol	WJJ symbol
1	1	$\begin{pmatrix}1\\1\end{pmatrix}$
m_Z	m	$\begin{pmatrix}m\\1\end{pmatrix}$
2_{XY}	2	$\begin{pmatrix}2\\1\end{pmatrix}$
2_{ZT}	$2^{\blacktriangledown}$	$\begin{pmatrix}m\\\bar{1}\end{pmatrix}$
$3^{\pm 1}_{XY}$	3	$\begin{pmatrix}3\\1\end{pmatrix}$
$4^{\pm 1}_{XY}$	4	$\begin{pmatrix}4\\1\end{pmatrix}$
$\dot{6}^{\pm 1}_{XY}$	6	$\begin{pmatrix}6\\1\end{pmatrix}$
$2_{ZT}4^{\pm 1}_{XY}$	$(24)^{\blacktriangledown}$	$\begin{pmatrix}\bar{4}\\\bar{1}\end{pmatrix}$
$2_{ZT}6^{\pm 1}_{XY}$	$(26)^{\blacktriangledown}$	$\begin{pmatrix}\bar{3}\\\bar{1}\end{pmatrix}$
$2_{ZT}3^{\pm 1}_{XY}$	$(23)^{\blacktriangledown}$	$\begin{pmatrix}\bar{6}\\\bar{1}\end{pmatrix}$
$\bar{1}_{XZT}$	$\bar{1}^{\blacktriangledown}$	$\begin{pmatrix}2\\\bar{1}\end{pmatrix}$
$\bar{1}_4$	$\bar{1}_4^{\blacktriangledown}$	$\begin{pmatrix}\bar{1}\\\bar{1}\end{pmatrix}$

external and the internal dimensions. Their WJJ symbols are usually directly deduced from the WPV ones by the previous correspondence of their generating PSOs, provided one outlines some supplementary remarks:

(i) the symbol '⊥' in WPV notations replaces the symbol '/' in WJJ notations;

(ii) for convenience, the respective arrangement of the PSOs is not always respected (VI-03, VI-04, VI-07, VII-09-03, VII-09-07);

(iii) the symbol of the PSG $2/m$ has been completed to $2/m\ \bar{1}^{\blacktriangledown}$, because the inversion axis $\bar{1}^{\blacktriangledown}$ can be a glide axis in the space group, and so justifies a notation for itself;

(iv) the notations of some PSOs are omitted in WJJ symbols when they are not necessary: 2 in IV-04 and $\bar{1}^{\blacktriangledown}$ in VII-08-05.

Here we can outline an important remark; when the WJJ symbol of a PSG has in its Z line only 1 values, and no $\bar{1}$ value, the fourth direction is invariant by all its PSOs and the corresponding PSG is a polar PSG of $\mathbb{E}^4$. Its WPV notation is then the same as the classical Hermann–Mauguin 3D notation of the basic structure (Veysseyre & Weigel, 1989).

(*c*) *Notations of the centring and of the Bravais classes*

From a crystallographic point of view, a centring derives from supplementary elementary translations with non-integer components introduced in the cell of the direct space or from systematic extinction conditions observed in the reciprocal space.

Now if we consider the different Bravais classes as they have been classified in de Wolff's approach, we can notice the very peculiar rôles of the 3D basic lattice on one hand and the internal direction on the other. Here a Bravais class is not defined as a rigorous Bravais type in $\mathbb{E}^4$, but (i) by the 3D Bravais type of its basic lattice, (ii) by the orientation of the modulation vector in this basic lattice (this distinction leads to the two monoclinic systems, either planar or axial) and (iii) by the rational components of the modulation wavevector. With all these considerations, a list of 24 Bravais classes has been established (de Wolff *et al.*, 1981).

On the other hand, the Bravais types of the 4D space have been listed and there are 16 for the 7 mono-incommensurate systems (Phan *et al.*, 1989). It becomes clear that some Bravais classes of the first classification are equivalent in the framework of the second one, since the internal fourth direction is not specified in the latter.

Let us take two examples and consider the WJJ Bravais classes 11 and 17 (first column of Table 3). The first one, $W^{P}{}^{m\,m\,m}_{1\,1\,\bar{1}}$ is characterized by a primitive orthorhombic basic lattice (**a**, **b**, **c**) and rational components $(1/2, 1/2, 0)$ of the modulation wavevector. The new lattice in direct 4D space is $(\mathbf{a}-1/2\mathbf{d}, \mathbf{b}-1/2\mathbf{d}, \mathbf{c}-\gamma\mathbf{d}, \mathbf{d})$. Now if we take $\mathbf{A}=2\mathbf{a}$, $\mathbf{B}=2\mathbf{b}$, $\mathbf{C}=\mathbf{c}-\gamma\mathbf{d}$, $\mathbf{D}=\mathbf{d}$ as new basic vectors, we note that the translations $(\mathbf{A}+\mathbf{B})/2$, $(\mathbf{A}+\mathbf{D})/2$ and $(\mathbf{B}+\mathbf{D})/2$ belong to the 4D lattice, and the new cell appears to be face centred [$F(1,2,4)$ in BBNWZ or $F(X, Y, T)$ in WPV notations].

The second one, $P^{F}{}^{m\,m\,m}_{1\,1\,\bar{1}}$ is characterized by a face-centred basic lattice (**a**, **b**, **c**) with additional translations $(\mathbf{a}+\mathbf{b})/2$, $(\mathbf{b}+\mathbf{c})/2$ and $(\mathbf{a}+\mathbf{c})/2$, and a purely irrational modulation wavevector $(0, 0, \gamma)$. The new cell in the direct 4D space is $(\mathbf{a}, \mathbf{b}, \mathbf{c}-\gamma\mathbf{d}, \mathbf{d})$. We know that, for a modulated structure, a 3D translation operation of vector $\boldsymbol{\nu}$ is equivalent to a translation $(\boldsymbol{\nu}, (-\mathbf{q}\,.\,\boldsymbol{\nu})\mathbf{d})$ in the 4D space. The extra centring translations become $(\mathbf{a}+\mathbf{b})/2$, $(\mathbf{a}+\mathbf{c}-\gamma\mathbf{d})/2$ and $(\mathbf{b}+\mathbf{c}-\gamma\mathbf{d})/2$ and correspond to face-centring translations [$F(1,2,3)$ in BBNWZ or $F(X, Y, Z)$ in WPV notations] in relation to the 4D cell.

These two classes correspond to the same 4D Bravais type F in crystal family IV, regardless of the choice of the axes. If we generalize the reflection conditions of such a Bravais type from the equivalent ones in 3D space, we obtain the conditions $(h+m=2n, k+m=2n')$ for $F(X, Y, T)$ and $(h+k=2n, k+l=2n')$ for $F(X, Y, Z)$ (we recall that m is the Miller

Table 2. *WPV and WJJ symbols for the mono-incommensurate PSGs of* $\mathbb{E}^4$

Family class	WPV symbol	WJJ symbol
I. Hexaclinic		
01-01	1	$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$
01-02	$\bar{1}_4^{\blacktriangledown}$	$\begin{pmatrix} \bar{1} \\ \bar{1} \end{pmatrix}$
II. Right hyperprism based on parallelepiped		
02-01	m	$\begin{pmatrix} m \\ 1 \end{pmatrix}$
02-02	$\bar{1}^{\blacktriangledown}$	$\begin{pmatrix} 2 \\ \bar{1} \end{pmatrix}$
02-03	$\bar{1}^{\blacktriangledown}\perp m$	$\begin{pmatrix} 2/m \\ \bar{1}\ 1 \end{pmatrix}$
III. Di-orthogonal parallelograms		
03-01	$\begin{cases} 2 \\ 2^{\blacktriangledown} \end{cases}$	$\begin{pmatrix} 2 \\ 1 \end{pmatrix}$ $\begin{pmatrix} m \\ \bar{1} \end{pmatrix}$
03-02	$2\perp 2^{\blacktriangledown}$	$\begin{pmatrix} 2/m \\ 1\ \bar{1} \end{pmatrix}$
IV. Orthogonal parallelogram rectangle		
04-01	$m, m, 2$	$\begin{pmatrix} m & m & 2 \\ 1 & 1 & 1 \end{pmatrix}$
04-02	$2^{\blacktriangledown}/m, \bar{1}^{\blacktriangledown}$	$\begin{pmatrix} m & m & 2 \\ \bar{1} & 1 & \bar{1} \end{pmatrix}$
04-03	$2, 1^{\blacktriangledown}, 1^{\blacktriangledown}$	$\begin{pmatrix} 2 & 2 & 2 \\ 1 & \bar{1} & \bar{1} \end{pmatrix}$
04-04	$2^{\blacktriangledown}\perp 2, m, m$	$\begin{pmatrix} m & m & m \\ \bar{1} & 1 & 1 \end{pmatrix}$
VI. Orthogonal parallelogram square		
07-01	$(24)^{\blacktriangledown}$	$\begin{pmatrix} \bar{4} \\ \bar{1} \end{pmatrix}$
07-02	4	$\begin{pmatrix} 4 \\ 1 \end{pmatrix}$
07-03	$2^{\blacktriangledown}\perp 4$	$\begin{pmatrix} 4/m \\ 1\ \bar{1} \end{pmatrix}$
07-04	$(24)^{\blacktriangledown}, m, \bar{1}^{\blacktriangledown}$	$\begin{pmatrix} \bar{4} & 2 & m \\ \bar{1} & \bar{1} & 1 \end{pmatrix}$
07-05	$4, \bar{1}^{\blacktriangledown}, \bar{1}^{\blacktriangledown}$	$\begin{pmatrix} 4 & 2 & 2 \\ 1 & \bar{1} & \bar{1} \end{pmatrix}$
07-06	$4, m, m$	$\begin{pmatrix} 4 & m & m \\ 1 & 1 & 1 \end{pmatrix}$
07-07	$2^{\blacktriangledown}\perp 4, m, m$	$\begin{pmatrix} 4/m & m & m \\ 1\ \bar{1} & 1 & 1 \end{pmatrix}$
VII. Orthogonal parallelogram hexagon		
08-01	3	$\begin{pmatrix} 3 \\ 1 \end{pmatrix}$
08-02	$(26)^{\blacktriangledown}$	$\begin{pmatrix} \bar{3} \\ \bar{1} \end{pmatrix}$
08-03	$3, m$	$\begin{pmatrix} 3 & m \\ 1 & 1 \end{pmatrix}$
08-04	$3, \bar{1}^{\blacktriangledown}$	$\begin{pmatrix} 3 & 2 \\ 1 & \bar{1} \end{pmatrix}$
08-05	$(26)^{\blacktriangledown}, m, \bar{1}^{\blacktriangledown}$	$\begin{pmatrix} \bar{3} & m \\ \bar{1} & 1 \end{pmatrix}$
09-01	6	$\begin{pmatrix} 6 \\ 1 \end{pmatrix}$
09-02	$2^{\blacktriangledown}\perp 3$	$\begin{pmatrix} \bar{6} \\ \bar{1} \end{pmatrix}$
09-03	$2^{\blacktriangledown}\perp 6$	$\begin{pmatrix} 6/m \\ 1\ \bar{1} \end{pmatrix}$
09-04	$6, m, m$	$\begin{pmatrix} 6 & m & m \\ 1 & 1 & 1 \end{pmatrix}$
09-05	$6, \bar{1}^{\blacktriangledown}, \bar{1}^{\blacktriangledown}$	$\begin{pmatrix} 6 & 2 & 2 \\ 1 & \bar{1} & \bar{1} \end{pmatrix}$
09-06	$2^{\blacktriangledown}\perp 3, m, \bar{1}^{\blacktriangledown}$	$\begin{pmatrix} \bar{6} & m & 2 \\ \bar{1} & 1 & \bar{1} \end{pmatrix}$
09-07	$2^{\blacktriangledown}\perp 6, m, m$	$\begin{pmatrix} 6/m & m & m \\ 1\ \bar{1} & 1 & 1 \end{pmatrix}$

index corresponding to the satellites in the diffraction pattern). These conditions correspond to the respective reflection conditions listed for the Bravais classes 11 and 17.

Some Bravais classes are a little more complicated since they simultaneously induce a non-primitive basic lattice and rational components of the modulation wavevector, for example, in the orthorhombic system, the Bravais class 14, $L^{C}{}^{m\,m\,m}_{1\,1\,\bar{1}}$.

The basic 3D lattice has **a**, **b** and **c** as basic cell vectors and $(\mathbf{a}+\mathbf{b})/2$ as an additional translation. The modulation wavevector is $(1, 0, \gamma)$. As a consequence, the 4D lattice has basis vectors $(\mathbf{a}-\mathbf{d}, \mathbf{b}, \mathbf{c}-\gamma\mathbf{d}, \mathbf{d})$. The vector **a** is still a lattice vector and if we keep it as first basis vector, we must introduce the new additional translation $(\mathbf{a}+\mathbf{b}-\mathbf{d})/2$, associated with the 3D translation $(\mathbf{a}+\mathbf{b})/2$; it is characteristic of a body-centred lattice $I(X, Y, T)$. Moreover, we can outline that the reflection condition $(h+k+m=2n)$ listed for this Bravais class corresponds to a typical body-centred-lattice reflection condition.

For most of the WJJ Bravais classes, it is no particular problem to derive the equivalent WPV Bravais type. The correspondence is listed in Table 3, with respect to the different settings including the fourth direction.

There are only two classes which cannot be directly deduced, the Bravais classes 18, $L^{F}{}^{m\,m\,m}_{1\,1\,\bar{1}}$, and 20, $W_1^{P4/}{}^{m\,m\,m}_{\bar{1}\,1\,1}$. For the first one, if we apply the same process as previously, we simultaneously obtain two body centrings $I(X, Y, T)$ and $I(X, Z, T)$ and a face centring $S(Y, Z)$, which are coherent with the corresponding reflection conditions $(h+k+m=2n, k+l=2n')$. But this Bravais type is not valid as a 4D Bravais type in the system orthogonal parallelogram rectangle; and in fact, the body centring $I(X, Z, T)$

Table 3. *Correspondence between WJJ, BBNWZ and WPV symbols of the Bravais lattices of* $\mathbb{E}^4$; *equivalent WJJ Bravais classes are bracketed together*

WJJ symbol*	BBNWZ symbol†	WPV symbol‡
Triclinic		Hexaclinic
01-P^P	I-01-02-01	P
Planar monoclinic		Right hyperprism based on parallelepiped(X, Y, T)
02-P^P	II-02-03-01	P
{03-C^P	II-02-03-02	{$S(Z, T)$
{04-P^B		{$S(X, Z)$
Axial monoclinic		Di-orthogonal parallelograms(XY)(ZT)
05-P^P	III-03-02-01	P
{06-A^P	III-03-02-02	{$S(X, T)$
{07-P^B		{$S(X, Z)$
08-B^B	III-03-02-03	$D(X, Z)(Y, T)$
Orthorhombic		Orthogonal parallelogram(ZT) rectangle(XY)
09-P^P	IV-04-04-01	P
13-P^C	IV-04-04-02	$S(X, Y)$
{10-B^P	IV-04-04-03	{$S(Y, T)$
{15-P^A		{$S(Y, Z)$
{12-P^I	IV-04-04-04	{$I(X, Y, Z)$
{14-L^C		{$I(X, Y, T)$
{16-A^A	IV-04-04-05	{$D(X, T)(Y, Z)$
{18-L^F		{$D(Y, Z)(X, Z+T)$
{11-W^P	IV-04-04-06	{$F(X, Y, T)$
{17-P^F		{$F(X, Y, Z)$
Tetragonal		Orthogonal parallelogram(ZT) square(XY)
19-P^P	VI-07-07-01	P
{20-W^P	VI-07-07-02	{$I(X+Y, X-Y, T)$
{21-P^I		{$I(X, Y, Z)$
Trigonal hexagonal		Orthogonal parallelogram(ZT) hexagon(XY)
{22-P^R	VII-08-05-01	{$R(X, Y, Z)$
{23-R^P		{$R(X, Y, T)$
24-P^P	VII-09-07-02	P

* One recalls that the symbols P, B, C, L, W and R correspond respectively to rational components of the modulation vector of (0, 0, 0), (0, 1/2, 0), (0, 0, 1/2), (1, 0, 0), (1/2, 1/2, 0) and (1/3, 1/3, 0). The number which precedes the WJJ symbol corresponds to the WJJ classification of the Bravais classes.

† The BBNWZ symbol refers to the holohedry of the considered Bravais type of $\mathbb{E}^4$.

‡ The setting of the axes has been defined again to be consistent with the WJJ setting, *i.e.* T is the internal direction. One recalls that the centring $D(X, Z)(Y, T)$ corresponds to the three simultaneous centrings $S(X, Z)$, $S(Y, T)$ and $Z(X, Y, Z, T)$.

is not a valid one with the angular relations between the three basis vectors $\mathbf{a}, \mathbf{c}-\gamma\mathbf{d}$ and $\mathbf{d}$ (they form a monoclinic cell which cannot be body centred). Now if we consider that the fourth direction is not a specific one, we can replace $\mathbf{d}$ by $\mathbf{d}'=\mathbf{c}+\mathbf{d}$, the centring $I(X, Z, T)$ becomes $S(X, T')$, $I(X, Y, T)$ becomes $Z(X, Y, Z, T')$ and the Bravais type becomes $D(Y, Z)(X, T')$, with $T' = Z + T$. In this case, the new axis $\mathbf{d}'$ is a combination of an internal and an external direction, and such a choice is forbidden in WJJ notations.

For the second one, W^P, similar considerations would give a face-centred $F(X, Y, T)$ cell (see, for example, the WJJ Bravais class 11). But in the tetragonal system we can choose a new set of axes $(A' = a + b, B' = a - b)$ and $F(X, Y, T)$ becomes $I(X', Y', T)$ which is compatible with the crystal system orthogonal parallelogram square (of course, a tetragonal cell cannot have all faces centred).

(*d*) *Notations of the space symmetry groups* (*SSGs*) *of* $\mathbb{E}^4$

From the previous considerations, it is now easy to derive the general correspondence of the WJJ and WPV notations of the SSGs of $\mathbb{E}^4$. The notations of the translation parts of the symmetry operators are the following:

(i) In WPV notations, a subscript indicates the orientation and the modulus of the translation vector, whatever its direction. (For simplification, the notation '/2' is omitted and is the standard value of the translation vector along the considered direction.)

(ii) In WJJ notations, in the external space, the notations are the Hermann–Mauguin notations of the 3D SSGs, and in the internal direction, a notation of the τ value of the phase shift is given by one of the letters s, t, q or h in the Z line of the symbol, according to the modulus of the translation vector.

Since there is a clear distinction between internal and external spaces in WJJ notation, which is not explicit in WPV notation, it becomes obvious that some different WJJ SSGs will be equivalent to the same WPV SSG, but with a different setting of the axes. We can here outline three different types of equivalence, which appear when one of the external directions is equivalent to the internal one with respect to all the PSOs of the SSG.

(i) Equivalence related to the translation vectors of the space symmetry operation; for example, the

WJJ SSG $P^{P}{}^{b}_{1}$ and $P^{P}{}^{m}_{s}$ will be written in WPV notation $Pm_{\mathbf{b}}$ and $Pm_{\mathbf{d}}$; in the same way, $P^{P}{}^{2_1}_{1}$ and $P^{P}{}^{2}_{s}$ will be written $P2_{\mathbf{a}}$ and $P2_{\mathbf{d}}$.

(ii) Equivalence related to the choice of the axes of a rotation plane in $\mathbb{E}^4$; for example, $P^{P}{}^{m}_{\bar 1}$ and $P^{P}{}^{2}_{1}$ will be written $P2^{\blacktriangledown}$ and $P2$.

(iii) Equivalence related to a centring; for example, $P^{B}{}^{m}_{1}$ and $C^{P}{}^{m}_{1}$ refer to a face centring which will be written respectively $S(X, Z)m$ and $S(Z, T)m$ in WPV notations.

Some physical examples of incommensurate structures

Some incommensurate structures have already been determined and their symmetry has generally been described in the four-dimensional formalism with the WJJ notation, which is the most closely related to the corresponding average structure and to the distinction between internal and external spaces. It is now interesting to consider their real four-dimensional SSG with their general WPV notation and to compare these notations.

In the introduction we have already detailed the example of γ-Na_2CO_3, with the equivalent WJJ and WPV notations $P^{C}{}^{2/}_{\bar 1}{}^{m}_{s}$ and $S(X, Y)\bar{1}^{\blacktriangledown}\perp m_{\mathbf{d}}$. In order to clarify the physical meaning of the different axes and to keep the setting chosen for the average structure, it is possible to add the components of the modulation vector and the orientation of the internal direction to the previously described WJJ or WPV symbol. The full symbols would be

$$P^{C}{}^{2/}_{\bar 1}{}^{m}_{1}(\alpha, 0, \gamma) \text{ and } S(X, Y)\bar{1}^{\blacktriangledown}\perp m_{\mathbf{d}}(\alpha\mathbf{a}^* + \gamma\mathbf{c}^*, \mathbf{d}).$$

Let us now take the example of the structural family A_2BX_4. The structure of K_2SeO_4 has been given in the WJJ space group $P^{P}{}^{n}_{\bar 1}{}^{a}_{s}{}^{m}_{s}$ $(\alpha, 0, 0)$ (Yamada, Ono & Ikeda, 1984). This group does not appear in the first table of the WJJ notations (de Wolff *et al.*, 1981), but it has been shown that it is equivalent to the space group $P^{P}{}^{n}_{\bar 1}{}^{a}_{1}{}^{m}_{s}$ $(1-\alpha, 0, 0)$ with a different choice of the modulation vector (Yamamoto *et al.*, 1985). These two symbols can be translated in WPV notation by

$$2^{\blacktriangledown}_{\mathbf{b}+\mathbf{c}}\perp 2_{\mathbf{a}},\ m_{\mathbf{a}+\mathbf{d}},\ m_{\mathbf{d}}(\alpha\mathbf{a}^*, \mathbf{d})$$

and

$$2^{\blacktriangledown}_{\mathbf{b}+\mathbf{c}}\perp 2_{\mathbf{a}+\mathbf{d}},\ m_{\mathbf{a}},\ m_{\mathbf{d}}[(1-\alpha)\mathbf{a}^*, \mathbf{d}].$$

In the same family, the group $P^{P}{}^{m}_{s}{}^{c}_{1}{}^{n}_{\bar 1}$ $(0, 0, \gamma)$ has been proposed for the modulated structure of $[N(CH_3)_4]_2CoCl_4$ (Fjaer, 1985) or of $[N(CH_3)_4]_2$-$ZnCl_4$ (Madariaga, Zuñiga, Pérez-Mato & Tello, 1987); it is equivalent to $P^{P}{}^{n}_{\bar 1}{}^{a}_{1}{}^{m}_{s}$ $(\alpha, 0, 0)$ in a different setting. Nevertheless it is not the same group as that of K_2SeO_4 because of the choice of the modulation vector and it must be noted in the WPV notation as

$$2^{\blacktriangledown}_{\mathbf{b}+\mathbf{a}}\perp 2_{\mathbf{c}},\ m_{\mathbf{c}},\ m_{\mathbf{d}}(\gamma\mathbf{c}^*, \mathbf{d}).$$

Another example which involves a centring is the modulated structure of CuAu II (Yamamoto, 1982) which has been refined with the space group $L^{F}{}^{m}_{1}{}^{m}_{\bar 1}{}^{m}_{1}$ $(0, \beta, 0)$. Its WPV notation is

$$D(Z, T)(X, Y+Z)2^{\blacktriangledown}\perp 2,\ m,\ m(\beta\mathbf{b}^*, \mathbf{d}).$$

In the same way, the NC-type pyrrhotite, $Fe_{1-x}S$ admits the superspace group $W^{P}{}^{n}_{q}{}^{a}_{q}{}^{2_1}_{1}(1/2, 1/2, \gamma)$ (Yamamoto & Nakazawa, 1982) or

$$F(X, Y, T)m_{\mathbf{c}+(\mathbf{b}+\mathbf{d})/4},\ m_{(\mathbf{a}+\mathbf{d})/4},\ 2_{\mathbf{c}}(\gamma\mathbf{c}^*, \mathbf{d}).$$

This group is equivalent in a different setting to $U^{P}{}^{2_1}_{1}{}^{n}_{q}{}^{b}_{q}(\alpha, 1/2, 1/2)$ or

$$F(Y, Z, T)2_{\mathbf{a}},\ m_{\mathbf{a}+(\mathbf{c}+\mathbf{d})/4},\ m_{(\mathbf{b}+\mathbf{d})/4}(\alpha\mathbf{a}^*, \mathbf{d}),$$

which is the group proposed in the orthorhombic symmetry analysis of $BaMnF_4$ (Sciau, Grebille, Bérar & Lapasset, 1986). But this last compound has been shown to present more probably a monoclinic symmetry with space group $B^{P}{}^{2_1}_{1}(\alpha, 1/2, 0)$ or $S(Y, T)2_{\mathbf{a}}(\alpha\mathbf{a}^*, \mathbf{d})$ (Sciau, Lapasset, Grebille & Bérar, 1988).

A last example can be given in the tetragonal or orthogonal parallelogram square system. The incommensurate structure of $NbTe_4$ has been refined in the space group $W^{P}{}^{4/}_{1}{}^{m}_{\bar 1}{}^{c}_{1}{}^{a}_{1}(1/2, 1/2, \gamma)$ (van Smaalen, Bronsema & Mahy, 1986), which can be written $F(X, Y, T)2\perp 4,\ m_{\mathbf{c}},\ m_{\mathbf{a}}(\gamma\mathbf{c}^*, \mathbf{d})$.

The four-dimensional formalism has been proved also to be useful and adequate for the description of commensurate modulated structures (superstructures). In this case, all the components of the modulation vector are rational, and a new symbol has been proposed for the WJJ notations: T (van Smaalen, 1987). Some superstructures can be directly described with the superspace groups of the incommensurately modulated structures. Thus, the structure of phase III of $KFeF_4$ has been successfully described in the space group $T^{A}{}^{m}_{1}{}^{m}_{\bar 1}{}^{a}_{1}(0, 1/2, 0)$ (Sciau & Grebille, 1989) or $S(Y, Z)2^{\blacktriangledown}\perp 2_{\mathbf{d}},\ m_{\mathbf{a}+\mathbf{d}},\ m(\mathbf{b}^*/2, \mathbf{d})$. But one can also derive for these commensurate structures new space groups which are not contained in de Wolff's table (de Wolff *et al.*, 1981) and which have been listed by van Smaalen (1987). These new groups satisfy new orthogonality and centring conditions and so do not belong to the seven mono-incommensurate crystal systems of $\mathbb{E}^4$, but to the systems di-orthogonal rectangles, orthogonal rectangle square, di-orthogonal squares or orthogonal rectangle hexagon; they would justify further developments on the different centrings of these systems.

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