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APPENDIX

The construction of the $\bar{\varrho}$, $\bar{\varphi}$-chart

In Fig. 5 there is shown a central section of the Ewald sphere passing through the relp P, and containing the

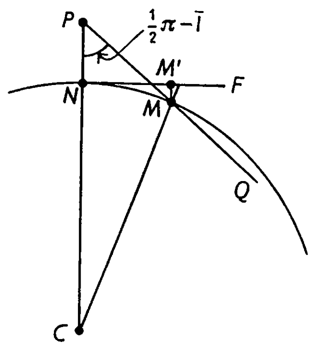

Fig. 5. Diagram showing the relation between the lengths $PM = R$, $PN = R_0$, $NM' = R'$ and $NC = G$.

rekha PQ. The angle CPQ is denoted $\frac{1}{2}\pi-\bar{\imath}$, and if PQ cuts Σ in M we have, from triangle CPM,

$$R^2-2R(G+R_0)\sin\bar{\imath}+R_0(2G+R_0) = 0\;. \tag{4}$$

Thus, being given $\bar{\imath}$ and R_0/G, the value of R can be calculated. R_0 is taken for convenience in plotting as 10 cm.

The circle on the R-chart corresponding to a given value of R has a radius R', where

$$R' = R\cos\bar{\imath}\;. \tag{5}$$

Thus R' corresponds to NM' in Fig. 5, where M' is the perpendicular projection of M on the tangent plane NF. Within the required accuracy, M' coincides with the projection of M from C on the tangent plane NF. To plot a point on the chart corresponding to particular value of $\bar{\varrho}$ and $\bar{\varphi}$ we first calculate $\bar{\imath}$ and an auxiliary angle $\bar{\psi}$ (Fig. 2) from the relations

$$\left.\begin{aligned}\sin\bar{\imath} &= \sin\bar{\varrho}\sin\bar{\varphi}\;,\\ \tan\bar{\psi} &= \tan\bar{\varrho}\cos\bar{\varphi}\;.\end{aligned}\right\} \tag{6}$$

The polar coordinates of the required point are thus R', $\bar{\psi}$ and its Cartesian coordinates are $R'\sin\bar{\psi}$, $R'\cos\bar{\psi}$.

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The Symmetry of Real Periodic Two-Dimensional Functions

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The symmetry of real periodic functions is considered, taking into account reversal symmetry elements which relate one point to another where the function has the same magnitude but opposite sign. There are 46 reversal space groups in two dimensions, and 3 in one dimension, which contain one or more of such symmetry elements. The number in three dimensions is not yet known. Reversal space groups can be denoted by symbols analogous to those of the Hermann–Mauguin space-group notation.

1. Introduction

It is well known that a periodic function which can be represented by a Fourier series

$$f(x, y, z) = \sum_h\sum_k\sum_l F(hkl)\exp\left[-2\pi i(hx+ky+lz)\right] \tag{1}$$

can be represented in projection on a plane perpendicular to the z direction by

$$f_0(x, y) = \sum_h\sum_k F(hk0)\exp\left[-2\pi i(hx+ky)\right]\;. \tag{2}$$

In crystal-structure analysis, a number of investigators (Clews & Cochran, 1949; Dyer, 1951*a*, *b*; Raeuchle & Rundle, 1952) have made practical use of the properties of a related two-dimensional function,

$$f_L(x, y) = \sum_h\sum_k F(hkL)\exp\left[-2\pi i(hx+ky)\right]\;. \tag{3}$$

Cochran & Dyer (1952) have suggested that functions such as (3) should be called generalized projections. In general the functions (1) and (2) are complex, although in crystallography, where they represent the electron density, they are entirely real and positive. Even in this case, however, f_L usually consists of a real and an imaginary component, so that $f_L = C_L + iS_L$. The functions C_L and S_L are real, but not everywhere positive.

All periodic functions must conform to the symmetry of one of the space groups, of which there are 230 in three dimensions, 17 in two dimensions, and 2 in one dimension. However, in order to describe fully the symmetry properties of periodic functions we require symmetry elements which are not taken into account in the formulation of the usual space groups. Crystallographers have not paid any attention to this point in the past, because they have been dealing with sets of points, or with functions such as the electron density, which is everywhere real and positive and whose symmetry can therefore be fully described in terms of mirror planes, centres of symmetry, etc. In dealing with generalized projections, however, one realises that, for example, centres of anti-symmetry, about which the function satisfies the condition $f_L(x, y) = -f_L(\bar{x}, \bar{y})$ are equally important. The situation may be stated quite generally as follows. In the usual space groups, a symmetry operator J relates a point r of a periodic function $f(\mathbf{r})$ to a point $\mathbf{r}' = \mathbf{r}.J$ such that $f(\mathbf{r}) = f(\mathbf{r}.J)$. What we shall call a reversal space group contains at least one corresponding reversal symmetry operator J^-, defined by the relations $\mathbf{r}' = \mathbf{r}.J^-$ and $f(\mathbf{r}) = -f(\mathbf{r}.J^-)$. Only a limited number of combinations of the operators J and J^- are consistent with periodicity. The writer has not attempted to enumerate the three-dimensional reversal space groups, but the number in two dimensions has been found to be 46, and in one dimension, 3. A notation is suggested which can be used to describe fully the symmetry of any real periodic two-dimensional function, and should be useful in describing generalized projections which occur in practical structure analysis.

2. Additional symmetry elements and point groups in a plane

In addition to the symmetry operators

$$1\ 2\ 3\ 4\ 6\ m\ g \tag{4}$$

which occur in the usual two-dimensional space groups, we require the reversal symmetry operators

$$2^-\ 4^-\ 6^-\ m^-\ g^-\ t^- . \tag{5}$$

The symbol 6^-, for example, indicates that rotation through an angle of 60°, followed by a change of sign, brings the function into self-coincidence. Similarly g^- denotes the action of a glide line g, followed by a change of sign, while t^- denotes a translation of one half of the repeat distance in any direction, followed by a change of sign. The diagrammatic representation of the symmetry elements (5) is shown in Fig. 1.

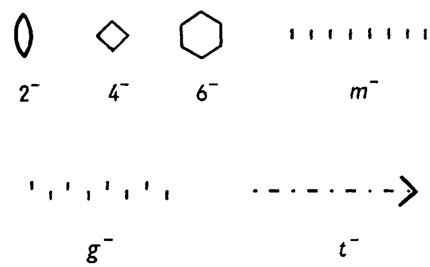

Fig. 1. Graphical representation of the symmetry elements 2^-, 4^-, 6^-, m^-, g^- and t^-.

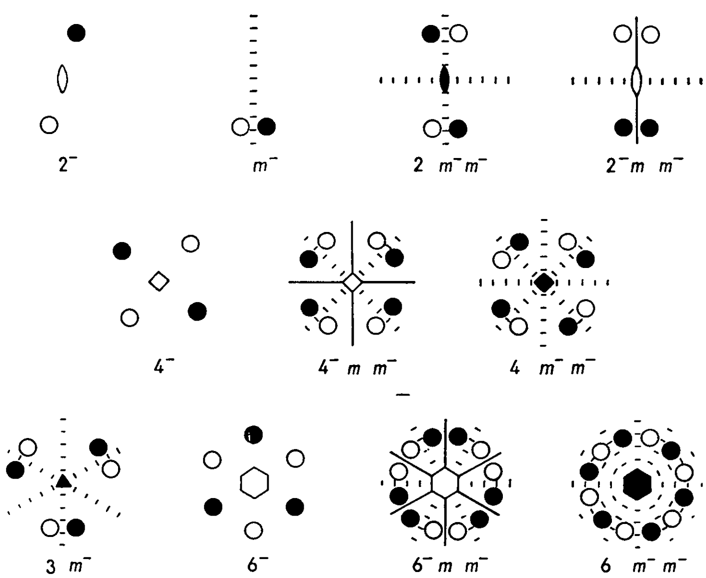

Fig. 2. The 11 reversal point groups in a plane.

It is well known that certain of the elements (4) can be combined to produce 10 point groups in a plane (Table 1). The addition of appropriate elements from (5) results in the appearance of 11 reversal point groups in a plane. They are listed in Table 2, and have already been described by Woods (1935*a*, *b*, *c*) as 'types of counterchange point-symmetry in occurring patterns'.

Table 1. *Point groups in a plane*

1	2	m	$2mm$	4	$4mm$	3	$3m$	6	$6mm$

Table 2. *Reversal point groups in a plane*

2^- m^- $2m^-m^-$ 2^-mm^- 4^- 4^-mm^- $4m^-m^-$ $3m^-$ 6^- 6^-mm^- $6m^-m^-$

The reversal point groups of Table 2 are illustrated in Fig. 2. The dark and open circles are related to one another as positive and negative.

3. Reversal space groups in two dimensions

By systematic replacement of the elements (4) by the corresponding elements of (5), and the addition of elements t^- to the usual two-dimensional space groups, as well as to those containing one or more of the corresponding reversal symmetry elements, the existence of 46 reversal space groups in two dimensions, in the sense of our definition, can be demonstrated. These space groups are listed in Table 3, and are described by symbols analogous to the Hermann–Mauguin symbols for the usual space groups. The meaning of the separate symbols such as m^- and g^- has already been defined. They are given their customary positional values, in that the first position after the lattice symbol, or after an axis when one is given, represents a symmetry line perpendicular to the x direction, while the significance of that in the second position varies according to the point group, but in exactly the same way as in the usual two-dimensional space groups. The combination $m+m^-$ denotes that m and m^- are parallel and separated from one another by one-quarter of the repeat distance in a direction perpendicular to the symmetry lines, as in $cm \equiv pm+g$. The set-up of the space-group symbols of Table 3 has been chosen to correspond to the diagrams in a paper by Weber (1929), which is briefly discussed in the next section. Two representative reversal space groups are shown in Figs. 3 and 4.

Table 3. *Reversal space groups in two dimensions*

I Number	II Symbol	III Figure	IV System
1	pt^-	3	Oblique
2	$p2^-$	2	
3	$p2t^-$	11	
4	pm^-	8	Rectangular
5	pg^-	9	
6	$pm+t^-$	21	
7	$pg+t^-$	22	
8	$pm+m^-$	23	
9	$pm+g^-$	26	
10	$pg+m^-$	25	
11	$pg+g^-$	24	
12	cm^-	10	
13	$cm+m^-$	27	
14	pmm^-	12	
15	pmg^-	13	
16	pgm^-	15	
17	pgg^-	16	
18	pm^-m^-	28	
19	pg^-m^-	29	
20	pg^-g^-	30	
21	$pmm+m^-$	34	
22	$pmg+g^-$	37	
23	$pgm+m^-$	32	
24	$pgg+g^-$	36	
25	$pm+g^-m+g^-$	38	
26	$pm+g^-g+m^-$	35	
27	$pg+m^-g+m^-$	33	
28	cmm^-	14	
29	cm^-m^-	31	
30	$cm+m^-m+m^-$	39	
31	$p4^-$	48	Square
32	$p4t^-$	54	
33	$p4^-mm^-$	56	
34	$p4^-m^-m$	51	
35	$p4m^-m^-$	52	
36	$p4g^-m^-$	58	
37	$p4^-gm^-$	57	
38	$p4^-g^-m$	55	
39	$p4m+g^-m+m^-$	60	
40	$p4g+m^-m+m^-$	59	
41	$p3m^-1$	44	Hexagonal
42	$p31m^-$	45	
43	$p6^-$	41	
44	$p6^-mm^-$	47	
45	$p6^-m^-m$	46	
46	$p6m^-m^-$	63	

Column III gives in each case the corresponding figure in the paper of Weber (1929). In Fig. 37 of that paper the x and y axes should be interchanged, while in Figs. 56 and 57 new axes should be chosen with x running from top left to bottom right. In some cases, for the sake of clearness, a longer symbol than is absolutely necessary has been given in the above table: for example, No. 30 could be written as $cm\,m+m^-$, and No. 37 as $p4^-g$.

4. Relation to other work

A generalization of plane-group theory made by Alexander & Herrmann (1928, 1929) and by Weber (1929) consists essentially in regarding the two sides of the plane as distinct. With this distinction, the number of plane groups is increased from 17 to 80. Of these, 46 are identical with reversal space groups in two dimensions, in the sense that the upper side of a plane may be equated with positive, and the lower side with negative. Of the remaining 34, 17 are identical with the usual 17 two-dimensional space groups, while the final 17 have no counterpart among reversal space groups in two dimensions, since in them upper and lower sides of the plane are occupied simultaneously at the same point, and this would

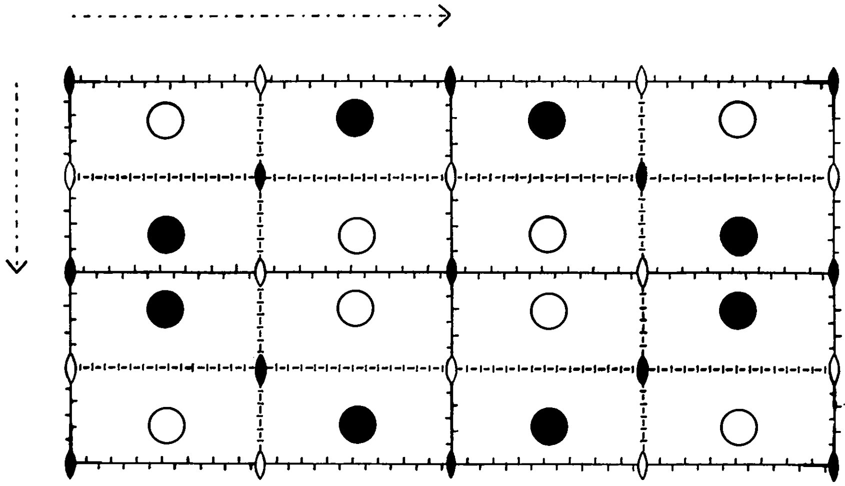

Fig. 3. The reversal space group $c\,m{+}m^-\,m{+}m^-$. Note that m and g^-, as well as g and m^-, occur superimposed.

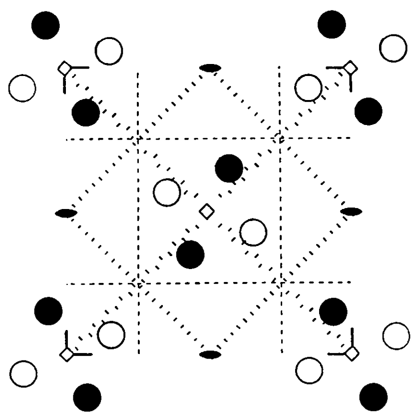

Fig. 4. The reversal space group $p\,4^-\,g\,m^-$.

correspond to a function which was simultaneously positive and negative, i.e. zero everywhere in all 17 instances.

Prof. Lonsdale has pointed out to me that the reversal space groups discussed in this paper could be described by means of the symbols for the usual 230 space groups. For example $p\,m^- \equiv P\,2$ where $x = 0$ or $z = 0$; $p\,m^-\,g^- \equiv P\,2\,2\,2_1$ where $x = 0$ or $y = 0$, etc. This symbolism would give a correct formal representation, but only by invoking a third dimension to describe what are essentially two-dimensional patterns; and would give no indication of the relation between reversal space groups in two dimensions and those in three dimensions, which remain to be investigated and which cannot be described without the use of reversal symmetry operators.

In one dimension, if we denote the usual space groups by $p\,1$, and $p\,m$, the reversal space groups are $p\,t^-$, $p\,m^-$ and $p\,m^-\,t^-$.

I should like to conclude by thanking Prof. K. Lonsdale and Dr N. F. M. Henry for some very constructive criticism of this paper.

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