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THE SUBGROUPS OF FINITE INDEX OF THE SPACE GROUPS: DETERMINATION VIA CONVENTIONAL COORDINATE SYSTEMS.

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Dedicated to B. D., J. R. M., C. L. C., J. F. D. and A. S. for their friendship in many circumstances.

Many papers covering space-subgroup derivations, group-subgroup relations and space-subgroup tables have been published (NEUBÜSER & WONDRATSCHEK, 1966 a, b; BOYLE & LAWRENSON, 1972 a, b; BÄRNIGHAUSEN 1975; BERTAUT 1976 a, b; ...). Unfortunately the existing tables of subgroups list in most cases maximal subgroups only. Moreover, for "klassengleiche" subgroups often only the type of subgroups is listed, not the subgroups themselves; however several maximal subgroups of a space group may belong to the same space-group type.

Let us look at an example. Consider a space group of type p2mm characterized by its conventional coordinate system (O, A, B: origin and basis vectors) and let be the maximal subgroups of type c2mm of index 2 (o, a, b: conventional coordinate system). The most part of the tables point out that the subgroup type c2mm is obtained when doubling the conventional cell parameters (a = 2A, b = 2B); indeed there are four distinct subgroups c2mm of index 2, they correspond to the following non-redundant dispositions of origin o (X_o, Y_o: coordinates of o with respect to O, A, B) (Figures 1 and 2):

$X_o = Y_o = 0$; $X_o = 0$, $Y_o = 1/2$; $X_o = 1/2$, $Y_o = 0$; $X_o = Y_o = 1/2$.

These four origin dispositions are not equivalent as to the relationship between structure and derivative structures. For instance, consider the next 2-dimensional structure, the space group of which is p2mm (Figure 1) (Cf. International Tables for X-ray Crystallography, 1952):

	4	I	1	$X, Y; \bar{X}, Y; \bar{X}, \bar{Y}; X, \bar{Y}.$
	2	F	m	$X, 1/2; \bar{X}, 1/2.$
	1	A	mm	$0, 0.$

The derivative structures of space-group type c2mm connected with the four origin dispositions are given as follows (Figure 2 a, b, c, d) (BILLIET, SAYARI & ZARROUK, 1978 b):

a) c2mm: $a = 2A$, $b = 2B$, $X_o = Y_o = 0$. $(0, 0; 1/2, 1/2)+$

I	8	f	1	$x, y; \bar{x}, y; \bar{x}, \bar{y}; x, \bar{y}.$ $(x \approx X/2, y \approx 1/2 + Y/2)$
				$x, y; \bar{x}, y; \bar{x}, \bar{y}; x, \bar{y}.$ $(x \approx X/2, y \approx Y/2)$
F	8	f	1	$x, y; \bar{x}, y; \bar{x}, \bar{y}; x, \bar{y}.$ $(x \approx X/2, y \approx 1/4)$
A	2	b	mm	$0, 1/2.$
	2	a	mm	$0, 0.$

b) c2mm: $a = 2A$, $b = 2B$, $X_o = 0$, $Y_o = 1/2$. $(0, 0; 1/2, 1/2)+$

I	8	f	1	$x, y; \bar{x}, y; \bar{x}, \bar{y}; x, \bar{y}.$ $(x \approx 1/2 + X/2, y \approx 3/4 + Y/2)$
	8	f	1	$x, y; \bar{x}, y; \bar{x}, \bar{y}; x, \bar{y}.$ $(x \approx X/2, y \approx 3/4 + Y/2)$
F	4	d	m	$x, 0; \bar{x}, 0.$ $(x \approx 1/2 + X/2)$
	4	d	m	$x, 0; \bar{x}, 0.$ $(x \approx X/2)$
A	4	e	m	$0, y; 0, \bar{y}.$ $(y \approx 0)$

c) c2mm: $a = 2A$, $b = 2B$, $X_o = 1/2$, $Y_o = 0$. $(0, 0; 1/2, 1/2)+$

I	8	f	1	$x, y; \bar{x}, y; \bar{x}, \bar{y}; x, \bar{y}.$ $(x \approx 1/4 + X/2, y \approx Y/2)$
	8	f	1	$x, y; \bar{x}, y; \bar{x}, \bar{y}; x, \bar{y}.$ $(x \approx 3/4 + X/2, y \approx Y/2)$
F	8	f	1	$x, y; \bar{x}, y; \bar{x}, \bar{y}; x, \bar{y}.$ $(x \approx 1/4 + X/2, y \approx 1/4)$
A	4	d	m	$x, 0; \bar{x}, 0.$ $(x \approx 1/4)$

d) c2mm: $a = 2A$, $b = 2B$, $X_o = Y_o = 1/2$. $(0, 0;\ 1/2, 1/2)+$

	8	f	1	$x, y;\ \bar{x}, y;\ \bar{x}, \bar{y};\ x, \bar{y}.$
I				$(x \approx 1/4 + X/2,\ Y \approx 1/4 + Y/2)$
	8	f	1	$x, y;\ \bar{x}, y;\ \bar{x}, \bar{y};\ x, \bar{y}.$
				$(x \approx 1/4 + X/2,\ Y \approx 1/4 - Y/2)$
	4	d	m	$x, 0;\ \bar{x}, 0.$ $(x \approx 1/4 + X/2)$
F	4	d	m	$x, 0;\ \bar{x}, 0$ $(x \approx 3/4 + X/2)$
A	4	c	2	$1/4, 1/4;\ 1/4, 3/4.$

Indeed these four derivative structures are very different. The first is consistent with a double ordering through positions I and A together with slight shiftings of positions I and F. The second results from a double ordering on positions I and F together with slight shiftings of positions I, F and A. As to the third, it follows from an ordering through positions I together with slight shiftings of positions I, F and A. The later is consistent with a double ordering of positions I and F together with slight shiftings of only positions I and F.

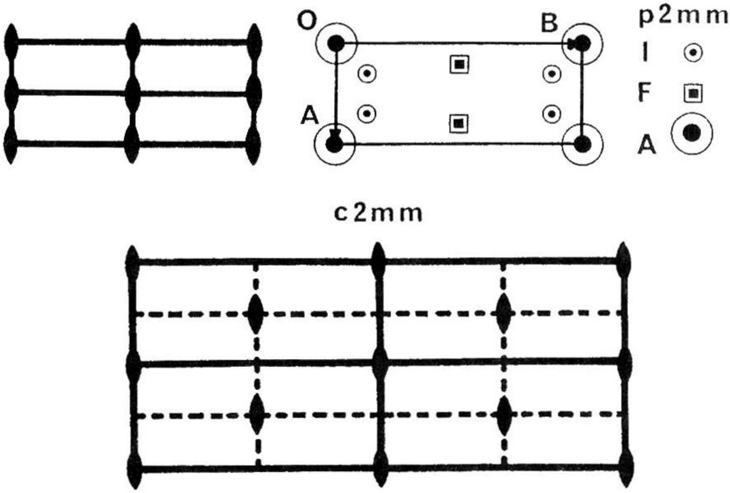

Figure 1.

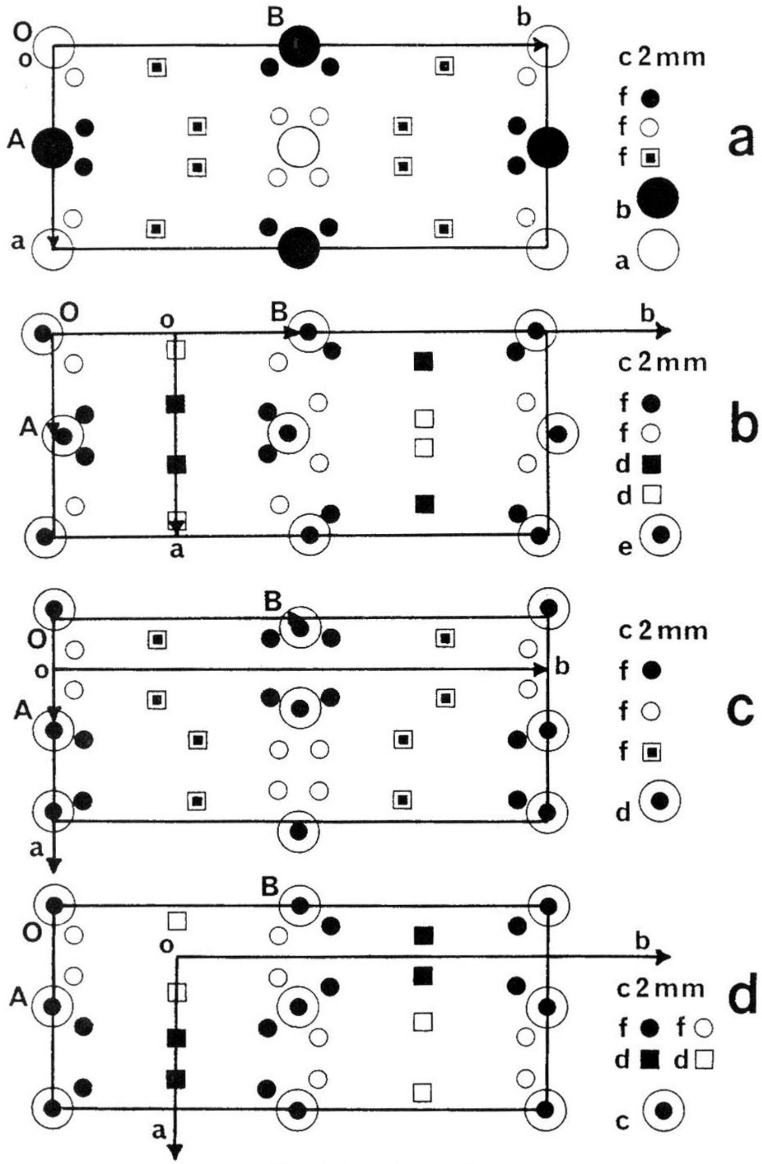

Figure 2 a, b, c, d.

Thus, for derivative-structure applications, it is necessary to obtain all distinct subgroups of a space group (*). This may be done in two steps.

FIRST STEP: DETERMINE ALL CONVENTIONAL COORDINATE SYSTEMS OF ALL SUBGROUPS OF A SPACE GROUP.

For all the space groups of each space-group type a type of conventional coordinate systems is used in the International Tables for X-ray Crystallography (1952). Instead of deriving all possible subgroups g of a certain type s from a space group G of type S, one may derive all possible conventional coordinate systems (o, a, b) of subgroups g from the conventional coordinate system (O, A, B) of G. There may be obtained, however, several of these coordinate systems (an infinite number in fact) which belong to the same subgroup. This is done in our previous papers (BILLIET, 1973; SAYARI & BILLIET, 1977; BILLIET, 1977; BILLIET, SAYARI & ZARROUK, 1978 a; SAYARI, BILLIET & ZARROUK, 1978; BILLIET, 1978; BERTAUT & BILLIET, 1978; BILLIET, 1979; BERTAUT & BILLIET, 1979; BILLIET & ROLLEY - LE COZ, 1980) where are determined all possible dispositions of vectors a, b and origin o.

$$(a,\ b) = (A,\ B)T;\ \mathrm{Det}T > 0;\ \begin{bmatrix} X_0 \\ Y_0 \end{bmatrix}.$$

There are two special cases:

s = S, DetT > 1: the subgroups g are said to be isosymbolic to the space group G (BILLIET, 1973);

s = S, DetT = 1: then g = G and the coordinate systems (o, a, b) are other conventional coordinate systems of G; any space group possesses an infinity of distinct conventional coordinate systems.

Example 1: G(O, A, B) is a space group c2mm. All conventional coordinate systems (o, a, b) of all subgroups p2 are given by the following conditions (SAYARI, BILLIET & ZARROUK, 1978):

(*) Conjugated subgroups are related to equivalent derivative structures.

<u>vector conditions</u>:

$$(a,\ b) = (A,\ B) \begin{vmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{vmatrix}; \quad t_{11}t_{22} - t_{21}t_{12} \geqq 1/2;$$

either <u>i</u>) $2t_{11}$, $2t_{21}$, $2t_{12}$, $2t_{22}$ are all even,

or <u>ii</u>) $2t_{11}$, $2t_{21}$ are both even and $2t_{12}$, $2t_{22}$ are both odd,

or <u>iii</u>) $2t_{11}$, $2t_{21}$ are both odd and $2t_{12}$, $2t_{22}$ are both even,

or <u>iv</u>) $2t_{11}$, $2t_{21}$, $2t_{12}$, $2t_{22}$ are all odd.

<u>origin conditions</u>:

either <u>v</u>) $2X_0$, $2Y_0$ are integers,

or <u>vi</u>) $4X_0$, $4Y_0$ are odd integers.

<u>Example 2</u>: Consider now the space group g (p2) of conventional coordinate system (o, a, b). All conventional coordinate systems (o', a', b') of all isosymbolic subgroups g' (p2) are given by the following conditions:

$$(a',\ b') = (a,\ b) \begin{vmatrix} t'_{11} & t'_{12} \\ t'_{21} & t'_{22} \end{vmatrix}; \quad t'_{11}t'_{22} - t'_{21}t'_{12} > 1;$$

all coefficients t'_{ij} are integers, $2x_{0'}$ and $2y_{0'}$ are integers. If the matrix is unimodular ($t'_{11}t'_{22} - t'_{21}t'_{12} = 1$), the conventional coordinate system belongs to g (p2) not to a proper subgroup of g (p2).

<u>SECOND STEP: SELECT ONE CONVENTIONAL COORDINATE SYSTEM FOR EACH SUBGROUP.</u>

A standard conventional coordinate system is defined for each subgroup and the listing is restricted to these standard coordinate systems. In this way by evaluating the formulae for the possible standard coordinate systems of subgroups one gets a list of all possible subgroups of that type and a given index. The process is illustrated by the next example.

<u>Example 3</u>: Suppose a subgroup g (p2) of G (c2mm) given by a matrix T of example 1.

I/ This subgroup only possesses conventional coordinate systems, defined in vector dispositions, either by conditions <u>i</u>, or by conditions <u>ii</u>, <u>iii</u> and <u>iv</u> at once. Indeed starting from a coordinate system of type i, one obtains by any change of conventional coordinate system in g (p2) (Cf. Example 2) another coordinate system of type i (with $t'_{11}t'_{22} - t'_{21}t'_{12} = 1$):

$$\begin{vmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{vmatrix} \times \begin{vmatrix} t'_{11} & t'_{12} \\ t'_{21} & t'_{22} \end{vmatrix} = \begin{vmatrix} n_{11}t'_{11} + n_{12}t'_{21} & n_{11}t'_{12} + n_{12}t'_{22} \\ n_{21}t'_{11} + n_{22}t'_{21} & n_{21}t'_{12} + n_{22}t'_{22} \end{vmatrix} \quad (n_{ij} \in \mathbb{Z}).$$

On the other hand, starting from a system of type iii, one obtains by a suitable change a system of type ii:

$$\begin{vmatrix} n_{11} + 1/2 & n_{12} \\ n_{21} + 1/2 & n_{22} \end{vmatrix} \times \begin{vmatrix} 0 & 1 \\ -1 & 0 \end{vmatrix} = \begin{vmatrix} -n_{12} & n_{11} + 1/2 \\ -n_{22} & n_{21} + 1/2 \end{vmatrix} \quad (n_{ij} \in \mathbb{Z}).$$

Starting from a system of type iv, one obtains a system of type ii:

$$\begin{vmatrix} n_{11} + 1/2 & n_{12} + 1/2 \\ n_{21} + 1/2 & n_{22} + 1/2 \end{vmatrix} \times \begin{vmatrix} 1 & 0 \\ -1 & 1 \end{vmatrix} = \begin{vmatrix} n_{11} - n_{12} & n_{12} + 1/2 \\ n_{21} - n_{22} & n_{22} + 1/2 \end{vmatrix} \quad (n_{ij} \in \mathbb{Z}).$$

II/ We consider now a subgroup g (p2) given by a system of type i. By an appropriate change into g one can obtain a new coordinate system given by a triangular matrix (BILLIET & ROLLEY - LE COZ, 1980):

$$\begin{vmatrix} n_{11} & n_{12} \\ n_{21} & n_{22} \end{vmatrix} \times \begin{vmatrix} n_{22}/D(n_{21}, n_{22}) & f \\ -n_{21}/D(n_{21}, n_{22}) & e \end{vmatrix} =$$

$$\begin{vmatrix} (n_{11}n_{22} - n_{12}n_{21})/D(n_{21}, n_{22}) & n_{11}f + n_{12}e \\ 0 & n_{21}f + n_{22}e \end{vmatrix} = \begin{vmatrix} p_1 & q_1 \\ 0 & p_2 \end{vmatrix} = T_I;$$

with $D(n_{21}, n_{22})$ greatest common divisor of n_{21} and n_{22}; $n_{22}/D(n_{21}, n_{22})$ and $n_{21}/D(n_{21}, n_{22})$ are coprime; then it is possible to find two integers e, f at least such that (Bezout relation):

$$en_{22}/D(n_{21}, n_{22}) + fn_{21}/D(n_{21}, n_{22}) = 1;$$

furthermore e and f may be chosen in such a way that the coefficients of the matrix T_I fulfil the following conditions:

$$p_1, p_2, q_1 \text{ integers; } p_1, p_2 > 0 \text{ and } -p_1/2 < q_1 \leq p_1/2. \qquad (I)$$

If now we consider a subgroup g (p2) given by a system of type ii, it is possible to obtain a new system expressed by a triangular matrix:

$$\begin{vmatrix} n_{11} & n_{12} + 1/2 \\ n_{21} & n_{22} + 1/2 \end{vmatrix} \times \begin{vmatrix} (2n_{22} + 1)/D(n_{21}, 2n_{22} + 1) & f \\ -2n_{21}/D(n_{21}, 2n_{22} + 1) & e \end{vmatrix} =$$

$$\begin{vmatrix} (2n_{11}n_{22} + n_{11} - 2n_{12}n_{21} - n_{21})/D(n_{21}, 2n_{22} + 1) & n_{11}f + (n_{12} + 1/2)e \\ 0 & n_{21}f + (n_{22} + 1/2)e \end{vmatrix} =$$

$$\begin{vmatrix} p_1 & q_1 + 1/2 \\ 0 & p_2 + 1/2 \end{vmatrix} = T_{II};$$

it is possible to find two integers e and f so that:

$$e(2n_{22} + 1)/D(n_{21}, 2n_{22} + 1) - 2fn_{21}/D(n_{21}, 2n_{22} + 1) = 1;$$

e is necessarily odd; moreover e and f may be chosen so that the coefficients of the matrix T_{II} fulfil the following conditions:

$$p_1, p_2, q_1 \text{ are integers; } p_1 > 0;\ p_2 \geqq 0 \text{ and } -(p_1 + 1)/2 < q_1 \leqq (p_1 - 1)/2. \qquad \text{(II)}$$

As a conclusion, <u>each</u> subgroup g (p2) is connected with exactly <u>one</u> standard conventional coordinate system, the vectors of which are define either by matrix T_I and conditions (I), or by matrix T_{II} and conditions (II).

III/ We are going to select one origin for each subgroup. Firstly consider a subgroup g (p2) defined by the vector conditions (I). Suppose an origin o of g. The coordinates of any other possible origin o' of g fulfil the following relations (BILLIET, 1973; BILLIET, SAYARI & ZARROUK, 1978 a):

$$\begin{vmatrix} X_{o'} \\ Y_{o'} \end{vmatrix} = \begin{vmatrix} p_1 & q_1 \\ 0 & p_2 \end{vmatrix} \times \begin{vmatrix} x_{o'} \\ y_{o'} \end{vmatrix} + \begin{vmatrix} X_o \\ Y_o \end{vmatrix} = \begin{vmatrix} X_o \\ Y_o \end{vmatrix} + \begin{vmatrix} p_1x_{o'} + q_1y_{o'} \\ p_2y_{o'} \end{vmatrix}$$

Now $2x_{o'}$ and $2y_{o'}$ are integers (Cf. example 2), then the origins of g are <u>either</u> all relevant to conditions <u>v</u>, <u>or</u> all relevant to conditions <u>vi</u> of example 1. If o is relevant to conditions <u>v</u> it is possible to choose $y_{o'}$ and then $x_{o'}$ so that:

$$0 \leqq Y_{o'} < p_2/2 \text{ and then } 0 \leqq X_{o'} < p_1/2 \text{ with } 2X_{o'},\ 2Y_{o'} \text{ integers.} \qquad \text{(III)}$$

If o is relevant to conditions <u>vi</u> it is possible to choose $y_{o'}$ and then $x_{o'}$ so that:

$$1/4 \leqq Y_{o'} < 1/4 + p_2/2 \text{ and then } 1/4 \leqq X_{o'} < 1/4 + p_1/2 \text{ with } 4X_{o'},\ 4Y_{o'} \text{ odd integers.} \qquad \text{(IV)}$$

As a conclusion, <u>each</u> subgroup g (p2) of type (I) is connected with exactly <u>one</u> standard conventional coordinate system whose origin is defined either by conditions (III) or by conditions (IV).
As to the subgroups g (p2) whose vector disposition is defined by conditions (II), each of them possesses origins relevant to conditions <u>v</u> <u>and</u> origins relevant to conditions <u>vi</u>.

$$\begin{vmatrix} X_{o'} \\ Y_{o'} \end{vmatrix} = \begin{vmatrix} p_1 & q_1 + 1/2 \\ 0 & p_2 + 1/2 \end{vmatrix} \times \begin{vmatrix} x_{o'} \\ y_{o'} \end{vmatrix} + \begin{vmatrix} X_o \\ Y_o \end{vmatrix} = \begin{vmatrix} X_o \\ Y_o \end{vmatrix} + \begin{vmatrix} p_1 x_{o'} + q_1 y_{o'} + y_{o'}/2 \\ p_2 y_{o'} + y_{o'}/2 \end{vmatrix}$$

Indeed if $2y_{o'}$ is even, o and o' are both relevant to the same conditions <u>v</u> or <u>vi</u>; if $2y_{o'}$ is odd, o belongs to conditions <u>v</u> (resp. <u>vi</u>) while o' belongs to conditions <u>vi</u> (resp. <u>v</u>). Thus it is possible to consider only origins of type <u>v</u> and it is possible to choose $y_{o'}$ (even) and then $x_{o'}$ so that

$$0 \leqq Y_{o'} < p_2/2 + 1/4 \text{ and then } 0 \leqq X_{o'} < p_1/2 \quad \text{with } 2X_{o'},\ 2Y_{o'} \text{ integers.} \qquad (V)$$

To conclude, <u>each</u> subgroup g (p2) of type (II) is connected with exactly <u>one</u> standard coordinate system whose origin is defined by conditions (V).

The process we have illustrated by example 3 may be extended to any space group: for <u>each</u> subgroup, it is possible to select, in vector disposition and origin disposition, exactly <u>one</u> standard conventional coordinate system relevant to special conditions.
<u>Example 4</u>: List of the standard coordinate systems (o, a, b) of all subgroups of a space group c2mm of conventional coordinate system (O, A, B), each standard coordinate system representing "its" subgroups; p_1, p_2, q_1, u, v are integers.

p1

1) $a = p_1A$, $b = (q_1 + 1/2)A + (p_2 + 1/2)B$, $X_o = Y_o = 0$ [$p_1 > 0$; $p_2 \geqq 0$; $-(p_1 + 1)/2 < q_1 \leqq (p_1 - 1)/2$]

2) $a = p_1A$, $b = q_1A + p_2B$, $X_o = Y_o = 0$ [p_1, $p_2 > 0$; $-p_1/2 < q_1 \leqq p_1/2$]

p2

1) $a = p_1A$, $b = (q_1 + 1/2)A + (p_2 + 1/2)B$, $X_o = u/2$, $Y_o = v/2$ [$p_1 > 0$; $p_2 \geqq 0$; $-(p_1 + 1)/2 < q_1 \leqq (p_1 - 1)/2$; $0 \leqq u < p_1$; $0 \leqq v < p_2 + 1/2$]

2) $a = p_1A$, $b = q_1A + p_2B$, $X_o = u/2$, $Y_o = v/2$ [$p_1, p_2 > 0$; $-p_1/2 < q_1 \leqq p_1/2$; $0 \leqq u < p_1$; $0 \leqq v < p_2$]

3) $a = p_1A$, $b = q_1A + p_2B$, $X_o = 1/4 + u/2$, $Y_o = 1/4 + v/2$ [$p_1, p_2 > 0$; $-p_1/2 < q_1 \leqq p_1/2$; $0 \leqq u < p_1$; $0 \leqq v < p_2$]

pm

1) $a = p_1A$, $b = p_2B$, $X_o = u/2$, $Y_o = 0$ [$p_1, p_2 > 0$; $0 \leqq u < p_1$]

2) $a = p_1B$, $b = -p_2A$, $X_o = 0$, $Y_o = v/2$ [$p_1, p_2 > 0$; $0 \leqq v < p_1$]

pg

1) $a = p_1A$, $b = (2p_2 + 1)B$, $X_o = 1/4 + u/2$, $Y_o = 0$ [$p_1 > 0$; $p_2 \geqq 0$; $0 \leqq u < p_1$]

2) $a = p_1A$, $b = 2p_2B$; $X_o = u/2$, $Y_o = 0$ [$p_1, p_2 > 0$; $0 \leqq u < p_1$]

3) $a = p_1B$, $b = -(2p_2 + 1)B$, $X_o = 0$; $Y_o = 1/4 + v/2$ [$p_1 > 0$, $p_2 \geqq 0$; $0 \leqq v < p_1$]

4) $a = p_1B$, $b = -2p_2A$, $X_o = 0$, $Y_o = v/2$ [$p_1, p_2 > 0$; $0 \leqq v < p_1$]

cm

1) $a = (2p_1 + 1)A$, $b = (2p_2 + 1)B$, $X_o = u/2$, $Y_o = 0$ [$p_1, p_2 \geqq 0$; $0 \leqq u < 2p_1 + 1$]

2) $a = 2p_1A$, $b = 2p_2B$, $X_o = u/2$, $Y_o = 0$ [$p_1, p_2 > 0$; $0 \leqq u < 2p_1$]

3) $a = (2p_1 + 1)B$, $b = -(2p_2 + 1)A$, $X_o = 0$; $Y_o = v/2$ [$p_1, p_2 \geqq 0$; $0 \leqq v < 2p_1 + 1$]

4) $a = 2p_1B$, $b = -2p_1A$, $X_o = 0$, $Y_o = v/2$ [$p_1, p_2 > 0$; $0 \leqq v < 2p_1$]

pmm

$a = p_1A$, $b = p_2B$, $X_o = u/2$, $Y_o = v/2$ [$p_1, p_2 > 0$; $0 \leqq u < p_1$; $0 \leqq v < p_2$]

pmg

1) $a = (2p_1 + 1)A$, $b = p_2B$, $X_o = 1/4 + u/2$, $Y_o = 1/4 + v/2$ $[p_1 \geqq 0;$ $p_2 > 0;$ $0 \leqq u < 2p_1 + 1;$ $0 \leqq v < p_2]$

2) $a = 2p_1A$, $b = p_2B$, $X_o = u/2$, $Y_o = v/2$ $[p_1, p_2 > 0;$ $0 \leqq u < 2p_1;$ $0 \leqq v < p_2]$

3) $a = (2p_1 + 1)B$, $b = -p_2A$, $X_o = 1/4 + u/2$, $Y_o = 1/4 + v/2$ $[p_1 \geqq 0;$ $p_2 > 0;$ $0 \leqq u < p_2;$ $0 \leqq v < 2p_1 + 1]$

4) $a = 2p_1B$, $b = -p_2A$, $X_o = u/2$, $Y_o = v/2$ $[p_1, p_2 > 0;$ $0 \leqq u < p_2;$ $0 \leqq v < 2p_2]$

pgg

1) $a = (2p_1 + 1)A$, $b = (2p_2 + 1)B$, $X_o = u/2$, $Y_o = v/2$ $[p_1, p_2 \geqq 0;$ $0 \leqq u < 2p_1 + 1;$ $0 \leqq v < 2p_2 + 1]$

2) $a = (2p_1 + 1)A$, $b = 2p_2B$, $X_o = 1/4 + u/2$, $Y_o = 1/4 + v/2$ $[p_1 \geqq 0;$ $p_2 > 0;$ $0 \leqq u < 2p_1 + 1;$ $0 \leqq v < 2p_2]$

3) $a = 2p_1A$, $b = (2p_2 + 1)B$, $X_o = 1/4 + u/2$, $Y_o = 1/4 + v/2$ $[p_1 > 0;$ $p_2 \geqq 0;$ $0 \leqq u < 2p_1;$ $0 \leqq v < 2p_2 + 1]$

4) $a = 2p_1A$, $b = 2p_2B$, $X_o = u/2$, $Y_o = v/2$ $[p_1, p_2 > 0;$ $0 \leqq u < 2p_1;$ $0 \leqq v < 2p_2]$

cmm

1) $a = (2p_1 + 1)A$, $b = (2p_2 + 1)B$, $X_o = u/2$, $Y_o = v/2$ $[p_1, p_2 \geqq 0;$ $(2p_1 + 1)(2p_1 + 1) > 1;$ $0 \leqq u < 2p_1 + 1;$ $0 \leqq v < 2p_2 + 1]$

2) $a = 2p_1A$, $b = 2p_2B$, $X_o = u/2$, $Y_o = v/2$ $[p_1, p_2 > 0;$ $0 \leqq u < 2p_1;$ $0 \leqq v < 2p_2]$

As an application of these tables, it is possible to determine easily the number of subgroups of a given index relevant to a given type.

Example 5: Suppose that we want to determine the subgroups of type p2 of index 4 of a group c2mm. The index $i_{g/G}$ of a space subgroup g (o, a, b) of a space group (O, A, B) is given by the following relation:

$$i_{g/G} = i_{h/H}.\mathrm{DetT}.M/m \; ;$$

$i_{h/H}$ is the index of the symmetry-class group h of g with reference to the symmetry-class group H of G; M and m are the numbers of lattice points of the Bravais lattices of G and g which are respectively contained into the conventional unit cells (O, A, B) and (o, a, b) (BILLIET, 1973; BILLIET, SAYARI & ZARROUK, 1978 a). In the present case $i_{h/H} = 2$, M = 2, m = 1 and then the matrix determinant must be equal to 1. Let us now evaluate the formulae giving the standard coordinate system associated with each subgroup p2 of a group c2mm (Cf. Example 4).

Formula 1: Since DetT = 1, the values permissible for the parameters are: $p_1 = 2$; $p_2 = 0$; $q_1 = 0, -1$; $u = 0, 1$; $v = 0$. Consequently there are four subgroups; each of them is given by "its" standard coordinate system:

No I $\quad a = 2A,\ b = A/2 + B/2,\ X_o = Y_o = 0$

No II $\quad a = 2A,\ b = A/2 + B/2,\ X_o = 1/2,\ Y_o = 0$

No III $\quad a = 2A,\ b = -A/2 + B/2,\ X_o = Y_o = 0$

No IV $\quad a = 2A,\ b = -A/2 + B/2,\ X_o = 1/2,\ Y_o = 0.$

Formula 2: The values permissible for the parameters are: $p_1 = 1$; $p_2 = 1$ $q_1 = 0$; $u = 0$; $v = 0$. There is one subgroup given by the following coordinate system:

No V $\quad a = A,\ b = B,\ X_o = Y_o = 0.$

Formula 3: The permissible parameters are: $p_1 = 1$; $p_2 = 1$; $q_1 = 0$; $u = 0$ $v = 0$. There is one subgroup of standard coordinate system:

No VI $\quad a = A,\ b = B,\ X_o = Y_o = 1/4.$

All considerations may be extended to 3-dimensional space groups (BILLIET, 1980).

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Abstract

This paper is relevant to phase-transition applications. For the study of the relationship between a crystal structure and its derivative structures, it is necessary to exactly determine each space subgroup of a space group. A method is given to select one standard conventional coordinate system for any subgroup: it is illustrated by the tables of the selected standard coordinate systems for all subgroups of a 2-dimensional space group c2mm. All considerations may be extended to 3-dimensional space groups.