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Determination of n-Dimensional Space Groups by Means of an Electronic Computer

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A method is presented to determine the n-dimensional space groups if the arithmetic crystal classes are known. It considers space groups as group extensions and gives a relation between the nonequivalent extensions and a set of vectors in a certain linear vector space. In this way we transform the group extension problem into a problem of linear algebra. In fact the method can be used to determine the nonequivalent extensions of a free Abelian group by an arbitrary finitely generated group. The algorithm has been used to determine four-dimensional space groups by means of an electronic computer.

1. INTRODUCTION

The Euclidean group $IO(n)$ in n dimensions is the group of n-dimensional inhomogeneous linear transformations which leave the distance of any two points invariant. It contains as a subgroup the group of n-dimensional translations R^n and the orthogonal group $O(n)$.[1] An n-dimensional space group G is a subgroup of $IO(n)$ such that its intersection with R^n, $U = G \cap R^n$, (1) is isomorphic to Z^n, the additive group of n-tuples of integers, and (2) is generated by n linearly independent translations. It can easily be shown that U is an invariant subgroup of G and that the factor group G/U is isomorphic to the point group K, which is the subgroup of $O(n)$ consisting of all elements α occurring in elements $\{\alpha \mid u\}$ of G. In the theory of groups this situation is well known. It means that G is an extension of Z^n by K. (For those who are not familiar with group extensions some important concepts are explained in the appendix.[2]) The mapping $\varphi : K \to GL(n, Z)$ which is associated with the extension is a monomorphism, which means that $\varphi(K)$ is a faithful n-dimensional integral representation of K. Moreover, K is finite. The situation can be visualized in the exact sequence

$$1 \longrightarrow Z^n \xrightarrow{\kappa} G \longrightarrow K \longrightarrow 1. \quad (\varphi)$$

[1] The elements of $IO(n)$ can be written as $\{\alpha \mid t\}$ with $\alpha \in O(n)$ and $t \in R^n$.

[2] There also some other group-theoretical notions, used in this paper, are defined.

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On the other hand, each extension of Z^n by a finite group K with a monomorphism $\varphi : K \to GL(n, Z)$ can be imbedded as a space group in $IO(n)$ [1]. Therefore all n-dimensional space groups can be obtained from a knowledge of all extensions of this kind. According to the analysis given by Ascher and Janner [1], it is sufficient to determine all nonisomorphic extensions of Z^n for one representative of each arithmetic crystal class, i.e., of each conjugacy class of finite subgroups of $GL(n, Z)$.

For a given set of representatives of the arithmetic crystal classes the problem is reduced to the determination of all nonisomorphic extensions with these groups $\varphi(K)$. We treat here the first step, the determination of all nonequivalent extensions. Two extensions are called equivalent if there exists an isomorphism $\psi : G \to G'$, which restricted to U is the identity and which induces the identity transformation on G/U, i.e., for which the diagram

$$\begin{array}{ccccccccc} 1 & \longrightarrow & Z^n & \longrightarrow & G & \longrightarrow & K & \longrightarrow & 1 \\ & & \| & & \downarrow{\scriptstyle\psi} & & \| & & \\ 1 & \longrightarrow & Z^n & \longrightarrow & G' & \longrightarrow & K & \longrightarrow & 1 \end{array}$$

is commutative. (A diagram is called commutative if it does not matter in which way one runs through the diagram along the arrows.) The nonisomorphic extensions may then be found if one knows the normalizer of $\varphi(K)$ in $GL(n, Z)$ [2], which is the subgroup of $GL(n, Z)$ of all elements A such that $A\varphi(K)\, A^{-1} = \varphi(K)$.

To determine all nonequivalent extensions one can make use of a theorem by Hall [3]. The extensions are determined by a set of generators and defining relations. Suppose K is generated as an abstract group by elements $\alpha_1, \ldots, \alpha_\nu$ with defining relations $\phi_i(\alpha_1, \ldots, \alpha_\nu) = \epsilon$ $(i = 1, \ldots, t)$. Consider the decomposition of the extension G in cosets of Z^n and choose in each coset a representative. The representative of the coset which is mapped by σ on $\alpha \in K$ is denoted by $r(\alpha)$. Then each element $g \in G$ can uniquely be written as (we use the additive notation for G and Z^n)

$$g = a + r(\alpha) \qquad (a \in Z^n, \alpha \in K).$$

Because $r(\alpha) + r(\beta) = m(\alpha, \beta) + r(\alpha\beta)$ for some element $m(\alpha, \beta) \in Z^n$, the group G is generated by $a_1, \ldots, a_n, r(\alpha_1), \ldots, r(\alpha_\nu)$, where $a_1, \ldots, a_n$ form a basis for Z^n. Because the elements $\phi_i(r(\alpha_1), \ldots, r(\alpha_\nu)) \in G$ are mapped by σ on the unit of K, there exist elements $g_1, g_2, \ldots, g_t$ in Z^n such that

$$\phi_i(r(\alpha_1), \ldots, r(\alpha_\nu)) = g_i \qquad (i = 1, \ldots, t).$$

These relations, together with the relations

$$r(\alpha) + a - r(\alpha) = \varphi(\alpha)a \qquad (\text{all } \alpha \in K, \quad \text{all } a \in Z^n),$$

determine G completely. However not every set $\{g_1, ..., g_t\}$ of elements of Z^n determines an extension. A necessary and sufficient condition on these elements can be found as follows. The integral group ring of K consists of all elements $\sum_\alpha m_\alpha \alpha$, where m_α are integers. The elements of the integral group ring operate on $u \in Z^n$ by

$$\left(\sum_\alpha m_\alpha\right) u = \sum_\alpha m_\alpha(\varphi(\alpha)\, u). \tag{1}$$

Now suppose that another set of coset representatives is chosen. Then one has $r'(\alpha) = u(\alpha) + r(\alpha)$ (all $\alpha \in K$; $u(\alpha) \in Z^n$). Then there exist elements $\pi_i(\alpha_j)$ of the integral group ring of K such that

$$\phi_i(r'(\alpha_1), ..., r'(\alpha_\nu)) = \sum_{j=1}^{\nu} \pi_i(\alpha_j)\, u(\alpha_j) + g_i\,.$$

Because of relation (1) an element of the integral group ring corresponds for fixed $\varphi(K)$ to a $n \times n$ matrix. Denote nt by p and $n\nu$ by q. Define a p-dimensional supervector build from $g_1, ..., g_t \in Z^n$,

$$\phi = \begin{pmatrix} g_1 \\ \vdots \\ g_t \end{pmatrix} \in Z^p,$$

and a $p \times q$ matrix,

$$\Pi = \begin{pmatrix} \pi_1(\alpha_1) & \cdots & \pi_1(\alpha_\nu) \\ \vdots & & \vdots \\ \pi_t(\alpha_1) & \cdots & \pi_t(\alpha_\nu) \end{pmatrix}.$$

Using the theorem mentioned before one can show [2] that ϕ determines an extension if and only if ϕ belongs to the discrete point set $\Pi R^q \cap Z^p$, i.e., all points in Z^p which can be obtained by the supermatrix from a vector in the real linear space R^q. Moreover ϕ and ϕ' determine equivalent extensions if and only if $\phi - \phi'$ is an element of the point set ΠZ^q. If one defines the sum of two relation vectors ϕ and ϕ' by their vector sum the elements of $\Pi R^q \cap Z^p$ form an Abelian group. A subgroup of this group is formed by all elements of ΠZ^q. Therefore to determine all nonequivalent extensions of Z^n by a finite group K one has to determine the factor group

$$(\Pi R^q \cap Z^p)/\Pi Z^q. \tag{2}$$

This Abelian group is isomorphic to the groups $\mathrm{Ext}(K, Z^n, \varphi) \cong H_\varphi{}^2(K, Z^n)$

which are well known in the theory of group extensions. The present group extension problem may be solved by the determination of the group (2). In this way we have transformed the group extension problem to a problem in linear algebra. We give here an algorithm for its solution which is well suited for treatment by a computer. We note that the same method can be used for the determination of the nonequivalent extensions of Z^n by an arbitrary finitely generated group, which is not necessarily finite or for which φ is not a monomorphism.

2. Determination of the Nonequivalent Extensions

To determine the elements of the set (2) one applies automorphisms $P \in GL(p, Z)$ and $Q \in GL(q, Z)$ such that the matrix $P\Pi Q$ has the form

$$\Pi' = P\Pi Q = \begin{pmatrix} d_1 & & & 0 \\ & d_2 & & \\ & & \ddots & \\ 0 & & & d_q \end{pmatrix}, \qquad d_i \geqslant 0. \tag{3}$$

This may be achieved as follows. Suppose the elements of Π are zero in the first $k - 1$ rows and columns, possibly with exception of the diagonal places. Then consider the k-th row. If there is only one nonzero element in this row, say on place (k, l), interchange the k-th and l-th columns. If there are more than one nonzero elements, either one of the row elements is a common divisor to all other row elements, or such a common divisor does not occur. In the first case, if a common divisor occurs in the l-th column, subtract this column as many times from the other ones as necessary to make all elements in the k-th row zero except the l-th one. Then interchange the k-th and l-th columns. In the other case consider two nonzero elements in the k-th row and apply the Euclidean algorithm to these elements. This means that one subtracts the column with the element of smaller absolute value as many times from the other one as necessary to make the resulting element in the k-th row smaller in absolute value than the element in the former column. Proceeding in this way one obtains zero in one column and the g.c.d. in the other one. This can be continued with other pairs of elements of the k-th row till only at most one nonzero element is left in this row. This element can be brought to the k-th column.

In the same way one proceeds in the k-th column. After this procedure the elements in the k-th row are either still zero or nonzero elements have been produced. In the former case continue with the $(k + 1)$-th row, in the latter case repeat the algorithm for the k-th row and column. Because the number of prime factors is finite, one reaches in a finite number of steps the situation where both k-th row and column have atmost one nonzero element on the (k, k) place.

The given procedure results in a matrix which has the required form (3). If E_{ij} is a matrix with only one nonzero element (which is equal to 1) on the (i, j) place, all steps in the procedure are given by right or left multiplication by matrices,

$$X_{ij} = 1 + E_{ij} ,$$
$$N_{ii} = 1 - 2E_{ii} ,$$
$$Y_{ij} = 1 + E_{ij} + E_{ji} - E_{ii} - E_{jj} ,$$

where $i, j = 1,..., p$ for left multiplication and $i, j = 1,..., q$ for right multiplication. The product of all matrices occurring in right multiplications is denoted by Q, the product of the other matrices by P. The matrices P and Q satisfy relation (3).

Consider now the set

$$(\Pi' R^q \cap Z^p)/\Pi' Z^q. \tag{4}$$

The elements of this set are given by

$$\phi' = \sum_{i=1}^{q} n_i \epsilon_i ,$$

where ϵ_i is an element of Z^p with i-th component equal to one and everywhere else zero; n_i is an integer given by

$$n_i = \begin{cases} 0 & \text{if } \ d_i = 0 \text{ or } 1, \\ 0,\ 1,..., d_i - 1 & \text{otherwise.} \end{cases}$$

If ϕ' is an element of the set (4), $\phi = P^{-1}\phi'$ is an element of (2). Hence the nonequivalent extensions are given by the relation vectors

$$\phi = P^{-1}\phi' = \sum_{i=1}^{q} n_i P^{-1} \epsilon_i . \tag{5}$$

Define a $p \times q$ matrix A with elements

$$A_{ij} = \delta_{ij} \times \begin{cases} 1 & \text{if } \ d_i > 1, \\ 0 & \text{if } \ d_i = 0 \text{ or } 1. \end{cases}$$

The columns e_i $(i = 1,..., q)$ of $P^{-1}A$ are generators for the group (2) if we identify $d_i e_i$ and zero. The Abelian group (2) is a direct product of cyclic groups C_{m_i} (m_i are the numbers d_i which are greater than one). The cyclic group C_{m_i} is generated by e_i and has order m_i. In other words, the numbers d_i greater than one are the torsion numbers of the group (2), hence of Ext(K, Z^n, φ).

The split extensions, which are equivalent to the semidirect product and which give rise to the symmorphic space groups, correspond to

$$\phi = \sum_{i=1}^{q} m_i(d_i e_i) \quad (m_1, ..., m_q \text{ arbitrary integers}).$$

This subgroup is generated by the vectors $d_i P^{-1} \epsilon_i$ ($i = 1, ..., q$). These are the columns of $P^{-1}\Pi'$.

3. Nonprimitive Translations

Since K is finite and φ a monomorphism, G may be imbedded as an n-dimensional space group in $IO(n)$. Hence its elements may be written as $\{\alpha \mid u(\alpha)\}$, which is defined by

$$\{\alpha \mid u(\alpha)\} : r \to \alpha r + u(\alpha) \qquad (r \in R^n, u(\alpha) \in R^n, \alpha \in K).$$

The element $u(\alpha)$ corresponding to $\alpha \in K$ is defined up to an element of Z^n.

According to Ref. [2] a system of nonprimitive translations $\{u(\alpha)\}_{\alpha \in K}$ is already determined by $u(\alpha_1), ..., u(\alpha_\nu)$ because of the relation

$$u(\alpha\beta) \equiv u(\alpha) + \alpha u(\beta) \qquad (\text{mod } Z^n).$$

If $u(\alpha_1), ..., u(\alpha_\nu)$ determine a system of nonprimitive translations, a relation vector is given by

$$\begin{aligned} g_i &= \phi_i(r(\alpha_1), ..., r(\alpha_\nu)) \\ &= \phi_i(\{\alpha_1 \mid u(\alpha_1)\}, ..., \{\alpha_\nu \mid u(\alpha_\nu)\}). \end{aligned}$$

On the other hand, a system of nonprimitive translations is found as follows for a given relation vector ϕ.

Define a diagonal $q \times p$ matrix D by

$$D_{ij} = \begin{cases} d_i^{-1}\delta_{ij} & \text{if } d_i \neq 0, \\ 0 & \text{if } d_i = 0. \end{cases}$$

Then according to Ref. [2] there corresponds to a relation vector (5)

$$\phi = \sum_{i=1}^{q} n_i P^{-1} \epsilon_i$$

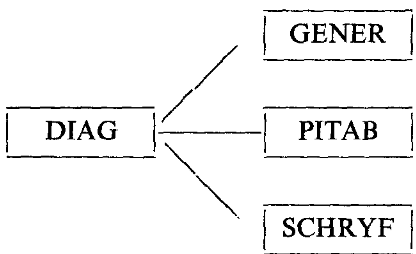
a system $u(\alpha_1),\ldots, u(\alpha_\nu)$ given by a vector $U \in R^q$,

$$\begin{pmatrix} u(\alpha_1) \\ \vdots \\ u(\alpha_\nu) \end{pmatrix} = U = QD\phi' = \sum_{i=1}^{q} n_i QD\epsilon_i \,.$$

Also the set of elements U corresponding to nonequivalent extensions can be given the structure of an Abelian group. It is isomorphic to $\mathrm{Ext}(K, Z^n, \varphi)$. The element U corresponding to $\phi = e_i$ is given by $QD\epsilon_i$, which is the i-th column of QD. Therefore the columns of QD generate the group of nonequivalent systems of nonprimitive translations if we identify d_i times the i-th column with zero. This result is in fact the same as that obtained by Zassenhaus [4]. The relation between his method and the present one is discussed in Ref. [2].

4. Program

A FORTRAN program has been written for the determination of the group (2) for given $\varphi(K)$. The program was restricted to $n \leqslant 4$ and to 25 isomorphism classes of the real $(3 + 1)$-reducible four-dimensional crystallographic point groups. These correspond to the three-dimensional magnetic groups. However this restriction is not essential.



GENER. The group $\varphi(K)$ may be given by its isomorphism class and its generating matrices. As two groups $\varphi(K)$ and $\varphi'(K)$, which are conjugated in $GL(n, R)$ but not in $GL(n, Z)$, are linked by a matrix T from $GL(n, R)$, it is sufficient to give the generating matrices of one representative of each geometric crystal class (i.e., conjugacy class in $GL(n, R)$) and a conjugation matrix T for each representative point group from an arithmetic crystal class in the same geometric crystal class. The subroutine GENER calculates $\varphi(\alpha_j) = T\bar{\varphi}(\alpha_j)\, T^{-1}$, where $\bar{\varphi}(\alpha_1),\ldots, \bar{\varphi}(\alpha_\nu)$ are generators for the representative group $\bar{\varphi}(K)$ of the geometric crystal class.

PITAB. For each isomorphism class the integral group ring elements $\pi_i(\alpha_j)$ are known. Because of relation (1) they can be represented by $n \times n$ matrices.

For given elements $\pi_i(\alpha_j) = \sum_{\alpha \in K} m_\alpha^{ij} \alpha$ these matrices are given by

$$\varphi(\pi_i(\alpha_j)) = \sum_{\alpha \in K} m_\alpha^{ij} \varphi(\alpha).$$

The matrices $\varphi(\pi_i(\alpha_j))$ are calculated for given m_α^{ij} and with the $\varphi(\alpha_j)$ from GENER. From these matrices $\varphi(\pi_i(\alpha_j))$ the supermatrix Π is constructed by the subroutine PITAB.

DIAG. The main program diagonalizes the matrix Π according to the procedure given in Section 2. It keeps the matrices Π', $P^{-1}A$, P^{-1}, and QD.

SCHRYF. This subroutine prints the matrices $P^{-1}A$, $P^{-1}\Pi'$, and QD, which give the nonequivalent relation vectors, the split extensions, and the nonequivalent systems of nonprimitive translations. Finally it prints the diagonal elements of Π' which are greater than one. These give the torsion numbers of $\mathrm{Ext}(K, Z^n, \varphi)$.

A typical example is given by the three-dimensional arithmetic crystal class $P4/m$. Its isomorphism class is $C_4 \times C_2$ and a point group from this class is generated by

$$\varphi(\alpha_1) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad \varphi(\alpha_2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

A group $C_4 \times C_2$ is generated by α_1 and α_2 with defining relations $\alpha_1{}^4 = \alpha_2{}^2 = \alpha_1\alpha_2\alpha_1^{-1}\alpha_2^{-1} = \epsilon$. Therefore $\nu = 2$, $t = 3$. The integral group ring elements $\pi_i(\alpha_j)$ are given by

$$\pi_1(\alpha_1) = 1 + \alpha_1 + \alpha_1{}^2 + \alpha_1{}^3, \qquad \pi_2(\alpha_2) = 1 + \alpha_2\,,$$

$$\pi_3(\alpha_1) = 1 - \alpha_2\,, \qquad \pi_3(\alpha_2) = \alpha_1 + \alpha_2\,.$$

The other ones are zero.

The program gives for the matrices $P^{-1}A$, $P^{-1}\Pi'$, QD, respectively,

0 0 0 0 0 0	0 0 0 0 0 0	0 0 0 0 0 0 0 0 0
0 0 0 0 0 0	0 0 0 0 0 0	0 0 0 0 0 0 0 0 0
2 0 0 0 0 0	4 0 0 0 0 0	$\frac{1}{2}$ 0 0 0 0 0 0 0 0
0 1 0 0 0 0	0 2 2 0 0 0	0 $\frac{1}{2}$ 1 0 0 0 0 0 0
0 1 0 0 0 0	0 2 0 0 0 0	0 $\frac{1}{2}$ 0 0 0 0 0 0 0
0 0 0 0 0 0	0 0 0 0 0 0	0 0 0 0 0 0 0 0 0
0 0 0 0 0 0	0 0 1 0 0 0	
0 1 0 0 0 0	0 2 1 0 0 0	
1 0 0 0 0 0	2 0 0 0 0 0	

Therefore the group $\mathrm{Ext}(K, Z^n, \varphi)$ is isomorphic to $C_2 \times C_2$. Its four elements are given, either by the relations

$$\begin{array}{rcccc} & \text{(i)} & \text{(ii)} & \text{(iii)} & \text{(iv)} \\ 4r(\alpha_1) = & \begin{pmatrix}0\\0\\0\end{pmatrix} & \begin{pmatrix}0\\0\\2\end{pmatrix} & \begin{pmatrix}0\\0\\0\end{pmatrix} & \begin{pmatrix}0\\0\\2\end{pmatrix} \\ 2r(\alpha_2) = & \begin{pmatrix}0\\0\\0\end{pmatrix} & \begin{pmatrix}0\\0\\0\end{pmatrix} & \begin{pmatrix}1\\1\\0\end{pmatrix} & \begin{pmatrix}1\\1\\0\end{pmatrix} \\ r(\alpha_1) + r(\alpha_2) - r(\alpha_1) - r(\alpha_2) = & \begin{pmatrix}0\\0\\0\end{pmatrix} & \begin{pmatrix}0\\0\\1\end{pmatrix} & \begin{pmatrix}0\\1\\0\end{pmatrix} & \begin{pmatrix}0\\1\\1\end{pmatrix} \end{array}$$

or by the nonprimitive translations

$$\begin{array}{rcccc} u(\alpha_1) = & \begin{pmatrix}0\\0\\0\end{pmatrix} & \begin{pmatrix}0\\0\\\frac{1}{2}\end{pmatrix} & \begin{pmatrix}0\\0\\0\end{pmatrix} & \begin{pmatrix}0\\0\\\frac{1}{2}\end{pmatrix} \\ u(\alpha_2) = & \begin{pmatrix}0\\0\\0\end{pmatrix} & \begin{pmatrix}0\\0\\0\end{pmatrix} & \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\0\end{pmatrix} & \begin{pmatrix}\frac{1}{2}\\\frac{1}{2}\\0\end{pmatrix} \end{array}$$

Comparing these groups with the space groups in the International Tables for *x*-ray crystallography [7] one finds that the first one is the group *nr* · 83 ($P4/m$ or C_{4h}^1). It is a symmorphic group. Our second group is *nr* · 84 ($P4_2/m$ or C_{4h}^2) in the tables as one finds comparing the nonprimitive translations. The third one is group *nr* · 85 ($P4/n$ or C_{4h}^4) up to a change of origin. A change of origin f causes a change in the nonprimitive translations given by $u'(\alpha) = u(\alpha) + (1 - \alpha)f$. In the same way our last group corresponds to *nr* · 86 ($P4_2/n$ or C_{4h}^4) in the tables after a change of origin.

The program has run on the IBM 360/40 computer of the University of Nijmegen for all three-dimensional and (3 + 1)-reducible four-dimensional crystal classes [5]. For the three-dimensional case we have taken one representative from each of the 73 arithmetic crystal classes. The number of nonequivalent extensions with these 73 groups is 305. In order to obtain the nonisomorphic extensions one can apply the techniques explained in Ref. [2]. However, in this case identification of the isomorphic groups is easily made without knowledge of the complete normalizers. It turns out that among the 305 nonequivalent extensions there are 219 nonisomorphic ones. It has been verified that each of these 219 nonisomorphic groups corresponds to one of the 219 groups in the International Tables, in the way sketched for the example. Proceeding to the four-dimensional case one finds for the 412 four-dimensional (3 + 1)-reducible crystal classes a number of

11,187 nonequivalent extensions. For each crystal class it is possible to determine the nonisomorphic extensions, but this was not done in a systematic fashion. The calculation and the results are published as a technical report [6].

After we did these calculations we obtained a computer program by H. Brown, who uses the Zassenhaus algorithm for his calculation. It turned out that his program gives the same nonprimitive translations as does our own program.

Appendix

A group B is called an *extension* of a group A by a group C if B contains an invariant subgroup A' isomorphic to A such that B/A' is isomorphic to C. In the following we take for A an Abelian group. Although B is in general not an Abelian group we use for the groups A and B the additive notation. One can decompose B in right cosets of A',

$$B = \bigcup_i (A' + g_i).$$

The right cosets $(A' + g_i)$ are the elements of the factor group B/A'. Therefore one can write $g_i = r(\alpha_i)$, where r is a one-to-one mapping of C into B. The elements $r(\alpha)$, with $\alpha \in K$, are the *coset representatives.* Any element b of B can be written in a unique way as $b = a + r(\alpha)$ for some $a \in A'$ and $\alpha \in K$. An element $r(\alpha)$ determines an inner automorphism of B by $b \to r(\alpha) + b - r(\alpha)$. In particular, $r(\alpha)$ determines an automorphism $\varphi(\alpha)$ of A' by $\varphi(\alpha)a = r(\alpha) + a - r(\alpha)$, because A' is an invariant subgroup of B. This mapping of C into the group of automorphisms of A' does not depend on the choice of the coset representatives. If $r'(\alpha) = a(\alpha) + r(\alpha)$ with $a(\alpha) \in A'$ are other coset representatives, one has $\varphi'(\alpha)a = r'(\alpha) + a - r'(\alpha) = a(\alpha) + r(\alpha) + a - r(\alpha) - a(\alpha) = \varphi(\alpha)a$, because A' is Abelian. As A and A' are isomorphic groups φ is also a mapping of C into the group of automorphisms of A.

The group A' is a subgroup of B. Therefore, there is a one-to-one homomorphism of A into B (a *monomorphism* $\kappa : A \to B$). On the other hand the mapping σ which assigns to each element of B the coset to which it belongs, i.e., $\sigma(a + r(\alpha)) = \alpha$, is a homomorphism of B onto C (an *epimorphism* $\sigma : B \to C$). Moreover, the image Im $\kappa = A'$ is exactly the kernel of σ, which is the subgroup of B which is mapped on the unit element of C. A sequence of groups connected by homomorphisms $\cdots G_1 \xrightarrow{\Psi_1} G_2 \xrightarrow{\Psi_2} G_3 \cdots$ is called *exact* at G_2 if Im $\Psi_1 =$ Ker Ψ_2. Therefore we have an exact sequence

$$1 \longrightarrow A \xrightarrow[\kappa]{} B \xrightarrow[\sigma]{} C \longrightarrow 1.$$

Notice that the exactness at A means that κ is a monomorphism, whereas the exactness at C means that σ is an epimorphism. In general the mapping $r : C \to B$ is not a homomorphism. If there is a choice of coset representatives such that $r(\alpha) + r(\beta) = r(\alpha\beta)$, the elements $r(\alpha)$ form a group isomorphic to C. In that case the extension splits and B is called the *semidirect product* of A and C. A symmorphic space group G is a semidirect product, because here the point group K is a subgroup of G.

Some other notions which require perhaps a definition are the following. Let H be a subgroup of G and g an element of G. Then gHg^{-1} is again a subgroup of G, called a conjugate subgroup. All subgroups of G conjugate to H form the *conjugacy class* of H. As this is an equivalence class (conjugation is an equivalence relation) the set of subgroups of G can be decomposed in nonoverlapping conjugacy classes. The arithmetic crystal classes are the conjugacy classes of arithmetic point groups in the group $GL(n, Z)$. If $gHg^{-1} = H$ the element g is a normalizer element of H. All normalizer elements of H form the *normalizer* of H in G. If G is the normalizer of H, i.e., if $gHg^{-1} = H$ for any $g \in G$, the group H is an *invariant* subgroup. For a group G a set of elements is called a *set of generators* if any element of G can be written as a product of generators. In general there are relations between the generators, which means that the unit element can be written as a product of generators. As an example consider a finite group. Any element, hence any generator is of finite order. Therefore for a generator g one has $g^n = 1$ for some integer n. If a set of relations completely determines a group it is called a set of *defining relations*. A very simple example is the following. For a finite group we can take all elements as generators. Then the multiplication table gives a set of defining relations. If $ab = c$, one has $abc^{-1} = 1$.

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