

## The Symmetry of the Rotation Function

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### Abstract

The correlation of two Patterson functions whose relative orientation is expressed in Eulerian coordinates gives rise to the rotation function, which possesses space-group symmetry. If the  $z$  axis is the first and last axis of Eulerian rotation then the space group of the rotation function depends only on the parity of the Patterson symmetry axes parallel and perpendicular to  $z$ . Symmetry axes in other orientations do not produce space-group effects. Nine different cross-rotation space groups occur in 16 settings. Self-rotation gives rise to additional symmetry in the rotation function and results in a further four space groups. The symmetry of a rotation function parameterized in any other coordinate system may be studied by examining the symmetries of the functions occurring in the relevant rotation matrix.

### Introduction

The rotation function (Rossmann & Blow, 1962) has found widespread use in defining molecular orientations when multiple copies of the same or similar molecular fragments occur in different crystallographic environments in the same or different crystals. The interpretation of the rotation function in Eulerian angles often requires an understanding of the space-group symmetry of the rotation map. Tollin, Main & Rossmann (1966) showed how the general equivalent positions of a rotation-function space group could be derived from combinations of rotation point-group symmetry operations. Rao, Jih & Hartsuck (1980) automated this approach by employing a Fortran computer program to generate exhaustively the cross-rotation equivalent positions that could arise from Patterson functions of non-cubic symmetry.

The purpose of this paper is to give a more general discussion of rotation-function symmetry showing how it depends on the parity of the Patterson-function axes parallel and perpendicular to  $z$ . Self-rotation functions possess extra symmetry, which appears hitherto to have been ignored in the literature. A formal derivation of the space-group symmetry of the rotation function is best carried out using the methods of group theory, which are discussed in the Appendix.

### Origin of rotation-function symmetry

The space-group symmetry of the rotation function, when expressed in Eulerian angles, can arise from three possible causes.

(1) The two-to-one relationship between triplets of Eulerian angles  $[(\alpha, \beta, \gamma)$  and  $(\pi + \alpha, -\beta, \pi + \gamma)]$  and the same rotation gives rise to a plane of symmetry in the rotation function.

(2) The point-group symmetry of the Patterson functions involved in the rotation study gives rise to space-group symmetry provided that the functions are appropriately oriented with respect to the Eulerian axes.

(3) In the case of self-rotation, the identity between the two Patterson functions itself produces rotation-function symmetry.

In order to discuss these cases in more detail, a convention for the use of Eulerian angles must be carefully established. We choose that used by Crowther (1972) in his fast rotation function program. We consider a right-handed set of Cartesian axes  $x$ ,  $y$  and  $z$ . The Patterson density  $P(\mathbf{x})$  is rotated first through  $\gamma$  about the  $z$  axis, then through  $\beta$  about the  $y$  axis and then through  $\alpha$  about the  $z$  axis. Rotations about the stationary axes are clockwise as viewed from the origin. For visualizing the effect of a series of rotations it may be easier to consider the Patterson density as stationary. In this case the above rotation may be described as a rotation of the coordinate system counterclockwise first through  $\gamma$  about the  $z$  axis, then through  $\beta$  about the new  $y$  axis and finally through  $\alpha$  about the new  $z$  axis. The effect of the rotation on the coordinates of a point is determined by premultiplication by the matrix  $R$  where

$$R = \begin{bmatrix} \cos \alpha \cos \beta \cos \gamma & -\cos \alpha \cos \beta \sin \gamma & \cos \alpha \sin \beta \\ -\sin \alpha \sin \gamma & -\sin \alpha \cos \gamma & \\ \sin \alpha \cos \beta \cos \gamma & -\sin \alpha \cos \beta \sin \gamma & \sin \alpha \sin \beta \\ +\cos \alpha \sin \gamma & +\cos \alpha \cos \gamma & \\ -\sin \beta \cos \gamma & \sin \beta \sin \gamma & \cos \beta \end{bmatrix}. \quad (1)$$

The lengths of the unit-cell edges of the orthogonal Eulerian cell in the directions  $\alpha$ ,  $\beta$  and  $\gamma$  will be called  $a$ ,  $b$  and  $c$  respectively. Care should be taken not to confuse these unit-cell parameters with the cell dimensions of the Patterson functions.

The rotation function  $F(\alpha, \beta, \gamma)$  may be expressed by the integral

$$F(\alpha, \beta, \gamma) = \int P_0(\mathbf{x})P_1(R\mathbf{x}) dV,$$

where  $P_0$  and  $P_1$  will be referred to respectively as the stationary and rotated Patterson functions. The integration is usually performed over a spherical region of space centred on the origin. If  $P_0$  and  $P_1$  belong to proper point groups with symmetry elements expressed by matrices  $S^0$  and  $S^1$  then

$$\begin{aligned} F(\alpha, \beta, \gamma) &= \int P_0(S^0\mathbf{x})P_1(RS^1\mathbf{x}) dV \\ &= \int P_0(\mathbf{x})P_1([S^0]^T RS^1\mathbf{x}) dV. \end{aligned} \quad (2)$$

If we write

$$R(\alpha', \beta', \gamma') = (S^0)^T R(\alpha, \beta, \gamma) S^1 \quad (3)$$

then under certain circumstances  $(\alpha', \beta', \gamma')$  is related to  $(\alpha, \beta, \gamma)$  by a space-group operation. These circumstances are investigated in the Appendix where the important result is proved that only Patterson rotation axes parallel to the  $z$  axis and rotation axes of even order perpendicular to the  $z$  axis can give rise to rotation-function space-group symmetry.

In the space-group-symmetry derivations given below one of  $S^0$  or  $S^1$  will be set equal to the identity matrix  $I$ . The space-group symmetry elements produced in this way may be combined together to yield the symmetry generated from  $(S^0)^T RS^1$  by using the relationship

$$(S^0)^T RS^1 = (S^0)^T [IRS^1]I. \quad (4)$$

If both  $S^0$  and  $S^1$  are set equal to  $I$  then (3) is satisfied by two sets of Eulerian angles that give identical rotations.

$$R(\alpha, \beta, \gamma) = R(\pi + \alpha, -\beta, \pi + \gamma). \quad (5)$$

This may be verified by considering the rotations performed on the axes or by direct substitution of the angles into the matrix elements of  $R$ .

#### Symmetry elements in $P_0$ and $P_1$

Axes of symmetry parallel to  $z$  determine the magnitude of the Eulerian cell dimensions  $a$  and  $c$  and thus determine the nature of the plane of symmetry relating  $(\alpha, \beta, \gamma)$  to the general equivalent position  $(\pi + \alpha, -\beta, \pi + \gamma)$ . If a rotation axis is of order  $p$  then a positive rotation about  $z$  of  $2\pi/p$  is represented by the matrix

$$S(2\pi/p) = \begin{bmatrix} \cos 2\pi/p & -\sin 2\pi/p & 0 \\ \sin 2\pi/p & \cos 2\pi/p & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (6)$$

If function  $P_0$  has an axis of order  $p_0$  then by considering the rotations involved or by matrix multiplication

Table 1. *Rotation-function symmetry elements as a function of axial parity*

$p_0$  and  $p_1$  are the orders of the rotation axes parallel to  $z$  in the stationary and rotated functions respectively. The table indicates how the nature of the glide or mirror plane produced in the rotation function perpendicular to  $\mathbf{b}$  depends on the parities of  $p_0$  and  $p_1$ .

	$p_0 = 2n + 1$	$p_0 = 2n$
$p_1 = 2n + 1$	$\frac{n}{a}$	$\frac{c}{m}$
$p_1 = 2n$	$\frac{n}{a}$	$\frac{c}{m}$

we see that

$$R(\alpha - 2\pi/p_0, \beta, \gamma) = S_0^T(2\pi/p_0)R(\alpha, \beta, \gamma). \quad (7)$$

By putting  $S_1$  as the identity matrix in (2) and using (7) we see that

$$F(\alpha - 2\pi/p_0, \beta, \gamma) = F(\alpha, \beta, \gamma). \quad (8)$$

We deduce from this equation that an axis of order  $p_0$  parallel to  $z$  in the stationary function gives a rotation-function unit-cell dimension  $a = 2\pi/p_0$ . Similar reasoning from the equation

$$R(\alpha, \beta, \gamma + 2\pi/p_1) = R(\alpha, \beta, \gamma)S_1(2\pi/p_1) \quad (9)$$

shows that an axis of order  $p_1$  parallel to  $z$  in the rotated function gives rise to a cell dimension  $c = 2\pi/p_1$ .

The above arguments show that the dimensions of the rotation-function unit cell are  $(2\pi/p_0, 2\pi, 2\pi/p_1)$ . The general equivalent position  $(\pi + \alpha, -\beta, \pi + \beta)$  in (5) is related to  $(\alpha, \beta, \gamma)$  by symmetry that depends on the parity of  $p_0$  and  $p_1$ . For example, if  $p_0$  is even and  $p_1$  is odd then  $(\pi + \alpha, -\beta, \pi + \gamma)$  is congruent to  $(\alpha, -\beta, \pi/p_1 + \gamma)$  modulo  $(2\pi/p_0, 2\pi, 2\pi/p_1)$  and therefore represents a  $c$  glide plane perpendicular to  $\mathbf{b}$  and passing through the origin. The nature of the planes of symmetry arising from the four combinations of parity of  $p_0$  and  $p_1$  is shown in Table 1.

We now consider axes oriented perpendicular to  $z$ . The Appendix shows that only twofold axes in this position give rise to space-group symmetry. All axes of even order contain twofold axes as suboperators and therefore all axes of even order give rise to the same space-group effects when oriented perpendicular to  $z$ . Consider a twofold axis in the  $xy$  plane making an angle  $\varphi$  to the  $y$  axis, where  $\varphi$  is measured in a clockwise direction about  $z$ . The twofold rotation may be represented by the matrix

$$S(\varphi) = \begin{bmatrix} -\cos 2\varphi & -\sin 2\varphi & 0 \\ -\sin 2\varphi & \cos 2\varphi & 0 \\ 0 & 0 & -1 \end{bmatrix}. \quad (10)$$

The space-group effects produced by such a twofold axis in  $P_0$  or  $P_1$  may be seen from the following equations:

$$R(2\varphi - \alpha, \pi + \beta, \gamma) = S_0^T(\varphi)R(\alpha, \beta, \gamma) \quad (11)$$

$$R(\alpha, \pi + \beta, -2\varphi - \gamma) = R(\alpha, \beta, \gamma)S_1(\varphi). \quad (12)$$

Equation (11) shows that a twofold axis perpendicular to  $z$  in the stationary function gives rise to a  $b$  glide plane perpendicular to  $a$  and intersecting the  $a$  axis at  $\alpha = -\varphi$ . Similarly, (12) shows that a twofold axis perpendicular to  $z$  in the rotated function produces a  $b$  glide plane perpendicular to  $c$  and intersecting the  $c$  axis at  $\gamma = \varphi$ .

Thus the presence in  $P_0$  (or  $P_1$ ) of an axis of even order perpendicular to  $z$  gives rise to  $b$  glide planes perpendicular to  $a$  (or  $c$ ). The addition of these planes to the monoclinic space group determined by the parities of  $p_0$  and  $p_1$  yields an orthorhombic space group.

### Cross-rotation space groups

The arguments in the preceding section show how the nature and orientation of the planes of symmetry in the rotation function and the relevant cell dimensions may be derived from the nature of the rotation axes parallel and perpendicular to  $z$  in the Patterson functions. These symmetry elements combine together to yield nine possible cross-rotation-function space groups, which occur in 16 settings relative to the Eulerian axes as shown in the matrix in Table 2. Monoclinic space groups occur when no axis of even order is perpendicular to  $z$  in either Patterson function. When such axes do occur then orthorhombic symmetry results.

Many of the rotation space-group settings differ from the standard setting shown in *International Tables for Crystallography* (1983). The relevant origin may also be non-standard in the case of the orthorhombic space groups. The orientation of a twofold axis in a Patterson rotation group such that it is parallel to  $x$  (or  $y$ ) causes the origin to lie on the line of intersection of the glide plane perpendicular to  $b$  with the relevant  $b$  glide plane perpendicular to  $a$  (or  $c$ ).

The effect of interchanging the functions associated with  $P_0$  or  $P_1$  yields a rotation function defined by

$$F'(\alpha, \beta, \gamma) = \int P_0(R\mathbf{x})P_1(\mathbf{x}) dV \\ = \int P_0(\mathbf{x})P_1(R^T\mathbf{x}) dV. \quad (13)$$

Because a transposed matrix  $R^T$  corresponds to equal and opposite Eulerian rotations carried out in the reverse order we see that

$$R^T(\alpha, \beta, \gamma) = R(-\gamma, -\beta, -\alpha) \quad (14)$$

and thus

$$F'(\alpha, \beta, \gamma) = F(-\gamma, -\beta, -\alpha). \quad (15)$$

This shows that  $F$  and  $F'$  are related by a twofold rotation and accounts for the different settings of the same space group that occur in the transposed positions in Table 2.

Table 2. *Matrix of cross-rotation space groups as a function of axial parity*

$P_0$  is the stationary function and  $P_1$  is the rotated function. In the respective functions  $p_0$  and  $p_1$  are the orders of the axes parallel to  $z$  and  $q_0$  and  $q_1$  are the orders of the axes perpendicular to  $z$ . Cell dimensions are  $a = 2\pi/p_0$ ,  $b = 2\pi$ ,  $c = 2\pi/p_1$ . Numbers in parentheses are the space-group numbers in *International Tables for Crystallography* (1983).

		$q_0 = 2n+1$		$q_0 = 2n$	
		$p_0 = 2n+1$	$p_0 = 2n$	$p_0 = 2n+1$	$p_0 = 2n$
$P_1$	$p_1 = 2n+1$	$Pn$ (7)	$Pc$ (7)	$Pbn2_1$ (33)	$Pbc2_1$ (29)
	$p_1 = 2n$	$Pa$ (7)	$Pm$ (6)	$Pba2$ (32)	$Pbm2$ (28)
$q_1 = 2n+1$	$p_1 = 2n+1$	$P2_1nb$ (33)	$P2cb$ (32)	$Pbnb$ (56)	$Pbcb$ (54)
	$p_1 = 2n$	$P2_1ab$ (29)	$P2mb$ (28)	$Pbab$ (54)	$Pbmb$ (49)

### Self-rotation space groups

The self-rotation function is the auto-correlation of the Patterson function; the Patterson functions  $P_0$  and  $P_1$  are identical and have the same initial orientation. The rotation functions  $F$  and  $F'$  are therefore identical. From (15) we see that

$$F(\alpha, \beta, \gamma) = F(-\gamma, -\beta, -\alpha). \quad (16)$$

Physically interpreted this means that equal and opposite rotations carried out in the reverse order give rise to identical correlations. Self-rotation therefore introduces a new general equivalent position  $(-\gamma, -\beta, -\alpha)$  into the rotation space group, which corresponds to a twofold axis through the origin and parallel to  $[10\bar{1}]$ . Applying the symmetry operation indicated in (5) to this new position shows that  $(\pi - \gamma, \beta, \pi - \alpha)$  is also a new general equivalent position of the rotation-function space group. This corresponds to a diagonal mirror plane through  $(\pi, 0, 0)$  and perpendicular to  $[10\bar{1}]$ . Thus sections of constant  $\beta$  in self-rotation functions exhibit characteristic diagonal mirror lines.

The fact that self-rotation itself gives rise to extra symmetry does not seem to have been hitherto recognized in the literature. Several authors who have undertaken self-rotation studies have quoted one of the four space groups appropriate to the cross rotation of different functions of the same symmetry (Rossmann & Blow, 1962; Rossmann, Ford, Watson & Banaszak, 1972; Ammon, Murphy, Sjolín, Wlodawer, Holcenberg & Roberts, 1983). These cross-rotation space groups occur along the leading diagonal of the space-group matrix in Table 2. The correct self-rotation space groups are obtained by adding a diagonal mirror plane to these four groups. The resulting space group depends again on the parity of the axes parallel and perpendicular to  $z$ . The addition of diagonal mirrors to the two monoclinic space groups produces

Table 3. Matrix of self-rotation space groups as a function of axial parity

Rotation axes parallel and perpendicular to  $z$  have orders  $p$  and  $q$  respectively. The cell dimensions of the primitive cell are  $a = c = 2\pi/p$ ,  $b = 2\pi$ . The centred cells for the two space groups not based on a primitive lattice have unit-cell vectors  $\mathbf{a}' = \mathbf{a} - \mathbf{c}$ ,  $\mathbf{b}' = \mathbf{b}$  and  $\mathbf{c}' = \mathbf{a} + \mathbf{c}$ . Numbers in parentheses are the space-group numbers in *International Tables for Crystallography* (1983).

	$p = 2n + 1$	$p = 2n$
$q = 2n + 1$	$B'ma'2$ (39)	$B'mm2$ (38)
$q = 2n$	$P4_2/nbm$ (138)	$P4_2/mbm$ (132)

orthorhombic space groups based on a non-primitive lattice. The space-group unit cell is related to the primitive cell by the transformations

$$\begin{aligned} \mathbf{a}' &= \mathbf{a} - \mathbf{c} \\ \mathbf{b}' &= \mathbf{b} \\ \mathbf{c}' &= \mathbf{a} + \mathbf{c}. \end{aligned} \quad (17)$$

The addition of diagonal mirrors to the orthorhombic space groups produces tetragonal space groups based on a primitive Bravais lattice. The self-rotation space groups are displayed in Table 3.

#### Rotation conventions

The convention used in this paper regarding the application of Eulerian angles may be termed a  $zyz$  convention so as to indicate the order in which the new axes are chosen for successive rotations.

The earlier work on the rotation function (Rossmann & Blow, 1962) employed a  $zxz$  convention and rotation functions computed in this system will have the same space-group symmetry but a shift of origin in the  $\alpha\gamma$  plane relative to a calculation carried out using the order  $zyz$ .

A fundamentally different class of Eulerian conventions arises when the first and last axes of rotation differ. Such conventions have been widely employed in crystallography (Sussman, Holbrook, Church & Kim, 1977; Scheringer, 1963) but do not appear to have been used in the context of the rotation function. With these conventions the rotation-function space groups arise in different circumstances, which are described in the Appendix.

In this paper the two Patterson functions  $P_0$  and  $P_1$  have been called stationary and rotated respectively. This designation is consistent with Crowther & Dodson (1981) but consideration of (13), (14) and (15) shows that the arguments in this paper would remain unchanged if  $P_1$  were regarded as stationary and the Eulerian rotations were carried out on  $P_0$  in the order  $\alpha\beta\gamma$  and in a counterclockwise sense. Many authors (e.g. Rao *et al.*, 1980) view the operation of Crowther's (1972) program in this way and therefore

quote space groups in settings that occur in transposed positions in Table 2 relative to the settings appropriate to the  $P_0$  stationary convention.

#### Discussion

We may summarize the relationship between the Patterson-function rotation symmetry and the rotation-function space-group symmetry elements in the following statements where  $p_0$  and  $p_1$  are the orders of the axes parallel to  $z$  in the stationary and rotated functions respectively.

(1) The dimensions of the primitive Eulerian cell are  $a = 2\pi/p_0$ ,  $b = 2\pi$  and  $c = 2\pi/p_1$ .

(2) A plane of symmetry always exists perpendicular to  $\mathbf{b}$  and passes through the origin. The nature of this plane of symmetry depends on the parity of  $p_0$  and  $p_1$  in a way shown in Table 1.

(3) Axes of even order perpendicular to  $z$  in the stationary or rotated functions give rise to  $b$  glide planes perpendicular to  $\mathbf{a}$  or  $\mathbf{c}$  respectively. Such a glide plane only passes through the origin if the corresponding Patterson axis is parallel to  $y$ .

(4) Self-rotation introduces a diagonal mirror plane into the rotation function, which passes through the origin and is perpendicular to  $[101]$ .

The practical implication of these statements is that a Patterson rotation axis produces the most helpful rotation space-group symmetry when oriented parallel to  $z$ . In these circumstances it produces pure translational symmetry. When a Patterson symmetry axis is oriented perpendicular to  $z$ , space-group symmetry only results when the axis is of even order and in this case if the order is greater than two then only the twofold component produces space-group symmetry. The  $b$  glide plane produced by this orientation is less convenient than the translational symmetry produced by orientation of the symmetry axis along  $z$ . It must be clearly understood that the  $x$ ,  $y$  and  $z$  axes in this discussion are the Cartesian axes about which Eulerian rotation takes place and may not be parallel to the crystallographic axes having the same labels. This is especially true in the case of monoclinic Patterson functions where the unique crystallographic axis is usually chosen to be parallel to  $y$ .

The above discussion is also applicable when a Patterson function has axes of pseudosymmetry that may be either intermolecular or intramolecular. Such a pseudo-axis when oriented parallel to  $z$  will enable rotation-function peaks corresponding to the solution and the pseudo-solution to be viewed on the same  $\beta$  section where they will have the same Eulerian distortion.

Considerations other than symmetry may sometimes be relevant when deciding how to orient a Patterson function with respect to Eulerian axes. Rotation-function space is considerably distorted near the sections  $\beta = 0$  and  $\beta = \pi$  where the angles

$\alpha$  and  $\gamma$  are degenerate. The occurrence of peaks close to these sections may make interpretation inconvenient and in such cases reorienting a Patterson function may aid interpretation even if some Patterson symmetry no longer produces such useful effects.

When the rotation symmetry of a Patterson function belongs to a cyclic or dihedral point group then alignment parallel to  $z$  of the principal symmetry axis ensures that each axis gives rise to space-group symmetry in the rotation function. However, in the case of the cubic rotation groups 23 and 432, it is not possible to align the axes so that they are simultaneously all parallel or perpendicular to  $z$ . Hence, not all the symmetry axes will produce space-group effects in any given rotation function. For example, if a Patterson function of rotation group 432 is aligned with a fourfold axis parallel to  $z$  then only the 422 subgroup will be effective in producing rotation-function space-group symmetry. Each threefold axis will give rise to sets of three points within the asymmetric unit of the rotation function where the function is equal valued. This situation is analogous to the occurrence of non-crystallographic threefold axes in the crystal unit cell. In order that one of the threefold axes shall produce rotation-function symmetry the Patterson function must be oriented with a threefold axis parallel to  $z$ , in which case symmetry appropriate to point group 32 will result.

A similar problem exists when the Patterson function exhibits icosahedral symmetry 532 within the radius of integration. In this case the subgroups 52 or 3 produce rotation-function space-group effects according to whether a fivefold or threefold axis is parallel to  $z$ .

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## APPENDIX

The purpose of this Appendix is to give a group-theoretical description of the origin of rotation-function space-group symmetry and to establish the conditions under which symmetry elements in the Patterson function can produce space-group effects in the Eulerian rotation function.

The group of operations  $D$  that leaves the rotation function invariant is given by the direct product of the point groups  $Q_0$  and  $Q_1$  of the two Patterson functions.

$$D = Q_0 \times Q_1. \quad (A1)$$

As we are only concerned with proper rotations we may take  $Q_0$  and  $Q_1$  to be the relevant proper rotation groups. Each element of  $D$  consists of a pair of symmetry operations ( $S_0, S_1$ ) performed respectively

on each Patterson function. The group  $D$  is not a point group and is not, in general, isomorphic with a point group. For example, if the rotation point group of both Patterson functions is 3 then  $D$  is a non-cyclic group of order 9. No such non-cyclic point group exists. It should be noted that the group  $D$  is independent of both the relative initial orientation of the two Patterson functions and of the angular system used to express the relative rotations.

The parameterization of proper rotations in terms of a system of Eulerian angles (or spherical coordinates) gives rise to a rotation-function space group  $G$ , which is related to  $D$  by a homomorphic mapping  $f: G \rightarrow D$ . The nature of this homomorphism is described below and the condition for a Patterson symmetry element to give rise to symmetry elements in  $G$  is determined by finding the condition for an element of  $D$  to have a pre-image in  $G$ .

Let us denote space-group symmetry operations by  $(R|\tau_1, \tau_2, \tau_3)$  where  $R$  is a rotation and  $\tau_1, \tau_2$  and  $\tau_3$  are translations parallel to  $\mathbf{a}, \mathbf{b}$  and  $\mathbf{c}$  in Eulerian space. The group of operations  $H$  that leaves a rotation function invariant when applied to Eulerian angles is given by

$$H = \{E|2n_1\pi, 2n_2\pi, 2n_3\pi\} \\ + \{m|(2n_1+1)\pi, 2n_2\pi, (2n_3+1)\pi\}. \quad (A2)$$

$E$  represents the identity operation,  $m$  represents a reflection in a plane perpendicular to  $\mathbf{b}$  and  $n_1, n_2$  and  $n_3$  are any integers.  $H$  is the kernel of  $f$  and is an invariant subgroup of  $G$ . Each coset of  $G$  with respect to  $H$  has an image in  $D$  and the factor group  $G/H$  maps one-to-one into  $D$ .

In order to illustrate the above relationships, consider the rotation of an asymmetric function against a monoclinic Patterson with its twofold axis along  $z$ . In this case the group  $D$  has two elements ( $E, E$ ) and ( $E, 2$ ). The pre-image of ( $E, E$ ) is  $H$ . From (8) one pre-image of ( $E, 2$ ) is  $(E|\pi, 2\pi, 2\pi)$ . The coset  $C$  of pre-images is therefore

$$C = H(E|\pi, 2\pi, 2\pi) \\ = \{E|(2n_1+1)\pi, 2n_2\pi, 2n_3\pi\} \\ + \{m|2n_1\pi, 2n_2\pi, (2n_3+1)\pi\}. \quad (A3)$$

The rotation-function space group may be written as the sum of  $H$  and its cosets. In this example  $G = H + C$ , which yields the space group  $Pc$  with unit-cell lengths  $(\pi, 2\pi, 2\pi)$ . The factor group  $G/H$  consists of the two elements  $E$  and  $C$ . This factor group is isomorphic with  $D$  because all the Patterson-function symmetry is expressed as rotation space-group symmetry. In general this is not the case and we need to determine from matrix representations the conditions for an element of  $D$  to have a pre-image in  $G$ .

The nine elements of the rotation matrix  $R$  form the basis of a nine-dimensional matrix representation

{ $T$ } of  $D$ . With the direct-product notation (Falicov, 1966) the  $9 \times 9$  matrices are given by the direct products

$$T_{(ij)(jk)} = S_{(ji)}^0 S_{(kl)}^1 \quad (A4)$$

and (3) can be rewritten

$$R_{(il)}(\alpha', \beta', \gamma') = \sum_j \sum_k T_{(ij)(jk)} R_{(jk)}(\alpha, \beta, \gamma). \quad (A5)$$

We need to determine the subset of matrices  $\{U\} \subseteq \{T\}$  that are such that  $(\alpha', \beta', \gamma')$  is related to  $(\alpha, \beta, \gamma)$  by space-group symmetry. To find  $\{U\}$  we first note from (1) that the elements of  $R$  may be written in terms of three functions  $g$ ,  $h$  and  $k$  each possessing a different space-group symmetry,

$$R = \begin{bmatrix} g(\alpha, \beta, \gamma) & g(\alpha, \beta, \gamma + \pi/2) & h(\alpha, \beta) \\ g(\alpha - \pi/2, \beta, \gamma) & g(\alpha - \pi/2, \beta, \gamma + \pi/2) & h(\alpha - \pi/2, \beta) \\ h(\gamma, \beta) & h(\gamma + \pi/2, \beta) & k(\beta) \end{bmatrix}. \quad (A6)$$

Each matrix  $U$  must form a linear combination of elements of  $R(\alpha, \beta, \gamma)$  to yield a function that is of appropriate symmetry since space-group operations on  $(\alpha, \beta, \gamma)$  may rotate or translate the functions in the rotation matrix but cannot alter their symmetry with respect to  $(\alpha, \beta, \gamma)$ . In order to preserve symmetry a matrix  $U$  can only form linear combinations of those functions in  $R$  of the same symmetry. Hence matrices in  $\{U\}$  only form linear combinations of the first and second columns (or rows) of  $R$  and this implies that the matrices in  $\{S\}$  must possess the canonical form

$$S = \begin{bmatrix} a & b & 0 \\ c & d & 0 \\ 0 & 0 & e \end{bmatrix} \quad (A7)$$

and the orthogonality conditions require that  $ad - bc = e = \pm 1$ .

If  $e = +1$ ,  $S$  represents a rotation about  $z$  and if  $e = -1$  then  $S$  represents a twofold rotation perpendicular to  $z$ . Hence, only axes of symmetry parallel to  $z$  and twofold axes perpendicular to  $z$  give rise to rotation-function space-group symmetry when the definition of Eulerian angles leads to a rotation matrix of functional symmetry as shown in (A6).

The self-rotation symmetry may be treated by extending the above theory and the general result is that self-rotation introduces extra space-group symmetry when functions of the same symmetry occur in transposed positions in the matrix  $R$ . The above argu-

ments may also be used to investigate Eulerian systems where the first and third rotations are about different axes. In these cases the same rotation-function space groups arise but in different circumstances. In an  $xyz$  convention the canonical form of  $\{S^0\}$  is associated with  $z$  as in the  $zyz$  system but the canonical form of  $\{S^1\}$  implies rotational symmetry about  $x$  or a twofold axis perpendicular to  $x$ . Self-rotation does not introduce extra symmetry because the  $xyz$  convention prevents the Eulerian rotations being carried out in the reverse order. Instead the self-rotation space groups of Table 3 occur in the cross rotation of two identical Patterson functions that have initial orientations differing by a rotation of  $\pi/2$  about the  $y$  axis. Thus the conditions for symmetry in the rotation function are less simple when the first and last axes of Eulerian rotation are different and the conventional choice, where these axes are identical, represents the optimum Eulerian system for rotation-function studies.

The rotation function has been expressed in terms of spherical polar coordinates but inspection of the relevant rotation matrix (Rossmann & Blow, 1962) shows that no rows (or columns) have corresponding functions of the same symmetry. Such functions only occur in transposed positions, hence only self-rotation can introduce extra space-group symmetry in this coordinate system.

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