numerators and respective denominators (terms can be considered as statistically independent). The correlation coefficient ρ has then been calculated for the test structures; it is shown in the last column of Table 2. It is seen that ρ_{10+13} is slightly better than ρ_{10} but the improvement is not really significant.

Concluding remarks

A probabilistic theory has been presented that is based on the representation of a given triplet phase by a family of special quintet phases. The information contained in the basis and in the cross terms of such quintets is used for estimating the triplet phase. The formulation is quite general and includes the well known P_{10} formula as a particular case. The final formula, called P_{13}, proved more efficient than the Cochran (1955) formula; in particular, it is able, as well as P_{10}, to recognize negative triplets. A strong correlation has been found between P_{10} and P_{13}, both from the theoretical point of view and in practical applications. The additional information exploited by P_{13} does not seem to be of sufficient quality for substantially improving the efficiency of P_{10} and, in addition, P_{13} is much more time consuming. Does this theory demonstrate the limits to which one can go with the embedding scheme? It is too early to conclude thus.

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Derivation of Wyckoff Positions of *N*-Dimensional Space Groups. Theoretical Considerations

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Abstract

An algorithm to calculate Wyckoff positions of n-dimensional space groups is developed and a detailed theoretical background is supplied. The algorithm is based on concepts of symmetry support and of translational normalizer

1. Introduction

It has become attractive to view quasicrystals as objects whose structure can be derived from a higher-dimensional crystal. This approach is based on the fact that the bright spots occurring in a diffraction pattern of a quasicrystal can be indexed by a finite number n, $n > 3$, of integers and that the positions and intensities of Bragg peaks display a point symmetry forbidden in three-dimensional crystals. The corresponding Z-module of rank n, sometimes called Fourier module (Janssen, 1991) of the related density function, can be interpreted as the reciprocal lattice of a certain n-dimensional lattice T, invariant under the symmetry group L of the diffraction pattern, where L is a representative of some Laue class. Usually, from L and from the statistical distribution of intensities, one is able to derive the point symmetry G. The n-dimensional lattice T together with the point group G define an arithmetic class (G, T) of n-dimensional space groups. Within such an arithmetic class, one will find the possible candidates that can be used for building up a structure model of the quasicrystal in question. The problem is that, up to now, there has been no generally accepted systematic description of positions of atoms in quasicrystals, which, in the case of crystals, is provided by the Wyckoff positions. Since there exists a relationship between crystal structures in n dimensions and quasicrystals, Wyckoff positions of n-dimensional space groups are of interest.

In three dimensions, the Wyckoff positions of space groups were originally derived by P. Niggli (1919). Later, they were redetermined by R. W. G. Wyckoff (1922). They are given in *International Tables for Crystallography* (1983) (hereafter *IT*, 1983) in a standard form.

In this paper, we present an algorithm to derive Wyckoff positions of an n-dimensional space group $\mathcal{G}$. The algorithm consists of the following three steps:

In the first step, we calculate all finite cyclic subgroups of a given space group $\mathcal{G}$ that leave fixed some point of a chosen elementary parallelepiped, defined by n generating vectors of the lattice of $\mathcal{G}$. In the second step, these cyclic subgroups are used for generating the non-trivial stabilizers of all points within the elementary parallelepiped. In the third step, equivalence classes of these stabilizers under $\mathcal{G}$ are determined. Each of these equivalence classes yields one Wyckoff position of $\mathcal{G}$.

The first step is the most involved and is dealt with in §§ 2, 3 and 4. In §§ 2 and 3, the concepts of symmetry supports and translational normalizers are employed to give lemmas to be used in deriving the required cyclic subgroups. These lemmas are used in § 4 to provide a method to determine all finite cyclic subgroups of $\mathcal{G}$ having a chosen cyclic point group C. An algorithm to derive Wyckoff positions of $\mathcal{G}$ is given in § 5.

The present algorithm has been implemented in a computer program which is available on request from the authors.

2. Symmetry supports and projection operators

We will consider an n-dimensional space group $\mathcal{G}$ and a point group G isomorphic to the factor group $\mathcal{G}/T$, where T is the translational subgroup (lattice) of $\mathcal{G}$. We denote by O the origin of the n-dimensional Euclidean space E_n and by V_n the difference space of E_n, *i.e.* the vector space associated with E_n, where each vector $v \in V_n$ represents one class of ordered pairs of points, $\{[x, y];\ y = v + x\}$. Accordingly, one can put $E_n \equiv x + V_n$ for an arbitrary point $x \in E_n$. Similarly, any manifold M of E_n can be written as $z + V$, where the point $z \in M$ can be chosen quite arbitrarily and V is the difference space of the manifold M. A 'Wyckoff position' is defined as the set of all points that have equivalent stabilizers under the space group $\mathcal{G}$.

In order to determine the Wyckoff positions of $\mathcal{G}$, the concept of symmetry support is employed:

Let $\mathcal{F}$ be a subgroup of $\mathcal{G}$. The manifold of E_n that is left fixed by $\mathcal{F}$ is called the symmetry support of $\mathcal{F}$ (Engel, 1986) and will be denoted as $\mathrm{Supp}\,(\mathcal{F})$. If $\mathcal{F}$ contains non-zero translations then its symmetry support is empty. If not, $\mathcal{F}$ is of finite order and it must fix at least one point of E_n. Furthermore, it is clear that the symmetry support of the trivial group $\mathcal{C}_1$, which consists of the identity alone, is the whole space E_n, *i.e.* $\mathrm{Supp}\,(\mathcal{C}_1) = E_n$. We note that a finite subgroup of $\mathcal{G}$ is uniquely determined by its point group and its symmetry support.

Given two subgroups, $\mathcal{F}_1$ and $\mathcal{F}_2$, of $\mathcal{G}$, one has

$$\mathcal{F}_1 \subseteq \mathcal{F}_2 \Rightarrow \mathrm{Supp}\,(\mathcal{F}_1) \supseteq \mathrm{Supp}\,(\mathcal{F}_2). \qquad (1)$$

It follows directly that

$$\mathrm{Supp}\,(\mathcal{F}_1 \cup \mathcal{F}_2) = \mathrm{Supp}\,(\mathcal{F}_1) \cap \mathrm{Supp}\,(\mathcal{F}_2), \qquad (2)$$

where $\mathcal{F}_1 \cup \mathcal{F}_2$ is to be understood as a group formed by all possible products of a finite number of elements belonging either to $\mathcal{F}_1$ or to $\mathcal{F}_2$. We note that if $\mathcal{F}_1$ and $\mathcal{F}_2$ are finite subgroups of $\mathcal{G}$ and if $\mathrm{Supp}\,(\mathcal{F}_1) \cap \mathrm{Supp}\,(\mathcal{F}_2) = \emptyset$ then the group $\mathcal{F}_1 \cup \mathcal{F}_2$ cannot be a finite subgroup of $\mathcal{G}$ and so $\mathcal{F}_1 \cup \mathcal{F}_2$ must contain some non-zero translation belonging to T. We note that Weigel, Veysseyre, Phan, Effantin & Billiet (1984) give the geometrical supports of the point-group operations.

In order to determine the Wyckoff positions of a space group $\mathcal{G}$, one has to know the stabilizers of all points in E_n. Owing to the translational symmetry, however, it is sufficient to compute the stabilizers of those points lying within some characteristic cell associated with the lattice T, such as the Voronoï domain (the Wigner–Seitz cell) $\Omega(0)$ of the origin O or, alternatively, the closed parallelepiped $\Theta(0)$ spanned by the n vectors chosen as the lattice basis of T and placed so that its centre coincides with the origin O. We prefer the latter possibility. Our algorithm to find the stabilizers of all points within $\Theta(0)$ is based on the well known basic fact that every finite group can be generated by its cyclic subgroups. A cyclic group is any group in which there exists an element such that all other group elements are powers of it.

The basic idea to determine the stabilizer of a given point $x \in \Theta(0)$ is the following: There is always at least one cyclic subgroup of $\mathcal{G}$, say $\mathcal{C}^1$, that fixes the point x, though it may consist only of the identity. If another cyclic group $\mathcal{C}^2 \subseteq \mathcal{G}$ leaves the point x fixed and is not a subgroup of $\mathcal{C}^1$, then the group $\mathcal{C}^1 \cup \mathcal{C}^2$ is a proper supergroup of $\mathcal{C}^1$ which, according to (2), must fix x too. Taking $\mathcal{C}^1 \cup \mathcal{C}^2$ instead of $\mathcal{C}^1$, one can look for a cyclic group $\mathcal{C}^3 \subseteq \mathcal{G}$ that will now play the role of

$\mathcal{C}^2$ in the preceding step. Proceeding in such a way, one successively generates an ascending chain (3) of finite groups fixing the point x.

$$\mathcal{C}^1 \subset \mathcal{C}^1 \cup \mathcal{C}^2 \subset (\mathcal{C}^1 \cup \mathcal{C}^2) \cup \mathcal{C}^3 \subset \dots \quad (3)$$

This chain is finite since every finite subgroup $\mathcal{F}$ of $\mathcal{G}$ is isomorphic to some subgroup of the point group G. The last group in the chain is the stabilizer of x and its symmetry support is the intersection of the symmetry supports of the distinct cyclic groups occurring in this chain.

We note that, given an arbitrary set $\{g_1, ..., g_s\}$, $s \geq 1$, of generating elements of a finite group, one can always construct an ascending chain analogous to (3) using the cyclic groups $C^1, ..., C^i, ..., C^s$, where C^i consists of all powers of the ith generator. In Appendix 2, we give an algorithm to determine consecutively all elements of $C^1 \cup C^2$, $(C^1 \cup C^2) \cup C^3$ *etc.* and finally all elements of the finite group.

The cyclic subgroups of $\mathcal{G}$ and their symmetry supports can conveniently be determined by the use of two linear operators, defined for each cyclic subgroup of the point group G. Consider an element g of the point group G and denote its order by m. This element generates a cyclic subgroup of G that has just m elements: $I \equiv g^0 = g^m, g, g^2, ..., g^{m-1}$; we denote it by C_m. We introduce the following linear operators which map the lattice T homomorphically into itself.

$$\overline{P} = I + g + g^2 + \dots + g^{m-1} \quad (4)$$
$$\overline{Q} = I - g. \quad (5)$$

The operators, $\overline{P}$ and $\overline{Q}$, belong to the commutative group ring associated with C_m and define an orthogonal splitting of V_n into a sum of two subspaces invariant under the action of C_m (see Appendix 1). Accordingly, one can write

$$V_n = V^0 + V^1 \quad (6)$$

where (*cf.* lemma $A1.1$) we put

$$V^0 \equiv \operatorname{Im} \overline{P} = \operatorname{Ker} \overline{Q}, \quad V^1 \equiv \operatorname{Ker} \overline{P} = \operatorname{Im} \overline{Q}.$$

One defines kernel $\operatorname{Ker} \overline{P} \equiv \{t \in V_n; \overline{P}t = 0\}$ and image $\operatorname{Im} \overline{P} \equiv \{\overline{P}t; t \in V_n\}$. The vector space V^0 is the greatest subspace of V_n on which the group C_m acts in a trivial manner; the superscript 0 is used to indicate the trivial action. The other space, V^1, is the orthogonal complement of V^0 in V_n. For example, if g is a fourfold rotation in three dimensions, then the space V^0 is one-dimensional and parallel to the direction of the rotational axis, while the space V^1 is two-dimensional and perpendicular to the rotational axis.

We note that V^0 is a difference space of the symmetry support of each such finite cyclic subgroup of $\mathcal{G}$, if any, that has C_m as its point group.

We define the projection operator $P : V_n \longrightarrow V^0$ as follows:

$$P = (1/m)\overline{P}. \quad (7)$$

The projection operator $I - P : V_n \longrightarrow V^1$, which is complementary to P, can be expressed as a product of two linear operators, $\overline{Q}$ and $\overline{\overline{Q}}$:

$$I - P = \overline{Q} \cdot \overline{\overline{Q}}, \quad (8)$$

where $\overline{\overline{Q}}$ is given by

$$\overline{\overline{Q}} = \begin{cases} I & g = I \\ (1/m)[I + (I+g) + (I+g+g^2) + \dots \\ \quad + (I + g + g^2 + \dots + g^{m-2})] & g \neq I. \end{cases} \quad (9)$$

We note that for $g \equiv I$ one has $I - P = \overline{Q} = 0$ so that $\overline{\overline{Q}}$ can be any linear operator on V_n; in this case, we choose $\overline{\overline{Q}}$ to be the identity operator.

The linear operator $\overline{\overline{Q}} : V_n \longrightarrow V_n$ leaves both subspaces, V^0 and V^1, invariant. The action of this operator on V_n is faithful (*cf.* lemma $A1.2$), *i.e.* for every $v \in V_n$, there is just one vector $w \in V_n$ such that $v = \overline{\overline{Q}}w$.

Consider the three-dimensional fourfold rotation along the z axis, *i.e.*

$$g = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

A straightforward computation yields the projection operators

$$P = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad I - P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Applying the projection operators to an arbitrary vector $v = (v_x, v_y, v_z) \in V_3$, one determines the subspaces V^0 and V^1. One has $Pv = (0, 0, v_z)$ and $(I - P)v = (v_x, v_y, 0)$. Using the definitions (5) and (9), one finds

$$\overline{Q} = \begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \overline{\overline{Q}} = \frac{1}{2}\begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 3 \end{pmatrix}.$$

The following statement, which is implied by the decomposition of the projection operator $I - P$, proves to be useful (*cf.* § 4) for determining the origin of the symmetry support of a finite cyclic subgroup of $\mathcal{G}$.

Lemma 2.1

For every $t \in V^1$, there exists a vector $\tau \in V^1$ such that $t = \overline{Q}\,\tau$. It holds that $\tau = \overline{\overline{Q}}\,t$.

By assumption, $Pt = 0$ and hence $(I - P)t = t$. The statement then directly follows from (8) and from the invariance of V^1 under C_m.

3. Projections of the translational group T and translational normalizer

The projection operator P also provides valuable information on some properties of the translational subgroup T. Such information (to be given below) will play a central role in determining whether $\mathcal{G}$ contains a finite cyclic subgroup with the point group C_m or not.

The application of the projection operators P and $I - P$ to T yields the translational groups T^0 and T^1, respectively. Intersecting T with T^0 and T^1, one obtains two subgroups, T_0 and T_1, respectively. The groups T^0 and T^1 as well as T_0 and T_1 have only the zero translation in common and it holds that $T_0 + T_1 \subseteq T \subseteq T^0 + T^1$. If one of the two inclusions turns out to be an equality then T^0 coincides with T_0, T^1 with T_1 and T is the direct sum of T_0 and T_1. In the general case, however, T is only a subdirect product of T^0 and T^1 and the following three factor groups are mutually isomorphic (Hall, 1959):

$$T/(T_0 + T_1) \simeq T^0/T_0 \simeq T^1/T_1. \qquad (10)$$

By lemma A1.3, both $T_0 + T_1$ and $T^0 + T^1$ are n-dimensional lattices. Consequently, all factor groups in (10) are finite.

A subgroup $\overline{T} \subseteq T$ is a direct summand of T if the factor group $T/\overline{T}$ is torsion free, *i.e.* no element of $T/\overline{T}$ is of finite order. This condition implies that there exists at least one subgroup $\overline{\overline{T}} \subseteq T$ such that $\overline{T} \cap \overline{\overline{T}} = \{0\}$ and $T = \overline{T} + \overline{\overline{T}}$. We remark that even if $T \neq T_0 + T_1$, T_0 as well as T_1 is a direct summand of T. However, direct summands $\overline{T}_1$ and $\overline{T}_0$ of T such that $T_0 \cap \overline{T}_1 = \overline{T}_0 \cap T_1 = \{0\}$ and $T_0 + \overline{T}_1 = \overline{T}_0 + T_1 = T$ are not invariant under C_m. An algorithm to determine generating vectors of T_0 and T_1 is described in Appendix 3.

Writing the coset decomposition of $T \bmod (T_0 + T_1)$ as

$$T = \bigcup_{j=0}^{r} t_j + (T_0 + T_1) \qquad (11)$$

and expressing each representative vector t_j as the sum of its components in V^0 and V^1, *i.e.* $t_j = t_j^0 + t_j^1$, one directly obtains the coset decompositions $T^0 \bmod T_0$ and $T^1 \bmod T_1$:

$$T^0 = \bigcup_{j=0}^{r} t_j^0 + T_0, \quad T^1 = \bigcup_{j=0}^{r} t_j^1 + T_1. \qquad (12)$$

One comes to the following conclusion where, for typographical brevity, we denote the components of a vector $v \in V_n$ in the subspaces V^0 and V^1 by $v^0 \equiv P\,v$ and $v^1 \equiv (I - P)\,v$, respectively, so that $v = v^0 + v^1$.

Conclusion 3.1

Given $v_1, v_2 \in T$, then

$$v_1^0 - v_2^0 \in T_0 \Leftrightarrow v_1^1 - v_2^1 \in T_1 \Leftrightarrow v_1 \in v_2 + (T_0 + T_1).$$

The translational normalizer of the space group $\mathcal{G}$ is defined to consist of all those vectors $v \in V_n$ that fulfil the condition $(I - g)v \in T$ for each $g \in G$. Since the translational normalizer is determined completely by the point group G and the translational group T, we denote it as $\mathrm{Trn}\,(G, T)$. It follows from this definition that the action of any vector of $\mathrm{Trn}\,(G,T)$ on $\mathcal{G}$ (the action being that of conjugation) will transform $\mathcal{G}$ into itself, *i.e.* $\{I|v\}\{g|u\}\{I|-v\} \in \mathcal{G}$ for any $v \in \mathrm{Trn}\,(G,T)$ and any $\{g|u\} \in \mathcal{G}$. Consequently, the translational normalizer $\mathrm{Trn}\,(G,T)$ is the translational subgroup of both the Euclidean and affine normalizers of the space group $\mathcal{G}$, and also of any other space group having the point group G and translational subgroup T. The definition of translational normalizers together with further detailed information can be found in Kopský (1993).

In the case where $G \equiv C_m$, one has $(I - g)v \in \mathrm{Im}\,\overline{Q} \equiv V^1$ and $\mathrm{Ker}\,\overline{Q} \equiv V^0 \subseteq \mathrm{Trn}\,(C_m, T)$. In order to determine the translational normalizer, one has to find only those vectors $v \in V^1$ for which $(I - g)v \equiv t_1 \in T_1$. From lemma 2.1, $v = \overline{\overline{Q}}t_1$ so that all such vectors belong to the translational group $\overline{\overline{Q}}\,T_1$. It follows that:

Lemma 3.2

The translational normalizer $\mathrm{Trn}\,(C_m, T)$ is the direct sum of the vector space V^0 (viewed as an additive Abelian group) and the translational group $\overline{\overline{Q}}\,T_1$, *i.e.*

$$\mathrm{Trn}\,(C_m, T) = \overline{\overline{Q}}\,T_1 + V^0. \qquad (13)$$

For the discrete part $\overline{\overline{Q}}\,T_1$ of $\mathrm{Trn}\,(C_m, T)$, one has $\overline{\overline{Q}}\,T_1 \supseteq T^1 \supseteq T_1$.

For the reader's convenience, the group–subgroup relationships between the translational groups occurring above are presented in a diagramatic form (see Fig. 1).

A subgroup $\mathcal{G}'$ of a space group $\mathcal{G}$ is called an equitranslational subgroup (t subgroup) if it contains the entire translational subgroup T of $\mathcal{G}$. $\mathcal{G}' \subseteq \mathcal{G}$ is an equiclass subgroup (k subgroup) of $\mathcal{G}$ if the factor groups $\mathcal{G}/T$ and $\mathcal{G}'/T'$, where $T' \equiv \mathcal{G}' \cap T$, are mutually isomorphic. By Hermann's well known theorem on subgroups of space groups (Hermann, 1929), every subgroup of $\mathcal{G}$, either finite or infinite, that has a point group C_m is contained in an equitranslational subgroup of $\mathcal{G}$, say $\mathcal{H}$, that is an equiclass supergroup of that subgroup. By definition, $\mathrm{Trn}\,(C_m, T)$ is a translational normalizer of $\mathcal{H}$ so that any vector $\tau \in \mathrm{Trn}\,(C_m, T)$ transforms $\mathcal{H}$ into itself.

Assume that $\mathcal{G}$ contains a finite subgroup $\mathcal{C}_m$ that is simultaneously an equiclass subgroup of $\mathcal{H}$. The very sense of the decomposition (13) consists in the following: Owing to the trivial action of C_m on V^0, any vector $\tau_0 \in V^0$ transforms $\mathcal{C}_m$ into itself. Any other vector $\tau' \in \mathrm{Trn}\,(C_m, T)$, when applied to $\mathcal{C}_m$, yields another finite equiclass subgroup of $\mathcal{H}$. This implies that there are just as many distinct finite equiclass subgroups of $\mathcal{H}$ as there are vectors in the discrete part of $\mathrm{Trn}\,(C_m, T)$. We shall see that this statement is a direct consequence of an equation to be satisfied by the generating symmetry operation of $\mathcal{C}_m$.

4. Finite cyclic subgroups of $\mathcal{G}$

It is known that all elements of an arbitrary finite subgroup of $\mathcal{G}$ belong to distinct cosets in the coset decomposition

$$\mathcal{G} = \{I|0\}T + \{g_2|u_2\}T + \ldots + \{g_i|u_i\}T + \ldots + \{g_p|u_p\}T, \tag{14}$$

where p is the order of the point group G. Therefore, in order to find the finite cyclic subgroups of $\mathcal{G}$, one has to determine those cosets in (14) that contain symmetry operations of finite order. It is sufficient, however, to check only those cosets $\{g_{i_j}|u_{i_j}\}T$ for which the rotational parts g_{i_j} generate distinct cyclic subgroups of G.

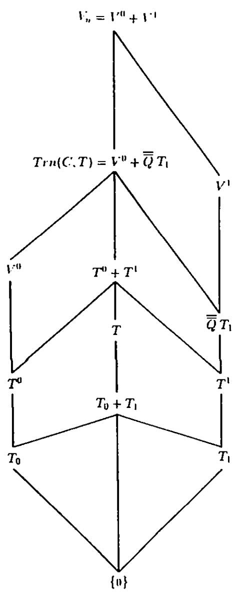

Fig. 1. Group–subgroup relationships between translational groups T and $\overline{\overline{Q}}T_1$.

The only element of finite order in the coset $\{I|0\}T$ is $\{I|0\}$, which forms the trivial cyclic group $\mathcal{C}_1$. The group $\mathcal{C}_1$ corresponds to the Wyckoff position of lowest symmetry.

A method to establish the occurrence of an element of finite order in the other cosets in (14) is as follows:

Let us consider the ith coset $\{g_i|u_i\}\,T$, $i \geq 2$. In this coset, there will be a symmetry operation of finite order if a translation $t \in T$ can be chosen such that

$$\{g_i|u_i + t\}^{m_i} = \{I|0\}, \tag{15}$$

where m_i is the order of the cyclic subgroup C_{m_i} of G generated by the rotational part g_i. With $\overline{P}_i \equiv I + g_i + g_i^2 + \ldots + g_i^{m_i - 1}$, the condition (15) can be rewritten as

$$\overline{P}_i\,(u_i + t) = 0. \tag{16}$$

According to the preceding section, the operators $\overline{P}_i$ and $\overline{Q}_i \equiv (I - g_i)$ define an orthogonal splitting of V_n into a sum of two complementary subspaces $V^1 \equiv \mathrm{Ker}\,\overline{P}_i = \mathrm{Im}\,\overline{Q}_i$ and $V^0 \equiv \mathrm{Im}\,\overline{P}_i = \mathrm{Ker}\,\overline{Q}_i$, where the corresponding projection operators are $P_i \equiv \frac{1}{m_i}\overline{P}_i$ and $I - P_i$, respectively. It holds that any translation of T must occur in one of finitely many cosets of the coset decomposition $T \bmod (T_0 + T_1)$:

$$T = \bigcup_{j=0}^{r_i} t_j + (T_0 + T_1). \tag{$\overline{11}$}$$

We state:

Lemma 4.1

The coset $\{g_i|u_i\}T$ contains a symmetry operation of finite order only if there is a coset $t_{j_1} + (T_0 + T_1)$ for which the following condition holds:

$$P_i(u_i + t_{j_1}) \in T_0. \tag{17}$$

If such a coset exists, it is unique.

The proof is straightforward: one can replace $\overline{P}_i$ in (16) with the projection operator P_i and $t \in t_{j_1} + (T_0 + T_1)$ for some j_1.

The uniqueness of the coset $t_{j_1} + (T_0 + T_1)$ to which all solutions of (16) belong follows from conclusion 3.1.

Suppose that we find a coset $t_{j_1} + (T_0 + T_1)$ for which (17) is true, *i.e.* $t_0 \equiv P_i\,(u_i + t_{j_1}) \in T_0$. Then, $t = t_{j_1} - t_0$ is a solution of (16) and $\{g_i|u_i + t\}$ generates a finite subgroup of $\mathcal{G}$. According to lemma 2.1, there exists a vector $\xi_i \in V^1$ such that $u_i + t = (I - g_i)\xi_i \equiv$

$\overline{Q}_i \xi_i$. One has

$$\xi_i = \overline{\overline{Q}}_i (u_i + t), \quad (18)$$

where the operator $\overline{\overline{Q}}_i$ is defined analogously to (9). Hence, we conclude that the element $\{g_i|u_i + t\}$ generates a cyclic group $\mathcal{C}_{m_i}$ of order m_i which leaves a point $x_i \equiv O + \xi_i$ of E_n fixed. Moreover, taking into account that the subspace of V_n on which g_i acts trivially is just V^0, one has

$$\mathrm{Supp}\,(\mathcal{C}_{m_i}) = x_i + V^0. \quad (19)$$

We note that the norm $||\xi_i||$ of vector ξ_i yields the distance of manifold $\mathrm{Supp}\,(\mathcal{C}_{m_i})$ from the origin O because ξ_i is orthogonal to all vectors of V^0. We establish that whenever we express a manifold of E_n as a (formal) sum of one of its points and an associated difference space, then this point will be chosen as the origin of the manifold.

In addition to $\{g_i|u_i + t\}$, the coset $\{g_i|u_i\}T$ contains infinitely many symmetry operations of order m_i, namely $\{g_i|u_i + t + t'_1\}$, $t'_1 \in T_1$. Since P_i projects the whole space V^1 onto the zero vector 0, it follows that, for every $t'_1 \in T_1$, the translation $t' \equiv t + t'_1$ also satisfies (16). For convenience, the cyclic group generated by the symmetry operation $\{g_i|u_i + t + t'_1\}$, $t'_1 \in T_1$, will be denoted by $\mathcal{C}_{m_i}(t'_1)$. The symmetry support of $\mathcal{C}_{m_i}(t'_1)$ is just a copy of $\mathrm{Supp}\,(\mathcal{C}_{m_i})$, being parallel to it and shifted with respect to it by $\overline{\overline{Q}}_i t'_1 \in V^1$, *i.e.*

$$\begin{aligned}\mathrm{Supp}\,(\mathcal{C}_{m_i}(t'_1)) &= O + \overline{\overline{Q}}_i (u_i + t + t'_1) + V^0 \\ &\equiv \mathrm{Supp}\,(\mathcal{C}_{m_i}) + \overline{\overline{Q}}_i t'_1. \end{aligned} \quad (19a)$$

This corresponds to the fact that

$$\{g_i|u_i + t + t'_1\} = \{I|\overline{\overline{Q}}_i t'_1\}\,\{g_i|u_i + t\}\,\{I| - \overline{\overline{Q}}_i t'_1\}. \quad (20)$$

Equations (19*a*) and (20) imply

Theorem 4.2

The set of all finite cyclic subgroups of $\mathcal{G}$, being generated by an element of the coset $\{g_i|u_i\}T$, as well as the set of their symmetry supports form an orbit under the discrete part $\overline{\overline{Q}}_i T_1$ of the translational normalizer $\mathrm{Trn}\,(C_{m_i}, T)$; the action, in the former case, being taken as conjugation.

It is convenient to split both orbits under T_1. The main advantage of such a splitting consists in the fact that one easily recognizes whether the symmetry support $\mathrm{Supp}\,(\mathcal{C}_{m_i}(t'_1))$ is in the same suborbit as $\mathrm{Supp}\,(\mathcal{C}_{m_i})$ or not. If so, the shift vector $\overline{\overline{Q}}_i (t'_1)$ belongs to T_1 and, hence, this vector must have integral components, if expressed in terms of the chosen lattice basis of T. Moreover, if $\overline{\overline{Q}}_i(t'_1) \in T_1$ then the groups $\mathcal{C}_{m_i}(t'_1)$ and $\mathcal{C}_{m_i}$ are conjugate subgroups of $\mathcal{G}$ and, therefore, their symmetry supports must belong to the same Wyckoff position. We note that if a symmetry support is found to be an interior point of the parallelepiped $\Theta(0)$ then all other symmetry supports within the same suborbit will not intersect $\Theta(0)$. Otherwise, if the intersection is not empty, it must contain at least one point of some lower-dimensional face of $\Theta(0)$. Then the corresponding suborbit may contain another manifold that intersects $\Theta(0)$. There can be at most 2^{n_1}, $n_1 \equiv \dim V^1$, such manifolds since there is at most 2^{n_1} translation vectors in T_1 that can bring such a face into an equivalent face of $\Theta(0)$. We remark that every lower-dimensional face of the parallelepiped is exposed and so it contains no interior point. In such a case when $T \neq T_0 + T_1$, it may also happen that no symmetry support of a certain suborbit will intersect $\Theta(0)$.

In order to split both orbits into suborbits under T_1, one has only to decompose the discrete part of the translational normalizer $\mathrm{Trn}\,(C_{m_i}, T) \bmod T_1$. We write

$$\overline{\overline{Q}}_i T_1 = (\tau_1 + T_1) \cup (\tau_2 + T_1) \cup \ldots \cup (\tau_{s_i} + T_1), \quad (21)$$

where s_i is the index of T_1 in $\overline{\overline{Q}}_i T_1$, *i.e.* $s_i = [\overline{\overline{Q}}_i T_1 : T_1]$. The number of distinct suborbits under T_1 is then equal to s_i and, as a representative of the jth suborbit, $j \in \{1, ..., s_i\}$, one can choose the manifold $(O + \xi_i + \tau_j) + V^0 \equiv (O + \sigma_{ij}) + V^0$, which is the symmetry support of the cyclic group $\mathcal{C}_{m_i}(\overline{\overline{Q}}_i \tau_j) = \{I|\tau_j\}\,\mathcal{C}_{m_i}\,\{I|-\tau_j\} \equiv \mathcal{C}^{(j)}_{m_i}$, *i.e.* $\mathrm{Supp}\,(\mathcal{C}^{(j)}_{m_i}) = (O + \sigma_{ij}) + V^0$.

With the use of the representative manifold $(O + \sigma_{ij}) + V^0$ of the jth suborbit, it is straightforward to obtain those manifolds of the suborbit that intersect $\Theta(0)$. One has to find all vectors $t'_{ij} \in T_1$, if any, for which there exists a vector $\omega_{ij} \in V^0$ such that $O + \sigma_{ij} + t'_{ij} + \omega_{ij} \in \Theta(0)$. Each such vector t'_{ij} then determines a manifold $(O + \sigma_{ij} + t'_{ij}) + V^0$ with the required property.

We notice that the s_i suborbits may belong to s_i distinct Wyckoff positions if $(I - P_i)T \equiv T^1 = T_1$, *i.e.* if $T = T_0 + T_1$. Otherwise, the number of distinct Wyckoff positions to which these suborbits belong must be less than s_i. The reason is the following:

A cyclic subgroup of $\mathcal{G}$ that is a conjugate of $\mathcal{C}_{m_i}$ by means of a translation $t' \in T$ can also be obtained if the conjugation is performed with the projection $(I - P_i)t' \in T^1$ of t' instead. Consequently, the s_i suborbits can belong at most to $d_i \equiv [\overline{\overline{Q}}_i T_1 : T^1]$ distinct Wyckoff positions and one has $s_i = d_i \cdot [T : (T_0 + T_1)]$ [*cf.* (10)]. One may then conclude:

Conclusion 4.3

The cyclic subgroups of $\mathcal{G}$, generated by a symmetry operation of the ith coset in (14), and leaving some point of $\Theta(0)$ fixed, can be classified at most into $s_i \equiv [\overline{\overline{Q}}_i T_1 : T_1]$ orbits of subgroups conjugated to each other by some translation of T_1. The corresponding symmetry supports can belong to at most $d_i \equiv [\overline{\overline{Q}}_i T_1 : T^1]$ distinct Wyckoff positions.

5. An algorithm to compute Wyckoff positions in n dimensions

The present algorithm to compute the Wyckoff positions of an n-dimensional space group $\mathcal{G}$ is based on equality (2). It implies [*cf.* text related to (3)] that the symmetry support of the stabilizer of an arbitrary point $x \in E_n$ is given by the intersection of the symmetry supports of all cyclic subgroups of that stabilizer. We remark that only those cyclic subgroups that generate the stabilizer are necessary. Consequently, one can determine the stabilizers of all points within the elementary cell $\Theta(0)$ by consecutive intersecting of the symmetry supports of all those cyclic subgroups of $\mathcal{G}$ that leave some point of $\Theta(0)$ fixed. The algorithm consists of the following three main steps.

In the first step, for each cyclic subgroup $C \not\equiv C_1$ of the point group G, one determines if there is a finite subgroup of $\mathcal{G}$ with the point group C. If so, there exists an infinite set of finite cyclic subgroups of $\mathcal{G}$ having point group C. This set forms an orbit under the action of the discrete part of the translational normalizer $\mathrm{Trn}\,(C,T)$ and the symmetry supports of all groups involved in the orbit are parallel to each other. One conveniently divides this orbit into finitely many suborbits under T_1, which is the greatest common subgroup of the translational subgroup T and the discrete part of $\mathrm{Trn}\,(C,T)$. Within each suborbit one then finds those subgroups of $\mathcal{G}$ whose symmetry supports intersect the elementary cell $\Theta(0)$, using a representative manifold of the corresponding suborbit of symmetry supports (*cf.* § 4). As stated in the preceding section, each suborbit may contain a different number of such subgroups: either none, or only one subgroup whose symmetry support is an interior point of $\Theta(0)$, or else a finite number of subgroups leaving a point of a lower-dimensional face of $\Theta(0)$ fixed. As a result, one obtains a finite set of (finite) subgroups of $\mathcal{G}$ having point group C.

For convenience, we call the set of their symmetry supports a family or a C-family in order to indicate the corresponding point group. Having established families of symmetry supports for all non-trivial cyclic subgroups of G, if any, one arrives at a finite set of manifolds intersecting $\Theta(0)$. This set is used to generate the stabilizers of all points within $\Theta(0)$ by intersecting the manifolds involved. The splitting of the set into families is suitable since the intersection of any two symmetry supports within a family is *a priori* known to be empty, and thus only manifolds belonging to distinct families have to be intersected. We remark that, among the families of symmetry supports, inclusion relations may occur. For example, the symmetry support of the cyclic site-symmetry group C_4 of order four coincides with the symmetry support of its subgroup C_2 of order two. Consequently, the C_4-family is completely included in the C_2-family.

In the second step, one takes a pair of families, one after another, and successively intersects every symmetry support of one family with every symmetry support of the other family. If the intersection of the two symmetry supports in question is empty, another two symmetry supports are taken from the chosen pair of families and their intersection is checked. This process is repeated until a non-empty manifold is found. It may happen that such a manifold does not intersect the elementary cell $\Theta(0)$. It is then discarded and one continues intersecting the symmetry supports as described above until a manifold that intersects $\Theta(0)$ is obtained. Suppose that this manifold arises as an intersection of two symmetry supports from C^1- and C^2-families. There are two possibilities: either this manifold coincides with some of the supports computed previously or it is a new one. In both cases, one obtains a new finite group $\mathcal{F}' \subseteq \mathcal{G}$ whose symmetry support is the computed manifold. In the latter case, the point group F' of $\mathcal{F}'$ is just $C^1 \cup C^2$. In the former case, if the corresponding manifold was already obtained as an intersection of symmetry supports belonging to $\overline{C}^1$-, $\overline{C}^2$-, ..., $\overline{C}^i$-families, then F' is generated by cyclic groups $\overline{C}^1$, $\overline{C}^2$, ..., $\overline{C}^i$ and also by C^1 and C^2.

After having intersected each pair of symmetry supports belonging to distinct families, one obtains finitely many new symmetry supports. In the case where no new symmetry support is found, one goes to step three. Otherwise, each of these new symmetry supports is intersected again with all symmetry supports of those C-families for which C is not a subgroup of the corresponding point group in order to produce further new finite subgroups of $\mathcal{G}$ as well as further new symmetry supports. This procedure is repeated until no new symmetry support occurs.

In the third step, all the symmetry supports found are classified into equivalence classes of manifolds under the action of $\mathcal{G}$ using the following fact:

Two manifolds $(O + \xi_a) + V^a$ and $(O + \xi_b) + V^b$ are equivalent under $\mathcal{G}$ if and only if

(1) an element g of the point group G exists so that $gV^a = V^b$;

(2) for any symmetry operation $\{g|u\} \in \mathcal{G}$, a translation $t \in T$ can be chosen so that $u + g\xi_a - \xi_b + t \in V^b$.

Condition (1) is trivially satisfied if both V^a and V^b contain only the zero vector. Otherwise, the Gauss exchange routine (Nef, 1966) is used to check if the manifolds $O + gV^a$ and $O + V^b$ coincide.

Condition (2) can be verified by a straightforward computation. Given a basis $\{v_i; i = 1, \ldots, \dim V^b\}$ of

V^b, one has to find a vector $w \equiv \sum_{i=1}^{\dim V^b} x_i v_i \in V^b$, if any, which solves the following congruence:

$$u + g\,\xi_a - \xi_b + \sum_{i=1}^{\dim V^b} x_i v_i \equiv 0 \bmod T.$$

By definition, each such equivalence class of the symmetry supports represents one Wyckoff position. For each Wyckoff position of $\mathcal{G}$, a representative manifold $(O+\zeta) + V^0$ is chosen according to some fixed rules.

6. An illustrative example: space group $P\overline{3}2/m1$

In order to illustrate the algorithm, we apply it to the three-dimensional space group $P\overline{3}2/m1$ where the site symmetry $\overline{3}2/m1$ occurs at the origin O and the orientation of the threefold axis coincides with the positive direction of the z axis. For typographical brevity, instead of the notation used in *IT* (1983), we introduce the following symbols for the point-symmetry operations of $\overline{3}2/m1$: $\overline{3}^+ \equiv \overline{3}^+(0,0,z)$, $3^+ \equiv 3^+(0,0,z)$, $m \equiv m(x,\overline{x},z)$, $m' \equiv m(x,2x,z)$, $m'' \equiv m(2x,x,z)$, $2 \equiv 2(x,x,0)$, $2' \equiv 2(x,0,0)$, $2'' \equiv 2(0,y,0)$ and $\overline{1} \equiv \overline{1}(0,0,0)$. As generators of $P\overline{3}2/m1$, one can choose sixfold rotoinversion $\{\overline{3}^+|0\}$, reflection $\{m|0\}$ and translations by the basis vectors of the lattice T, $a \equiv (1,0,0)$, $b \equiv (0,1,0)$ and $c \equiv (0,0,1)$. One can write the coset decomposition of $P\overline{3}2/m1$ modulo translational subgroup T as follows:

$$\begin{aligned} P\overline{3}2/m1 = {} & \{1|0\}T + \{3^+|0\}T + \{3^-|0\}T + \{m|0\}T \\ & + \{m'|0\}T + \{m|0\}T + \{\overline{1}|0\}T \\ & + \{\overline{3}^+|0\}T + \{\overline{3}^-|0\}T + \{2|0\}T \\ & + \{2'|0\}T + \{2|0\}T. \end{aligned}$$

Since the space group chosen is a symmorphic one, the condition of lemma 4.1 is trivially satisfied for all coset representatives. Consequently, each non-trivial subgroup of the point group $\overline{3}2/m1$ occurs as a point group of infinitely many finite subgroups of $P\overline{3}2/m1$. The point group $\overline{3}2/m1$ contains ten cyclic subgroups $\overline{3}$, 3, m, m', m'', 2, $2'$, $2''$, $\overline{1}$ and 1 so that all finite cyclic subgroups of $P\overline{3}2/m1$ belong to ten mutually disjoint sets, each of which consists of groups with a given point group. Each such set can be represented by a group leaving the origin O fixed. The ten representative groups are generated by the following coset representatives: $\{\overline{3}^+|0\}$, $\{3^+|0\}$, $\{m|0\}$, $\{m'|0\}$, $\{m''|0\}$, $\{2|0\}$, $\{2'|0\}$, $\{2''|0\}$, $\{\overline{1}|0\}$ and $\{1|0\}$. We recall that (by theorem 4.2) a set of all finite cyclic subgroups with a point group C forms an orbit under the discrete part of the translational normalizer $\mathrm{Trn}\,(C,T)$. In order to find those groups of the orbit whose symmetry supports intersect the elementary cell $\Theta(0)$, one has first to determine the translational groups T^0, T^1, T_0, T_1 and the discrete part $\overline{\overline{Q}}T_1$ of $\mathrm{Trn}\,(C,T)$ and then to decompose $\overline{\overline{Q}}T_1$ into cosets in terms of T_1. The case $C \equiv C_1$ is trivial: $T^0 = T_0 = T$ and $T^1 = T_1 = \overline{\overline{Q}}T_1 = \{0\}$.

Consider the twofold rotation $2'$. Using definition (7) of the projection operator P, one finds

$$P = \frac{1}{2}\begin{pmatrix} 2 & -1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \text{and} \quad I - P = \frac{1}{2}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

Applying P and $I-P$ to the lattice basis $\{a,b,c\}$ of T, one obtains

$$\begin{aligned} P(-b) &= \frac{1}{2}Pa = \frac{1}{2}a, & (I-P)b &= \frac{1}{2}a + b, \\ Pc &= (I-P)a = 0, & (I-P)c &= c. \end{aligned}$$

Accordingly, $T^0 \equiv PT$ is generated by $a/2$ and $T^1 \equiv (I-P)T$ by $a/2+b$ and c. It follows that a generates $T_0 \equiv T \cap T^0$ and $\{a+2b, c\}$ is a basis of $T_1 \equiv T \cap T^1$. Since $\overline{\overline{Q}} = \frac{1}{2}I$, then vectors $a/2+b$, $c/2$ form a basis of the discrete part $\overline{\overline{Q}}T_1$ of translational normalizer $\mathrm{Trn}\,(2',T)$. The coset decomposition $\overline{\overline{Q}}T_1 \bmod T_1$ (22) implies that an orbit of all finite cyclic subgroups

$$\begin{aligned} \overline{\overline{Q}}T_1 = {} & (0+T_1) \cup (\frac{a}{2}+b+T_1) \cup (\frac{c}{2}+T_1) \\ & \cup (\frac{a}{2}+b+\frac{c}{2}+T_1) \end{aligned} \tag{22}$$

of $P\overline{3}2/m1$ with the point group $2'$ as well as an orbit of their symmetry supports splits under T_1 into four suborbits. Considering that a generates T_0, and thus also the difference space V^0 of all symmetry supports within the orbit, one directly writes down representative symmetry supports of the four suborbits: $(x,0,0)$, $(x+\frac{1}{2},1,0)$, $(x,0,\frac{1}{2})$ and $(x+\frac{1}{2},1,\frac{1}{2})$. The results for all ten cyclic point groups are summarized in Table 1.

With the use of translations $a+2b$, c generating T_1 and translation a generating T_0, it is straightforward to establish the $2'$-family of symmetry supports. Consider origins $(0,0,0)$, $(\frac{1}{2},1,0)$, $(0,0,\frac{1}{2})$ and $(\frac{1}{2},1,\frac{1}{2})$ of the representative manifolds. For each suborbit, one has to find all such translations $t = \eta a + k(a+2b) + lc \equiv (\eta+k, 2k, l)$, where η is real and k, l are integers, that bring the corresponding origin into a point of $\Theta(0)$. One can readily see that there exists a trivial solution $t = (0,0,0)$ for the first suborbit and two solutions $t_1 = (0,0,0)$ and $t_2 = (0,0,-1)$ for the third suborbit. For the second and the last suborbits there is no solution (note that $T \neq T_0 + T_1$). The $2'$-family then consists of three symmetry supports, $(x,0,0)$, $(x,0,\frac{1}{2})$ and $(x,0,-\frac{1}{2})$.

One can avoid a lot of superfluous calculations in the second step if pairs of cyclic subgroups of $\overline{3}2/m1$ are classified into equivalence classes in the following way. Given a point group G, two pairs of cyclic subgroups,

Table 1. *Translational groups specific to cyclic subgroups of* $\bar{3}2/m1$ *and representatives of orbits of symmetry supports*

Symbol of cyclic point group	Generating translations of T^0	T_0	T_1	T^1	$\overline{\overline{Q}}\,T_1$	Representative symmetry supports of suborbits under T_1
$\bar{3}$	0	=	a, b, c	=	$a, b, \frac{c}{2}$	$(0,0,0), (0,0,\frac{1}{2})$
3	c	=	a, b	=	$a(b), \frac{a-b}{3}$	$(0,0,z)$ $(\frac{1}{3},-\frac{1}{3},z), (-\frac{1}{3},\frac{1}{3},z)$
m	$\frac{a-b}{2}, c$	$a-b, c$	$a+b$	$\frac{a+b}{2}$	=	$(x,-x,z)$ $(x+\frac{1}{2},-x+\frac{1}{2},z)$
m'	$\frac{a+2b}{2}, c$	$a+2b, c$	a	$\frac{a}{2}$	=	$(x,2x,z)$ $(x+\frac{1}{2},2x,z)$
m''	$\frac{2a+b}{2}, c$	$2a+b, c$	b	$\frac{b}{2}$	=	$(2y,y,z)$ $(2y,y+\frac{1}{2},z)$
2	$\frac{a+b}{2}$	$a+b$	$a-b, c$	$\frac{a-b}{2}, c$	$\frac{a-b}{2}, \frac{c}{2}$	$(x,x,0), (x+\frac{1}{2},x-\frac{1}{2},0)$ $(x,x,\frac{1}{2}), (x+\frac{1}{2},x-\frac{1}{2},\frac{1}{2})$
$2'$	$\frac{a}{2}$	a	$a+2b, c$	$\frac{a+2b}{2}, c$	$\frac{a+2b}{2}, \frac{c}{2}$	$(x,0,0), (x+\frac{1}{2},1,0)$ $(x,0,\frac{1}{2}), (x+\frac{1}{2},1,\frac{1}{2})$
$2''$	$\frac{b}{2}$	b	$2a+b, c$	$\frac{2a+b}{2}, c$	$\frac{2a+b}{2}, \frac{c}{2}$	$(0,y,0), (1,y+\frac{1}{2},0)$ $(0,y,\frac{1}{2}), (1,y+\frac{1}{2},\frac{1}{2})$
$\bar{1}$	0	=	a, b, c	=	$\frac{a}{2}, \frac{b}{2}, \frac{c}{2}$	$(0,0,0), (\frac{1}{2},0,0), (0,\frac{1}{2},0), (0,0,\frac{1}{2})$ $(\frac{1}{2},\frac{1}{2},\frac{1}{2}), (0,\frac{1}{2},\frac{1}{2}), (\frac{1}{2},0,\frac{1}{2}), (\frac{1}{2},\frac{1}{2},0)$
1	a, b, c	=	0	=	=	(x,y,z)

(C^1, C^2) and $(\overline{C}^1, \overline{C}^2)$, are equivalent if they generate the same subgroup of G. For example, pair $(\bar{3}, m)$ is equivalent to $(m, 2')$ since both pairs generate the point group $\bar{3}2/m1$. Consequently, symmetry support of an equiclass finite subgroup of $P\bar{3}2/m1$ must occur as an intersection of certain two-symmetry supports that belong either to $\bar{3}$- and m-families or to m- and $2'$-families. We note that, for n-dimensional point groups of high order, the effort exerted for establishing such a classification may become comparable with the effort saved; moreover, one might classify not only pairs but also k-tuples, $k \geq 3$. In that case, one might find it more advantageous to apply the algorithm without introducing such a classification. Also, in the case of calculations performed by means of a computer, it seems to be suitable not to incorporate the classification into a computer program.

In our case, the nine non-trivial cyclic subgroups yield 36 pairs, which fall into six equivalence classes, corresponding to point groups $\bar{3}2/m1$, $3m1$, 321, $2/m$, $2'/m'$ and $2''/m''$. One can choose the following representative pairs: $(\bar{3}, m)$, $(3, m)$, $(3, 2')$, $(m, \bar{1})$, $(m', \bar{1})$ and $(m'', \bar{1})$. For each of these pairs, it is routine to obtain the intersections of manifolds that belong to two corresponding families. In fact, most of these intersections are almost obvious and they can be read directly from Table 1.

All points of the $\bar{3}$-family and all lines of the 3-family lie in the plane $(x, -x, z)$ of the m-family. Accordingly, the $\bar{3}$-family coincides with the $\bar{3}2/m1$-family and the 3-family with the $3m1$-family. For the pair $(3, 2')$, only line $(0,0,z)$ of the 3-family has a non-empty intersection with the lines of the $2'$-family; as a result, however, one obtains all points of the $\bar{3}2/m1$-family. It is straightforward to decide which of the 25 points of the $\bar{1}$-family belong to the planes of the m-, m'- and m''-families. One need not consider three points belonging to the $\bar{3}2/m1$-family: $(0,0,0)$, $(0,0,\frac{1}{2})$ and $(0,0,-\frac{1}{2})$. Finally, one obtains all families of symmetry supports that correspond to stabilizers of points within $\Theta(0)$. The results are given in Table 2.

One may also determine which symmetry supports of a C-family are equivalent under $P\bar{3}2/m1$. For that purpose, one can apply the criteria stated at the end of § 5, but in a slightly different form: one supplies condition (1) with an additional requirement that an element $g \in G$ must satisfy $gCg^{-1} = C$. Consequently, one divides the C-family into subsets of equivalent manifolds. For each family, we give the representative manifolds of all such subsets in the last column of Table 2.

In the last step, by applying the original criteria of § 5 to the representative manifolds, one establishes the Wyckoff positions of space group $P\bar{3}2/m1$.

Table 2. *Families of symmetry supports of subgroups of* $32/m1$

Symbol of point group	Family of symmetry supports	Representative manifolds
$\bar{3}2/m1$	$(0,0,0); (0,0,\frac{1}{2}), (0,0,-\frac{1}{2})$	$(0,0,0); (0,0,\frac{1}{2})$
$3m1$	$(0,0,z); (\frac{1}{3},-\frac{1}{3},z), (-\frac{1}{3},\frac{1}{3},z)$	$(0,0,z); (\frac{1}{3},-\frac{1}{3},z)$
$2/m$	$\pm(\frac{1}{2},\frac{1}{2},0), \pm(\frac{1}{2},-\frac{1}{2},0)$; $\pm(\frac{1}{2},\frac{1}{2},\frac{1}{2}), \pm(-\frac{1}{2},\frac{1}{2},\frac{1}{2}), \pm(\frac{1}{2},-\frac{1}{2},\frac{1}{2}), \pm(\frac{1}{2},\frac{1}{2},-\frac{1}{2})$	$(\frac{1}{2},\frac{1}{2},0); (\frac{1}{2},\frac{1}{2},\frac{1}{2})$
$2'/m'$	$\pm(\frac{1}{2},0,0); \pm(\frac{1}{2},0,\frac{1}{2}), \pm(\frac{1}{2},0,-\frac{1}{2})$	$(\frac{1}{2},0,0); (\frac{1}{2},0,\frac{1}{2})$
$2''/m''$	$\pm(0,\frac{1}{2},0); \pm(0,\frac{1}{2},\frac{1}{2}), \pm(0,\frac{1}{2},-\frac{1}{2})$	$(0,\frac{1}{2},0); (0,\frac{1}{2},\frac{1}{2})$
m	$(x,-x,z), (x+\frac{1}{2},-x+\frac{1}{2},z), (x-\frac{1}{2},-x-\frac{1}{2},z)$	$(x,-x,z)$
m'	$(x,2x,z), (x+\frac{1}{2},2x,z), (x-\frac{1}{2},2x,z)$	$(x,2x,z)$
m''	$(2y,y,z), (2y,y+\frac{1}{2},z), (2y,y-\frac{1}{2},z)$	$(2y,y,z)$
2	$(x,x,0), (x+\frac{1}{2},x-\frac{1}{2},0), (x-\frac{1}{2},x+\frac{1}{2},0)$; $(x,x,\frac{1}{2}), (x+\frac{1}{2},x-\frac{1}{2},\frac{1}{2}), (x-\frac{1}{2},x+\frac{1}{2},\frac{1}{2})$, $(x,x,-\frac{1}{2}), (x+\frac{1}{2},x-\frac{1}{2},-\frac{1}{2}), (x-\frac{1}{2},x+\frac{1}{2},-\frac{1}{2})$	$(x,x,0); (x,x,\frac{1}{2})$
$2'$	$(x,0,0); (x,0,\frac{1}{2}), (x,0,-\frac{1}{2})$	$(x,0,0); (x,0,\frac{1}{2})$
$2''$	$(0,y,0); (0,y,\frac{1}{2}), (0,y,-\frac{1}{2})$	$(0,y,0); (0,y,\frac{1}{2})$
1	(x,y,z)	(x,y,z)

7. Concluding remarks

The algorithm presented is dimension independent and as such it can be used for the determination of Wyckoff positions of any space group in an arbitrary dimension n. As shown in § 6, one can perform the corresponding computations by hand, in which case certain modifications may prove useful. However, for dimensions higher than three, especially when the point group of a given space group has a high order, it is more suitable to accomplish such calculations by means of a computer. For that reason, a computer program in C has been written. It can serve two purposes: either one can use this program to analyse one's individual problems or, if needed, one can also calculate all Wyckoff positions for a given collection of higher-dimensional space groups. In this connection, we note that the determination of Wyckoff positions of four-dimensional space groups is now a feasible project.

In order to run the program, one has to meet the following software and hardware requirements. One must have a C compiler that complies with the ANSI C standard. The hardware requirements depend on the space dimension and also on the order of an occurring point group. If the dimension $n \leq 3$ or if $n \geq 4$ and the order of the point group of a space group in question is relatively small, the program may run on a PC-486 (also a 386 may be used) with 1–2 Mbyte RAM. In other cases, one will need a workstation with at least 32 Mbyte RAM (we recommend 64 Mbyte RAM).

We note that the use of Wyckoff positions in analysing a diffraction pattern is very limited. The special extinction conditions occurring for the Wyckoff positions of high symmetry are rarely met in practice. In our opinion, the best use of the investigation of Wyckoff positions is for a complete understanding of the space groups. This is a prerequisite for any crystal-structure determination. Quasicrystals are three dimensional and a possible model is a projection of a slice through a higher-dimensional crystal of suitable symmetry. The projection corresponds to an intersection of Fourier space.

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APPENDIX 1
Orthogonal splittings of V_n under a finite cyclic point group

In this Appendix, we supply the proofs of statements used in §§ 2 and 3. We will consider a finite cyclic point group generated by a symmetry operation g of order $m \geq 2$; it will be denoted as C_m. With the cyclic group

C_m there is associated a commutative group ring whose elements are sums of the form $\sum_{j=0}^{m-1} z_j g^j$, where each z_j is an integer. Such a sum is a linear operator acting on the vector space V_n according to the prescription $(\sum_{j=0}^{m-1} z_j g^j) \cdot v = \sum_{j=0}^{m-1} z_j (g^j \cdot v)$ for an arbitrary $v \in V_n$. We choose the following m linear operators from the commutative group ring.

$$\overline{P} = I + g + g^2 + \ldots + g^{m-1} \qquad (A1.1)$$

$$\overline{Q^{(j)}} = I - g^j, \quad j = 1, \ldots, m-1. \qquad (A1.2)$$

A straightforward computation shows that

$$\overline{P}^2 \equiv \overline{P} \cdot \overline{P} = m\overline{P} \qquad (A1.3)$$

$$\overline{P} \cdot \overline{Q^{(j)}} = \overline{Q^{(j)}} \cdot \overline{P} = 0, \quad j = 1, \ldots, m-1. \quad (A1.4)$$

The m linear operators given by ($A1.1$) and ($A1.2$) yield m splittings ($A1.5$) of V_n into two orthogonal subspaces each, which, owing to the commutativity of the group ring, are invariant under the action of C_m.

$$\begin{aligned} V_n &= \operatorname{Ker}\overline{P} + \operatorname{Im}\overline{P} \\ &= \operatorname{Ker}\overline{Q^{(j)}} + \operatorname{Im}\overline{Q^{(j)}} \quad j = 1, \ldots, m-1. \quad (A1.5) \end{aligned}$$

The subspace $\operatorname{Ker}\overline{P}$ of V_n consists of all those vectors that $\overline{P}$ maps onto the zero vector and the subspace $\operatorname{Im}\overline{P}$ contains the images of all vectors from V_n. The meaning of $\operatorname{Ker}\overline{Q^{(j)}}$ and $\operatorname{Im}\overline{Q^{(j)}}$ is analogous.

We note that if an integer $0 < j_1 < m$ has no common divisor with m except 1, *i.e.* if each element of C_m can be expressed as a power of g^{j_1}, then the only vector involved simultaneously in $\operatorname{Ker}\overline{P}$ and $\operatorname{Ker}\overline{Q^{(j_1)}}$ is the zero vector 0. This can be proved as follows:

Assume that $v \in \operatorname{Ker}\overline{Q^{j_1}} \cap \operatorname{Ker}\overline{P}$, *i.e.* $\overline{Q^{j_1}}v = \overline{P}v = 0$. Hence, $g^{j_1}v = v$. Since $\overline{P} = I + g^{j_1} + {g^{j_1}}^2 + \ldots + {g^{j_1}}^{m-1}$, then $\overline{P}v \equiv mv = 0$. Taking into account ($A1.4$), one has

Lemma $A1.1$

If $0 < j_1 < m$ and m are mutually prime, then

$$\operatorname{Ker}\overline{P} = \operatorname{Im}\overline{Q^{(j_1)}} \quad \text{and} \quad \operatorname{Im}\overline{P} = \operatorname{Ker}\overline{Q^{(j_1)}}. \quad (A1.6)$$

The action of C_m on $\operatorname{Im}\overline{P}$ is trivial.

The assumption of this lemma is obviously fulfilled by $j_1 = 1$. Hence, $g \cdot t = t$ for any $t \in \operatorname{Im}\overline{P}$ and the second part of the lemma follows.

It may happen that the greatest common divisor d of an integer $0 < j_2 < m$ and of m is greater than 1. If so, one introduces the operator $\overline{P^{(d)}} \equiv I + g^d + (g^d)^2 + \ldots + (g^d)^{m/d-1}$ and, by analogous reasoning, one finds that $\operatorname{Ker}\overline{P^{(d)}} = \operatorname{Im}\overline{Q^{(j_2)}}$, $\operatorname{Im}\overline{P^{(d)}} = \operatorname{Ker}\overline{Q^{(j_2)}}$. The subgroup $C_{m/d}$ of C_m, generated by the element g^d, acts on $\operatorname{Im}\overline{P^{(d)}}$ in a trivial way. By ($A1.6$), it also holds that $\operatorname{Ker}\overline{P} \supseteq \operatorname{Im}\overline{Q^{(j_2)}} \equiv \operatorname{Ker}\overline{P^{(d)}}$ and $\operatorname{Im}\overline{P} \subseteq \operatorname{Ker}\overline{Q^{(j_2)}} \equiv \operatorname{Im}\overline{P^{(d)}}$. Since $\operatorname{Im}\overline{P}$ as well as $\operatorname{Im}\overline{P^{(d)}}$ are the greatest subspaces of V_n on which, in corresponding order, C_m and $C_{m/d}$ act trivially, all splittings in ($A1.5$) are orthogonal. Only relatively few of these m splittings are mutually distinct:

The number of distinct splittings of V_n in ($A1.5$) equals at most the number of all subgroups of C_m excluding the trivial one to which a trivial splitting $\{0\} + V_n$ corresponds.

Using ($A1.3$), we define the projection operators P and Q as follows:

$$P = (1/m)\overline{P} \qquad (A1.7)$$

$$Q = (1/m)\sum_{j=1}^{m-1} \overline{Q^{(j)}}. \qquad (A1.8)$$

It is easy to check that the projection operator Q is complementary to P, *i.e.*

$$Q = I - P. \qquad (A1.8a)$$

One has $\operatorname{Ker}P = \operatorname{Ker}\overline{P} = \operatorname{Im}\overline{Q} = \operatorname{Im}Q$ and $\operatorname{Ker}Q = \operatorname{Ker}\overline{Q} = \operatorname{Im}\overline{P} = \operatorname{Im}P$. Moreover, since $\overline{Q^{(j)}} = (I-g)\,(I+g+\ldots+g^{j-1})$, for each j, Q can be expressed as a product of two operators, $\overline{Q}$ and $\overline{\overline{Q}}$,

$$Q = \overline{Q} \cdot \overline{\overline{Q}}, \qquad (A1.9)$$

where we have put $\overline{Q} \equiv \overline{Q^{(1)}}$ and $\overline{\overline{Q}}$ is given as

$$\begin{aligned} \overline{\overline{Q}} = (1/m)[I + (I+g) + (I+g+g^2) + \ldots \\ + (I + g + g^2 + \ldots + g^{m-2})]. \qquad (A1.10) \end{aligned}$$

After making some rearrangements in (A1.10), one gets an alternative expression for $\overline{\overline{Q}}$:

$$\overline{\overline{Q}} = \begin{cases} \frac{1}{2}I, & m = 2 \\ \frac{1}{2}[(\overline{P} - I) + \overline{Q} \cdot R], & m \geq 3, \end{cases} \qquad (A1.11)$$

where the linear operator R is defined as

$$R = \sum_{j=0}^{m-1} \alpha_j g^j$$

$$\alpha_{m-1} = -1, \quad \alpha_{m-2} = 0,$$

$$\alpha_k = \alpha_{m-3-k} = (k+1)(m-2-k)/m, \quad 0 \leq k < m/2. \quad (A1.12)$$

*Lemma A*1.2

The linear operator $\overline{\overline{Q}}$ is regular, *i.e.* $\overline{\overline{Q}} \in GL(V_n)$.

For $m = 2$, the proof is obvious. Let $m \geq 3$ and assume $v \in \operatorname{Ker} \overline{\overline{Q}}$, *i.e.* $\overline{\overline{Q}}v = 0$. Writing $v = Pv + Qv$, from $(A1.9)$, one finds, by assumption, that $v = Pv$. Equalities $(A1.11)$ and $(A1.4)$ imply that $\overline{\overline{Q}}v \equiv \overline{\overline{Q}}Pv = (m-1)/2v = 0$ and the statement follows.

Consider now an n-dimensional lattice $T \subseteq V_n$ generated by $a_1, ..., a_n$. One can always produce free Abelian groups $T_0 \equiv T \cap V^0$, $T^0 \equiv PT$, $T_1 \equiv T \cap V^1$ and $T^1 \equiv QT$. The groups T_0 and T_1 as well as the groups T^0 and T^1 have only the zero vector in common and so one can form the direct sums $T_0 + T_1$ and $T^0 + T^1$. It follows directly that $T_0 + T_1 \subseteq T \subseteq T^0 + T^1$. Among the projections $Pa_1, ..., Pa_n$ and $Qa_1, ..., Qa_n$ that generate T^0 and T^1, respectively, there are always $\dim V^0$ and $\dim V^1$ linearly independent vectors. However, the number of free generators of T^0 and/or T^1 may be, in contrast to T, greater than the number of linearly independent vectors involved so that the corresponding group will not be a discrete subgroup of V_n.

*Lemma A*1.3

If C_m is a subgroup of the Bravais group of T, then $T_0 + T_1$ as well as $T^0 + T^1$ are n-dimensional lattices.

By assumption, T is C_m invariant so that the linear operators $\overline{P}$ and $\overline{Q}$ map T homomorphically onto subgroups $T_0' \equiv \overline{P}T$ and $T_1' \equiv \overline{Q}T$. The commutativity of the group ring implies that both T_0' and T_1' are invariant under the action of C_m. By the definition of the projection operators, we have $T^0 = 1/m\, T_0'$ and $T^1 = \overline{\overline{Q}}T_1'$. Therefore, if $b_1, ..., b_{n_0}$ freely generate T_0', then $1/m\, b_1, ..., 1/m\, b_{n_0}$ freely generate T^0. Furthermore, if $c_1, ..., c_{n_1}$ freely generate T_1' then $\overline{\overline{Q}}c_1, ..., \overline{\overline{Q}}c_{n_1}$ freely generate T^1. On the other hand, since $a_1, ..., a_n$ is a basis of V_n, the projections $Pa_1, ..., Pa_n$ must generate not only T^0 but also V^0. Hence, $n_0 = \dim V^0$. By an analogous argument for the projections $Qa_1, ..., Qa_n$, we have $n_1 = \dim V^1$. Since T_0' and T^0 have equal rank and $T_0' \subseteq T_0 \subseteq T^0$, it follows that the group T_0 must also be freely generated by n_0 vectors; by an analogous reasoning, one finds that the group T_1 is freely generated by n_1 vectors. Considering that all the groups in question are C_m invariant and that $n_0 + n_1 = n$, it follows that $T_0' + T_1'$, $T_0 + T_1$ and $T^0 + T^1$ are n-dimensional lattices invariant under C_m.

We note that an alternative proof is given by Engel (1986) using theorem 7.2, according to which the lattice vectors freely generating T_0' and T_1' form a basis of V^0 and V^1, respectively. The lemma then directly follows from the definition $(A1.7)$ of P and the decomposition $(A1.9)$ of Q.

APPENDIX 2
Generation of a two-generator subgroup of a finite group

In order to determine all the elements of a finite group G given by means of $s > 1$ generators, say $g_1, \ldots, g_s$, one has to compute for each integer $k \geq 2$ all products $g_{i_1} \cdots g_{i_k}$ of the g's up to some integer k_0. The existence of such an integer follows from the finite order of G. Proceeding in this way, for each $k \leq k_0$, one has to compute s^k products of the given generators. Even for a small number s of generators and a not too large value of k, the number s^k will be quite large. Moreover, some of the elements of G will be produced many times. Such an algorithm would be very inefficient. Therefore, we supply a step-by-step algorithm for $s = 2$ that reduces superfluous calculations; this algorithm can easily be extended to the case of an arbitrary s, which is shown at the end of this Appendix. In order to present such an algorithm, we first introduce a possible method of proceeding in the case of two generators only. This will serve as a basis for establishing a more efficient algorithm.

Consider a finite group G and choose two elements of it, say g^1 and g^2, such that neither of them is a power of the other. All powers of g^1 and g^2 form cyclic subgroups of G, say C^1 and C^2, respectively. The two cyclic groups generate a subgroup $C^1 \cup C^2$ of G, each element of which can be expressed as a finite product of symmetry operations, belonging either to C^1 or to C^2. Such a product can always be rearranged into a form in which all even positions are occupied by elements of one group while elements of the other group occur on the odd positions.

We denote by $B_1^{(k)}$, $k \geq 2$, the set of all products $h_1 h_2 \ldots h_k$, where $h_k, h_{k-2}, \ldots \in C^1$ and $h_{k-1}, h_{k-3}, \ldots \in C^2$, and by $B_2^{(k)}$, $k \geq 2$, the set of all products of the above form, where, in turn, $h_k, h_{k-2}, \ldots \in C^2$ and $h_{k-1}, h_{k-3}, \ldots \in C^1$. Furthermore, we put $B_1^{(1)} \equiv C^1$ and $B_2^{(1)} \equiv C^2$. One has the following recursive relations among the B's.

$$\begin{aligned} B_1^{(2l)} &= \{h^2 B_1^{(2l-1)}; h^2 \in C^2\} = \{B_2^{(2l-1)} h^1; h^1 \in C^1\} \\ B_1^{(2l+1)} &= \{h^1 B_1^{(2l)}; h^1 \in C^1\} \quad = \{B_2^{(2l)} h^1; h^1 \in C^1\} \\ B_2^{(2l)} &= \{B_1^{(2l-1)} h^2; h^2 \in C^2\} = \{h^1 B_2^{(2l-1)}; h^1 \in C^1\} \\ B_2^{(2l+1)} &= \{B_1^{(2l)} h^2; h^2 \in C^2\} \quad = \{h^2 B_2^{(2l)}; h^2 \in C^2\}, \\ & \qquad l \geq 1. \qquad (A2.1) \end{aligned}$$

These recursive relations enable one to determine all sets $B_1^{(k)}$ and $B_2^{(k)}$ in a step-by-step manner, using the groups C^1 and C^2 and, for $k > 2$, also the set $B_1^{(k-1)}$, which was computed in the preceding step. Considering that the identity belongs to both groups C^1 and C^2, one has

$$\begin{aligned} B_1^{(k)} &\subseteq B_1^{(k+1)}, \quad B_1^{(k)} \subseteq B_2^{(k+1)}, \\ B_2^{(k)} &\subseteq B_1^{(k+1)}, \quad B_2^{(k)} \subseteq B_2^{(k+1)}. \end{aligned} \qquad (A2.2)$$

Consequently,

$$B_1^{(k)} \cup B_2^{(k)} \subseteq B_1^{(k+1)} \cap B_2^{(k+1)}. \quad (A2.3)$$

Being a subgroup of a finite group G, the group $C^1 \cup C^2$ is also finite and, hence, there exists an integer k_0 such that each element of $C^1 \cup C^2$ must be expressible as a product of at most k_0 elements belonging to either C^1 or C^2. In view of (A2.2) and (A2.3), one has

$$C^1 \cup C^2 \subseteq B_1^{(k_0)} \cup B_2^{(k_0)} \subseteq B_1^{(k_0+1)} \cap B_2^{(k_0+1)}. \quad (A2.4)$$

We assume k_0 to be the minimal integer for which (A2.4) is satisfied. Then, after k_0 steps in each of which the sets $B_1^{(k)}$ and $B_2^{(k)}$, $1 \le k \le k_0$, are determined, one obtains all the elements of the group $C^1 \cup C^2$.

Owing to the inclusions (A2.2), all those elements of $C^1 \cup C^2$ that were already determined in the kth step will be recalculated in any further step. To avoid superfluous calculations, we introduce reduced sets $\overline{B}_1^{(k)}$ and $\overline{B}_2^{(k)}$ for each k in the following way:

The set $\overline{B}_1^{(1)}$ is obtained from C^1 by deleting identity element I and the set $\overline{B}_2^{(1)}$ contains all those elements of C^2 that are not involved in C^1. For $k \ge 2$, we define $\overline{B}_2^{(k)}$ to be the set of all elements of $B_2^{(k)}$ that do not occur in $B_1^{(k-1)} \cup B_2^{(k-1)}$ and $\overline{B}_1^{(k)}$ to be the set of all elements of $B_1^{(k)}$ that are contained neither in $B_1^{(k-1)} \cup B_2^{(k-1)}$ nor in $B_2^{(k)}$. Consequently, relations (A2.2) will no longer be valid for the barred sets. Instead of (A2.1), one has

$$\begin{aligned}
\overline{B}_1^{(2l)} &\subseteq \{h^2\overline{B}_1^{(2l-1)}; h^2 \in \overline{B}_2^{(1)}\}, \{\overline{B}_2^{(2l-1)}h^1; h^1 \in \overline{B}_1^{(1)}\}\\
\overline{B}_1^{(2l+1)} &\subseteq \{h^1\overline{B}_1^{(2l)}; h^1 \in \overline{B}_1^{(1)}\}, \{\overline{B}_2^{(2l)}h^1; h^1 \in \overline{B}_1^{(1)}\}\\
\overline{B}_2^{(2l)} &\subseteq \{\overline{B}_1^{(2l-1)}h^2; h^2 \in \overline{B}_2^{(1)}\}, \{h^1\overline{B}_2^{(2l-1)}; h^1 \in \overline{B}_1^{(1)}\}\\
\overline{B}_2^{(2l+1)} &\subseteq \{\overline{B}_1^{(2l)}h^2; h^2 \in \overline{B}_2^{(1)}\}, \{h^2\overline{B}_2^{(2l)}; h^2 \in \overline{B}_2^{(1)}\},\\
& \qquad l \ge 1. \quad (A2.5)
\end{aligned}$$

We emphasize that there are two convenient ways to obtain the barred sets: compute either the sets in the left column or in the right column in (A2.5). If we choose the left column, then we have to omit from $B_1^{(k)}$ all those elements simultaneously contained in $B_2^{(k)}$ since, owing to the recursive relations, these elements will yield, when multiplied, elements of $B_2^{(k)}$ in the next step. If the right column is chosen, one has to interchange the roles of $B_1^{(k)}$ and $B_2^{(k)}$. The definition of the barred sets together with relations (A2.4) and (A2.5) directly imply:

Lemma A2.1

Let k_1 be the smallest integer for which at least one of the sets $\overline{B}_1^{(k_1)}$ and $\overline{B}_2^{(k_1)}$ is empty. If both sets are empty, put $k_0 \equiv k_1 - 1$; otherwise, $k_0 \equiv k_1$. Then,

$$C^1 \cup C^2 = \left(\bigcup_{k=1}^{k_0} \overline{B}_1^{(k)} \cup \overline{B}_2^{(k)}\right) \cup \{I\}.$$

Accordingly, after k_0 steps in each of which all the products of k elements, $1 \le k \le k_0$, involved either in $\overline{B}_1^{(k)}$ or in $\overline{B}_2^{(k)}$ are computed, one obtains all elements of $C^1 \cup C^2$.

We note that, instead of the cyclic subgroups C^1 and C^2 of G, any two subgroups F^1 and F^2 of G can be used to obtain all the elements of the group $F^1 \cup F^2$. Using this fact, one can directly extend the above algorithm to the case of $s > 2$ generators $g_1, \ldots, g_s$. In the first step, one proceeds as described above with $g^1 \equiv g_1$ and $g^2 \equiv g_2$ in order to obtain a subgroup $C^1 \cup C^2$ generated by the first two generators. Then, one checks whether g_3 belongs to $C^1 \cup C^2$ or not. If it does, one takes the next generator. If not, one repeats the first step with $F^1 \equiv C^1 \cup C^2$ and $F^2 \equiv C^3 = \{I = (g_3)^{m_3}, g_3, (g_3)^2, \ldots, (g_3)^{m_3-1}\}$ in order to generate the group $(C^1 \cup C^2) \cup C^3$. Proceeding in such a way with the remaining generators of the finite group G, one finally obtains all group elements.

APPENDIX 3
An algorithm to determine free generators of a subgroup of a free Abelian group

We consider a free Abelian group A of rank n, freely generated by $a_1, ..., a_n$. Let B denote a subgroup of A generated by $b_1, ..., b_{m'}$. As is any subgroup of A, B is also a free Abelian group of rank $m \le m'$. According to the fundamental theorem on subgroups of free Abelian groups (Magnus, Karrass & Solitar, 1966), there exist free generators $\overline{a}_i$, $i = 1, ..., n$, for A and m non-zero integers $d_1, ..., d_m$, where d_j divides d_{j+1}, such that $d_j\overline{a}_j$, $j = 1, ..., m$, freely generate B. This implies that there is a unique direct summand $D \supseteq B$ of A in which B is of finite index. The direct summand D is freely generated by $\overline{a}_j$, $j = 1, ..., m$, so that the index $[D : B]$ equals the product of all the d's, *i.e.* $[D : B] = d_1 \times \ldots \times d_m$, and the finite factor group D/B is isomorphic to the direct product of cyclic groups C_{d_j}, $j = 1, ..., m$, *i.e.*

$$D/B \simeq C_{d_1} \times \ldots \times C_{d_m}. \quad (A3.1)$$

The orders of these cyclic groups are invariants of D/B.

Magnus, Karrass & Solitar (1966) give an algorithm to establish the above-mentioned generators $\overline{a}_i$, $i = 1, ..., n$, of A and the m integers d_j, $j = 1, ..., m$. We remark that the original purpose of the algorithm was to convert a presentation of a given group (as a factor group of a free group by a normal subgroup spanned by defining relators) into a pre-Abelian presentation.

Consider a non-trivial cyclic subgroup $C \equiv \{I \equiv g^0 = g^k, g, g^2, \ldots, g^{k-1}; k \geq 2\}$ of the point group G of the given space group $\mathcal{G}$. One can use this algorithm to determine vectors freely generating the direct summands T_0 and T_1 of the translational subgroup T of $\mathcal{G}$ starting from generating vectors of their subgroups of finite index, $T_0' \equiv \overline{P}T$ and $T_1' \equiv \overline{Q}T$, respectively (*cf.* proof of lemma $A1.3$). However, it is not necessary to have vectors freely generating T_0 and T_1 that possess the above properties concerning the integers $d_1, \ldots, d_m$. Therefore, to cut out some calculations involved, we modify the algorithm to obtain an alternative set of free generators $\overline{a}_i$, $i = 1, ..., n$, of A together with the corresponding m integers e_j, $j = 1, ..., m$, such that the m elements $\overline{\overline{b}}_j \equiv e_j \overline{\overline{a}}_j$ freely generate B. The integers $e_1, \ldots, e_m$ are not supposed to satisfy any particular condition; their product must, of course, be equal to the product of all the d's since it gives the index of B in D. Instead of ($A3.1$), one has

$$D/B \simeq C_{e_1} \times \ldots \times C_{e_m}, \qquad (A3.2)$$

which is one possibility, among others, of expressing the finite Abelian group D/B as a product of m cyclic subgroups.

The algorithm is based on the so-called Nielsen transformations (Magnus, Karrass & Solitar, 1966) that take one m'-tuple of elements of A into another m'-tuple such that both m'-tuples generate the same subgroup of A. m' may be any positive integer and is said to be the rank of the Nielsen transformation in question. In order to define Nielsen transformations, one introduces first the concept of elementary Nielsen transformations (Magnus, Karrass & Solitar, 1966). One usually considers three (or four) standard kinds of elementary Nielsen transformations; two kinds will be given below explicitly. Under a Nielsen transformation, one then understands an operation, bringing an m'-tuple of elements of A into another such m'-tuple, which can be produced by a sequence of a finite number of elementary Nielsen transformations.

We note that this algorithm represents also a constructive proof of the existence of the free generators for A, B and D as mentioned above. According to this proof (Magnus, Karrass & Solitar, 1966), there exists a Nielsen transformation of the n-tuple $[a_1, \ldots, a_n]$ and a simultaneous Nielsen transformation of the m'-tuple $[b_1, \ldots, b_{m'}]$, which yields the generators in question. In fact, this algorithm provides a way of obtaining each of these two Nielsen transformations as a finite sequence of elementary Nielsen transformations.

In the modified algorithm, we use the two following kinds of elementary Nielsen transformation

Consider an arbitrary m'-tuple $[b_1, ..., b_{m'}]$ of elements of A. The elementary Nielsen transformations $\mathcal{B}_{k,l}$ and $\overline{\mathcal{B}}_{k,l}$ act on this m'-tuple as follows:

$$\mathcal{B}_{k,l} : [b_1, \ldots, b_k, \ldots, b_{m'}] \longrightarrow [b_1, \ldots, b_k + b_l, \ldots, b_{m'}]$$
$$\overline{\mathcal{B}}_{k,l} : [b_1, \ldots, b_k, \ldots, b_{m'}] \longrightarrow [b_1, \ldots, b_k - b_l, \ldots, b_{m'}] \qquad (A3.3)$$

where $k, l = 1, \ldots, m'$, $k \neq l$.

The elementary Nielsen transformations can conveniently be translated into matrix form. Following Magnus, Karrass & Solitar (1966), we introduce a titled $n \times m'$ integral matrix $R = (r_{ij})$,

$$b_j = \sum_{i=1}^{n} r_{ij} a_i, \quad j = 1, ..., m'.$$

The following titles are introduced for each row and for each column: b_j for the jth column, and a_i for the ith row. Then, one can write the matrix R as

$$R = \begin{array}{c} \\ a_1 \\ \vdots \\ a_j \\ \vdots \\ a_n \end{array} \begin{array}{c} \begin{array}{ccccc} b_1 & \ldots & b_k & \ldots & b_{m'} \end{array} \\ \begin{pmatrix} r_{11} & \ldots & r_{1k} & \ldots & r_{1m'} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ r_{j1} & \ldots & r_{jk} & \ldots & r_{jm'} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ r_{n1} & \ldots & r_{nk} & \ldots & r_{nm'} \end{pmatrix} \end{array}.$$

We remark that this matrix is simply a translation of the so-called titled exponent sum matrix defined in the original algorithm (Magnus, Karrass & Solitar, 1966) for the case of free Abelian groups.

To each elementary Nielsen transformation, applied either to the a's or to the b's, there corresponds a unique transformation of the titled matrix. If $\mathcal{B}_{.,.}$ is performed on the a's, then just two rows are affected:

$$\mathcal{B}_{i,j} : \begin{cases} a_i \rightarrow a_i + a_j \\ r_{jk} \rightarrow r_{jk} - r_{ik}, \quad k = 1, \ldots, m'. \end{cases} \qquad (A3.4)$$

In the case of the b's only one column is changed:

$$\mathcal{B}_{k,l} : \begin{cases} b_k \rightarrow b_k + b_l \\ r_{jk} \rightarrow r_{jk} + r_{jl}, \quad j = 1, \ldots, n. \end{cases} \qquad (A3.5)$$

One can directly obtain analogous expressions for $\overline{\mathcal{B}}_{.,.}$.

In terms of the titled matrix R, the problem is to find such a sequence of transformations $\mathcal{B}_{.,.}$ and $\overline{\mathcal{B}}_{.,.}$ that will take the titled matrix R into a new titled matrix $\overline{R}$ that has as many non-zero entries as the rank m of the matrix with the titles omitted. The non-zero entries, say $e_1 \equiv r_{j_1 k_1}, \ldots, e_m \equiv r_{j_m k_m}$, will identify those free generators $\overline{\overline{a}}_{j_1}, \ldots, \overline{\overline{a}}_{j_m}$ of A that generate the direct summand D of A that contains B as a subgroup of finite index; the elements $\overline{\overline{b}}_{k_1} \equiv e_1 \overline{\overline{a}}_{j_1}, \ldots, \overline{\overline{b}}_{k_m} \equiv e_m \overline{\overline{a}}_{j_m}$ then freely generate B.

The algorithm to obtain the resulting titled matrix $\overline{R}$, starting from the titled matrix R, consists of m steps in each of which an integer e_i and a free generator $\overline{\overline{a}}_{j_i}$ of T, $i \in \{1,\ldots,m\}$, are produced. We describe the first step.

We suppose that at least one of the b's is non-zero to exclude the trivial case. We choose an entry r_{ij} of R as follows:

(1) Its absolute value is equal to the minimum of the absolute values of all non-zero entries of R. If there are several such entries, condition (2) is applied.

(2) Its column subscript j is not less than the column subscripts of other entries satisfying condition (1). If the jth column contains several such entries, say $r_{i_1j},\ldots,r_{i_kj}$, condition (3) is applied.

(3) Its row subscript i is the greatest of the row subscripts $i_1,\ldots,i_k$.

Selecting an element r_{ij} of R will be called a full-matrix choice procedure.

Then, we repeatedly apply the elementary Nielsen transformations $\mathcal{B}_{k,j}$ or $\overline{\mathcal{B}}_{k,j}$ to the b's and their transforms (*i.e.* we either add or subtract the jth column to or from the kth column, respectively) for such $k \neq j$ for which $|r_{ik}| \geq \frac{1}{2}|r_{ij}|$ until all the entries of the ith row are, in absolute value, less than or equal to $\frac{1}{2}|r_{ij}|$. After each elementary Nielsen transformation, the column titles are appropriately changed according to (A3.5).

Next, we select a new non-zero entry $r_{ij'}$ of the ith row applying conditions (1) and (2) to the ith row. We call this way of selecting an entry of R a column choice procedure relative to the ith row.

Using again the elementary Nielsen transformations $\mathcal{B}_{k,j}$ or $\overline{\mathcal{B}}_{k,j}$, one makes all entries of the ith row, in absolute value, less than or equal to $\frac{1}{2}|r_{ij'}|$ and one changes simultaneously the column titles in an appropriate manner. Then, one applies the column choice procedure relative to the ith row to select a new entry of the ith row and repeats the above procedure with that entry. In such a way, one proceeds until, after a finite number of steps, only one non-zero entry of the ith row is left, say $r_{i\bar{j}}$; its absolute value is equal to the greatest common divisor of all entries of the ith row. If there is no other non-zero entry in the $\bar{j}$th row, the step is over. One has $e_1 \equiv |r_{i\bar{j}}|$ and $\overline{\overline{a}}_{j_1} \equiv a_i$ (since the row titles have not changed).

Otherwise, one applies the elementary Nielsen transformations $\mathcal{B}_{k,i}$ or $\overline{\mathcal{B}}_{k,i}$ to the a's to make all entries of the $\bar{j}$th column less than or equal to $\frac{1}{2}|r_{i\bar{j}}|$. One proceeds in the same way as above, but with the roles of rows and columns interchanged, and transforms the row titles according to (A3.4). Instead of the column-choice procedure relative to the ith row, one analogously introduces a row choice procedure relative to the $\bar{j}$th column. As a result, one obtains only one non-zero entry in the $\bar{j}$th column, say $r_{\bar{i}\bar{j}}$; its absolute value equals the greatest common divisor of all entries of the ith row and $\bar{j}$th column. If $r_{\bar{i}\bar{j}}$ is the only non-zero entry in the $\bar{i}$th row, then the step is over so that $e_1 \equiv |r_{\bar{i}\bar{j}}|$ and $\overline{\overline{a}}_{j_1}$ is given by the title of the $\bar{i}$th row.

Otherwise, one repeats the whole procedure starting with the $\bar{i}$th row as an initial one. After finitely many steps, one arrives at an entry $r_{\bar{\bar{i}}\bar{\bar{j}}}$, which is the only non-zero entry in the $\bar{\bar{i}}$th row as well as in the $\bar{\bar{j}}$th column; its absolute value is equal to the greatest common divisor of all the entries occurring in the rows and columns to which the column- or row-choice procedure was applied. One then has $e_1 \equiv |r_{\bar{\bar{i}}\bar{\bar{j}}}|$ and $\overline{\overline{a}}_{j_1}$ is given by the title of the $\bar{\bar{i}}$th row.

Since after this step one obtains one row and one column, each containing only one non-zero entry so that the zero entries form in most cases a more or less symmetric cross, we call this a cross-nulling procedure.

Using a cross-nulling procedure, one transforms the matrix $R \equiv R^{(0)}$ into a titled matrix R'. From R' we omit both the row and column that constitute a 'cross' in order to get a new titled matrix $R^{(1)}$ upon which the next step is performed. As above, we use the full-matrix choice procedure to choose a starting entry of $R^{(1)}$ and then perform the cross-nulling procedure with $R^{(1)}$. After m steps, where m is the rank of R, one arrives at a titled matrix $R^{(m)}$, which must contain only zero entries. As a result, one obtains the required m integers $e_1,\ldots,e_m$ and n new free generators of T, m of which are determined in the m steps, and the remaining $n-m$ ones are given by the row titles of $R^{(m)}$. The m new generators freely generate the corresponding direct summand of T, either T_0 or T_1.

We note that the titled matrix $\overline{R}$ into which the original matrix R is transformed under simultaneous Nielsen transformations of the a's and of the b's is composed of the 'crosses' (and the corresponding titles), omitted in the above way, and of the titled matrix $R^{(m)}$.

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