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Determination of Planar Group Orientation in Patterson Methods

BY C. C. WILSON

Neutron Division, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, England

AND P. TOLLIN

Carnegie Laboratory of Physics, University of Dundee, Dundee DD1 4HN, Scotland

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Abstract

An adaptation of the $I(\theta, \varphi)$ function for location of planar group orientation is presented. More accurate determination of this orientation is found to be possible in some cases using the modified functions, based on rings and hoops rather than disks in Patterson space. In some examples incorrect orientations are corrected by the new functions. A possible extension to the simultaneous detection of several small group orientations in one molecule, based on bond length selection, is discussed.

Introduction

The $I(\theta, \varphi)$ function was defined by Tollin & Cochran (1964). The philosophy of the function is to recognize that in a planar group the vectors between pairs of atoms in that group will all lie in one plane in Patterson space. By placing a disk of dimensions approximating to those of the planar group at the origin in Patterson space, one can rotate this disk in the two spherical polar coordinates θ and φ , the integral of the Patterson function over the disk being maximized when the disk is in the same orientation as the planar group.

The $I(\theta, \varphi)$ function is

$$I(\theta, \varphi) = \int_{\mathbf{r}} P(\mathbf{r})t(\mathbf{r}) d\mathbf{r} \quad (1)$$

where

$$t(\mathbf{r}) = \begin{cases} 1 & \text{on disk} \\ 0 & \text{elsewhere.} \end{cases}$$

One may use the facts that the transform of $P(\mathbf{r})$ is $|F(\mathbf{h})|^2$ and that of a disk is related to the first-order Bessel function $J_1(x)$ and exploit Parseval's theorem to evaluate this (apart from constant factors) as

$$I(\theta, \varphi) = \sum_{\mathbf{h}} |F_{\mathbf{h}}|^2 2\pi R^2 J_1(2\pi RS) / 2\pi RS \quad (2)$$

where S is the distance of the reciprocal-lattice point \mathbf{h} from the normal to the disk, R is the disk radius, and $J_1(x)$ is the first-order Bessel function. In practice the $|F_{\mathbf{h}}|^2$ values are replaced by sharpened structure factors $|F_{\mathbf{h}}^s|^2$ in the calculations.

Since its definition, this function has been found to locate the orientation of planar groups with accuracy in many cases. However, there are occasions when the located orientation is either very inaccurate or incorrect when $I(\theta, \varphi)$ is calculated.

Investigation of cases where these problems have arisen has suggested three possible contributing factors.

(1) Overemphasis of the contributions of some high-order [$\sin(\theta)/\lambda$] reflections, caused by the sharpening procedure applied to the $|F_{\mathbf{h}}|^2$.

(2) Possible asymmetry in the large origin peak in the Patterson function, especially in cases where the asymmetric unit is large and only a small portion is planar.

(3) When the orientation of the group is close to one of the extrema of the $I(\theta, \varphi)$ function (e.g. close to $\theta = 90^\circ$) an 'averaged' orientation of the group and a symmetry-related group may be found. For example in the TAA example (below) the correct θ value is $\sim 80^\circ$, but the $I(\theta, \varphi)$ indicates $\sim 90^\circ$ - in this orthorhombic example there is also a peak at $\theta \sim 100^\circ$, by symmetry. This ambiguity is caused by intergroup vectors.

The simplest way of dealing with factor (1) is to use data from a restricted range of $(\sin \theta)/\lambda$ as used in other Patterson-methods techniques (Wilson & Tollin, 1988), but in this case cutting off the outer [higher $(\sin \theta)/\lambda$] data. The use of $|E_{\mathbf{h}}|^2$ values does not in general eliminate oversharpening problems, as noted elsewhere (Wilson & Tollin, 1988). Problems can be encountered in trying to eliminate factor (2) by attempting to remove a particularly large and asymmetric origin peak from the Patterson function

by analytic means. This can be unreliable and lead to ambiguities, and often some residual contribution can be left which will confuse the later calculations.

A novel approach to improving the calculation of the $I(\theta, \varphi)$ function is suggested in this paper, where modifications have been made to the disk model used in the original $I(\theta, \varphi)$ function.

Modifying the disk model

The original $I(\theta, \varphi)$ function uses a disk as model, with defining equation

$$f(\mathbf{r}) = \begin{cases} 1 & |\mathbf{r}| < R \\ 0 & |\mathbf{r}| > R \end{cases} \quad (3)$$

with Fourier transform (Champeny, 1973)

$$F(\mathbf{k}) = 2\pi R^2 J_1(kR)/kR. \quad (4)$$

If we wish to exclude vectors of less than a particular length in the Patterson summation (akin to a very primitive origin removal plus additional terms), the function defined in (5) would suffice. This function is a 'top hat' function in one dimension, representing a 'ring' in Patterson space defined by

$$f(\mathbf{r}) = \begin{cases} 0 & |\mathbf{r}| < R_2 \\ 1 & R_2 < |\mathbf{r}| < R_1 \\ 0 & |\mathbf{r}| > R_1. \end{cases} \quad (5)$$

This function can be regarded as the difference of two functions of type (3), with radii R_1 and R_2 respectively, and for the combined function $f(\mathbf{r}) = f_1(\mathbf{r}) - f_2(\mathbf{r})$, the Fourier transform is simply the difference between the transforms of the individual functions,

$$F(\mathbf{k}) = 2\pi [R_1^2 J_1(kR_1)/kR_1 - R_2^2 J_1(kR_2)/kR_2]. \quad (6)$$

The expression (6) can be regarded as the Fourier transform of a Patterson-space ring of inner radius R_2 and outer radius R_1 .

From this it is obvious that we can define a 'ring $I(\theta, \varphi)$ ' function I_R as

$$I_R(\theta, \varphi) = \sum_{\mathbf{h}} |F_{\mathbf{h}}^s|^2 2\pi S [R_1^2 J_1(2\pi R_1 S)/2\pi R_1 S - R_2^2 J_1(2\pi R_2 S)/2\pi R_2 S]. \quad (7)$$

This is one of the functions investigated here.

As an alternative approach, one can define a 'hoop' in Patterson space at a particular radius R by the equation

$$f(\mathbf{r}) = (2\pi Ra)^{-1} [R < r < (R + a); a \ll R] \quad (8)$$

with Fourier transform (Champeny, 1973)

$$F(k) = J_0(kR). \quad (9)$$

Hence one can define the 'hoop $I(\theta, \varphi)$ ' function I_H

as

$$I_H(\theta, \varphi) = \sum_{\mathbf{h}} |F_{\mathbf{h}}^s|^2 J_0(2\pi RS). \quad (10)$$

This function is again investigated here.

As a final modification of the hoop $I(\theta, \varphi)$ function, one can convolute a Gaussian envelope onto the hoop in Patterson space, which by the properties of Fourier transforms implies multiplying by a Gaussian in reciprocal space. Hence the 'modulated' hoop $I(\theta, \varphi)$ function I_{HM} has the form

$$I_{HM}(\theta, \varphi) = \sum_{\mathbf{h}} |F_{\mathbf{h}}^s|^2 J_0(2\pi RS) \exp[-(2\pi S)^2/4a^2] \quad (11)$$

where the parameter a defines the amount of 'spreading out' of the hoop. In the cases examined here a was chosen to be $2-10 \text{ \AA}^{-1}$.

$I(\theta, \varphi)$ function tests

A series of tests was made on the following compounds, using each of the four functions $I(\theta, \varphi)$, $I_H(\theta, \varphi)$, $I_{HM}(\theta, \varphi)$ and $I_R(\theta, \varphi)$ as models for planar group orientation:

(A) 2',3',5'-Tri-*O*-acetyladenosine (TAA) (Wilson, Tollin & Howie, 1986). $C_{16}H_{19}N_5O_7$; planar fragment is C_5N_5 ($p^2 = 0.33$, $p_1^2 = 0.083$). Correct planar group orientation is $(\theta, \varphi) \sim (80^\circ, 16^\circ)$.

(B) 2',3',5'-Tri-*O*-acetylguanosine (TAG) (Wilson, Low & Tollin, 1985). $C_{16}H_{19}N_5O_8$; planar fragment is C_5N_5O ($p^2 = 0.36$, $p_1^2 = 0.18$). Correct planar group orientation is $(\theta, \varphi) \sim (54^\circ, 180^\circ)$.

(C) 3-Methylxanthine (MX) (Low, Tollin, Brand & Wilson, 1986). $C_5H_6N_4O_2$; planar fragment is $C_5N_4O_2$ ($p^2 = 0.89$, $p_1^2 = 0.22$). Correct planar group orientation is $(\theta, \varphi) \sim (56^\circ, 174^\circ)$.

(D) 2',3',5'-Tri-*O*-acetyluridine (TAU) (Low & Wilson, 1984). $C_{15}H_{18}N_2O_6$; planar fragment is $C_4N_2O_2$ ($p^2 = 0.29$, $p_1^2 = 0.073$). Correct planar group orientation is $(\theta, \varphi) \sim (54^\circ, 90^\circ)$.

(E) 3-Deazauracil (DAZA) (Low & Wilson, 1983). $C_5H_5NO_2$; planar fragment is C_5NO_2 ($p^2 = 0.95$, $p_1^2 = 0.24$). Correct planar group orientation is $(\theta, \varphi) \sim (43^\circ, 55^\circ)$.

The tests were carried out using a range of model radii for each compound. In the case of the ring function $I_R(\theta, \varphi)$, the inner ring radius is set to $(R - 0.1) \text{ \AA}$, the outer to $(R + 0.1) \text{ \AA}$. The results of the extensive $I(\theta, \varphi)$ function tests carried out are contained in Table 1. All calculations were carried out using the program *PATMET* (Wilson & Tollin, 1986), on the Neutron Division VAX 8600 at Rutherford Appleton Laboratory.

In an overall view of the results indicated in Table 1, the first impression is that the results from the modified $I(\theta, \varphi)$ functions are somewhat inconclusive. No single function seems to give unequivocally

Table 1. Results of tests of traditional and modified $I(\theta, \varphi)$ functions

Compound	Ranking of correct solution [deviation of solution from correct orientation (°)]				
	R	I	I_H	I_{HM}	I_R
TAA ($c = 8.42 \text{ \AA}$) ($80^\circ, 16^\circ$)	2.1	×	×	×	×
	2.4	×	1 (7)	1 (7)	×
	2.8	×	1 (3)	1 (3)	2 (6)
	4.1	×	×	×	1 (5)
	4.5	×	×	×	2 (2)
TAG ($a = 7.41 \text{ \AA}$) ($54^\circ, 180^\circ$)	2.4	1 (0)	(0)	1 (0)	1 (7)
	2.8	1 (0)	1 (0)	1 (0)	1 (6)
	4.1	1 (0)	1 (0)	1 (0)	1 (3)
	4.5	1 (0)	1 (0)	1 (0)	1 (3)
MX ($a = 3.74 \text{ \AA}$) ($56^\circ, 174^\circ$)	2.1	1 (6)	1 (8)	1 (7)	2 (4)
	2.4	1 (7)	1 (7)	1 (7)	1 (0)
	2.8	1 (4)	1 (3)	1 (3)	1 (0)
	3.2	1 (6)	×	×	1 (2)
	3.5	1 (3)	×	×	1 (0)
TAU ($a = 7.49 \text{ \AA}$) ($54^\circ, 90^\circ$)	1.4	×	×	×	×
	2.1	×	×	×	×
	2.4	×	1 (8)	1 (6)	×
	2.8	1 (8)	1 (4)	1 (0)	×
	3.2	1 (6)	1 (2)	1 (2)	×
	4.0	1 (0)	×	×	×
DAZA ($b = 5.28 \text{ \AA}$) ($43^\circ, 55^\circ$)	4.5	1 (2)	×	×	×
	1.4	1 (8)	1 (5)	1 (5)	1 (9)
	2.1	1 (6)	3 (5)	3 (5)	1 (8)
	2.4	1 (5)	3 (4)	3 (1)	1 (6)
	2.8	1 (2)	1 (2)	1 (2)	1 (2)
	3.2	1 (2)	1 (2)	1 (2)	1 (2)
4.0	1 (2)	×	×	1 (3)	
4.5	1 (2)	3 (5)	2 (4)	1 (2)	

better results than the others. There are, however, some general trends which seem to be reasonably well borne out by these results.

(i) The hoop $I_H(\theta, \varphi)$ and modulated hoop $I_{HM}(\theta, \varphi)$ functions give very similar results, and appear to work best at smaller R values.

(ii) The ring $I_R(\theta, \varphi)$ is better for larger R values, but in general is the least consistent of the functions. This may be a consequence of the fact that this function is a sum (difference) of two Bessel function terms and any rounding or 'ripple' errors will thus be magnified. Rather surprisingly, increasing the width of the annulus ($R \pm \Delta R$) where $\Delta R > 0.1 \text{ \AA}$ does not seem to alleviate the problems of the ring function. Again, this may be attributable to the difference nature of the calculation.

(iii) The disk function [the traditional $I(\theta, \varphi)$] seems to be the most consistent form of the calculation in these examples. This behaviour is of course in keeping with the fact that this function has been successful since its inception (Tollin & Cochran, 1964).

$I(\theta, \varphi)$ results and interatomic vectors

A further attempt to interpret the inconsistent results of the modified $I(\theta, \varphi)$ functions has been made in terms of interatomic vector density. Table 2 contains a list of approximate interatomic vectors in the planar

Table 2. Interatomic vector distributions for the five organic test structures, (A)–(E) (magnitudes in \AA)

(A) TAA	(B) TAG	(C) MX	(D) TAU	(E) DAZA
2.1 :10	2.4 :26	2.1 :10	1.4 :14	1.4 :16
2.4 :20	2.8 :6	2.4 :24	2.1 :2	2.1 :0
2.8 :6	4.1 :6	2.8 :6	2.4 :18	2.4 :20
4.1 :8	4.5 :8	3.2 :2	2.8 :6	2.8 :6
4.5 :6		3.5 :20	3.2 :0	3.2 :0
			4.0 :4	4.0 :4
			4.5 :2	4.5 :0

portion of each of these compounds, grouped around a set of average values. As can be seen from this table, the median density of interatomic vectors in compounds (A)–(E) tends to occur around 2.4 \AA , apart from bond vectors which of course pack around $\sim 1.4 \text{ \AA}$. In addition, in the purine compounds (A), (B) and (C) there is a relatively high density of vectors at around 4.1 \AA .

One would expect from these considerations that for the hoop and ring $I(\theta, \varphi)$ functions, 1.4 \AA would be a good radius to try (although this may be somewhat close to the origin peak if this is extensive), 2.4 \AA should perhaps be the optimum in all these structures and for the purine bases 4.1 \AA may also give good results.

Some of these indications do indeed seem to emerge in certain of the results, but disappointingly once again a clear pattern does not:

(i) TAA $I_H(\theta, \varphi)$ and $I_{HM}(\theta, \varphi)$ give the correct orientation at $R = 2.1, 2.4 \text{ \AA}$ but for none of the other radii attempted.

(ii) TAA $I_R(\theta, \varphi)$ is only correct at $R = 4.1 \text{ \AA}$.

(iii) MX $I_R(\theta, \varphi)$ fails for $R \leq 2.1 \text{ \AA}$ (correct for $R = 2.4 \text{ \AA}$).

(iv) TAU $I_H(\theta, \varphi)$ and $I_{HM}(\theta, \varphi)$ are correct for $R \geq 2.4 \text{ \AA}$, but fail for $R = 4.0 \text{ \AA}$.

There remain ambiguities where, although the correct solution is indicated in most of the calculations, these are often not the highest or even the second-highest peaks in the $I(\theta, \varphi)$ map. For example, the DAZA $I_H(\theta, \varphi)$ calculation with $R = 2.4 \text{ \AA}$ indicates the correct solution as the third-highest peak.

It should be noted that no significant improvement in these results is obtained when $|E_n|^2 - 1$ values are used as coefficients in the summation in place of $|F_n^s|^2$.

Discussion

While the results in the examples studied are somewhat inconsistent, the general impression is that the $I(\theta, \varphi)$ function can be calculated satisfactorily using a disk, hoop or ring rotating in Patterson space and that the reciprocal-space Bessel functions $J_1(x)/x$, $\Delta[J_1(x)/x]$ and $J_0(x)$ can all be used to locate coplanar interatomic vectors. There is no clear indication as to which of the functions is the best in all cases, there being examples when each of the models

seems to produce the best results. The original disk $I(\theta, \varphi)$ function of Tollin & Cochran (1964) would seem to be at least as good as the others studied here, on average. However, the analysis of radius of model against interatomic vector distribution does suggest one application which the original disk model would not encompass, which will now be outlined.

Finding the orientation of several groups in one molecule

In the examples studied above, the orientation of one dominant planar group was detected using the range of $I(\theta, \varphi)$ functions described. These examples were taken from small-molecule organic structures. In these, the range of bond lengths present in the molecule tends to be rather small, and the distribution of coplanar interatomic vectors tends to adopt a fairly familiar pattern (see Table 2). In these circumstances, whatever the choice of model radius, the $I(\theta, \varphi)$ function will tend to find the orientation of the largest planar fragment. If, however, one studied a molecule where two distinct planar groups had significantly different distributions of interatomic vectors, then some selectivity of plane location may be possible according to the choice of model radius. For example, in an octahedrally coordinated ligand configuration, if the axial bonds are 3.0 Å long but the equatorial are as short as 1.4 Å (Fig. 1), then the interatomic vector distributions corresponding to the two perpendicular planes (i) including two axial, two equatorial ligands and (ii) including four equatorial ligands, will be significantly different (Table 3). If one selected appropriate radii for the model (in this case either a hoop or ring in Patterson space) it might be possible to detect preferentially one or other of these planes. In this simple case, of course, and in other similar idealized examples such as tetrahedral or trigonal bipyramidal, it might be expected [and has been found using both simulated and real data (Wilson, unpublished)] that the major planar orientations would be found, with differing heights, in the traditional (disk) $I(\theta, \varphi)$ calculation. However, the

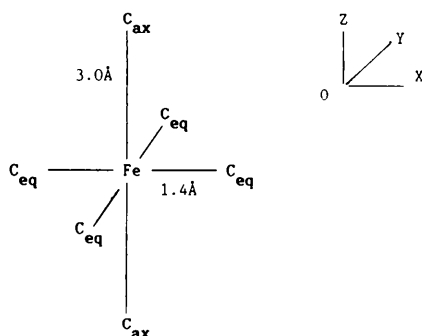


Fig. 1. Idealized octahedral structure used to simulate data for tests with disk and hoop functions. The interatomic vector distribution for this structure is given in Table 3.

Table 3. *Interatomic vector distributions, expected $I(\theta, \varphi)$ peaks and results for disk and modulated hoop $I(\theta, \varphi)$ ($a = 4 \text{ \AA}^{-1}$) calculations on ideal octahedral structure (simulated neutron data)*

Atoms	Vector distribution	Expected $I(\theta, \varphi)$ peak
1, 4, 5, 6, 7	$\begin{Bmatrix} 1.4:4 \\ 2.0:4 \\ 2.8:2 \end{Bmatrix}$	(0, 0)
1, 2, 3, 5, 6	$\begin{Bmatrix} 1.4:2 \\ 2.8:1 \\ 3.0:2 \\ 3.3:4 \end{Bmatrix}$	(90, 0)
1, 2, 3, 4, 7	$\begin{Bmatrix} 1.4:2 \\ 2.8:1 \\ 3.0:2 \\ 3.3:4 \end{Bmatrix}$	(90, 90)

From this one would expect $R = 1.4 \text{ \AA}$ to give a peak at (0, 0), $R = 3.2 \text{ \AA}$ to give a peak at (90, 0) and (90, 90), and $R = 2.0 \text{ \AA}$ to peak at (0, 0)

Results:

$R = 1.4 \text{ \AA}$ - Disk: 1st (0, 0) 99, 2nd (90, 90) 78, 3rd (90, 0) 36.

Hoop: 1st (0, 0) 99, 2nd (90, 90) 39, 3rd (90, 0) 32.

Both give correct answer but hoop is more clear cut

$R = 3.2 \text{ \AA}$ - Disk: 1st (0, 0) 99, 2nd (90, 90) 73, 3rd (90, 0) 36.

Hoop: 1st (90, 90) 99, 2nd (90, 0) 67, 3rd (0, 0) 38.

Disk is wrong, hoop selects the correct answer for $\sim 3 \text{ \AA}$ vectors

$R = 2.0 \text{ \AA}$ - Disk: 1st (0, 0) 99, 2nd (90, 90) 40, 3rd (90, 0) 19.

Hoop: 1st (0, 0) 99, 2nd (90, 90) 34, 3rd (90, 0) 11.

Again both correct but hoop more clear cut

extension to more complicated structures such as zeolite frameworks where the Si-O tetrahedra may be of interest would probably require the use of hoops or rings.

A calculation using simulated neutron data for the octahedral model shown in Fig. 1 has been performed using disk and modulated hoop models in the $I(\theta, \varphi)$ function. The results are summarized in Table 3, along with the expected planes for various sets of interatomic vectors present in the model. These results quite clearly indicate the improvements obtainable by the selective nature of the hoop function, where the $\sim 3 \text{ \AA}$ vectors lead to the enhancement of $\theta = 90^\circ$, $\varphi = 0^\circ, 90^\circ$ peaks in the hoop calculation, but the disk calculation gives (θ, φ) values of $(0^\circ, 0^\circ)$, being dominated by the 1.4, 2.1 Å vectors present in the overall system. In addition, the hoop function tends to have smaller secondary peaks than those calculated using the disk.

A further consideration in these calculations, possibly more relevant to possible applications of these functions to neutron data but also of interest in X-ray applications, is the necessity for optimal sharpening of structure-factor data by either analytical or maximum entropic (with implied 'smoothest' distribution) means. Examination of the effects of various sharpening schemes is under study (David & Wilson, work in progress) as part of the continuation of this work.

Concluding remarks

Modifications to the $I(\theta, \varphi)$ function for the location of planar group orientation exploiting hoops and

rings rather than disks have been examined and the results show that all three models can be utilized in determination of this orientation. However, no unambiguous indication of which is the best function to use emerges. This may indeed mean that all models used, which by their nature are gross approximations to the actual structure under study, suffer equally from this approximation, with local variations in particular calculations favouring one or the other. The reasonable results obtained using the 'selective' hoop and ring models in the simulated cases suggest that further pursuance of the location of several planar groups simultaneously and selectively (on bond lengths/interatomic vector distributions) may be fruitful and work is continuing on this possible development of the ideas advanced here.

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Full Tables of Colour Space Groups with Colour-Preserving Translations

BY J. N. KOTZEV AND D. A. ALEXandroVA

Faculty of Physics, Sofia University, 5 Anton Ivanov Blvd, Sofia BG-1126, Bulgaria

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Abstract

All 2571 permutational colour space groups $G^{(P)} \equiv T^{(1)}\hat{G}^{(P)}$ isostructural to the 230 space groups are tabulated and classified. The method for constructing these groups is described. The permutational representation $D_G^{H'}$ associated with each $G^{(P)}$ is given in order to make the physical applications easier. The group-theoretical criteria of the Landau theory have been checked in connection with the colour space-group application in phase transition analysis. Comparison with the results of other authors is given.

1. Introduction

The theory of crystallographic colour groups is a relatively new group-theoretical approach in the description of the structure and physical properties of crystals (see Shubnikov & Koptsik, 1974). Many problems of solid-state physics connected with the determination of the relationships between the symmetry group of the crystal, its subgroups, factor groups and their representations can effectively be solved using the colour-group theory and the corresponding tables of groups. The interpretation of the Landau theory of continuous phase transitions in terms of the permutational colour groups can be given as an example. It is based on the results of Koptsik & Kotzev (1974*a, b*), and Kotzev (1975) and is published in a series of papers (Kotzev, Litvin & Birman,

1982; Litvin, Kotzev & Birman, 1982; Kotzev, Koptsik & Rustamov, 1983).

A historical review of the colour-symmetry theory is given in the monograph of Shubnikov & Koptsik (1974) and the recent article by Schwarzenberger (1984). Therein a comprehensive list of the most important papers in this field (including the works of Heesch, Shubnikov, Belov, Wondratschek, van der Waerden & Burckhardt, Zamorzaev *etc.*) can be found. The most general theory covering all possible kinds of generalized (colour) groups was advanced by Koptsik & Kotzev (1974*a, b*) (see also Koptsik, 1975; Kotzev, 1975, 1980).

The groups to be discussed in the present paper are a special type of colour group, the *P*-type permutational colour groups, or 'colour groups' for short.

Unfortunately, the derivation and tabulation of all the colour groups is too complicated. The number of the colour *point* groups is finite and all these groups have been derived and published (*e.g.* Shubnikov & Koptsik, 1974; Koptsik & Kotzev, 1974*a*; Harker, 1976; Litvin, Kotzev & Birman, 1982). The colour *space* groups can be subdivided into two types: (i) groups with colour-preserving translation subgroup $T^{(1)}$ - their number is finite and all of them have been derived by Kotzev & Alexandrova (1986); and (ii) groups $T^{(n_1)}\hat{G}^{(n_2)}$ with colour translation subgroup $T^{(n_1)}$ containing a maximal colour-preserving one $T^{(1)}$ of index $n_1 \geq 2$. The list of these groups is finite for