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Rotation-Function Space Groups

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Abstract

Space groups of the 100 possible rotation functions which do not involve cubic crystallographic symmetry have been derived. All 100 belong to one of 16 basic space groups, but many possess additional translational symmetry. Asymmetric units for Eulerian coordinates and for θ_+, θ_- coordinates are tabulated.

Introduction

Since its conception in 1962, the rotation function (Rossmann & Blow, 1962) has been used in many laboratories to determine the orientation of a known molecule in a different crystal or to define non-crystallographic rotational symmetry within a crystal. Tollin, Main & Rossmann (1966) developed a method for calculating the symmetry of the rotation function. We have now applied that method to all possible combinations of non-cubic space groups. One hundred such pairs exist, but several combinations yield the same symmetry elements so that there are only 16 possible space groups for all the rotation functions from non-cubic space groups. Lattman (1972) suggested a modification of the coordinate system for the rotation function. We also tabulate asymmetric units for the rotation space groups in the Lattman θ_+, θ_- coordinate system.

Derivation of the rotation space groups

As explained by Tollin *et al.* (1966), the symmetry of the rotation function can be deduced by exhaustive combination of all equivalent positions in the proper rotation groups of the two Patterson functions which are being compared. The three Eulerian angles θ_1, θ_2 and θ_3 are used to form a three-dimensional coordinate system. The unit cell is 2π along each axis since θ and $2\pi + \theta$ are the same rotation. Each equivalent rotation is considered an equivalent position in the rotation space. Fortunately, the rotation space groups thus formed are members of the crystallographic space group set described in *International Tables for X-ray Crystallography* (1969). Table 1 lists the symmetry elements in Eulerian angles for the proper rotation groups of the nine non-cubic Laue groups. Each group includes the operation $\pi + \theta_1, -\theta_2, \pi + \theta_3$, which is an identity operation in the Eulerian system.

Since the Eulerian rotation matrix is not Hermitian, reversing the order of the Patterson functions in the rotation function does not produce the same rotation-

Table 1. *Symmetry elements S_i and $_jS$ for all proper rotation groups except cubic ones*

This table is compiled from Tables 1 and 2 of Tollin *et al.* (1966).

Laue group	Proper rotation group	Symmetry elements* S_i	Symmetry elements $_jS$
$\bar{1}$	1	$\pi+\theta_1, -\theta_2, \pi+\theta_3$	$\pi+\theta_1, -\theta_2, \pi+\theta_3$
$2/m$	2	$\pi+\theta_1, -\theta_2, \pi+\theta_3$	$\pi+\theta_1, -\theta_2, \pi+\theta_3$
(*b* axis unique)		$\pi-\theta_1, \pi+\theta_2, \theta_3$	$\theta_1, \pi+\theta_2, \pi-\theta_3$
$2/m$†	2	$\pi+\theta_1, -\theta_2, \pi+\theta_3$	$\pi+\theta_1, -\theta_2, \pi+\theta_3$
(*c* axis unique)		$\pi+\theta_1, \theta_2, \theta_3$	$\theta_1, \theta_2, \pi+\theta_3$
mmm	222	$\pi+\theta_1, -\theta_2, \pi+\theta_3$	$\pi+\theta_1, -\theta_2, \pi+\theta_3$
		$\pi-\theta_1, \pi+\theta_2, \theta_3$	$\theta_1, \pi+\theta_2, \pi-\theta_3$
		$\pi+\theta_1, \theta_2, \theta_3$	$\theta_1, \theta_2, \pi+\theta_3$
$4/m$	4	$\pi+\theta_1, -\theta_2, \pi+\theta_3$	$\pi+\theta_1, -\theta_2, \pi+\theta_3$
		$-\pi/2+\theta_1, \theta_2, \theta_3$	$\theta_1, \theta_2, \pi/2+\theta_3$
$4/mmm$	422	$\pi+\theta_1, -\theta_2, \pi+\theta_3$	$\pi+\theta_1, -\theta_2, \pi+\theta_3$
		$\pi-\theta_1, \pi+\theta_2, \theta_3$	$\theta_1, \pi+\theta_2, \pi-\theta_3$
		$-\pi/2+\theta_1, \theta_2, \theta_3$	$\theta_1, \theta_2, \pi/2+\theta_3$
$\bar{3}$	3	$\pi+\theta_1, -\theta_2, \pi+\theta_3$	$\pi+\theta_1, -\theta_2, \pi+\theta_3$
		$-2\pi/3+\theta_1, \theta_2, \theta_3$	$\theta_1, \theta_2, 2\pi/3+\theta_3$
$\bar{3}m$	321	$\pi+\theta_1, -\theta_2, \pi+\theta_3$	$\pi+\theta_1, -\theta_2, \pi+\theta_3$
		$\pi-\theta_1, \pi+\theta_2, \theta_3$	$\theta_1, \pi+\theta_2, \pi-\theta_3$
		$-2\pi/3+\theta_1, \theta_2, \theta_3$	$\theta_1, \theta_2, 2\pi/3+\theta_3$
$6/m$	6	$\pi+\theta_1, -\theta_2, \pi+\theta_3$	$\pi+\theta_1, -\theta_2, \pi+\theta_3$
		$-\pi/3+\theta_1, \theta_2, \theta_3$	$\theta_1, \theta_2, \pi/3+\theta_3$
$6/mmm$	622	$\pi+\theta_1, -\theta_2, \pi+\theta_3$	$\pi+\theta_1, -\theta_2, \pi+\theta_3$
		$\pi-\theta_1, \pi+\theta_2, \theta_3$	$\theta_1, \pi+\theta_2, \pi-\theta_3$
		$-\pi/3+\theta_1, \theta_2, \theta_3$	$\theta_1, \theta_2, \pi/3+\theta_3$

* Proper rotation-group symmetry elements S_i and $_jS$ are applied successively to generate a rotation-function symmetry element $_jS_i$. S_i is an element in the Patterson map which is rotated.

† The two monoclinic settings (*b* axis or *c* axis unique) are not separate Laue groups but are treated individually here since they produce different results in the rotation function.

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function equivalent positions. Consequently, we treat reverse order in the rotation function as an independent case even though the two arrangements do yield related equivalent positions (Tollin *et al.*, 1966).

As an example, suppose the Patterson map to be rotated (P_1) has Laue symmetry $P6/m$ and the other Patterson map (P_2) has symmetry $P2/m$ with the twofold rotation axis parallel to **b**. From Table 1, the Laue group symmetry elements S_i and ${}_jS$ are:

$$S_1\ (\theta_1,\theta_2,\theta_3) \rightarrow (\pi+\theta_1, -\theta_2, \pi+\theta_3);$$
$$S_2\ (\theta_1,\theta_2,\theta_3) \rightarrow (-\pi/3+\theta_1, \theta_2, \theta_3);$$
$${}_1S\ (\theta_1,\theta_2,\theta_3) \rightarrow (\pi+\theta_1, -\theta_2, \pi+\theta_3);$$
$${}_2S\ (\theta_1,\theta_2,\theta_3) \rightarrow (\theta_1, \pi+\theta_2, \pi-\theta_3).$$

An exhaustive combination of these S_i and ${}_jS$ results in 24 unique rotation-function symmetry elements ${}_jS_i$. Multiple application of the sixfold rotation element is required to generate all possible equivalent positions. Another example of this type of treatment has already been given (Tollin *et al.*, 1966). For each of the 24 ${}_jS_i$ below, one of the combinations of S_i's and ${}_jS$'s which yield each ${}_jS_i$ is shown in parentheses. Other combinations exist which yield the same equivalent position ${}_jS_i$:

θ_1,	θ_2,	θ_3	
θ_1,	$-\theta_2$,	$\pi+\theta_3$	$(S_2.S_2.S_2.S_1)$
θ_1,	$\pi+\theta_2$,	$\pi-\theta_3$	$({}_2S)$
θ_1,	$\pi-\theta_2$,	$-\theta_3$	$(S_2.S_2.S_2.S_1.{}_2S)$
$\pi/3+\theta_1$,	θ_2,	θ_3	$(S_2.S_2.S_2.S_2.S_2)$
$\pi/3+\theta_1$,	$-\theta_2$,	$\pi+\theta_3$	$(S_2.S_2.S_1)$
$\pi/3+\theta_1$,	$\pi+\theta_2$,	$\pi-\theta_3$	$(S_2.S_2.S_2.S_2.S_2.{}_2S)$
$\pi/3+\theta_1$,	$\pi-\theta_2$,	$-\theta_3$	$(S_2.S_2.S_1.{}_2S)$
$2\pi/3+\theta_1$,	θ_2,	θ_3	$(S_2.S_2.S_2.S_2)$
$2\pi/3+\theta_1$,	$-\theta_2$,	$\pi+\theta_3$	$(S_2.S_1)$
$2\pi/3+\theta_1$,	$\pi+\theta_2$,	$\pi-\theta_3$	$(S_2.S_2.S_2.S_2.{}_2S)$
$2\pi/3+\theta_1$,	$\pi-\theta_2$,	$-\theta_3$	$(S_2.S_1.{}_2S)$
$\pi+\theta_1$,	θ_2,	θ_3	$(S_2.S_2.S_2)$
$\pi+\theta_1$,	$-\theta_2$,	$\pi+\theta_3$	(S_1)
$\pi+\theta_1$,	$\pi+\theta_2$,	$\pi-\theta_3$	$(S_2.S_2.S_2.{}_2S)$
$\pi+\theta_1$,	$\pi-\theta_2$,	$-\theta_3$	$(S_1.{}_2S)$
$4\pi/3+\theta_1$,	θ_2,	θ_3	$(S_2.S_2)$
$4\pi/3+\theta_1$,	$-\theta_2$,	$\pi+\theta_3$	$(S_2.S_2.S_2.S_2.S_2.S_1)$
$4\pi/3+\theta_1$,	$\pi+\theta_2$,	$\pi-\theta_3$	$(S_2.S_2.{}_2S)$
$4\pi/3+\theta_1$,	$\pi-\theta_2$,	$-\theta_3$	$(S_2.S_2.S_2.S_2.S_2.S_1.{}_2S)$
$5\pi/3+\theta_1$,	θ_2,	θ_3	(S_2)
$5\pi/3+\theta_1$,	$-\theta_2$,	$\pi+\theta_3$	$(S_2.S_2.S_2.S_2.S_1)$
$5\pi/3+\theta_1$,	$\pi+\theta_2$,	$\pi-\theta_3$	$(S_2.{}_2S)$
$5\pi/3+\theta_1$,	$\pi-\theta_2$,	$-\theta_3$	$(S_2.S_2.S_2.S_2.S_1.{}_2S)$.

This rotation-function space group of 24 equivalent positions is made up of a basic group of four rotations plus five related groups which are identical except for consecutive translation by $\pi/3$ along the θ_1 axis. In the basic set the space group $P2cb$ can be recognized by examining the symmetry properties shown in brackets below:

θ_1, θ_2, θ_3
θ_1, $-\theta_2$, $\pi+\theta_3$ (*c* glide perpendicular to **b**)
θ_1, $\pi+\theta_2$, $\pi-\theta_3$ (*b* glide perpendicular to **c**)
θ_1, $\pi-\theta_2$, $-\theta_3$ (2-fold axis along **a**).

For every rotation space group, there are several consistent choices of the range of the asymmetric unit. But when the rotation function is calculated as a function of θ_+ and θ_- in sections of constant θ_2 (Lattman, 1972), it is advantageous to minimize the range of θ_2. For this reason, we chose the asymmetric unit for this example to be:

$$0 \le \theta_1 < \pi/3$$
$$0 \le \theta_2 \le \pi/2$$
$$0 \le \theta_3 < 2\pi.$$

We wrote a Fortran computer program which listed all possible combinations of a group of input symmetry elements. From these lists the equivalent positions for each rotation-function space group were deduced.

Our numbering of the possible rotation-function space groups is listed in Table 2. Once the number of a specific rotation-function space group is known from Table 2, its characteristics can be easily found in Table 3, in which all the possible rotation-function space groups, except those involving cubic Laue groups, are listed. In the 100 unique combinations of Laue groups, there are only 16 basic rotation-function space groups, whose equivalent positions are listed in Table 4. All rotation-function space groups are either one of the 16 listed in Table 4 or one of the 16 basic groups plus translation along the θ_1 and/or the θ_3 axis. This translation is not a linear translation in real space, but rather it is a rotation about an axis. Translation along θ_2 does not occur.

In Table 3, the number of equivalent positions is greater in most cases than the number of equivalent

Table 2. *Numbering of the rotation-function space groups*

The Laue group of the rotated Patterson map P_1 is chosen from the left column and the Laue group of P_2 is chosen from the upper row.

	$\bar{1}$	$2/m$ *b* axis unique	$2/m$ *c* axis unique	*mmm*	$4/m$	$4/mmm$	$\bar{3}$	$\bar{3}m$	$6/m$	$6/mmm$
$\bar{1}$	1	11	21	31	41	51	61	71	81	91
$2/m$ *b* axis unique	2	12	22	32	42	52	62	72	82	92
$2/m$ *c* axis unique	3	13	23	33	43	53	63	73	83	93
mmm	4	14	24	34	44	54	64	74	84	94
$4/m$	5	15	25	35	45	55	65	75	85	95
$4/mmm$	6	16	26	36	46	56	66	76	86	96
$\bar{3}$	7	17	27	37	47	57	67	77	87	97
$\bar{3}m$	8	18	28	38	48	58	68	78	88	98
$6/m$	9	19	29	39	49	59	69	79	89	99
$6/mmm$	10	20	30	40	50	60	70	80	90	100

Table 3. *Rotation-function space groups*

No. of the rotation space group	No. of equivalent positions[a]	Symbol[b]	Translation along the θ_1 axis[c]	Translation along the θ_3 axis[c]	Range of the asymmetric unit[d]
1	2	*Pn*	2π	2π	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < 2\pi$
2	4	*Pbn*2_1	2π	2π	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi$
3	4	*Pc*	π	2π	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < 2\pi$
4	8	*Pbc*2_1	π	2π	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi$
5	8	*Pc*	$\pi/2$	2π	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < 2\pi$
6	16	*Pbc*2_1	$\pi/2$	2π	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi$
7	6	*Pn*	$2\pi/3$	2π	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < 2\pi$
8	12	*Pbn*2_1	$2\pi/3$	2π	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi$
9	12	*Pc*	$\pi/3$	2π	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < 2\pi$
10	24	*Pbc*2_1	$\pi/3$	2π	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi$
11	4	*P*2_1*nb*	2π	2π	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi$
12	8	*Pbnb*	2π	2π	$0 \le \theta_1 \le \pi/2$ $0 \le \theta_2 < \pi$ $0 \le \theta_3 < 2\pi$
13	8	*P2cb*	π	2π	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi$
14	16	*Pbcb*	π	2π	$0 \le \theta_1 \le \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi$
15	16	*P2cb*	$\pi/2$	2π	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi$
16	32	*Pbcb*	$\pi/2$	2π	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 < \pi$ $0 \le \theta_3 \le \pi/2$
17	12	*P*2_1*nb*	$2\pi/3$	2π	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi$
18	24	*Pbnb*	$2\pi/3$	2π	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 < \pi$ $0 \le \theta_3 \le \pi/2$
19	24	*P2cb*	$\pi/3$	2π	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi$
20	48	*Pbcb*	$\pi/3$	2π	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 < \pi$ $0 \le \theta_3 \le \pi/2$
21	4	*Pa*	2π	π	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi$
22	8	*Pba2*	2π	π	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi$
23	8	*Pm*	π	π	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi$
24	16	*Pbm2*	π	π	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi$
25	16	*Pm*	$\pi/2$	π	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi$
26	32	*Pbm2*	$\pi/2$	π	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi$
27	12	*Pa*	$2\pi/3$	π	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi$
28	24	*Pba2*	$2\pi/3$	π	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi$
29	24	*Pm*	$\pi/3$	π	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi$
30	48	*Pbm2*	$\pi/3$	π	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi/2$ $0 < \theta_3 < \pi$
31	8	*P*2_1*ab*	2π	π	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi$
32	16	*Pbab*	2π	π	$0 \le \theta_1 \le \pi/2$ $0 \le \theta_2 < \pi$ $0 \le \theta_3 < \pi$
33	16	*P2mb*	π	π	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi$
34	32	*Pbmb*	π	π	$0 \le \theta_1 \le \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi$
35	32	*P2mb*	$\pi/2$	π	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi$
36	64	*Pbmb*	$\pi/2$	π	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 \le \pi/2$
37	24	*P*2_1*ab*	$2\pi/3$	π	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi$
38	48	*Pbab*	$2\pi/3$	π	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 \le \pi/2$
39	48	*P2mb*	$\pi/3$	π	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi$
40	96	*Pbmb*	$\pi/3$	π	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 \le \pi/2$
41	8	*Pa*	2π	$\pi/2$	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi/2$
42	16	*Pba2*	2π	$\pi/2$	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/2$
43	16	*Pm*	π	$\pi/2$	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi/2$
44	32	*Pbm2*	π	$\pi/2$	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/2$
45	32	*Pm*	$\pi/2$	$\pi/2$	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi/2$
46	64	*Pbm2*	$\pi/2$	$\pi/2$	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/2$
47	24	*Pa*	$2\pi/3$	$\pi/2$	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi/2$
48	48	*Pba2*	$2\pi/3$	$\pi/2$	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/2$
49	48	*Pm*	$\pi/3$	$\pi/2$	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi/2$
50	96	*Pbm2*	$\pi/3$	$\pi/2$	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/2$
51	16	*P*2_1*ab*	2π	$\pi/2$	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/2$
52	32	*Pbab*	2π	$\pi/2$	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 \le \pi/4$

Table 3 (*cont.*)

Table 3 (*cont.*)

No. of the rotation space group	No. of equivalent positions[a]	Symbol[b]	Translation along the θ_1 axis[c]	Translation along the θ_3 axis[c]	Range of the asymmetric unit[d]
53	32	*P2mb*	π	$\pi/2$	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/2$
54	64	*Pbmb*	π	$\pi/2$	$0 \le \theta_1 \le \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/2$
55	64	*P2mb*	$\pi/2$	$\pi/2$	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/2$
56	128	*Pbmb*	$\pi/2$	$\pi/2$	$0 \le \theta_1 \le \pi/4$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/2$
57	48	*P2₁ab*	$2\pi/3$	$\pi/2$	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/2$
58	96	*Pbab*	$2\pi/3$	$\pi/2$	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 \le \pi/4$
59	96	*P2mb*	$\pi/3$	$\pi/2$	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/2$
60	192	*Pbmb*	$\pi/3$	$\pi/2$	$0 \le \theta_1 \le \pi/6$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/2$
61	6	*Pn*	2π	$2\pi/3$	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < 2\pi/3$
62	12	*Pbn2₁*	2π	$2\pi/3$	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi/3$
63	12	*Pc*	π	$2\pi/3$	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < 2\pi/3$
64	24	*Pbc2₁*	π	$2\pi/3$	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi/3$
65	24	*Pc*	$\pi/2$	$2\pi/3$	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < 2\pi/3$
66	48	*Pbc2₁*	$\pi/2$	$2\pi/3$	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi/3$
67	18	*Pn*	$2\pi/3$	$2\pi/3$	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < 2\pi/3$
68	36	*Pbn2₁*	$2\pi/3$	$2\pi/3$	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi/3$
69	36	*Pc*	$\pi/3$	$2\pi/3$	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < 2\pi/3$
70	72	*Pbc2₁*	$\pi/3$	$2\pi/3$	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi/3$
71	12	*P2₁nb*	2π	$2\pi/3$	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi/3$
72	24	*Pbnb*	2π	$2\pi/3$	$0 \le \theta_1 \le \pi/2$ $0 \le \theta_2 < \pi$ $0 \le \theta_3 < 2\pi/3$
73	24	*P2cb*	π	$2\pi/3$	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi/3$
74	48	*Pbcb*	π	$2\pi/3$	$0 \le \theta_1 \le \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi/3$
75	48	*P2cb*	$\pi/2$	$2\pi/3$	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi/3$
76	96	*Pbcb*	$\pi/2$	$2\pi/3$	$0 \le \theta_1 \le \pi/4$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi/3$
77	36	*P2₁nb*	$2\pi/3$	$2\pi/3$	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi/3$
78	72	*Pbnb*	$2\pi/3$	$2\pi/3$	$0 \le \theta_1 \le \pi/6$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < 2\pi/3$
79	72	*P2cb*	$\pi/3$	$2\pi/3$	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < 2\pi/3$
80	144	*Pbcb*	$\pi/3$	$2\pi/3$	$0 < \theta_1 \le \pi/6$ $0 \le \theta_2 < \pi/2$ $0 \le \theta_3 < 2\pi/3$
81	12	*Pa*	2π	$\pi/3$	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi/3$
82	24	*Pba2*	2π	$\pi/3$	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/3$
83	24	*Pm*	π	$\pi/3$	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi/3$
84	48	*Pbm2*	π	$\pi/3$	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/3$
85	48	*Pm*	$\pi/2$	$\pi/3$	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi/3$
86	96	*Pbm2*	$\pi/2$	$\pi/3$	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/3$
87	36	*Pa*	$2\pi/3$	$\pi/3$	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi/3$
88	72	*Pba2*	$2\pi/3$	$\pi/3$	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/3$
89	72	*Pm*	$\pi/3$	$\pi/3$	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi$ $0 \le \theta_3 < \pi/3$
90	144	*Pbm2*	$\pi/3$	$\pi/3$	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/3$
91	24	*P2₁ab*	2π	$\pi/3$	$0 \le \theta_1 < 2\pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/3$
92	48	*Pbab*	2π	$\pi/3$	$0 \le \theta_1 \le \pi/2$ $0 \le \theta_2 < \pi$ $0 \le \theta_3 < \pi/3$
93	48	*P2mb*	π	$\pi/3$	$0 \le \theta_1 < \pi$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/3$
94	96	*Pbmb*	π	$\pi/3$	$0 \le \theta_1 \le \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 \le \pi/2$
95	96	*P2mb*	$\pi/2$	$\pi/3$	$0 \le \theta_1 < \pi/2$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/3$
96	192	*Pbmb*	$\pi/2$	$\pi/3$	$0 \le \theta_1 \le \pi/4$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/3$
97	72	*P2₁ab*	$2\pi/3$	$\pi/3$	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/3$
98	144	*Pbab*	$2\pi/3$	$\pi/3$	$0 \le \theta_1 < 2\pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 \le \pi/6$
99	144	*P2mb*	$\pi/3$	$\pi/3$	$0 \le \theta_1 < \pi/3$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/3$
100	288	*Pbmb*	$\pi/3$	$\pi/3$	$0 \le \theta_1 \le \pi/6$ $0 \le \theta_2 \le \pi/2$ $0 \le \theta_3 < \pi/3$

[a] This is the number of equivalent positions in the rotation unit cell.

[b] Each symbol retains the order θ_1, θ_2, θ_3. The monoclinic space groups have the *b*-axis unique setting.

[c] This is a translation symmetry: *e.g.* for the case of $\pi/2$ translation along the θ_1 axis, $\theta_1, \theta_2, \theta_3$ goes to $\pi/2+\theta_1, \theta_2, \theta_3$ and $\pi+\theta_1, \theta_2, \theta_3$ and $3\pi/2+\theta_1, \theta_2, \theta_3$. All other equivalent positions in the basic rotation space group are similarly translated.

[d] Several consistent sets of ranges exist but the one with the minimum range of θ_2 is listed.

Table 4. *The* 16 *basic rotation-function space groups and their equivalent positions*

Pa	θ_1,	θ_2,	θ_3	$\pi+\theta_1$,	$-\theta_2$,	θ_3
Pc	θ_1,	θ_2,	θ_3	θ_1,	$-\theta_2$,	$\pi+\theta_3$
Pm	θ_1,	θ_2,	θ_3	θ_1,	$-\theta_2$,	θ_3
Pn	θ_1,	θ_2,	θ_3	$\pi+\theta_1$,	$-\theta_2$,	$\pi+\theta_3$
*Pbm*2	θ_1,	θ_2,	θ_3	θ_1,	$-\theta_2$,	θ_3
	$-\theta_1$,	$\pi+\theta_2$,	θ_3	$-\theta_1$,	$\pi-\theta_2$,	θ_3
*P*2*mb*	θ_1,	θ_2,	θ_3	θ_1,	$\pi+\theta_2$,	$-\theta_3$
	θ_1,	$-\theta_2$,	θ_3	θ_1,	$\pi-\theta_2$,	$-\theta_3$
Pbc2_1	θ_1,	θ_2,	θ_3	θ_1,	$-\theta_2$,	$\pi+\theta_3$
	$-\theta_1$,	$\pi+\theta_2$,	θ_3	$-\theta_1$,	$\pi-\theta_2$,	$\pi+\theta_3$
P2_1*ab*	θ_1,	θ_2,	θ_3	θ_1,	$\pi+\theta_2$,	$-\theta_3$
	$\pi+\theta_1$,	$-\theta_2$,	θ_3	$\pi+\theta_1$,	$\pi-\theta_2$,	$-\theta_3$
*Pba*2	θ_1,	θ_2,	θ_3	$\pi+\theta_1$,	$-\theta_2$,	θ_3
	$-\theta_1$,	$\pi-\theta_2$,	θ_3	$\pi-\theta_1$,	$\pi+\theta_2$,	θ_3
*P*2*cb*	θ_1,	θ_2,	θ_3	θ_1,	$\pi+\theta_2$,	$\pi-\theta_3$
	θ_1,	$-\theta_2$,	$\pi+\theta_3$	θ_1,	$\pi-\theta_2$,	$-\theta_3$
Pbn2_1	θ_1,	θ_2,	θ_3	$\pi+\theta_1$,	$-\theta_2$,	$\pi+\theta_3$
	$-\theta_1$,	$\pi-\theta_2$,	$\pi+\theta_3$	$\pi-\theta_1$,	$\pi+\theta_2$,	θ_3
P2_1*nb*	θ_1,	θ_2,	θ_3	θ_1,	$\pi+\theta_2$,	$\pi-\theta_3$
	$\pi+\theta_1$,	$-\theta_2$,	$\pi+\theta_3$	$\pi+\theta_1$,	$\pi-\theta_2$,	$-\theta_3$
Pbab	θ_1,	θ_2,	θ_3	θ_1,	$\pi+\theta_2$,	$-\theta_3$
	$\pi+\theta_1$,	$-\theta_2$,	θ_3	$\pi+\theta_1$,	$\pi-\theta_2$,	$-\theta_3$
	$-\theta_1$,	$-\theta_2$,	$-\theta_3$	$-\theta_1$,	$\pi-\theta_2$,	θ_3
	$\pi-\theta_1$,	θ_2,	$-\theta_3$	$\pi-\theta_1$,	$\pi+\theta_2$,	θ_3
Pbmb	θ_1,	θ_2,	θ_3	θ_1,	$\pi+\theta_2$,	$-\theta_3$
	θ_1,	$-\theta_2$,	θ_3	θ_1,	$\pi-\theta_2$,	$-\theta_3$
	$-\theta_1$,	$-\theta_2$,	$-\theta_3$	$-\theta_1$,	$\pi-\theta_2$,	θ_3
	$-\theta_1$,	θ_2,	$-\theta_3$	$-\theta_1$,	$\pi+\theta_2$,	θ_3
Pbcb	θ_1,	θ_2,	θ_3	θ_1,	$\pi+\theta_2$,	$\pi-\theta_3$
	θ_1,	$-\theta_2$,	$\pi+\theta_3$	θ_1,	$\pi-\theta_2$,	$-\theta_3$
	$-\theta_1$,	$-\theta_2$,	$-\theta_3$	$-\theta_1$,	$\pi-\theta_2$,	$\pi+\theta_3$
	$-\theta_1$,	θ_2,	$\pi-\theta_3$	$-\theta_1$,	$\pi+\theta_2$,	θ_3
Pbnb	θ_1,	θ_2,	θ_3	θ_1,	$\pi+\theta_2$,	$\pi-\theta_3$
	$\pi+\theta_1$,	$-\theta_2$,	$\pi+\theta_3$	$\pi+\theta_1$,	$\pi-\theta_2$,	$-\theta_3$
	$-\theta_1$,	$-\theta_2$,	$-\theta_3$	$-\theta_1$,	$\pi-\theta_2$,	$\pi+\theta_3$
	$\pi-\theta_1$,	θ_2,	$\pi-\theta_3$	$\pi-\theta_1$,	$\pi+\theta_2$,	θ_3

positions dictated by the space-group symbol which is listed. This is due to the translation along the θ_1 and/or the θ_3 axis as indicated. In all instances where the basic rotation space group is *Pa*, *Pc*, *Pm* or *Pn* the asymmetric unit has θ_2 limits $0 \le \theta_2 \le \pi$. With a few exceptions (rotation space groups 12, 16, 18, 20, 32, 72 and 78), the other rotation space groups have θ_2 limits $0 \le \theta_2 \le \pi/2$. In the seven exceptions listed, an upper limit of π for θ_2 was required in order for a continuous asymmetric unit to be chosen. If the basic rotation-function space group is not *Pbmb*, *Pbab*, *Pbcb* or *Pbnb* then the θ_1 and θ_3 limits on the asymmetric unit are equal to the allowed translations in θ_1 and θ_3. For these four basic rotation-function space groups of highest symmetry θ_1 or θ_3 limits less than the θ_1 and θ_3 translations are possible.

Crowther (1972) has used a definition of the rotation angles (α, β and γ) in his fast rotation function program which is different from that adopted by Rossmann & Blow (1962). However, a simple relationship exists between the two systems, *viz*: $\theta_1 = \alpha + \pi/2$, $\theta_2 = \beta$ and $\theta_3 = \gamma - \pi/2$. Moreover, Crowther's program always computes ranges of α and γ from 0 to $2\pi/p$, where p is the rotational symmetry along the axis about which the α rotation takes place. The symmetry of the Patterson map which is rotated affects the range of α, and the symmetry of the stationary Patterson map affects the range of γ. This treatment is equivalent to acknowledging the translational symmetry which we observed in the equivalent positions of the rotation-function space groups. Therefore, the asymmetric units tabulated in Table 3 are appropriate for determining the range of β required to cover the unique portion of rotation space. Crowther's program reindexes monoclinic data to the *c*-axis unique setting so those rotation space groups involving the *b*-axis unique setting will not occur. When the rotation space-group symmetry is *Pbab*, *Pbmb*, *Pbcb* or *Pbnb* the asymmetric unit listed in Table 3 is smaller in θ_1 or θ_3 than is deduced from consideration of the translational symmetry only.

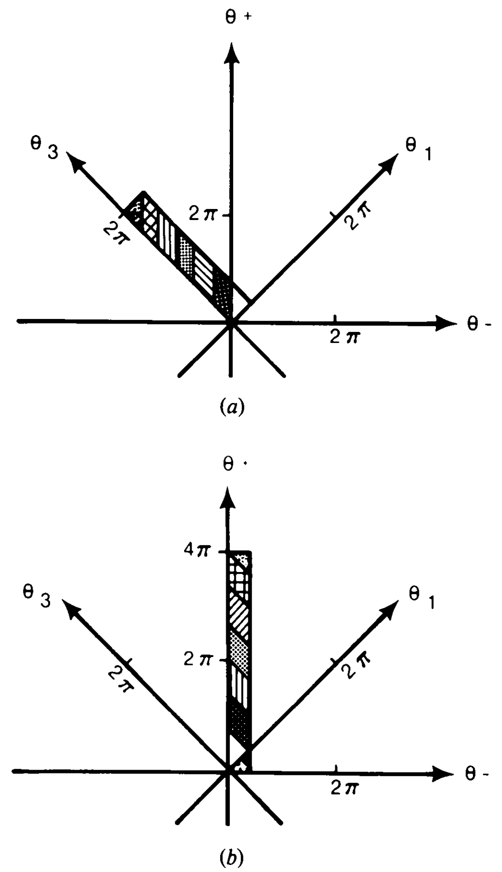

Fig. 1. Derivation of asymmetric unit in θ_+, θ_- space for rotation space group 19. θ_1 translation is $\pi/3$, θ_3 translation is 2π, and θ_+ translation is 4π. Each segment of the asymmetric unit in (*a*) is moved by allowed translations parallel to θ_1 or θ_3 to the similarly marked segment in (*b*). This transfer does not involve θ_2. Consequently, the Eulerian space asymmetric unit of $0 \le \theta_1 \le \pi/3$, $0 \le \theta_2 \le \pi/2$, $0 \le \theta_3 \le 2\pi$ becomes $0 \le \theta_+ < 4\pi$, $0 \le \theta_2 \le \pi/2$, $0 \le \theta_- \le \pi/3$ in θ_+, θ_- *space*.

However, in all instances but one, the $\theta_2(\beta)$ range required will be that which is tabulated. The one exception is space group 78 where we chose a contiguous asymmetric unit $0 \le \theta_1 \le \pi/6$, $0 \le \theta_2 \le \pi$, $0 \le \theta_3 < 2\pi/3$. A β range from 0 to $\pi/2$ will suffice for Crowther's treatment since the α and γ will both range from 0 to $2\pi/3$. In the rotation space groups of symmetry *Pbab*, *Pbmb*, *Pbcb* and *Pbnb* there will be more than one copy of the asymmetric unit in the output.

Derivation of asymmetric units in θ_+, θ_- space

Lattman (1972) showed that if the coordinates of the rotation function are θ_+, θ_2 and θ_- where $\theta_+ = \theta_1 + \theta_3$ and $\theta_- = \theta_1 - \theta_3$, then the coordinates are locally orthogonal and the sample points are associated with equal volumes so that more symmetrical peaks occur. He also presented a graphical means for determining the asymmetric unit in θ_+, θ_- space. Fig. 1 demonstrates the application of this method to rotation space group 19, which served as an example above. In this method, translations of portions of the asymmetric unit are allowed along the θ_1 and θ_3 axes as dictated by the rotation space group and listed in Table 3. Translations in the θ_+ direction sometimes are required. The translational equivalent in θ_+ is twice the translation which is a multiple of both the θ_1 and the θ_3 translations. For example, if the θ_1 translation is $\pi/3$ and the θ_3 translation is $\pi/2$, π is a multiple of both of these so that a 2π translation in θ_+ is allowed.

In order to derive the asymmetric units of all of the rotation space groups in θ_+, θ_- space, the rotation-function space groups are best arranged according to translational symmetry in θ_1 and θ_3. Our results for the 100 rotation-function space groups are given in Table 5. In all instances but two (rotation space groups 58 and 76), the minimum asymmetric unit in θ_+, θ_- space may run in θ_- from 0 to an upper limit which is equal to the translational symmetry in θ_1 or θ_3, whichever is smaller. In a majority of cases, a rectangular,

Table 5. *Asymmetric units in θ_+, θ_- space*

The rotation space groups are divided according to translational symmetry in θ_1 (horizontal) and θ_3 (vertical). Within each square, the first line lists the numbers of the four rotation space groups which have the indicated translational symmetry. If the list is followed by † the true asymmetric unit for all four space groups is smaller than the rectangular unit listed, while if the list is followed by * such is the case only for the last rotation space group listed. If only one set of θ_+, θ_- limits is listed it applies to all four space groups; when a second set of limits is listed it applies only to the fourth space group listed. The θ_2 limits are the same as shown in Table 3 with two exceptions. Rotation space groups 12 and 78, marked with §, have limits $0 \le \theta_2 \le \pi/2$ in θ_+, θ_- space.

	$\pi/3$	$\pi/2$	$2\pi/3$	π	2π	θ_1
$\pi/3$	89,90,99,100* $0 \le \theta_+ < 2\pi/3$ $0 \le \theta_- \le \pi/3$	85,86,95,96† $-\pi/3 \le \theta_+ \le \pi$ $0 \le \theta_- \le \pi/3$ $-\pi/3 \le \theta_+ \le \pi/2$ $0 \le \theta_- \le \pi/3$	87,88,97,98* $0 \le \theta_+ < 4\pi/3$ $0 \le \theta_- \le \pi/3$	83,84,93,94* $0 \le \theta_+ < 2\pi$ $0 \le \theta_- \le \pi/3$ $-\pi/3 \le \theta_+ \le \pi$ $0 \le \theta_- \le \pi/3$	81,82,91,92* $0 \le \theta_+ < 4\pi$ $0 \le \theta_- \le \pi/3$ $-\pi/3 \le \theta_+ \le 3\pi$ $0 \le \theta_- \le \pi/3$	
$\pi/2$	49,50,59,60† $0 \le \theta_+ \le 4\pi/3$ $0 \le \theta_- \le \pi/3$ $0 \le \theta_+ \le 5\pi/6$ $0 \le \theta_- \le \pi/3$	45,46,55,56* $0 \le \theta_+ < \pi$ $0 \le \theta_- \le \pi/2$	47,48,57,58† $-\pi/2 \le \theta_+ \le 4\pi/3$ $0 \le \theta_- \le \pi/2$ $0 \le \theta_+ \le 7\pi/6$ $0 \le \theta_- \le 2\pi/3$	43,44,53,54* $0 \le \theta_+ < 2\pi$ $0 \le \theta_- \le \pi/2$ $-\pi/2 \le \theta_+ \le \pi$ $0 \le \theta_- \le \pi/2$	41,42,51,52* $0 \le \theta_+ < 4\pi$ $0 \le \theta_- \le \pi/2$	
$2\pi/3$	69,70,79,80* $0 \le \theta_+ < 4\pi/3$ $0 \le \theta_- \le \pi/3$	65,66,75,76† $0 \le \theta_+ \le 11\pi/6$ $0 \le \theta_- \le \pi/2$ $0 \le \theta_+ \le 7\pi/6$ $-\pi/6 \le \theta_- \le \pi/2$	67,68,77,78*§ $0 \le \theta_+ < 4\pi/3$ $0 \le \theta_- \le 2\pi/3$	63,64,73,74† $-2\pi/3 \le \theta_+ \le 2\pi$ $0 \le \theta_- \le 2\pi/3$ $-2\pi/3 \le \theta_+ \le \pi$ $0 \le \theta_- \le 2\pi/3$	61,62,71,72* $0 \le \theta_+ < 4\pi$ $0 \le \theta_- \le 2\pi/3$ $-2\pi/3 \le \theta_+ \le \pi$ $0 \le \theta_- \le 2\pi/3$	
π	29,30,39,40* $0 \le \theta_+ < 2\pi$ $0 \le \theta_- \le \pi/3$ $0 \le \theta_+ \le 4\pi/3$ $0 \le \theta_- \le \pi/3$	25,26,35,36* $0 \le \theta_+ < 2\pi$ $0 \le \theta_- \le \pi/2$ $0 \le \theta_+ \le 3\pi/2$ $0 \le \theta_- < \pi/2$	27,28,37,38† $0 \le \theta_+ \le 8\pi/3$ $0 \le \theta_- \le 2\pi/3$ $0 \le \theta_+ \le 5\pi/3$ $0 \le \theta_- \le 2\pi/3$	23,24,33,34* $0 \le \theta_+ < 2\pi$ $0 \le \theta_- \le \pi$	21,22,31,32* $0 \le \theta_+ < 4\pi$ $0 \le \theta_- \le \pi$ $0 \le \theta_+ \le \pi$ $-\pi \le \theta_- \le \pi$	
2π	9,10,19,20* $0 \le \theta_+ < 4\pi$ $0 \le \theta_- \le \pi/3$ $0 \le 0_+ \le 4\pi/3$ $0 \le \theta_- \le \pi/3$	5,6,15,16* $0 \le \theta_+ < 4\pi$ $0 \le \theta_- \le \pi/2$ $0 \le \theta_+ \le 3\pi/2$ $0 \le \theta_- \le \pi/2$	7,8,17,18* $0 \le \theta_+ < 4\pi$ $0 \le \theta_- \le 2\pi/3$ $0 \le \theta_+ \le 5\pi/3$ $0 \le 0_- \le 2\pi/3$	3,4,13,14* $0 \le \theta_+ < 4\pi$ $0 \le \theta_- \le \pi$	1,2,11,12*§ $0 \le \theta_+ < 4\pi$ $0 \le \theta_- \le 2\pi$	
θ_3						

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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