Table 2. *Descriptive symbols for* $SrGeO_3$

Substance $SrGeO_3$	BLs chosen	Full symbol (redundant)	Simplified symbol (nonredundant)	Number of equivalent BLs per repeat	Space group
(2*O*)	(*a*)(*b*)	$\|p_3p_0\|$	|30|	2	*Ccmm*
	(*c*)	$\|P_3P_0\|$			
(2*M*)	(*a*)(*b*)	$\|p_1p_2\|$	|12|	2	*C*2/*c*11
	(*c*)	$\|P_1P_2\|$			
(6*H*)	(*a*)(*b*)	$\|p_3p_4p_5p_0p_1p_2\|$	|3 4 5 0 1 2|	6	$P6_122$
	(*c*)	$\|P_3P_4P_5P_0P_1P_2\|$			

the *c* axis. They are accordingly assigned the characters $n = 0, 1, \ldots, 5$. The character 0 (or 6) denotes the vector parallel to $-\mathbf{a}$ of the orthogonal *C*-centered base a, $b = a\sqrt{3}$.

An example is given in Table 2.

B. Illustrative papers on polytypic substances with description of symbolism used

Astrophyllite
Zvyagin & Vrublevskaya (1976).

Kaolinite-type structures
Zvyagin (1964, 1967) (tri- and di-octahedral polytypes).
Dornberger-Schiff & Ďurovič (1975) (tri-, di- and mono-octahedral polytypes).

Mica
Zvyagin (1964, 1967) (tri-octahedral polytypes).
Takeda (1967) (tri-octahedral polytypes).
Dornberger-Schiff, Backhaus & Ďurovič (1982) (tri-, di- and mono-octahedral polytypes).

Vermiculites
Weiss & Ďurovič (1980).

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Graphic Representation and Nomenclature of the Four-Dimensional Crystal Classes. III. A Notation for the Crystal Classes

BY E. J. W. WHITTAKER

Department of Geology and Mineralogy, Oxford University, Parks Road, Oxford OX1 3PR, England

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Abstract

A Hermann–Mauguin type notation is devised for the 227 four-dimensional (geometric) crystal classes, and appropriate conventions are proposed for each of the 23 crystal families.

Introduction

In paper I of the series (Whittaker, 1983) the principle was demonstrated of representing graphically the symmetry of the four-dimensional crystal classes by means of the hyperstereogram. Such representations

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were produced for the first sixteen crystal classes, containing symmetry operations of order not greater than two. The possibility of visualizing the nature of the symmetry in this way suggested a symbolic nomenclature following the general principles of the Hermann–Mauguin notation, and such a notation was developed for the sixteen crystal classes that were illustrated. In paper II (Whittaker, 1984*a*) all the crystallographic symmetry operations of order greater than two were examined and their effects illustrated by means of hyperstereograms. This has helped to clarify their nature and their orientational characteristics, and for all of them unitary symbols have been introduced that are suitable for incorporation in a Hermann–Mauguin-type notation for the crystal classes. Hyperstereograms have now been prepared for all the 227 four-dimensional (geometric) crystal classes tabulated by Brown, Bülow, Neubüser, Wondratscheck & Zassenhaus (1978), and these will be published elsewhere (Whittaker, 1984*b*). On the basis of this work it has been possible to develop a complete notation for all these crystal classes, although it has proved desirable to introduce slight modifications into the original one devised for the first sixteen. It is the purpose of this paper to describe and tabulate this complete notation.

Principles of the notation

It was pointed out in paper I that the main difficulty in the way of a Hermann–Mauguin style nomenclature in four dimensions is that the orientation of a plane is not specifiable by the direction of a line perpendicular to it. The device was therefore adopted of splitting the symbol into two parts separated by a semicolon. The first part consisted of a sequence of positions each of which specified (according to a convention) the orientation of a line. Each such position could then be used to specify the orientation of an axis of rotation–inversion $\bar{n}$ or a mirror hyperplane m, or both by the usual notation $\bar{n}/m$, as in three dimensions. The second part consisted of a similar sequence of positions, each of which specified, according to a separate convention, the orientation of a plane. This general principle is retained here, but two modifications of detail have been found to be desirable as a result of the extension of the work.

1. In paper I the sequence of symbols specifying lines and hyperplanes was placed first, because it has the most direct analogy to three-dimensional Hermann–Mauguin symbols. However, out of the 227 crystal classes there are 120 that do not contain axes of symmetry or mirror hyperplanes, and only 17 that do not possess, or do not require the specification of, rotation planes. Moreover, it is the latter symbols which are usually the diagnostic ones for assigning a crystal class to a crystal system. It is therefore desirable to reverse the order of the two sequences and place that for the planes first.

2. Within the sequence of planes each position specified the orientation of one plane. However, even in the simple systems discussed in paper I it was already difficult to devise a systematic order for the axial planes, because wx, xy, yz, zw, wy, xz cannot all be listed in a straight forward cyclic order. As a result a rather cumbersome convention had to be adopted so that it should be possible to deduce which pairs of positions correspond to orthogonal (absolutely perpendicular) planes. This problem becomes still more important and difficult in the classes of higher symmetry, and the device has therefore been adopted of assigning each position to a pair of orthogonal planes separated by an oblique stroke. Thus the axial planes of family V (orthogonal) can be specified

$$wx/yz\ xy/zw\ yw/xz,$$

and the holosymmetric class 5/02, for example, can then be symbolized (in the full form) as 2/2 2/2 2/2 instead of 222222. This has three advantages: it permits the planes to be listed in strict cyclic order in terms of the planes specified by the 'numerators'; it makes clear which planes are orthogonal to one another; and it reduces by a factor of two the number of orientational positions to be specified. It is to be noted that there are in fact three other ways in which the axial planes could have been specified in pairs, by inverting them in different ways, that is

$$xy/zw\ yz/wx\ zx/yw$$

$$wy/xz\ yz/wx\ zw/xy$$

$$wx/yz\ xz/yw\ zw/xy.$$

These allot a special role to w, x, and y, respectively, in that in each set one axis is excluded from the 'numerators' and is present in all three 'denominators'. The preferred arrangement is that which allots this special role to z, because this axis has already been given a special role by the convention that it is projected to the centre of the hyperstereogram. It is therefore most natural, when one is looking at a hyperstereogram, to regard the three axes w, x, y as the ones to be considered in cyclic order.

As in three-dimensional crystallography it is necessary to introduce a different convention in each crystal family as to the orientation to be associated with each position in the symbol. These conventions are given in Table 2. Each direction is specified either by a coordinate axis (w, x, y or z) or by an axis symbol – a set of four integers in square brackets defining a vector in terms of the basis vectors of the axial system of the crystal family. Similarly, each plane is specified by a pair of such directions lying in it.

For this specification of conventional directions in each family to be meaningful it is of course necessary

Table 1. *The crystallographic axes adopted for the twenty three crystal families*

For each family there are potentially five lines containing the following information:
1. Any equivalences between the axes. (Absent if not required.)
2. The angle $\angle\ wx$.
3. The angles $\angle\ wy$ and $\angle\ xy$.
4. The angles $\angle\ wz$, $\angle\ xz$, and $\angle\ yz$. Equivalences between angles are indicated by the use of the same symbol in 2, 3 and 4.
5. Any relationships between the angles. (Absent if not required.)

Family I
Hexaclinic
α
$\beta\quad\gamma$
$\delta\quad\varepsilon\quad\zeta$

Family II
Triclinic
α
$\beta\quad\gamma$
90° 90° 90°

Family III
Diclinic
α
90° 90°
90° 90° ζ

Family IV
Monoclinic
α
90° 90°
90° 90° 90°

Family V
Orthogonal
90°
90° 90°
90° 90° 90°

Family VI
Tetragonal monoclinic
$y\equiv z$
α
90° 90°
90° 90° 90°

Family VII
Hexagonal monoclinic
$y\equiv z$
α
90° 90°
90° 90° 120°

Family VIII
Ditetragonal diclinic
$w\equiv x,\ y\equiv z$
90°
$\beta\quad\gamma$
$180°-\gamma\quad\beta\quad 90°$

Family IX
Ditrigonal diclinic
$w\equiv x,\ y\equiv z$
120°
$\beta\quad\gamma$
$\delta\quad\beta\quad 120°$
with $\cos\delta=\cos\beta-\cos\gamma$

Family X
Tetragonal orthogonal
$y\equiv z$
90°
90° 90°
90° 90° 90°

Family XI
Hexagonal Orthogonal
$y\equiv z$
90°
90° 90°
90° 90° 120°

Family XII
Ditetragonal monoclinic
$w\equiv x,\ y\equiv z$
90°
$\beta\quad 90°$
$90°\quad\beta\quad 90°$

Family XIII
Ditrigonal monoclinic
$w\equiv x,\ y\equiv z$
120°
$\beta\quad\gamma$
$\gamma\quad\beta\quad 120°$
with $\cos\gamma=-\frac{1}{2}\cos\beta$

Family XIV
Ditetragonal orthogonal
$w\equiv x,\ y\equiv z$
90°
90° 90°
90° 90° 90°

Family XV
Hexagonal tetragonal
$w\equiv x,\ y\equiv z$
90°
90° 90°
90° 90° 120°

Family XVI
Dihexagonal orthogonal
$w\equiv x,\ y\equiv x$
120°
90° 90°
90° 90° 120°

Family XVII
Cubic Orthogonal
$x\equiv y\equiv z$
90°
90° 90°
90° 90° 90°

Family XVIII
Octagonal
$w\equiv x\equiv y\equiv z$
α
$90°\quad\alpha$
$180°-\alpha\quad 90°\quad\alpha$

Family XIX
Decagonal
$w\equiv x\equiv y\equiv z$
α
$\beta\quad\alpha$
$\beta\quad\beta\quad\alpha$
with $\cos\beta=-0{\cdot}5-\cos\alpha$

Family XX
Dodecagonal
$w\equiv x\equiv y\equiv z$
90°
$120°\quad\gamma$
$\gamma\quad 120°\quad 90°$

Family XXI
Di-isohexagonal
$w\equiv x\equiv y\equiv z$
120°
90° 90°
90° 90° 120°

Family XXII
Icosagonal
$w\equiv x\equiv y\equiv z$
α
$\alpha\quad\alpha$
$\alpha\quad\alpha\quad\alpha$
with $\cos\alpha=-1/4$

Family XXIII
Hypercubic
$w\equiv x\equiv y\equiv z$
90°
90° 90°
90° 90° 90°

that the arrangement of the crystallographic axes adopted for that family be defined. This is done in Table 1. The numbering of the families follows Brown *et al.* (1978), as does the naming of all but three of them. In the names of families IX and XIII the term 'trigonal' has been substituted for 'hexagonal' because these families contain only systems with trigonal characteristics (see Table 3). Also, the name of family XXII has been changed from 'icosahedral' to 'icosagonal' to keep its derivation in line with the names (octagonal, decagonal *etc.*) of other families. The orientation of the axes has been changed in certain cases from that adopted by Brown *et al.* (1978); hexagonal-type axes have always been set at 120° rather than 60°, and orthogonal axes have been used throughout family XXIII.

Axes involving crypto-rotation planes

As defined so far the system of notation deals adequately with rotation planes, with *m* hyperplanes, and with $\bar{1}$ axes whose crypto-rotation planes have no defined orientation. Other axes of rotation–inversion ($\bar{3}$, $\bar{4}$ and $\bar{6}$) require the orientation of their crypto-rotation plane to be specified in some way. In fact, no problem arises in the case of $\bar{3}$ and $\bar{6}$ axes because both give rise to an overt threefold rotation plane coincident with their threefold or sixfold crypto-rotation plane. This is of course specified in the sequence of planes in the ordinary way, and the $\bar{3}$ or $\bar{6}$ symbol in the sequence of axes can always be identified with a specified threefold plane in which it lies in order to define it completely. This is not true

Table 2. *Conventions as to the orientations corresponding to the positions in the Hermann–Mauguin type symbols*

Family I
None

Family II
z

Family III
wx/yz

Family IV
wx/yz: $y\ z$

Family V
$wx/yz\ xy/wz\ yw/xz$; $w\ x\ y\ z$

Family VI
wx/yz; $w\ x\ y\ [0011]$

Family VII
wx/yz; $w\ x\ y\ [0021]$

Family VIII
w_0x_0/yz

Family IX
w_0x_0/yz

Family X
$wx/yz\ xy/zw\ w[0011]/x[00\bar{1}1]$; $w\ x\ y[0011]$

Family XI
$wx/yz\ xy/w[00\bar{1}1]\ yw/x[00\bar{1}1]$; $w\ x\ y\ [00\bar{1}1]$

Family XII
$w_0x_0/yz\ wy/xz$

Family XIII
$w_0x_0/yz\ wy/[1200][0012]$

Family XIV
$wx/yz\ xy/wz\ [1100][0011]/[1\bar{1}00][00\bar{1}1]$;
$w\ y\ [1100]\ [0011]$

Family XV
$wx/yz\ xy/w[0012]\ y[1100]/[1\bar{1}00][0012]$;
$w\ y\ [1100]\ [0012]$

Family XVI
$xz/yz\ xy/[2100][0012]$; $w\ y\ [2100]\ [0012]$

Family XVII
$wx/yz\ w[0111]^*\ w[0110]/z[0\bar{1}10]$: $w\ x\ [0110]$

Family XVIII
$w_0y_0/zx_0\ x[1010]/z[10\bar{1}0]$

Family XIX
(V) $y[0101]/[2111][010\bar{1}]$

Family XX
$w_0x_0/yz\ w_0y_0/xz\ y[0201]/[2010]$

Family XXI
$wx/yz\ z[\bar{1}\bar{1}00]/[1\bar{1}00][0021]\ w[0012]/y[1200]\ [1010][01\bar{1}1]/[10\bar{1}0][0111]\ [1010][0101]/[10\bar{1}0][010\bar{1}]$; $w\ y\ [2100]\ [0021]\ [1001]\ [\bar{1}001]\ [2121]$

Family XXII
(V) $wx^*\ y[0101]/[2111][010\bar{1}]\ y[1001]/[1211][100\bar{1}]$; $w\ [1\bar{1}00]\ [0212]$

Family XXIII
$wx/yz\ xy/wz\ z[1110]/[1\bar{1}00][10\bar{1}0]\ w[00\bar{1}1]/x[0011]\ [1100][0011]/[1\bar{1}00][00\bar{1}1]\ [1100][00\bar{1}1]/[1\bar{1}00][0011]\ [1010][0101]/[10\bar{1}0][0\bar{1}01]$
$[1010][0\bar{1}01]/[10\bar{1}0][0101]$; $w\ [1100]\ [1010]\ [1111]$.

In families VIII, IX, XII, XIII and XX w_0x_0 indicates a (crystallographically irrational) plane orthogonal to yz, and in family XX w_0y_0 similarly indicates a plane orthogonal to xz.

In family XVIII w_0, x_0, y_0 indicate (crystallographically irrational) axes such that y_0 lies in yz at 90° to z, x_0 lies in xyz at 90° to y_0 and z, and w_0 is orthogonal to x_0, y_0 and z.

* There are no rotation planes orthogonal to the orientations indicated thus.

of a $\bar{4}$ axis, and therefore the symbol ($\bar{4}$), in parentheses, is inserted in the appropriate position in the sequence of planes to complete the specification of the orientational characteristics of a $\bar{4}$ axis given in the sequence of axes. In one instance it is necessary (in order to avoid ambiguity) to denote by a subscript number, appended to the symbol of the $\bar{4}$ axis, the position in the sequence of planes in which its crypto-rotation plane is specified.

The point symmetry elements $\tilde{\bar{3}}$, $\tilde{\bar{4}}$ and $\tilde{\bar{6}}$

These symmetry elements also have a crypto-rotation plane whose orientation must be specified. When they occur alone the symbol $\tilde{\bar{3}}$, $\tilde{\bar{4}}$ or $\tilde{\bar{6}}$ is simply inserted in the appropriate position in the sequence of planes. When they arise from combinations of overt **3**, **4**, or **6** operations with a separately defined or implied $\tilde{\bar{1}}$ operation they are not specified.

The point symmetry elements III, I$\tilde{\bar{\text{I}}}$I, IV and VIII

Although a symmetry element of this type does not have a uniquely defined pair of orthogonal crypto-rotation planes, it is always compatible with its crypto-rotation planes lying on one (and only one) of the conventionally chosen pairs in a given crystal family. Thus the symbols III, I$\tilde{\bar{\text{I}}}$I and IV can be meaningfully placed at the appropriate positions among the sequence of planes in order to define the orientational characteristics of the corresponding symmetry operations. When these operations arise from mutually orthogonal pairs of overt rotation planes (3/3, 6/6, 4/4) they do not require any separate specification. The symbol I$\tilde{\bar{\text{I}}}$I is only used when it is present alone and not when it arises from the combination of a **III** operation with a separately defined or implied $\tilde{\bar{1}}$ operation. When both **III** and **IV** operations or two differently oriented **IV** operations, or an **VIII** and a differently oriented **IV** operation are present together in a class it is necessary to indicate whether they are of the same hand, of opposite hand, or of both hands. This is done by use of a subscript on the second symbol of the two (s for same, o for opposite), and no subscript indicates that there is no such restriction.

Where the **VIII** operation has to be specified its symbol occupies the position in the sequence of planes appropriate to that of the **IV** operation that is its square. The direction of the initial line of the graphical VIII symbol is not specified in the class symbol, but is defined by convention.

The point symmetry elements V and $\tilde{\bar{\text{V}}}$

In the two families in which these occur their orientational characteristics are specified by the conventions for the family. The V symbol is then placed before the sequence of plane symbols. Since the $\tilde{\bar{\text{V}}}$ operation

Table 3. *The Hermann–Mauguin type symbols of the 227 crystal classes*

Family I Hexaclinic

System 1

1/01	1
1/02	$\bar{1}$

Family II Triclinic

System 2

2/01	*m*
2/02	$\bar{1}$
2/03	$\bar{1}$/*m*

Family III Diclinic

System 3

3/01	2
3/02	2/2

Family IV Monoclinic

System 4

4/01	2; *m m*
4/02	–/2; $\bar{1}$ *m*
4/03	2; $\bar{1}$ $\bar{1}$
4/04	2/2; *m m*

Family V Orthogonal

System 5

5/01	–/2 –/2 –/2
5/02	2/2 2 2

System 6

6/01	–/2 –/2 –/2; *m m m* $\bar{1}$
6/02	–/2 –/2 –/2; $\bar{1}$ $\bar{1}$ $\bar{1}$ *m*
6/03	2/2 2 2; *m m m m*

Family VI Tetragonal monoclinic

System 7

7/01	$\bar{\bar{4}}$
7/02	4
7/03	4/2
7/04	$\bar{\bar{4}}$; – – $\bar{1}$ *m*
7/05	4; – – $\bar{1}$ $\bar{1}$
7/06	4; – – *m m*
7/07	4/2; – – *m m*

Family VII Hexagonal monoclinic

System 8

8/01	3
8/02	$\bar{\bar{3}}$
8/03	3; – – *m*
8/04	3; – – $\bar{1}$
8/05	$\bar{\bar{3}}$; – – $\bar{1}$/*m*

System 9

9/01	6
9/02	$\bar{\bar{6}}$
9/03	6/2
9/04	6; – – *m m*
9/05	6; – – $\bar{1}$ $\bar{1}$
9/06	$\bar{\bar{6}}$; – – *m* $\bar{1}$
9/07	6/2; – – *m m*

Family VIII Ditetragonal diclinic

System 10

10/01	IV

Family IX Ditrigonal diclinic

System 11

11/01	III
11/02	I$\bar{\bar{\mathrm{I}}}$I

Family X Tetragonal orthogonal

System 12

12/01	($\bar{4}$); – $\bar{4}$
12/02	($\bar{4}$)/2; $\bar{4}$ $\bar{4}$
12/03	(4) 2; – $\bar{4}$ – *m*
12/04	($\bar{4}$) –/2; – $\bar{4}$ – $\bar{1}$
12/05	($\bar{4}$)/2 2; $\bar{4}$ $\bar{4}$ – *m*

System 13

13/01	4; *m* $\bar{1}$
13/02	$\bar{\bar{4}}$; $\bar{1}$ $\bar{4}$/*m*
13/03	$\bar{\bar{4}}$ 2 2
13/04	4 2 –/2
13/05	4/2; *m m*
13/06	4 2 –/2; *m* $\bar{1}$ *m m*
13/07	$\bar{\bar{4}}$ 2 2; $\bar{1}$ $\bar{4}$/*m* $\bar{1}$ *m*
13/08	4 –/2 2; *m* $\bar{1}$ $\bar{1}$ $\bar{1}$
13/09	4/2 2 2
13/10	4/2 2 2; *m m m m*

Family XI Hexagonal orthogonal

System 14

14/01	3; $\bar{3}$
14/02	3; *m* $\bar{6}$
14/03	3 – 2
14/04	$\bar{\bar{3}}$; $\bar{1}$/*m* $\bar{6}$
14/05	3 – 2/2
14/06	3 – 2; $\bar{3}$ – *m*
14/07	3 – –/2; $\bar{3}$ – $\bar{1}$
14/08	3 – –/2; *m* $\bar{6}$ *m*
14/09	3 – 2; *m* $\bar{6}$ $\bar{1}$
14/10	3 – 2/2; *m* $\bar{6}$ *m*

System 15

15/01	6; *m*
15/02	$\bar{\bar{6}}$; *m m*
15/03	$\bar{\bar{6}}$; $\bar{3}$ $\bar{3}$
15/04	6 –/2 2
15/05	$\bar{\bar{6}}$ –/2 –/2
15/06	6 2 –/2; *m* $\bar{1}$ *m m*
15/07	$\bar{\bar{6}}$ –/2 –/2; *m m m* $\bar{1}$
15/08	6/2; *m m*
15/09	6 –/2 2; *m* $\bar{1}$ $\bar{1}$ $\bar{1}$
15/10	$\bar{\bar{6}}$ 2 2; $\bar{3}$ $\bar{3}$ *m* $\bar{1}$
15/11	6/2 2 2
15/12	6/2 2 2; *m m m m*

Family XII Ditetragonal monoclinic

System 16

16/01	IV 2/2

Family XIII Ditrigonal monoclinic

System 17

17/01	III –/2
17/02	III 2/2

Family XIV Ditetragonal orthogonal

System 18

18/01	IV/2/2
18/02	IV/($\bar{4}$)/2; $\bar{4}$ – *m*
18/03	($\bar{4}$)/($\bar{4}$) – 2; $\bar{4}$ $\bar{4}$
18/04	IV/2/2 2 2
18/05	IV/($\bar{4}$)/($\bar{4}$) 2 2; $\bar{4}$ $\bar{4}$ *m m*

System 19

19/01	($\bar{4}$)/4; $\bar{4}$ – $\bar{4}$
19/02	4/4
19/03	4/4; *m* – *m*
19/04	($\bar{4}$)/4 2; $\bar{4}$ – $\bar{4}$ *m*
19/05	4/4 2 2
19/06	4/4 2 2; *m m m m*

Family XV Hexagonal tetragonal

System 20

20/01	3/4
20/02	3/$\bar{\bar{4}}$
20/03	3/($\bar{4}$); – – – $\bar{4}$
20/04	3/4; – *m* – $\bar{1}$
20/05	6/4
20/06	3/4; $\bar{3}$ – $\bar{3}$
20/07	3/4 2 2
20/08	3/4; *m* – *m*
20/09	3/($\bar{4}$); – $\bar{4}$/*m*
20/10	3/$\bar{\bar{4}}$; $\bar{3}$ – *m*
20/11	3/4 2/2 2
20/12	3/($\bar{4}$) – 2; *m* $\bar{4}$
20/13	3/($\bar{4}$) – 2; $\bar{3}$ – – $\bar{4}$
20/14	6/($\bar{4}$); – $\bar{4}$ – $\bar{4}$
20/15	6/4; – *m* – *m*
20/16	3/4 2 2; $\bar{3}$ *m* $\bar{3}$ $\bar{1}$
20/17	3/4 –/2 –/2; *m m m* $\bar{1}$
20/18	6/4; *m* – *m*
20/19	6/4 2 2
20/20	3/$\bar{\bar{4}}$ 2 –/2; $\bar{3}$ *m m* $\bar{1}$
20/21	6/($\bar{4}$) – 2; *m* $\bar{4}$ – $\bar{4}$
20/22	6/4 2 2; *m m m m*

Family XVI Dihexagonal orthogonal

System 21

21/01	III/–/2
21/02	III/2/2
21/03	III/–/2 –/2
21/04	III/2/2 2

System 22

22/01	3/3
22/02	3/$\bar{\bar{3}}$
22/03	3/3; – – – *m*
22/04	3/3; – – – $\bar{3}$
22/05	3/3 –/2
22/06	3/$\bar{\bar{3}}$; – – – $\bar{1}$/*m*
22/07	3/3 2/2
22/08	3/3 2; – – *m m*
22/09	3/3 –/2; – – $\bar{3}$ *m*
22/10	3/3 2; – – $\bar{3}$ $\bar{3}$
22/11	3/3 2/2; – – *m m*

System 23

23/01	3/6
23/02	6/6
23/03	3/6; $\bar{3}$ – $\bar{3}$
23/04	3/6; *m* – *m*
23/05	3/6 –/2
23/06	3/6; – $\bar{3}$ – *m*
23/07	6/6; *m* – *m*
23/08	6/6 2
23/09	3/6 –/2; $\bar{3}$ $\bar{3}$ $\bar{3}$ *m*
23/10	3/6 –/2; *m m m* $\bar{3}$
23/11	6/6 2; *m m m m*

Family XVII Cubic orthogonal

System 24

24/01	2 3
24/02	2/2 3
24/03	($\bar{4}$) 3; $\bar{4}$ – *m*
24/04	($\bar{4}$) 3; – $\bar{4}$ $\bar{1}$
24/05	($\bar{4}$)/2 3; $\bar{4}$ $\bar{4}$ *m*

System 25

25/01	2 3; $\bar{3}$ *m*
25/02	2 3; *m*
25/03	4 3 2
25/04	$\bar{\bar{4}}$ 3 –/2
25/05	2/2 3; *m m*
25/06	4/2 3 2
25/07	4 3 2; $\bar{3}$ *m m*
25/08	($\bar{4}$) 3 –/2; $\bar{3}$ $\bar{4}$/*m* $\bar{1}$
25/09	($\bar{4}$) 3 –/2; $\bar{4}$/*m* $\bar{1}$ *m*
25/10	4 3 2; *m* $\bar{4}$ $\bar{1}$
25/11	4/2 3 2; *m m m*

Family XVIII Octagonal

System 26

26/01	VIII
26/02	VIII 2/2

Family XIX Decagonal

System 27

27/01	V
27/02	$\bar{\bar{\mathrm{V}}}$
27/03	V 2
27/04	V 2/2

Family XX Dodecagonal

System 28

28/01	IV III_o
28/02	IV III_o2/2

Family XXI Di-isohexagonal orthogonal

System 29

29/01	3/3 – – – 2
29/02	3/3 – – – 2/2
29/03	3/3 –/2 – –/2 2
29/04	3/3 ($\bar{4}$); – – – – $\bar{4}$
29/05	3/3 2/2 – 2 2
29/06	3/3 ($\bar{4}$)/2; – – – – $\bar{4}$ $\bar{4}$
29/07	3/3 ($\bar{4}$) – 2 2; $\bar{6}$ $\bar{6}$ *m m* $\bar{4}$
29/08	3/3 ($\bar{4}$) – 2 2; – – $\bar{3}$ $\bar{3}$ – $\bar{4}$
29/09	3/3 ($\bar{4}$)/2 – 2 2; $\bar{6}$ $\bar{6}$ *m m* $\bar{4}$ $\bar{4}$

Table 3 (*cont.*)

Family XXI (*cont.*)	
System 30	
30/01	III IV_s
30/02	III IV_o/2/2
30/03	III/2/2 IV_o – 2
30/04	III IV_s 2/2 – 2
30/05	3/3 IV
30/06	III/2/2 IV_o/2 2 2 2
30/07	6/6 IV – – 2
30/08	3/3 IV 2/2 2
30/09	3/3 IV/2/2
30/10	6/6 IV/2/2 2 2
30/11	6/6 ($\bar{4}$)/($\bar{4}$) 2; – – – – $\bar{4}$ $\bar{4}$ $\bar{4}$
30/12	3/3 IV/2/($\bar{4}$); $\bar{6}$ $\bar{6}$ *m m* – – $\bar{4}$
30/13	6/6 ($\bar{4}$)/($\bar{4}$) 2 2 2; *m m m m* $\bar{4}$ $\bar{4}$ $\bar{4}$
Family XXII Icosagonal	
System 31	
31/01	V – ($\bar{4}$); – – $\bar{4}$
31/02	V – ($\bar{4}$)/2; $\bar{4}$ – $\bar{4}$
31/03	V 3 2 2
31/04	V 3 ($\bar{4}$) ($\bar{4}$); $\bar{4}$ *m*
31/05	V 3 ($\bar{4}$) ($\bar{4}$); – $\bar{1}$ $\bar{4}$
31/06	V 3 2/2 2
31/07	V 3 ($\bar{4}$)/2 ($\bar{4}$); $\bar{4}$ *m* $\bar{4}$

Family XXIII Hypercubic	
System 32	
32/01	IV IV_s
32/02	VIII/2/2 IV_o
32/03	IV IV_s – 2/2
32/04	IV/2/2 IV_s – – – – – – 2
32/05	IV IV_s 3
32/06	VIII/2/2 IV_s – 2 – – – 2
32/07	VIII/2/2 2 – – 2 2
32/08	VIII/4/4 IV_o – – – – 2
32/09	($\bar{4}$)/($\bar{4}$) IV – – 2 ($\bar{4}$)/($\bar{4}$) 2; $\bar{4}$ – – $\bar{4}$
32/10	IV/2/2 IV/2 – –2 2 2 2
32/11	IV IV_s 3 2
32/12	4/4 IV/2 – 2 2 2 2 2
32/13	($\bar{4}$)/($\bar{4}$) ($\bar{4}$)/($\bar{4}$) – – 2 2; $\bar{4}_1$ *m* $\bar{4}$
32/14	($\bar{4}$)/($\bar{4}$) 2 – – ($\bar{4}$)/($\bar{4}$) ($\bar{4}$)/($\bar{4}$) 2 2; $\bar{4}$ *m* – $\bar{4}$
32/15	4/4 ($\bar{4}$)/($\bar{4}$) – 2 ($\bar{4}$)/($\bar{4}$) ($\bar{4}$)/($\bar{4}$) 2 2; – – $\bar{4}$ $\bar{4}$
32/16	IV/2/2 IV/2 3 – 2 2 2 2
32/17	4/4 ($\bar{4}$)/($\bar{4}$) – 2 ($\bar{4}$)/($\bar{4}$) ($\bar{4}$)/($\bar{4}$) 2 2; *m m* $\bar{4}$ $\bar{4}$
32/18	($\bar{4}$)/($\bar{4}$) ($\bar{4}$)/($\bar{4}$) 3 – – 2 2 2 2; *m* $\bar{4}$ $\bar{4}$
32/19	($\bar{4}$)/($\bar{4}$) ($\bar{4}$)/($\bar{4}$) 3 – ($\bar{4}$)/($\bar{4}$) ($\bar{4}$)/($\bar{4}$) ($\bar{4}$)/($\bar{4}$)($\bar{4}$)/($\bar{4}$); $\bar{4}$ *m m* $\bar{4}$
32/20	4/4 4/4 3 2 2 2 2 2
32/21	4/4 4/4 3 2 ($\bar{4}$)/($\bar{4}$) ($\bar{4}$)/($\bar{4}$) ($\bar{4}$)/($\bar{4}$) ($\bar{4}$)/($\bar{4}$); *m m m* $\bar{4}$

System 33	**Dodecagonal hypercubic**
33/01	IV IV_s III_o
33/02	VIII – III_o
33/03	IV IV_s III_s
33/04	IV IV_s III_o 2/2
33/05	IV/2/2 IV_s III_s – – – – 2
33/06	IV IV_s III_s 2/2
33/07	IV IV_s 3/3
33/08	IV/2/2 IV_s/2 III_s – – – 2 2
33/09	IV/2/2 IV_s III_s 2 – – – 2
33/10	4/4 IV III_s – – – – 4/4
33/11	IV IV_s 3/3 2/2
33/12	4/4 IV III_s 2 – – 4/4 2
33/13	IV/2/2 IV/2 3/3 – 2 2 2 2
33/14	($\bar{4}$)/($\bar{4}$) ($\bar{4}$)/($\bar{4}$) 3/3 – – – ($\bar{4}$)/($\bar{4}$) ($\bar{4}$)/($\bar{4}$); $\bar{4}$ *m m* $\bar{4}$
33/15	4/4 4/4 3/3 2 4/4 4/4 4/4 4/4
33/16	4/4 4/4 3/3 2 4/4 4/4 4/4 4/4; *m m m m*.

involves explicit V and $\bar{\bar{1}}$ operations it is only used if the remainder of the class symbol does not imply the $\bar{\bar{1}}$ operation (see below).

The point symmetry elements VI, XII, X$\bar{\bar{\mathrm{I}}}$I and XII′

These are never used in the class symbols because the corresponding operations are all expressible in terms of the products of simpler overt operations, as has been discussed in paper II (Whittaker, 1984*a*). The orientational characteristics of these overt components are therefore expressed by the appropriate positions of their symbols in the sequence of planes as discussed above.

The point symmetry element $\bar{\bar{1}}$

This symmetry element occurs by itself only in class 1/02, for which it is the only symbol. Elsewhere it arises either as a component of $\bar{\bar{3}}$, I$\bar{\bar{\mathrm{I}}}$I, IV, $\bar{\bar{\mathrm{V}}}$, or VIII, or from the presence of $\bar{1}/m$ in the sequence of axial symbols, or from the presence of a pair of orthogonal even-order rotation planes – 2/2, 4/2, 6/2, ($\bar{4}$)/2, 4/4, 6/4, ($\bar{4}$)/4, 6/6, 6/($\bar{4}$), or ($\bar{4}$)/($\bar{4}$). In none of these cases is $\bar{1}$ included explicitly in the symbol (*cf.* the corresponding treatment of $\bar{1}$ in three dimensions).

If the $\bar{\bar{1}}$ operation is present then every even-order rotation plane is accompanied by an orthogonal rotation plane of order 2 (or of higher even order), and every *m* hyperplane is accompanied by a perpendicular $\bar{1}$ axis. For the sake of brevity, once the first such orthogonal pair of even-order rotation planes has been recorded subsequent occurrences of twofold rotation planes that can be regarded as derived from the effect of the $\bar{\bar{1}}$ operation are omitted. Thus the class symbol 4/2 2/2 2/2 is simplified to 4/2 2 2. Similarly, $\bar{1}/m$ is simplified to *m* following an earlier implication of a $\bar{\bar{1}}$ operation either in the sequence of planes or in the sequence of axes. For the sake of clarity it has seemed preferable not to extend this system of omissions to the effects of $\bar{\bar{1}}$ operations implied by the symbols of point-symmetry elements.

Null symbols

In three-dimensional crystallography it is never necessary to use null symbols in the Hermann–Mauguin notation, unless it is desired to indicate a departure from normal conventions as in 1 1 2/*m* to denote a monoclinic class with the unique axis on *z*. However, in four dimensions the greater number of orientationally defined positions in the notation, and the presence of the two separately defined sequences for planes and axes, make it impracticable to avoid the use of null symbols. The symbol adopted is the dash (–). Its use is kept to a minimum by omitting it in trailing positions both in the sequence of planes and in the sequence of axes. In other words, it is only used when there is a following position in the sequence that is occupied. If either sequence is wholly null then the whole sequence (and the semicolon) is omitted. The null symbol (and the oblique stroke) is also omitted if the 'denominator position' of a pair of orthogonal planes is unoccupied.

Economy of symbols *versus* clarity

Although the specification of an excessive number of symmetry elements in a symbol of Hermann–Mauguin type can be confusing, reduction of the number to an absolute minimum can be mystifying. The symbols proposed, although reasonably concise, are therefore not claimed to have been condensed to the maximum possible extent.

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Maximum Entropy and the Foundations of Direct Methods*

BY G. BRICOGNE†

Department of Biochemistry, College of Physicians and Surgeons, Columbia University, 630 *West* 168*th Street, New York, NY* 10032, *USA*

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Abstract

A revision of the classical statistical methods of phase determination is presented which widens their theoretical foundations and consolidates their practical implementation, thus bringing about a major increase of their power. In a brief introductory survey (§ 1), the basic concepts and mathematical techniques of direct methods are analysed. Closer scrutiny (§ 2) reveals that severe inadequacies still impair the effectiveness of these methods. The asymptotic character of the series used to approximate joint distributions of structure factors demands that great caution be exercised to guarantee their accuracy, and this requirement can only be fulfilled if they are used within a multisolution algorithm in which the prior distribution of atoms is constantly updated so as to incorporate at every stage all the phase information assumed to that point. Further limitations follow from the traditional practice of approximating joint distributions by products of marginal distributions of single invariants. A scheme for simultaneously overcoming both difficulties is then proposed. The pivotal element of this scheme is a device, based on Jaynes's maximum-entropy principle, for exploiting the prior knowledge of some structure factors in the construction of the joint distributions of others conditional to that knowledge. Jaynes's maximum-entropy formalism is presented and systematically applied to the construction of the requisite non-uniform prior distributions of atoms in § 3. The problem of effectively approximating conditional distributions of very large numbers of structure factors is solved in § 4 by a novel technique of 'maximum-entropy inversion' of Karle–Hauptman matrices, and the result obtained is shown to generalize the most sophisticated probabilistic formulae hitherto obtained. This procedure is proved in § 5 to coincide with an enhancement of the standard method of asymptotic expansions by means of Daniels's saddlepoint approximation. Its relationship to determinantal methods is investigated in § 6. A numerical algorithm for implementing these ideas is presented in § 7, together with an application to data from the small protein Crambin, and a unified strategy for its use *ab initio* is described and discussed in § 8. It is concluded that the phase-determination strategy proposed here will expedite the realization of the full potential of probabilistic direct methods, and is likely to bring macromolecular structures within their reach.

Introduction

Thirty years ago Hauptman and Karle pioneered the use of sophisticated methods of probability theory for directly determining the phases of structure factors from the sole knowledge of their amplitudes (Hauptman & Karle, 1953). After an initial latency period, these probabilistic direct methods underwent a

* *Editorial Note*: Papers exceeding the normal length limitations of the journal are scrutinized particularly carefully to ensure they meet the stated goal of providing the maximum density of information consistent with clarity of presentation. Considerable reductions in length are often achievable in revision without loss of essential information. This very long paper, having passed all normal editorial procedures, constitutes a rare exception to the normal upper bound.

† Present address: LURE, Bâtiment 209C, 91405 Orsay CEDEX, France.

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