continuous asymmetric unit can be deduced in θ_+, θ_- space. For these cases the limits in θ_+ are from 0 to twice the translational symmetry in θ_1 or θ_3, whichever is larger. In the other instances where the asymmetric unit is not rectangular or not continuous, the asymmetric unit listed in Table 5 will contain some redundancy. A space-group-specific rotation-function computer program which only calculates the unique portions of the asymmetric units listed in Table 5 is certainly feasible.

Discussion

The rotation function is now being applied widely to elucidate macromolecular structures. Rotation functions are calculated either in terms of Eulerian angles θ_1, θ_2, θ_3 as described by Rossmann & Blow (1962) or in the quasi-orthogonal angles θ_+, θ_2 and θ_-. Sometimes, if an internal symmetry axis can be anticipated, the spherical polar angles φ and ψ and the azimuthal angle χ are used. However, the symmetry of the rotation function is more difficult to define in this system.

In several instances rotation-function space groups have been explicitly stated in the literature. These studies provide confirmation of our assignment of rotation-function space groups for space groups 12 (Rossmann & Blow, 1962), 22 (Wishner, Ward, Lattman & Love, 1975), 24 (Tollin, Main & Rossmann, 1966), 31 (Lattman & Love, 1970; Ward, Wishner, Lattman & Love, 1975), 32 (Burnett & Rossmann, 1971) and 34 (Rossmann, Ford, Watson & Banaszak, 1972). Although many of these workers did not choose asymmetric-unit limits the same as those listed in Tables 4 and 5, their choices are equivalent to ours. In a study which uses rotation space group 61, the space-group name is not given but the limits on θ_+, θ_2 and θ_- which were used are consistent with our asymmetric unit (Schmidt, Herriott & Lattman, 1974).

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Coloured Plane Groups

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Abstract

The 46 black and white plane groups are well known. The corresponding colour groups with more than two colours are extremely numerous. We give a listing of the 935 groups with N colours for N lying between 2 and 15 inclusive.

1. Introduction

Consider an n-dimensional space group G whose elements permute N colours transitively and let G_1 be the subgroup keeping the first colour fixed. Then the index of G_1 in G is N and the colours correspond naturally to the cosets. The effect of any member of G

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under group multiplication on the cosets is the same as its effect on the colours. For these reasons a *coloured space group with N colours* is defined to be a pair $G \supset G_1$ consisting of a space group G and a subgroup G_1, which is also a space group, of index N. The pairs $G \supset G_1$ and $G' \supset G'_1$ are equivalent if there is an isomorphism between G and G' which maps G_1 onto G'_1. This implies that there is actually an affine transformation f such that $G' = fGf^{-1}$ and $G'_1 = fG_1f^{-1}$. If $N = 2$ then $G \supset G_1$ is called a *black and white group*. These definitions go back to Heesch and Shubnikov; they can be found (in slightly different form) in the paper of van der Waerden & Burckhardt (1961).

There are two well known books by Shubnikov & Belov (1964) and by Loeb (1971) which discuss the case $N = 2$ in detail and which include coloured pictures illustrating various coloured place groups. Both give complete descriptions of the 46 black and white groups but for $N = 2$ the listings begun in these books are far from complete. In this paper we describe a method for obtaining a complete listing for any given value of N and give explicit results for all N up to 15. For further remarks on the significance of coloured groups in the enumeration of space groups and in the study of twinning we refer to Schwarzenberger (1980).

Other recent work on coloured space groups by Senechal (1975) and Harker (1976) has led to the development of arithmetic algorithms for the determination of coloured space groups. Senechal (1979) uses such an algorithm to count coloured plane groups for various values of N. When N is prime she shows that the number is 14, 15, 13, 16 when $N = 5, 7, 11, 1$ modulo 12 in agreement with our computations; when N is composite there were some discrepancies between our preliminary results even for $N = 4$. Meanwhile, Wieting (1980) has developed two quite different methods of computation: one using generators and relations for $N \leq 5$, and the other using pairs of plane ornamental groups for $N \leq 60$. Comparison of the preliminary results both of Senechal and of ourselves with the results of Wieting made us aware of several errors which have been corrected in the present version. We are grateful to Senechal and Wieting for their generous cooperation but accept sole responsibility for any errors which remain.

2. The Hermann decomposition

Let $G \supset G_1$ be a coloured group and $T \supset T_1$ the corresponding pair of lattices. These groups yield point groups $H = G/T$ and $H_1 = G_1/T_1$ with homomorphisms

$$\begin{array}{ccccccccc} 0 & \to & T & \to & G & \xrightarrow{p} & H & \to & 1 \\ & & \uparrow & & \uparrow & & \uparrow & & \\ 0 & \to & T_1 & \to & G_1 & \to & H_1 & \to & 1 \end{array}$$

where vertical arrows denote embeddings of subgroups. Following Hermann (1929) we call the coloured group $G \supset G_1$ *lattice equivalent* if $T = T_1$ and *class equivalent* if $H = H_1$. The main result, which is due to Hermann and holds for arbitrary dimension n, is:

Theorem. Any coloured group $G \supset G_1$ can be expressed uniquely as the composition of a lattice equivalent coloured group $G \supset G'$ and a class equivalent coloured group $G' \supset G_1$.

Proof. A subgroup G' of G satisfies the required conditions if and only if it has lattice T and $p(G') = H_1$. There is one and only one subgroup with these properties, namely $G' = p^{-1}(H_1)$. The pair $G \supset G'$ is then lattice equivalent of index r and the pair $G' \supset G_1$ is class equivalent of index s where $r \times s = N$.

Remark. If two coloured groups are equivalent then so are their lattice equivalent and class equivalent parts. The converse is not true (see § 4).

Table 1 lists the numbers of distinct coloured plane groups corresponding to various factorizations $N = r \times s$ for $n = 2$. An indication of the method used to obtain these results is given in §§ 3 and 4.

3. The lattice equivalent and class equivalent cases

The lattice equivalent coloured groups $G \supset G'$ are finite in number for given dimension n. To obtain the list for $n = 2$ it is sufficient to consider the possible pairs $H \supset H_1$ of point groups. For completeness, and for use in § 4, we list the 52 lattice equivalent coloured plane groups explicitly in Table 2. The class equivalent coloured groups $G' \supset G_1$ depend on the possible pairs $T \supset T_1$ of lattices. We consider these according to the Bravais type of T; the number which occur is infinite but is finite for given s. The groups $G' \supset G_1$ which occur depend on the choice of integers p, q; in the

Table 1. *Number of coloured plane groups with $N = r \times s$ colours for $N = 2, \ldots, 15$*

N	Lattice equivalent		Other		Class equivalent	Total
2	(2 × 1) 26				(1 × 2) 20	46
3	(3 × 1) 5				(1 × 3) 18	23
4	(4 × 1) 12		(2 × 2) 46		(1 × 4) 38	96
5					(1 × 5) 14	14
6	(6 × 1) 6	(3 × 2) 11		(2 × 3) 44	(1 × 6) 29	90
7					(1 × 7) 15	15
8	(8 × 1) 2	(4 × 2) 26		(2 × 4) 98	(1 × 8) 44	170
9			(3 × 3) 10		(1 × 9) 30	40
10				(2 × 5) 45	(1 × 10) 30	75
11					(1 × 11) 13	13
12	(12 × 1) 1	(6 × 2) 9 (4 × 3) 25		(2 × 6) 98 (3 × 4) 30	(1 × 12) 58	221
13					(1 × 13) 16	16
14				(2 × 7) 53	(1 × 14) 29	82
15				(3 × 5) 10	(1 × 15) 24	34
Total	52		505		378	935

Table 2. *The 52 lattice equivalent groups $G \supset G'$*

$r=2$	G	$P2$	Pm	Pg	Cm	Pmm	Pmg	Pgg	Cmm	$P4$
	G'	$P1$	$P1$	$P1$	$P1$	$P2$	$P2$	$P2$	$P2$	$P2$
	G	Pmm	Pmg	Pmg	Pgg	$P4mm$	$P4gm$	Cmm	$P4mm$	$P4gm$
	G'	Pm	Pm	Pg	Pg	Pmm	Pgg	Cm	Cmm	Cmm
	G	$P4mm$	$P4gm$	$P31m$	$P3m1$	$P6$	$P6mm$	$P6mm$	$P6mm$	
	G'	$P4$	$P4$	$P3$	$P3$	$P3$	$P31m$	$P3m1$	$P6$	
$r=3$	G	$P3$	$P6$	$P31m$	$P3m1$	$P6mm$				
	G'	$P1$	$P2$	Cm	Cm	Cmm				
$r=4$	G	Pmm	Pmg	Pgg	Cmm	$P4$	$P4mm$	$P4gm$		
	G'	$P1$	$P1$	$P1$	$P1$	$P1$	$P2$	$P2$		
	G	$P4mm$	$P4gm$	$P4mm$	$P4gm$	$P6mm$				
	G'	Pm	Pg	Cm	Cm	$P3$				
$r=6$	G	$P31m$	$P3m1$	$P6$	$P6mm$	$P6mm$	$P6mm$			
	G'	$P1$	$P1$	$P1$	$P2$	$Cm1$	$C1m$			
$r=8, 12$	G	$P4mm$	$P4gm$	$P6mm$						
	G'	$P1$	$P1$	$P1$						

tabulations which follow, the symbol for G_1 is placed below the symbol for G' to indicate existence of the corresponding coloured group $G' \supset G_1$.

(i) $T = P$ *parallelogram*

Each sublattice P_1 is determined by the highest common factor d = h.c.f.(p,q) of a factorization $s = pq$. For $s \leq 15$ the possible values of d are 1 (for all s), 2 (for s = 4, 8, 12) and 3 (for s = 9). Each value of d gives two coloured groups:

$$G' = P1 \quad P2$$
$$G_1 = P_11 \quad P_12$$

(ii) $T = P$ *rectangle* (*primitive orthogonal*)

Each primitive sublattice P_1 compatible with reflections is determined by a factorization $s = pq$ and generators $(p,0)$, $(0q)$ with respect to orthogonal coordinates. If $p \neq q$ there are eight coloured groups whereas if $p = q$ there are five because of the equivalences marked $\sim$:

G' –	p,q odd	$Pm1$	$P1m$	$Pg1$	$P1g$	Pgm	Pgm	Pmm	Pgg
	p,q even	$Pm1$	$P1m$	$Pm1$	$P1m$	Pmm	Pmm	Pmm	Pmm
	$p-q$ odd	$Pm1$	$P1m$	$Pm1$	$P1g$	Pmm	Pmg	Pmm	Pmg
G_1		$P_1m \sim$	P_1m	$P_1g \sim$	P_1g	$P_1gm \sim$	P_1mg	P_1mm	P_1gg.

Similarly each centred sublattice C_1 compatible with reflections is determined by a factorization $s = 2pq$ and generators $(2p,0)$, $(0,2q)$, (p,q). If $p \neq q$ there are three coloured groups reducing to two if $p = q$:

$$G' = Pm1 \quad P1m \quad Pmm$$
$$G_1 = C_1m \sim C_1m \quad C_1mm$$

(iii) $T = C$ *diamond* (*centred orthogonal*)

Each primitive sublattice P_1 compatible with reflections is determined by a factorization $s = 2pq$ and generators $(p,0)$, $(0,q)$. If $p \neq q$ there are eight coloured groups reducing to five if $p = q$:

$G' =$	$Cm1$	$C1m$	$Cm1$	$C1m$	Cmm	Cmm	Cmm	Cmm
$G_1 =$	$P_1m \sim$	P_1m	$P_1g \sim$	P_1g	$P_1mg \sim$	P_1gm	P_1mm	P_1gg.

Similarly each centred sublattice C_1 compatible with reflections is determined by a factorization $s = pq$ where p,q have the same parity and generators $(p,0)$, $(0,q)$, $(\tfrac{1}{2}p,\tfrac{1}{2}q)$. If $p \neq q$ there are three coloured groups reducing to two if $p = q$:

$$G' = Cm1 \quad C1m \quad Cmm$$
$$G_1 = C_1m \sim C_1m \quad C_1mm$$

(iv) $T = P$ *square*

The possible sublattices invariant under rotations of order 4 are

P_1 with generators $(p,0)$, $(0,p)$ and $s = p^2$

P_1 with generators $(2p,0)$, $(0,2p)$, (p,p) and $s = 2p^2$

P_1 with generators (p,q), $(-q,p)$ and $s = p^2 + q^2$, $p \neq q$

of which only the first two are invariant also under reflections. In the range $2 \leq s \leq 15$ the coloured groups which arise are:

$G' =$	$P4$	$P4mm$	$P4mm$	$P4gm$
$G_1 =$	P_14	P_14mm	P_14gm	P_14gm
$s =$	2, 4, 5, 8, 9, 10, 13	2, 4, 8, 9	2, 4, 8	9

(v) $T = P$ *hexagonal*

The possible sublattices invariant under rotations of order 3 or 6 are (with generators now expressed relative to inclined axes)

P_1 with generators $(p,0)$, $(0,p)$ and $s = p^2$

P_1 with generators $(3p,0)$, $(0,3p)$, (p,p) and $s = 3p^2$

P_1 with generators (p,q), $(-q,p+q)$ and
$$s = p^2 + pq + q^2 (p \neq q)$$

of which only the first two are invariant under reflections. In the range $2 \leq s \leq 15$ the coloured groups which arise are

$G' =$	$P3$	$P31m$	$P31m$	$P3m1$	$P3m1$	$P6$	$P6mm$
$G =$	P_13	P_131m	P_13m1	P_13m1	P_131m	P_16	P_16mm
$s =$	3, 4, 7, 9, 12, 13	4, 9	3, 12	4, 9	3, 12	3, 4, 7, 9, 12, 13	3, 4, 9, 12

Table 3. *Number of class equivalent groups $G' \supset G_1$ with s colours arranged according to Bravais type*

	G'	T_1	$s=$ 2	3	4	5	6	7	8	9	10	11	12	13	14	15
(i)	$P1$*		1	1	2	1	1	1	2	2	1	1	2	1	1	1
	$P2$*		1	1	2	1	1	1	2	2	1	1	2	1	1	1
(ii)	Pm	P_1	3	2	5	2	6	2	7	3	6	2	10	2	6	4
		C_1	1	–	2	–	2	–	3	–	2	–	4	–	2	–
	Pmm*	P_1	2	1	5	1	4	1	6	2	4	1	8	1	4	2
		C_1	1	–	1	–	1	–	2	–	1	–	2	–	1	–
	Pg		1	2	1	2	2	2	1	3	2	2	2	2	2	4
	Pmg		2	2	2	2	4	2	2	3	4	2	4	2	4	4
	Pgg		–	1	–	1	–	1	–	2	–	1	–	1	–	2
(iii)	Cm	P_1	2	–	4	–	4	–	6	–	4	–	8	–	4	–
		C_1	–	2	1	2	–	2	2	3	–	2	2	2	–	4
	Cmm*	P_1	3	–	4	–	4	–	7	–	4	–	8	–	4	–
		C_1	–	1	1	1	–	1	1	2	–	1	1	1	–	2
(iv)	$P4$		1	–	1	1	–	–	1	1	1	–	–	1	–	–
	$P4mm$		2	–	2	–	–	–	2	1	–	–	–	–	–	–
	$P4gm$		–	–	–	–	–	–	–	1	–	–	–	–	–	–
(v)	$P3$*		–	1	1	–	–	1	–	1	–	–	1	1	–	–
	$P6$		–	1	1	–	–	1	–	1	–	–	1	1	–	–
	$P31m$		–	1	1	–	–	–	–	1	–	–	1	–	–	–
	$P3m1$*		–	1	1	–	–	–	–	1	–	–	1	–	–	–
	$P6mm$		–	1	1	–	–	–	–	1	–	–	1	–	–	–
Total			20	18	38	14	29	15	44	30	30	13	58	16	29	24

* Consult Table 4 before using this information in conjunction with Table 2.

Table 4. *Coloured groups $G' \supset G_1$ giving inequivalent compositions $G \supset G' \supset G_1$ for $s = 2, \ldots, 7$*

G	r	$G' \supset G_1$	$s=2$	3	4	5	6	7
Pm, Pg, Pmg	2, 4	$P1 \supset P_11$	3	3	6	4	9	5
Pmm, Pgg, Cmm $P4, P4mm, P4gm$	4, 8		2	2	4	3	5	3
Cm	2		2	3	5	4	7	5
$P3, P31m, P3m1$ $P6, P6mm$	3, 6, 12		1	2	3	2	3	2
Pmm, Pmg	2	$P2 \supset P_12$	2	2	4	3	5	3
Pmg	2		3	3	6	4	9	5
$Cmm, P4, P4mm, P4gm$	2, 4		3	2	6	3	7	3
$P6, P6mm$	3, 6		2	2	7	2	6	2
$P4mm$	2	$Pmm \supset P_1mm$	1	1	3	1	2	1
		$Pmm \supset P_1mg$	1	0	3	0	2	0
		$Pmm \supset P_1gg$	0	0	2	0	0	0
		$Pmm \supset C_1mm$	2	0	3	0	3	0
$P6mm$	3	$Cmm \supset P_1mm$	1	0	2	0	2	0
		$Cmm \supset P_1mg$	2	0	4	0	4	0
		$Cmm \supset P_1gg$	1	0	2	0	2	0
		$Cmm \supset C_1mm$	0	2	2	2	0	2
$P6, P31m, P6mm$	2, 4	$P3 \supset P_13$	0	2	2	0	0	2
$P6mm$	2	$P3m1 \supset P_131m$	0	2	0	0	0	0
		$P3m1 \supset P_13m1$	0	0	2	0	0	0

Table 5. *Number of coloured groups $G \supset G_1$ with N colours corresponding to each plane group G for $N = 2, \ldots, 15$*

G	$N=2$	3	4	5	6	7	8	9	10	11	12	13	14	15
$P1$	1	1	2	1	1	1	2	2	1	1	2	1	1	1
$P2$	2	1	3	1	2	1	4	2	2	1	3	1	2	1
Pm	5	2	10	2	11	2	16	3	12	2	23	2	13	4
Pmm	5	1	13	1	9	1	21	2	10	1	25	1	10	2
Pg	2	2	4	2	5	2	7	3	6	2	11	2	7	4
Pmg	5	2	11	2	11	2	19	3	12	2	26	2	13	4
Pgg	2	1	4	1	4	1	7	2	5	1	9	1	5	2
Cm	3	2	7	2	7	2	13	3	8	2	17	2	9	4
Cmm	5	1	11	1	8	1	21	2	9	1	22	1	9	2
$P4$	2	0	5	1	2	0	9	1	4	0	9	1	3	0
$P4mm$	5	0	13	0	2	0	29	1	3	0	17	0	2	0
$P4gm$	3	0	7	0	2	0	13	1	3	0	10	0	2	0
$P3$	0	2	1	0	1	1	0	3	0	0	4	1	0	2
$P6$	1	2	1	0	5	1	2	3	0	0	9	1	2	2
$P31m$	1	2	1	0	5	0	2	3	0	0	7	0	2	2
$P3m1$	1	2	1	0	4	0	1	3	0	0	7	0	1	2
$P6mm$	3	2	2	0	11	0	4	3	0	0	20	0	1	2
Total	46	23	96	14	90	15	170	40	75	13	221	16	82	34

Finally, counting up the various ways of expressing $s = 2, \ldots, 15$ in terms of p, q we obtain the 378 class equivalent coloured plane groups enumerated in Table 3.

4. The mixed case

Previous sections have dealt with all coloured plane groups arising from factorizations $N = r \times s$ with $r = 1$ (class equivalent, $s \leq 15$) or $s = 1$ (lattice equivalent). Unless N is prime there are further coloured groups to be obtained from a careful comparison of Table 2 and Table 3. Thus, for each of the 52 lattice equivalent coloured groups $G \supset G'$ listed in Table 2, we determine from Table 3 the number of possible class equivalent groups $G' \supset G_1$ so as to obtain the total number of compositions $G \supset G' \supset G_1$. There is one difficulty: it may be necessary to distinguish between subgroups G_1 of G' which, although equivalent in G', are not equivalent in G (that is, the coloured groups $G' \supset G_1$ are equivalent although the compositions $G \supset G_1$ are not). An example may clarify this phenomenon. Consider the lattice equivalent coloured group $P6 \supset P2$ of index 3 from Table 2 and the unique class equivalent coloured group $P2 \supset P_12$ of index 2 from Table 3. The group $P6$ defines centres of rotation of order six (6 centres) and, between these, centres of rotation of order two (2 centres). Which of these occur as 2 centres for the group P_12? Either a mixture of 6 centres and 2 centres of $P6$ or else only 2 centres of $P6$, giving two distinct coloured groups $P6 \supset P_12$. Note that it is not possible for the 2 centres of P_12 to consist only of 6 centres of $P6$ (although this can happen when $P2 \supset P_12$ is of index 4 instead of index 2). In this way we obtain the entry 2 in the column of Table 4 for $s = 2$. Other entries of Table 4 are obtained by a similar argument. By using Tables 2, 3 and 4 together we obtain the figures in the middle column of Table 1.

For any of the seventeen plane groups G we may, using Tables 2, 3 and 4, find the total number of coloured groups $G \supset G_1$ of index $N = 2, \ldots, 15$. The results are listed in Table 5.

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