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Space-Group Notation with an Explicit Origin

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Abstract

A set of symbols based on the minimum subset of Seitz matrices required to generate the complete symmetry may be derived for each of the three-dimensional crystallographic space groups. This has a number of desirable properties including explicit information on the choice of origin. It also leads to a simple and general algorithmic procedure for generating equivalent positions.

Introduction

Two main systems of crystallographic space group names are in use today. Schönflies notation originated with the early derivation of space groups (Schönflies, 1891) and International notation came into general use with the 'old' *International Tables for X-ray Crystallography* (Bragg, von Laue & Hermann, 1935). Both the International and Schönflies notations appear in the current issue of *International Tables for X-ray Crystallography*, Vol. I (Henry & Lonsdale, 1972).

International space-group notation is commonly used in crystallography because it contains explicit information about the nature and the orientation of the symmetry elements in any particular space group. This notation invokes a sequence of alphanumeric characters which specify the Bravais-lattice type, the constituent symmetry elements and the orientation of elements with respect to the cell axes. *International Tables for X-ray Crystallography*, Vol. I, lists these symbols in a 'full' and 'short' format. The full symbol contains complete information on the nature and orientation of the symmetry elements, while the short symbol contains the minimum subset of this information necessary to describe uniquely the essential point group and diffraction symmetry of the space group.

The diffraction symmetry information appears in the International short symbol as those translational elements which give rise to systematic absences (see p. 549, *International Tables for X-ray Crystallography*, Vol. I). Translational information which relates the symmetry operators to a cell origin is not included. This omission is not surprising since the choice of origin is irrelevant in diffraction space, and it is from this direction that crystallographers have traditionally determined space-group symmetry.

It should be emphasized that from a group theoretical point of view the complete translational symmetry of each space group is *implicit* in the symmetry elements of the International symbol. However, the absence of *explicit* translational information in the space-group name places practical limitations on its use as a concise space-group descriptor. In the first place, most space groups have more than one possible origin. But origin specification is often desirable for easy comparison of symmetrically equivalent sites. *International Tables for X-ray Crystallography*, Vol. I, satisfies this requirement by listing the equivalent positions of each space group for a specific origin choice. Unfortunately, the selection of origins for the space groups as given in *International Tables for X-ray Crystallography* appears to have been arbitrary. This makes a consistent approach to generation of equivalent positions using the International notation unduly complicated.

The use of the International notation has several other disadvantages as a space-group descriptor. The implied directions of the pure and impure rotational elements vary according to the crystal system (see Table 3.3.2, *International Tables for X-ray Crystallography*, Vol. I). This further complicates the transcription of the International notation into the symmetry elements. Similarly the use of *redundant* symmetry information in the space-group names of certain crystal classes, but not of others, precludes a consistent procedure using these names to generate a complete set of symmetry elements for each of the space groups.

The space-group names described in this paper have the following properties:

(*a*) they contain explicit translational information which completely specifies the space-group origin;

(*b*) they contain no redundant symmetry information (*i.e.* they invoke a minimum subset of symmetry operators required to generate all elements);

(*c*) they explicitly distinguish centrosymmetric from noncentrosymmetric space groups;

(*d*) they provide direct information about the number of symmetry elements in the space group; and

(*e*) a very simple set of rules defines the implicit *directions* of rotational elements.

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Seitz matrix formalism

Each space group is composed of a unique set of symmetry operators in three-dimensional space. These operators are conveniently represented by 4 × 4 Seitz matrices (Seitz, 1936; Bradley & Cracknell, 1972) of the form

$$S = \left[\begin{array}{ccc:c} r_{11} & r_{12} & r_{13} & t_1 \\ r_{21} & r_{22} & r_{23} & t_2 \\ r_{31} & r_{32} & r_{33} & t_3 \\ \hdashline 0 & 0 & 0 & 1 \end{array}\right] \quad (1)$$

$$= \left[\begin{array}{c:c} R & \mathbf{t} \\ \hdashline 0 & 1 \end{array}\right] \quad (2)$$

$$= \{R/\mathbf{t}\}, \quad (3)$$

where R is the 3 × 3 matrix defining the rotation operation and $\mathbf{t}$ is the vector defining the translation operation. The allowed values for $r_{11}, r_{12}, \ldots, r_{13}$ are 0, +1 or −1, and the elements t_1, t_2, t_3 are the fractions of the crystal unit cell 0, $\frac{1}{6}$, $\frac{1}{4}$, $\frac{1}{3}$, $\frac{1}{2}$, $\frac{2}{3}$, $\frac{3}{4}$, or $\frac{5}{6}$. That is, for a space group composed of n symmetry operators the binary product $S_i S_j = S_k$ must satisfy the condition that $1 \leq \{i,j,k\} \leq n$. It follows that there can exist subsets of Seitz matrices which also define uniquely the symmetry of a space group, and that enable the full set of symmetry operators to be generated simply by a process of binary multiplication. The *minimum* subset of Seitz matrices required to define a space group uniquely is the basis of the notation proposed in this paper and will be referred to henceforth as the set of *generator matrices*.

In *International Tables for X-ray Crystallography*, Vol. I, the complete set of symmetry operators for each space group is given as general equivalent positions expressed in the Jones Faithful representation **x** (= *x,y,z*; *etc.*). The relationship between these two representations is simply

$$x = r_{11}x + r_{12}y + r_{13}z + t_1, \quad (4)$$

$$y = r_{21}x + r_{22}y + r_{23}z + t_2, \quad (5)$$

$$z = r_{31}x + r_{32}y + r_{33}z + t_3, \quad (6)$$

where *x,y,z* are coordinates in fractions of unit-cell axes along the principal cell directions. Equations (4)–(6) may be more concisely expressed for the *i*th symmetry operation as

$$\mathbf{x}_i = R_i\,\mathbf{x} + \mathbf{t}_i \quad (7)$$

or simply

$$(\mathbf{x},1)_i = S_i(\mathbf{x},1). \quad (8)$$

The convenience of the Seitz matrix formalism can be illustrated by considering the relationship between symmetry operations in real and reciprocal space. Each space group defines a set of symmetry operations in reciprocal space, referred to as equivalent reflections **h** (= *h,k,l*; *etc.*). The *i*th equivalent reflection $\mathbf{h}_i$ and corresponding phase shift Δ_i (in cycles $1{\cdot}0 = 2\pi$) may be expressed in Seitz notation as

$$(\mathbf{h},\Delta)_i = (\mathbf{h},0)\,S_i. \quad (9)$$

This is equivalent to the equations

$$h = r_{11}h + r_{21}k + r_{31}l, \quad (10)$$

$$k = r_{12}h + r_{22}k + r_{32}l, \quad (11)$$

$$l = r_{13}h + r_{23}k + r_{33}l, \quad (12)$$

and

$$\Delta = t_1 h + t_2 k + t_3 l. \quad (13)$$

Computer application of Seitz matrices

Every form of space-group symmetry is defined uniquely by the associated Seitz matrices. Information such as special positions in real space, site reflection multiplicities, systematic absences, intensity reinforcement factors, and structure seminvariant relationships may be obtained directly from these matrices. Computationally it is of significant practical value to use these matrices as the sole source of space-group information. Thus a space group need be specified only once, after which all subsequent symmetry considerations can be handled automatically. The advantages of this approach in the use of space-group symmetry include user convenience, minimization of input errors and reduced computer storage requirements.

In many cases of existing crystallographic computer software this approach to space-group definition has been adopted. Some computer programs require as input the complete set of n symmetry operators as either equivalent positions $\mathbf{x}_i$ (Stewart, 1976; Main, Woolfson & Germain, 1971) or as R_i matrices and $\mathbf{t}_i$ vectors (Ahmed, Hall, Pippy & Huber, 1966). For higher-symmetry space groups this is a tedious and error-prone task. The use of equivalent positions is also dependent upon whether the crystal settings used are those listed in *International Tables for X-ray Crystallography*, Vol. I.

Clearly it would be more desirable to specify the space-group symmetry in terms of a unique but simple name. This has been attempted in some programs which depend upon the short form of the International space-group name (Larson, 1969; Burzlaff, Böhme & Jomm, 1977). However, because of the difficulties of origin definition and the order and choice of symbols referred to above, a large and relatively complex program segment is needed to generate from these names the complete set of equivalent positions given in *International Tables for X-ray Crystallography*, Vol. I.

Proposed space-group notation

The notation proposed in this paper results from an attempt to combine the computational advantages of an abbreviated name with the precise definition of a space group provided by its Seitz matrices. It is thus in essence a symbolic representation of the minimum set of Seitz matrices required to generate all the symmetry elements of each space group.

The proposed space-group notation has the general format:

$$L[N_T^A]_1\,[N_T^A]_2\,[N_T^A]_3.$$

L is the lattice symbol which specifies the pure translational symmetry associated with the elementary rotation matrix E and the inversion matrix $-E$. These are described in detail in Table 1.

N_T^A is a combined symbol which describes the Seitz matrix to be used as a generator. T is the symbol denoting the translation vector **t** (see Table 2) and N^A is the symbol specifying the rotation matrix R with respect to an axis 'A' (see Tables 3, 4 and 5). The general form of N_T^A is such that N is either a positive integer (1, 2, 3, 4 or 6) designating the order of a *proper* rotation, or a negative integer ($\bar{1}$, $\bar{2}$, $\bar{3}$, $\bar{4}$ or $\bar{6}$) designating the order of an *improper* rotation. The axis symbols are limited to x, y, z, '', ' and * to denote symmetry operations in the **a**, **b**, **c**, **a** + **b**$\circlearrowleft$, **a** − **b**$\circlearrowleft$ and **a** + **b** + **c**$\circlearrowleft$ directions, respectively.

The subscript symbol T is blank when **t** = (0,0,0) or some combination of alphanumeric symbols when specifying a fractional translation vector. For example, the subscript '*ad*' specifies the translation vector **t** = $(\frac{1}{2},0,0) + (\frac{1}{4},\frac{1}{4},\frac{1}{4}) = (\frac{3}{4},\frac{1}{4},\frac{1}{4})$. The subscript '2' of the combined symbol 3_2^z refers to translation vector $(0,0,\frac{2}{3})$.

Table 1. *Lattice symbol L*

The lattice symbol L of the space-group name specifies one or more generator matrices. Symbols with an overbar specify a centrosymmetric space group and two matrices related by an inversion centre. The number of generator matrices implied by each symbol is given as nS.

Noncentrosymmetric symbol	nS†	Centrosymmetric symbol	nS‡	Implied lattice translation **t**
P	1	$\bar{P}$	2	0,0,0
A	2	$\bar{A}$	4	0,0,0 $0,\frac{1}{2},\frac{1}{2}$
B	2	$\bar{B}$	4	0,0,0 $\frac{1}{2},0,\frac{1}{2}$
C	2	$\bar{C}$	4	0,0,0 $\frac{1}{2},\frac{1}{2},0$
I	2	$\bar{I}$	4	0,0,0 $\frac{1}{2},\frac{1}{2},\frac{1}{2}$
R	3	$\bar{R}$	6	0,0,0 $\frac{1}{3},\frac{2}{3},\frac{2}{3}$ $\frac{2}{3},\frac{1}{3},\frac{1}{3}$
F	4	$\bar{F}$	8	0,0,0 $0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$

† Implies $R = E$.

‡ Implies $R = E$ and $-E$, where $E \equiv \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$ and $-E = \begin{pmatrix} \bar{1} & & \\ & \bar{1} & \\ & & \bar{1} \end{pmatrix}$.

Table 2. *Translation symbol T*

The subscript symbol T specifies the translation component of each generator matrix. Alphabetic symbols specify fractional translations along a fixed direction. Numeric symbols specify translations as a fraction of the rotation order N and in the direction of the implied or explicitly defined axis.

Subscript symbol	Translation vector **t**	Subscript symbol	Translation vector **t**
a	$\frac{1}{2},0,0$	1 in 3_1	$\frac{1}{3}$
b	$0,\frac{1}{2},0$	2 in 3_2	$\frac{2}{3}$
c	$0,0,\frac{1}{2}$	1 in 4_1	$\frac{1}{4}$
n	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	3 in 4_3	$\frac{3}{4}$
u	$\frac{1}{4},0,0$	1 in 6_1	$\frac{1}{6}$
v	$0,\frac{1}{4},0$	2 in 6_2	$\frac{1}{3}$
w	$0,0,\frac{1}{4}$	4 in 6_4	$\frac{2}{3}$
d	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$	5 in 6_5	$\frac{5}{6}$

Table 3. *Rotation symbol N^A for principal axes*

The symbol N^A specifies the order of rotation (N) and the axial direction of rotation superscript A. This table lists N for the three principal unit-cell directions. Improper rotations are specified by an overbar. $R(\bar{n}) = -R(n)$.

Symbol	Rotation axis	Rotation component R $N=2$	$N=3$	$N=4$	$N=6$
N^x	**a**	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}$
N^y	**b**	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ \bar{1} & 0 & 1 \end{pmatrix}$
N^z	**c**	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Table 4. *Rotation symbol N^A for face-diagonal axes*

The symbols for face-diagonal twofold rotations are 2′ and 2″. The face-diagonal rotation matrices R are implied by the preceding rotor symbol which defines the unique axis.

Category	Preceded by N^x		Preceded by N^y		Preceded by N^z	
Symbol	2′	2″	2′	2″	2′	2″
Rotation axis	**b** − **c**	**b** + **c**	**a** − **c**	**a** + **c**	**a** − **b**	**a** + **b**
Rotation matrix R	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & \bar{1} & 0 \end{pmatrix}$	$\begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 \\ 0 & \bar{1} & 0 \\ 1 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$	$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}$

Table 5. *Rotation symbol N^A for body-diagonal axes*

The symbol for the body-diagonal threefold rotation is 3*. This defines the matrix for the **a** + **b** + **c** direction.

Symbol	Rotation axis	Rotation matrix R
3*	**a** + **b** + **c**	$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$

Some typical examples of Seitz matrices specified by N_T^A symbols are:

$$\bar{2}_c^x \equiv \begin{pmatrix} \bar{1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & \frac{1}{2} \\ 0 & 0 & 0 & 1 \end{pmatrix}; \quad 3^* \equiv \begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix};$$

$$4_{vw}^z \equiv \begin{pmatrix} 0 & \bar{1} & 0 & 0 \\ 1 & 0 & 0 & \frac{1}{4} \\ 0 & 0 & 1 & \frac{1}{4} \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Implied order for symmetry axes

The explicit form of the matrix symbols N_T^A means that space-group definition is essentially independent of the order they appear in the names.† It is desirable, however, to standardize the *order* of the matrix symbols for a number of practical reasons. It aids in the recognition of a space-group name and most importantly it facilitates an overall simplification of the notation. A simple set of rules for ordering the N_T^A symbols can enable most axis designations to be *implied* rather than *declared* explicitly with the symbol A.

The proposed space-group names listed in Table 6 use the following rules to define implicitly the direction of symmetry operations.

When the axis symbol A is omitted

the *first* symbol N_T refers to the axis direction **c**;
the *subsequent* N_T symbols refer to the axis direction
a if $N = 2$ preceded by $N = 2$ or 4,
a − **b** if $N = 2$ preceded by $N = 3$ or 6,
and **a** + **b** + **c** if $N = 3$.

In addition to their simplicity, these rules have several important advantages over those governing the International notation. Firstly, they are self-defining and independent of the crystal system; secondly, the unique axis for all space groups is implied to be along **c**; and thirdly, there is no need for redundant symbols to satisfy an implied axis order.

There is one further important difference. The proposed notation distinguishes quite clearly between the two alternative axial systems possible for some trigonal space groups. The primitive definition is used for the rhombohedral axes, while the R-centred cell is identified explicitly for hexagonal axes. The use of two names for a single space group is consistent both with the change in symmetry operators expected with a change in axial assignment, and with the self-defining nature of the proposed notation.

† The exception being the face-diagonal symbols which must be preceded by a symbol defining a unique axis.

Generation of equivalent positions

Step 1: *Decode space-group symbols*

The generation of a complete set of equivalent positions for a given space group is a relatively straightforward procedure. The first step is to decode the space-group symbols into the 'generator' matrices. This process is illustrated with a number of examples. In each example the number of generator matrice m is simply the *sum* of the Seitz matrices contributed by each component of the space group name. For instance, in example (ii) the lattice symbol $\bar{I}$ contributes four Seitz matrices, two from the I centre and two from the inversion $\bar{1}$. Similarly, the number of equivalent positions n for any space group comes directly from the *product* of the symmetry operations implied from each component of the space-group name. Again, in example (ii) the fourfold operator contributes four equivalent positions, while 2_c contributes two.

(i) $P2_{ac}\bar{2}$ (No. 31, $Pmn2_1$) decodes into m = 3 Seitz matrices which generate n = 1.2.2 = 4 equivalent positions.

$$P\colon S_1 = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix};$$

$$2_{ac}\colon S_2 = \begin{pmatrix} \bar{1} & & & \frac{1}{2} \\ & \bar{1} & & 0 \\ & & 1 & \frac{1}{2} \\ & & & 1 \end{pmatrix}; \quad \bar{2}\colon S_3 = \begin{pmatrix} \bar{1} & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}.$$

(ii) $\bar{I}42_c$ (No. 140, $I4/mcm$) decodes into m = 6‡ Seitz matrices which generate n = 4.4.2 = 32 equivalent positions.

‡ In practice it is not necessary to add to the generator list those matrices due either to a centred cell or to an inversion centre. It is usually more convenient to exclude all matrices related by a centre or an inversion from the symmetry elements and flag these properties of the space group separately. Each full set of generator matrices is shown in these examples to illustrate the complete expansion of the lattice symbol.

$$\bar{I}: S_1 = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}, \quad S_2 = \begin{pmatrix} 1 & & & \frac{1}{2} \\ & 1 & & \frac{1}{2} \\ & & 1 & \frac{1}{2} \\ & & & 1 \end{pmatrix},$$

$$S_3 = \begin{pmatrix} \bar{1} & & & \\ & \bar{1} & & \\ & & \bar{1} & \\ & & & 1 \end{pmatrix}, \quad S_4 = \begin{pmatrix} \bar{1} & & & \frac{1}{2} \\ & \bar{1} & & \frac{1}{2} \\ & & \bar{1} & \frac{1}{2} \\ & & & 1 \end{pmatrix};$$

$$4: S_5 = \begin{pmatrix} & \bar{1} & & \\ 1 & & & \\ & & 1 & \\ & & & 1 \end{pmatrix}; \quad 2_c: S_6 = \begin{pmatrix} 1 & & & 0 \\ & \bar{1} & & 0 \\ & & \bar{1} & \frac{1}{2} \\ & & & 1 \end{pmatrix}.$$

(iii) $R32_c''$ (No. 161, $R3c$) decodes into m = 5† Seitz matrices which generate n = 3.3.2 = 18 equivalent positions.

$$R: S_1 = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}, \quad S_2 = \begin{pmatrix} 1 & & & \frac{2}{3} \\ & 1 & & \frac{1}{3} \\ & & 1 & \frac{1}{3} \\ & & & 1 \end{pmatrix},$$

$$S_3 = \begin{pmatrix} 1 & & & \frac{1}{3} \\ & 1 & & \frac{2}{3} \\ & & 1 & \frac{2}{3} \\ & & & 1 \end{pmatrix}; \quad 3: S_4 = \begin{pmatrix} & \bar{1} & & \\ 1 & \bar{1} & & \\ & & 1 & \\ & & & 1 \end{pmatrix};$$

$$\bar{2}_c'': S_5 = \begin{pmatrix} & \bar{1} & & 0 \\ \bar{1} & & & 0 \\ & & \bar{1} & \frac{1}{2} \\ & & & 1 \end{pmatrix}.$$

(iv) $P3^*\bar{2}_n'$ (No. 161, $R3c$) decodes into m = 3 Seitz matrices which generate n = 1.3.2 = 6 equivalent positions.

$$P: S_1 = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix};$$

$$3^*: S_2 = \begin{pmatrix} & & 1 & \\ 1 & & & \\ & 1 & & \\ & & & 1 \end{pmatrix}; \quad \bar{2}_n': S_3 = \begin{pmatrix} 1 & & & \frac{1}{2} \\ & & 1 & \frac{1}{2} \\ & 1 & & \frac{1}{2} \\ & & & 1 \end{pmatrix}.$$

(v) $\bar{P}423$ (No. 221, $Pm3m$) decodes into m = 5† Seitz matrices which generate n = 2.4.2.3 = 48 equivalent positions.

† See footnote ‡ on p. 520.

$$\bar{P}: S_1 = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}, \quad S_2 = \begin{pmatrix} \bar{1} & & & \\ & \bar{1} & & \\ & & \bar{1} & \\ & & & 1 \end{pmatrix};$$

$$4: S_3 = \begin{pmatrix} & \bar{1} & & \\ 1 & & & \\ & & 1 & \\ & & & 1 \end{pmatrix}; \quad 2: S_4 = \begin{pmatrix} 1 & & & \\ & \bar{1} & & \\ & & \bar{1} & \\ & & & 1 \end{pmatrix};$$

$$3: S_5 = \begin{pmatrix} & & 1 & \\ 1 & & & \\ & 1 & & \\ & & & 1 \end{pmatrix}.$$

Step 2: *Generate symmetry operators*

The second stage of the generation process is to multiply together the m matrices in the generator list to obtain new matrices. Each matrix so formed is added to the list, and used in turn to form further binary products. This process, applied exhaustively, results in the generation of a set of matrices representing all possible symmetry operations in a space group. Since the number of unique symmetry operations n is specified explicitly by the notation (see the above examples) the generation process may be curtailed as soon as the list count m reaches n.

An algorithmic procedure for matrix generation is given below. R is the 3 × 3 partition of the 4 × 4 S matrix and the m and n are counts that do not include matrices related by a centre or an inversion.

```
do i = 2 to m                          outer generator loop
{  do j = 2 to m                       inner generator loop
   {   S(m + 1) = S(i) * S(j)          form new Seitz matrix
       for k = 1 to m + 1              inner search loop
       {if R(m + 1) = +R(k)            test for unique rotation
        or R(m + 1) = -R(k) exit loop  matrix exit if not
       }m = max (m, k)                 extend list if unique
   }   if m = n exit loop              exit when list complete
}                                      end of generation process
```

The procedure assumes, of course, that the list of matrices supplied by the 'decode' step are sensible and correct. In practice, it is necessary to have additional steps in this procedure as a protection against user error. Usually these would test both the space-group symbols and the generated matrices for logical integrity.

In addition it is desirable to output the general equivalent positions in the Jones Faithful representation (*i.e.* *x*,*y*,*z*; *etc.*), and the systematic absence conditions for *hkl* diffraction data. Although not essential these provisions provide in both real and reciprocal space the symmetry data in more familiar form. In both cases this information may be derived directly from the Seitz matrices.

Table 6. *Proposed space-group names*

IT = *International Tables for X-ray Crystallography*

IT No.	International notation	Proposed notation
1	$P1$	$P1$
2	$P\bar{1}$	$P\bar{1}$
3	$P2$	$P2$
4	$P2_1$	$P2_c$
5	$B2$	$B2$
6	Pm	$P\bar{2}$
7	Pb	$P\bar{2}_b$
8	Bm	$B\bar{2}$
9	Bb	$B\bar{2}_b$
10	$P2/m$	$\bar{P}2$
11	$P2_1/m$	$\bar{P}2_c$
12	$B2/m$	$\bar{B}2$
13	$P2/b$	$\bar{P}2_b$
14	$P2_1/b$	$\bar{P}2_{bc}$
15	$B2/b$	$\bar{B}2_b$
16	$P222$	$P22$
17	$P222_1$	$P2_c2$
18	$P2_12_12$	$P22_{ab}$
19	$P2_12_12_1$	$P2_{ac}2_{ab}$
20	$C222_1$	$C2_c2$
21	$C222$	$C22$
22	$F222$	$F22$
23	$I222$	$I22$
24	$I2_12_12_1$	$I2_{ac}2_{ab}$
25	$Pmm2$	$P2\bar{2}$
26	$Pmc2_1$	$P2_c\bar{2}$
27	$Pcc2$	$P2\bar{2}_c$
28	$Pma2$	$P2\bar{2}_a$
29	$Pca2_1$	$P2_c\bar{2}_{ac}$
30	$Pnc2$	$P2\bar{2}_{bc}$
31	$Pmn2_1$	$P2_{ac}\bar{2}$
32	$Pba2$	$P2\bar{2}_{ab}$
33	$Pna2_1$	$P2_c\bar{2}_n$
34	$Pnn2$	$P2\bar{2}_n$
35	$Cmm2$	$C2\bar{2}$
36	$Cmc2_1$	$C2_c\bar{2}$
37	$Ccc2$	$C2\bar{2}_c$
38	$Amm2$	$A2\bar{2}$
39	$Abm2$	$A2\bar{2}_b$
40	$Ama2$	$A2\bar{2}_a$
41	$Aba2$	$A2\bar{2}_{ab}$
42	$Fmm2$	$F2\bar{2}$
43	$Fdd2$	$F2\bar{2}_d$
44	$Imm2$	$I2\bar{2}$
45	$Iba2$	$I2\bar{2}_c$
46	$Ima2$	$I2\bar{2}_a$
47	$Pmmm$	$\bar{P}22$
48	$Pnnn$	$\bar{P}2_{ab}2_{bc}$
49	$Pccm$	$\bar{P}22_c$
50	$Pban$	$\bar{P}2_{ab}2_b$
51	$Pmma$	$\bar{P}2_a2_a$
52	$Pnna$	$\bar{P}2_a2_{bc}$
53	$Pmna$	$\bar{P}2_{ac}2$
54	$Pcca$	$\bar{P}2_a2_{ac}$
55	$Pbam$	$\bar{P}22_{ab}$
56	$Pccn$	$\bar{P}2_{ab}2_{ac}$
57	$Pbcm$	$\bar{P}2_c2_b$
58	$Pnnm$	$\bar{P}22_n$
59	$Pmmn$	$\bar{P}2_{ab}2_a$
60	$Pbcn$	$\bar{P}2_n2_{ab}$
61	$Pbca$	$\bar{P}2_{ac}2_{ab}$
62	$Pnma$	$\bar{P}2_{ac}2_n$
63	$Cmcm$	$\bar{C}2_c2$
64	$Cmca$	$\bar{C}2_{bc}2$
65	$Cmmm$	$\bar{C}22$
66	$Cccm$	$\bar{C}22_c$
67	$Cmma$	$\bar{C}2_a2$
68	$Ccca$	$\bar{C}2_b2_{ac}$
69	$Fmmm$	$\bar{F}22$
70	$Fddd$	$\bar{F}2_{uv}2_{vw}$
71	$Immm$	$\bar{I}22$
72	$Ibam$	$\bar{I}22_c$
73	$Ibca$	$\bar{I}2_b2_c$
74	$Imma$	$\bar{I}2_b2$
75	$P4$	$P4$
76	$P4_1$	$P4_1$
77	$P4_2$	$P4_c$
78	$P4_3$	$P4_3$
79	$I4$	$I4$
80	$I4_1$	$I4_{1b}$
81	$P\bar{4}$	$P\bar{4}$
82	$I\bar{4}$	$I\bar{4}$
83	$P4/m$	$\bar{P}4$
84	$P4_2/m$	$\bar{P}4_c$
85	$P4/n$	$\bar{P}4_a$
86	$P4_2/n$	$\bar{P}4_{bc}$
87	$I4/m$	$\bar{I}4$
88	$I4_1/a$	$\bar{I}4_{ad}$
89	$P422$	$P42$
90	$P42_12$	$P4_{ab}2_{ab}$
91	$P4_122$	$P4_12_c$
92	$P4_12_12$	$P4_{3n}2_{nw}$
93	$P4_222$	$P4_c2$
94	$P4_22_12$	$P4_n2_n$
95	$P4_322$	$P4_32_c$
96	$P4_32_12$	$P4_{1n}2_{abw}$
97	$I422$	$I42$
98	$I4_122$	$I4_{1b}2_{bw}$
99	$P4mm$	$P4\bar{2}$
100	$P4bm$	$P4\bar{2}_{ab}$
101	$P4_2cm$	$P4_c\bar{2}_c$
102	$P4_2nm$	$P4_n\bar{2}_n$
103	$P4cc$	$P4\bar{2}_c$
104	$P4nc$	$P4\bar{2}_n$
105	$P4_2mc$	$P4_c\bar{2}$
106	$P4_2bc$	$P4_c\bar{2}_{ab}$
107	$I4mm$	$I4\bar{2}$
108	$I4cm$	$I4\bar{2}_{ab}$
109	$I4_1md$	$I4_{1b}\bar{2}$
110	$I4_1cd$	$I4_{1b}\bar{2}_c$
111	$P\bar{4}2m$	$P\bar{4}2$
112	$P\bar{4}2c$	$P\bar{4}2_c$
113	$P\bar{4}2_1m$	$P\bar{4}2_{ab}$
114	$P\bar{4}2_1c$	$P\bar{4}2_n$
115	$P\bar{4}m2$	$P\bar{4}\bar{2}$
116	$P\bar{4}c2$	$P\bar{4}\bar{2}_c$
117	$P\bar{4}b2$	$P\bar{4}\bar{2}_{ab}$
118	$P\bar{4}n2$	$P\bar{4}\bar{2}_n$
119	$I\bar{4}m2$	$I4\bar{2}$
120	$I\bar{4}c2$	$I4\bar{2}_c$
121	$I\bar{4}2m$	$I\bar{4}2$
122	$I\bar{4}2d$	$I\bar{4}2_{bw}$
123	$P4/mmm$	$\bar{P}42$
124	$P4/mcc$	$\bar{P}42_c$
125	$P4/nbm$	$\bar{P}4_a2_b$
126	$P4/nnc$	$\bar{P}4_a2_{bc}$
127	$P4/mbm$	$\bar{P}42_{ab}$
128	$P4/mnc$	$\bar{P}42_n$
129	$P4/nmm$	$\bar{P}4_a2_a$
130	$P4/ncc$	$\bar{P}4_a2_{ac}$
131	$P4_2/mmc$	$\bar{P}4_c2$
132	$P4_2/mcm$	$\bar{P}4_c2_c$
133	$P4_2/nbc$	$\bar{P}4_{ac}2_b$
134	$P4_2/nnm$	$\bar{P}4_{ac}2_{bc}$
135	$P4_2/mbc$	$\bar{P}4_c2_{ab}$
136	$P4_2/mnm$	$\bar{P}4_n2_n$
137	$P4_2/nmc$	$\bar{P}4_{ac}2_a$
138	$P4_2/ncm$	$\bar{P}4_{ac}2_{ac}$
139	$I4/mmm$	$\bar{I}42$
140	$I4/mcm$	$\bar{I}42_c$
141	$I4_1/amd$	$\bar{I}4_{bd}2$
142	$I4_1/acd$	$\bar{I}4_{bd}2_c$
143	$P3$	$P3$
144	$P3_1$	$P3_1$
145	$P3_2$	$P3_2$
146	$R3$	$R3$ $P3^*$
147	$P\bar{3}$	$\bar{P}3$
148	$R\bar{3}$	$\bar{R}3$ $\bar{P}3^*$
149	$P312$	$P32$
150	$P321$	$P32''$
151	$P3_112$	$P3_12$
152	$P3_121$	$P3_12''$
153	$P3_212$	$P3_22$
154	$P3_221$	$P3_22''$
155	$R32$	$R32''$ $P3^*2$
156	$P3m1$	$P3\bar{2}''$
157	$P31m$	$P3\bar{2}$
158	$P3c1$	$P3\bar{2}_c''$
159	$P31c$	$P3\bar{2}_c$
160	$R3m$	$R3\bar{2}''$ $P3^*\bar{2}$
161	$R3c$	$R3\bar{2}_c''$ $P3^*\bar{2}_n$
162	$P\bar{3}1m$	$\bar{P}32$
163	$P\bar{3}1c$	$\bar{P}32_c$
164	$P\bar{3}m1$	$\bar{P}32''$
165	$P\bar{3}c1$	$\bar{P}32_c''$
166	$R\bar{3}m$	$\bar{R}32''$ $\bar{P}3^*2$
167	$R\bar{3}c$	$\bar{R}32_c''$ $\bar{P}3^*2_n$
168	$P6$	$P6$
169	$P6_1$	$P6_1$
170	$P6_5$	$P6_5$
171	$P6_2$	$P6_2$
172	$P6_4$	$P6_4$
173	$P6_3$	$P6_c$
174	$P\bar{6}$	$P\bar{6}$
175	$P6/m$	$\bar{P}6$
176	$P6_3/m$	$\bar{P}6_c$
177	$P622$	$P62$
178	$P6_122$	$P6_12$
179	$P6_522$	$P6_52$
180	$P6_222$	$P6_22$
181	$P6_422$	$P6_42$
182	$P6_322$	$P6_c2$
183	$P6mm$	$P6\bar{2}$
184	$P6cc$	$P6\bar{2}_c$
185	$P6_3cm$	$P6_c\bar{2}$
186	$P6_3mc$	$P6_c\bar{2}_c$
187	$P\bar{6}m2$	$P\bar{6}2$
188	$P\bar{6}c2$	$P\bar{6}_c2$
189	$P\bar{6}2m$	$P\bar{6}\bar{2}$
190	$P\bar{6}2_c$	$P\bar{6}_c\bar{2}_c$
191	$P6/mmm$	$\bar{P}62$
192	$P6/mcc$	$\bar{P}62_c$
193	$P6_3/mcm$	$\bar{P}6_c2$
194	$P6_3/mmc$	$\bar{P}6_c2_c$
195	$P23$	$P223$
196	$F23$	$F223$
197	$I23$	$I223$
198	$P2_13$	$P2_{ac}2_{ab}3$
199	$I2_13$	$I2_{ac}2_{ab}3$
200	$Pm3$	$\bar{P}223$
201	$Pn3$	$\bar{P}2_{ab}2_{bc}3$
202	$Fm3$	$\bar{F}223$
203	$Fd3$	$\bar{F}2_{uv}2_{vw}3$
204	$Im3$	$\bar{I}223$
205	$Pa3$	$\bar{P}2_{ac}2_{ab}3$
206	$Ia3$	$\bar{I}2_{ac}2_{ab}3$
207	$P432$	$P423$
208	$P4_232$	$P4_n23$
209	$F432$	$F423$
210	$F4_132$	$F4_d23$
211	$I432$	$I423$
212	$P4_332$	$P4_{bdn}2_{ab}3$
213	$P4_132$	$P4_{bd}2_{ab}3$
214	$I4_132$	$I4_{bd}2_{ab}3$
215	$P\bar{4}3m$	$P\bar{4}23$
216	$F\bar{4}3m$	$F\bar{4}23$
217	$I\bar{4}3m$	$I\bar{4}23$
218	$P\bar{4}3n$	$P4_n23$
219	$F\bar{4}3c$	$F4_c23$
220	$I\bar{4}3d$	$I\bar{4}_{bd}2_{ab}3$
221	$Pm3m$	$\bar{P}423$
222	$Pn3n$	$\bar{P}4_a2_{bc}3$
223	$Pm3n$	$\bar{P}4_n23$
224	$Pn3m$	$\bar{P}4_{bc}2_{bc}3$
225	$Fm3m$	$\bar{F}423$
226	$Fm3c$	$\bar{F}4_n23$
227	$Fd3m$	$\bar{F}4_{vw}2_{vw}3$
228	$Fd3c$	$\bar{F}4_{ud}2_{vw}3$
229	$Im3m$	$\bar{I}423$
230	$Ia3d$	$\bar{I}4_{bd}2_{ab}3$

Comparison of generated equivalent positions with those in *International Tables for X-ray Crystallography*

The generation procedure outlined above will, except for some centred-space-group names, provide equivalent positions identical to those in *International Tables for X-ray Crystallography*, Vol. I. The exceptions arise when the non-centred subgroup of equivalent positions listed in *International Tables for X-ray Crystallography* is inconsistent with a sequential generation process. Differences occur only if matrices related by a centre or an inversion are not generated but implied. If all matrices are generated, they are identical to the complete set of equivalent positions *implied* in *International Tables for X-ray Crystallography*, Vol. I. It follows that the generated subgroup of symmetry elements is identically equivalent for the majority of symmetry requirements.

Nonconventional space-group settings

Constructing new space-group names for nonconventional settings is a relatively straightforward task. Rotations can be assigned to any direction with the axis symbol *A*. As discussed above, a matrix generation process will normally check the symbolic name and equivalent positions for logical integrity. In addition, the systematic absences derived from this process can be validated against the measured diffraction data. In general, the proposed notation is no more difficult to use with nonconventional settings than is the existing International notation, even when the tables of International notation to translate nonconventional settings for space groups in the monoclinic and orthorhombic systems (*International Tables for X-ray Crystallography*, Vol. I, Tables 6.2.1) are taken into account.

To illustrate the use of a nonconventional space-group setting, consider space group No. 41 in *International Tables for X-ray Crystallography*, Vol. I, pp. 547 and 549.

Notation			Reflection conditions
Axes	International	Proposed	
abc	*Aba2*	$A2\tilde{2}_{ab}$	$hkl\ \ k+l=2n$; $0kl\ \ k=2n$; $(l=2n)$; $h0l\ \ h=2n$; $(l=2n)$; $hk0\ \ (k=2n)$
cab	*B2cb*	$B2^{x}\tilde{2}^{y}_{bc}$	$hkl\ \ h+l=2n$; $0kl\ \ (l=2n)$; $h0l\ \ (h=2n);\ l=2n$; $hk0\ \ (h=2n);\ k=2n$
ac̄b	*Ac2a*	$A2^{y}\tilde{2}^{z}_{ac}$	$hkl\ \ k+l=2n$; $0kl\ \ (k=2n);\ l=2n$; $h0l\ \ (l=2n)$; $hk0\ \ h=2n;\ (k=2n)$

Different origin choice and order to *International Tables for X-ray Crystallography*

Any proposal for new space-group notation would be incomplete without some *a priori* consideration of how the space-group names might be tabulated; that is, if the particular origin choice and space-group order adopted in *International Tables for X-ray Crystallography*, Vol. I, was ignored.

Table 7 shows the result of an approach to space-group arrangement based on similarity of symmetry operators and the number of symmetry elements. The ordering is simple and consistent with recognized operator subgroups. The subgroups of space groups are arranged in approximate order of increasing symmetry.

Conclusion

The proposed space-group notation gives a precise description of space-group symmetry. The explicit definition of the space-group inversion centre and the clear separation of rotation, translation and axis-direction symbols provides direct and easily interpretable information about the symmetry of any group. The construction and format of the notation make it particularly suited to computer generation of symmetry information. Because it is a concise representation of symmetry in real space it should also be attractive to disciplines other than crystallography. Certainly the existing International notation is limited for many workers in non-crystallographic fields because the name itself cannot be readily interpreted in either real or reciprocal space. This deficiency could be one of the reasons why International notation has not gained wider acceptance in other scientific disciplines.

There is an ever-increasing use of computers in the collection and processing of scientific data. Tabulated information currently extracted from books will in the future be generated by computer in much the same way as sine, cosine and exponential values are today. Space-group information, which has traditionally been extracted from *International Tables for X-ray Crystallography*, Vol. I, will increasingly be computer-generated. The need for a simple and efficient procedure for performing this task is of prime importance.

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Table 7. *Proposed ordering of space groups*

IT = *International Tables for X-ray Crystallography.*

Proposed order	Proposed notation	IT order	Proposed order	Proposed notation	IT order	Proposed order	Proposed notation	IT order	Proposed order	Proposed notation	IT order
1	$P1$	1	58	$\bar{C}2_b2$	67	116	$\bar{P}4_c2$	131	173	$P6_4$	172
2	$\bar{P}1$	2	59	$\bar{C}2_b2_{ac}$	68	117	$\bar{P}4_c2_c$	132	174	$P6_5$	170
			60	$\bar{C}2_{bc}2$	64	118	$\bar{P}4_c2_{ab}$	135	175	$P62$	177
3	$P2$	3	61	$I22$	23	119	$\bar{P}4_n2_n$	136	176	$P6\bar{2}$	183
4	$P\bar{2}$	6	62	$I2\bar{2}$	44	120	$\bar{P}4_{ac}2_a$	137	177	$P6\bar{2}$	187
5	$P2_c$	4	63	$I2\bar{2}_a$	46	121	$\bar{P}4_{ac}2_b$	133	178	$P6\bar{2}$	189
6	$P\bar{2}_b$	7	64	$I2\bar{2}_c$	45	122	$\bar{P}4_{ac}2_{ac}$	138	179	$P6\bar{2}_c$	184
7	$\bar{P}2$	10	65	$I2_c\bar{2}$	24	123	$\bar{P}4_{ac}2_{bc}$	134	180	$P6_c2$	182
8	$\bar{P}2_c$	11	66	$\bar{I}22$	71	124	$I4$	79	181	$P6_c\bar{2}$	185
9	$\bar{P}2_b$	13	67	$\bar{I}22_c$	72	125	$I\bar{4}$	82	182	$P6_c2$	188
10	$\bar{P}2_{bc}$	14	68	$\bar{I}2_b\bar{2}$	74	126	$I4_{1b}$	80	183	$P6_c\bar{2}_c$	186
11	$B2$	5	69	$\bar{I}2_b2_c$	73	127	$I42$	97	184	$P6_c\bar{2}_c$	190
12	$B\bar{2}$	8	70	$F22$	22	128	$I4\bar{2}$	107	185	$P6_12$	178
13	$B\bar{2}_b$	9	71	$F2\bar{2}$	42	129	$I\bar{4}2$	121	186	$P6_22$	180
14	$\bar{B}2$	12	72	$F2\bar{2}_d$	43	130	$I4\bar{2}$	119	187	$P6_42$	181
15	$\bar{B}2_b$	15	73	$\bar{F}22$	69	131	$I4\bar{2}_c$	108	188	$P6_52$	179
			74	$\bar{F}2_{uv}2_{vw}$	70	132	$I4\bar{2}_c$	120	189	$\bar{P}6$	175
16	$P22$	16				133	$I4_{bd}2$	98	190	$\bar{P}6_c$	176
17	$P22_n$	18	75	$P4$	75	134	$I4_{bd}\bar{2}$	109	191	$\bar{P}62$	191
18	$P2\bar{2}$	25	76	$P\bar{4}$	81	135	$I4_{bd}2_c$	110	192	$\bar{P}62_c$	192
19	$P2\bar{2}_a$	28	77	$P4_1$	76	136	$I4_{bd}2_c$	122	193	$\bar{P}6_c\bar{2}$	193
20	$P2\bar{2}_c$	27	78	$P4_c$	77	137	$\bar{I}4$	87	194	$\bar{P}6_c2_c$	194
21	$P2\bar{2}_{ab}$	32	79	$P4_3$	78	138	$\bar{I}4_{ad}$	88			
22	$P2\bar{2}_{bc}$	30	80	$P42$	89	139	$\bar{I}42$	139	195	$P223$	195
23	$P2\bar{2}_n$	34	81	$P4\bar{2}$	99	140	$\bar{I}42_c$	140	196	$P2_{ac}2_{ab}3$	198
24	$P2_c2$	17	82	$P\bar{4}2$	111	141	$\bar{I}4_{bd}2$	141	197	$P423$	207
25	$P2_c2_n$	19	83	$P\bar{4}\bar{2}$	115	142	$\bar{I}4_{bd}2_c$	142	198	$P\bar{4}23$	215
26	$P2_c\bar{2}$	26	84	$P4\bar{2}_c$	103				199	$P4_n23$	208
27	$P2_c\bar{2}_a$	31	85	$P\bar{4}2_c$	112	143	$P3$	143	200	$P\bar{4}_n23$	218
28	$P2_c\bar{2}_{ac}$	29	86	$P\bar{4}\bar{2}_c$	116	144	$P3$	147	201	$P4_{bd}2_{ab}3$	213
29	$P2_c\bar{2}_n$	33	87	$P4\bar{2}_{ab}$	100	145	$P3_1$	144	202	$P4_{bdn}2_{ab}3$	212
30	$\bar{P}22$	47	88	$P4\bar{2}_{ab}$	113	146	$P3_2$	145	203	$\bar{P}223$	200
31	$\bar{P}22_c$	49	89	$P\bar{4}\bar{2}_{ab}$	117	147	$P32$	149	204	$\bar{P}2_{ac}2_{ab}3$	205
32	$\bar{P}22_{ab}$	55	90	$P4\bar{2}_n$	104	148	$P32''$	150	205	$\bar{P}2_{ab}2_{bc}3$	201
33	$\bar{P}22_n$	58	91	$P\bar{4}2_n$	114	149	$P3\bar{2}$	157	206	$\bar{P}423$	221
34	$\bar{P}2_a2_a$	51	92	$P\bar{4}\bar{2}_n$	118	150	$P3\bar{2}''$	156	207	$\bar{P}4_n23$	223
35	$\bar{P}2_a2_n$	60	93	$P4_c2$	93	151	$P3\bar{2}_c$	159	208	$\bar{P}4_a2_{bc}3$	222
36	$\bar{P}2_a2_{ab}$	57	94	$P4_c\bar{2}$	105	152	$P3\bar{2}_c''$	158	209	$\bar{P}4_{bc}2_{bc}3$	224
37	$\bar{P}2_a2_{bc}$	52	95	$P4_c\bar{2}_c$	101	153	$P3_12$	151	210	$I223$	197
38	$\bar{P}2_{ac}2$	53	96	$P4_c\bar{2}_{ab}$	106	154	$P3_12''$	152	211	$I2_{ac}2_{ab}3$	199
39	$\bar{P}2_{ac}2_c$	54	97	$P4_n2_n$	94	155	$P3_22$	153	212	$I\bar{4}23$	211
40	$\bar{P}2_{ac}2_{ab}$	61	98	$P4_n\bar{2}_n$	102	156	$P3_22''$	154	213	$I\bar{4}23$	217
41	$\bar{P}2_{ac}2_n$	62	99	$P4_12$	91	157	$\bar{P}32$	162	214	$I4_{bd}2_{ab}3$	214
42	$\bar{P}2_{ab}2_a$	59	100	$P4_32$	95	158	$\bar{P}32''$	164	215	$I\bar{4}_{bd}2_{ab}3$	220
43	$\bar{P}2_{ab}2_b$	50	101	$P4_{1n}2_n$	96	159	$\bar{P}32_c$	163	216	$\bar{I}223$	204
44	$\bar{P}_{ab}2_{ac}$	56	102	$P4_{3n}2_n$	92	160	$\bar{P}32_c''$	165	217	$\bar{I}2_{ac}2_{ab}3$	206
45	$\bar{P}2_{ab}2_{bc}$	48	103	$P4_{ab}2_{ab}$	90	161	$R3 \quad P3^*$	146	218	$\bar{I}\bar{4}23$	229
46	$C22$	21	104	$P4$	83	162	$R32'' \; P3^*2$	155	219	$\bar{I}4_{bd}2_{ab}3$	230
47	$C2\bar{2}$	35	105	$\bar{P}4_a$	85	163	$R3\bar{2}'' \; P3^*\bar{2}$	160	220	$F223$	196
48	$C2\bar{2}_c$	37	106	$\bar{P}4_c$	84	164	$R32_c'' \; P3^*\bar{2}_n$	161	221	$F423$	209
49	$C2_c\bar{2}$	20	107	$\bar{P}4_{bc}$	86	165	$\bar{R}3 \quad \bar{P}3^*$	148	222	$F\bar{4}23$	216
50	$C2_c\bar{2}$	36	108	$\bar{P}42$	123	166	$\bar{R}32'' \; \bar{P}3^*2$	166	223	$F\bar{4}_n23$	219
51	$C2^y\bar{2}$	38	109	$\bar{P}42_c$	124	167	$\bar{R}32_c'' \; \bar{P}3^*2_n$	167	224	$F4_d23$	210
52	$C2^y\bar{2}_a$	39	110	$\bar{P}4\bar{2}_{ab}$	127				225	$\bar{F}223$	202
53	$C2^y\bar{2}_c$	40	111	$\bar{P}42_n$	128	168	$P6$	168	226	$\bar{F}2_{uv}2_{vw}3$	203
54	$C2^y\bar{2}_{ac}$	41	112	$\bar{P}4_a2_a$	129	169	$P\bar{6}$	174	227	$\bar{F}\bar{4}23$	225
55	$\bar{C}22$	65	113	$\bar{P}4_a2_b$	125	170	$P6_1$	169	228	$\bar{F}4_n23$	226
56	$\bar{C}22_c$	66	114	$\bar{P}4_a2_{ab}$	130	171	$P6_2$	171	229	$\bar{F}4_{vw}2_{vw}3$	227
57	$\bar{C}2_c2$	63	115	$\bar{P}4_a2_{bc}$	126	172	$P6_3$	173	230	$\bar{F}4_{ud}2_{vw}3$	228

References

AHMED, F. R., HALL, S. R., PIPPY, M. E. & HUBER, C. P. (1966). *NRC Crystallographic Programs*. NRC, Ottawa.

BRADLEY, C. J. & CRACKNELL, A. P. (1972). *The Mathematical Theory of Symmetry in Solids*. Oxford: Clarendon Press.

BRAGG, W. H., VON LAUE, M. & HERMANN, C. (1935). *International Tables for the Determination of Crystal Structures*, Vol. I. Berlin: Borntraeger.

BURZLAFF, H., BÖHME, R. & JOMM, M. (1977). *CRYSTAN: A Crystallographic Program System for Minicomputers*. Univ. of Erlangen, Federal Republic of Germany.

HENRY, N. F. M. & LONSDALE, K. (1972). *International Tables for X-ray Crystallography*, Vol. I. Birmingham: Kynoch Press.
LARSON, A. (1969). *Acta Cryst.* A**25**, S1.
MAIN, P., WOOLFSON, M. M. & GERMAIN, G. (1971). *MULTAN: A Program for the Solution of Crystal Structures*. Univs. of York and Louvain.
SCHÖNFLIES, A. (1891). *Theory of Crystal Structure*. Leipzig: Teubner.
SEITZ, F. (1936). *Ann. Math.* **37**, 17–28.
STEWART, J. M. (1976). *The XRAY system of crystallographic programs*. Tech. Rep. TR 446. Computer Science Center, Univ. of Maryland.

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Diffracted Intensities From Partially Ordered Layer Structures With Layer Shift: Two Dimensional

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Abstract

A general expression for the diffracted intensities from an aggregate of partially disordered layer structures consisting of plane lattice layers displaced randomly along **a** and **b** by arbitrary fractions a/q_a and b/q_b has been worked out. The approach is similar to that of Wilson [*X-ray Optics* (1962). London: Methuen] and has been followed by Ray, De & Bhattacherjee [*Clay Miner.* (1980), **15**, 393]. The expression is very general in nature and is suitable for studying the variation of intensities from such crystallites with any amount of displacements. Numerical computations for several cases have been carried out and results discussed. It is concluded that the peak will broaden and background increase as the magnitudes and probabilities of disorder increase.

Introduction

In a previous publication (Ray, De & Bhattacherjee, 1980) a general expression for the diffracted intensities from a partially disordered layer structure with a displacement has been worked out. The displacement, as is commonly found in minerals, consists of a one-dimensional shift of a layer parallel to the adjacent layers by an arbitrary fraction b/q along the b axis, where q is any integer. This expression is quite suitable for investigating the nature of the diffraction pattern from the layer structure when the displacement is gradually changed by any fraction of the axial length **b** in this direction. It would be more general and interesting to study the effect on the diffraction pattern when the layer is displaced in two directions simultaneously by a/q_a and b/q_b along **a** and **b**, where q_a and q_b are both integers. As mentioned in the previous paper (Ray *et al.*, 1980) such situations are closer to reality and are likely to occur in several minerals with a layer type structure, which are prone to this type of disorder because of their structural characteristics. Wilson (1962) has also made an attempt to study the diffraction from hexagonal cobalt with displacements **a**/3 and 2**b**/3. However, a more general expression of the diffracted intensity from a disordered structure of the above type is expected to be very useful in distinguishing between conglomerations of layer crystallites with different types of displacement and perhaps to estimate the magnitude of the displacements. The present work aims at fulfilling this objective.

Theory

The present derivation is based primarily on the model of disordered crystals with plane lattice layers as described in the previous work (Ray *et al.*, 1980). Here too the layers are taken to be parallel to the **ab** plane with **c** perpendicular to the layer. The disorder consists of shifts of the layer parallel to itself by a/q_a and b/q_b along **a** and **b** respectively, where q_a and q_b are integers. All symbols used carry the usual meaning as in the previous publication (Ray *et al.*, 1980).

Let the shift of a layer be a/q_a along the a axis and the probability of such shift be α. Corresponding quantities in the b direction for a layer are taken to be

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