Crystallography of quasicrystals ; application to icosahedral symmetry

L.S. Levitov, J. Rhyner

J. Phys. France **49** (1988) 1835-1849 NOVEMBRE **1988**, PAGE 1835

Classification
Physics Abstracts
61.10D — 61.14D — 61.50E

Crystallography of quasicrystals ; application to icosahedral symmetry

L. S. Levitov (1) and J. Rhyner (2,3)

(1) L. D. Landau Institute for Theoretical Physics, USSR Academy of Sciences, Moscow, U.S.S.R.
(2) Institute for Theoretical Physics, ETH-Hönggerberg, CH-8093 Zürich, Switzerland
(3) Asea Brown Boveri, Corporate Research, CH-5405 Baden, Switzerland (*)

(Reçu le 11 mai 1988, accepté sous forme définitive le 28 juin 1988)

Résumé. — Les concepts de la cristallographie sont étendus aux structures quasicristallines et appliqués aux quasicristaux icosaédriques. On montre que les symétries de rotation d'ordre N bidimensionnelles sont compatibles avec les réseaux de Bravais en dimension $\varphi(N)$ (au moins), où $\varphi(N)$ est le nombre d'Euler, alors que pour la symétrie de l'icosaèdre tridimensionnelle, la dimension minimale est 6. La cristallographie de l'icosaèdre est traitée en détail. Une classification complète des structures périodiques en six dimensions avec symétrie icosaédrique est dérivée. Il est surprenant de voir qu'il n'y a que quelques types d'« objets cristallographiques » en 6 dimensions avec la symétrie de l'icosaèdre, en fait trois structures type réseaux de Bravais, deux groupes ponctuels et onze groupes d'espace inéquivalents. Le problème de l'équivalence des groupes d'espace icosaédriques est étudié en détail. Comme dans le cas des cristaux ordinaires à trois dimensions, les symétries de groupes d'espace non « symmorphes » conduisent à l'extinction des pics de Bragg. Ces extinctions sont calculées systématiquement.

Abstract. — Crystallographic concepts are extended to quasicrystalline structures and applied to icosahedral quasicrystals. 2-dimensional N-fold rotational symmetries are shown to be compatible with Bravais lattices in (at least) $\varphi(N)$ dimensions, where $\varphi(N)$ is the *Euler number,* while for 3-dimensional icosahedral symmetry the minimal dimension is 6. The case of icosahedral crystallography is worked out in detail. A complete classification of six-dimensional periodic structures with icosahedral symmetry is derived. There are surprisingly few types of 6-dimensional « crystallographic objects » with icosahedral symmetry, namely 3 Bravais lattice types, 2 point groups, and 11 inequivalent space groups. The problem of equivalence of icosahedral space groups is studied in detail. Similar to the case of ordinary 3-dimensional crystals, non-symmorphic space group symmetries lead to extinction of Bragg peaks. These extinctions are calculated systematically.

1. Introduction.

Quasicrystals are well known to have *crystallographically forbidden symmetries,* i.e. they have no underlying Bravais lattice. However, these noncrystallographic symmetries are compatible with Bravais lattices in higher-dimensional spaces (by some authors called *superlattices* and *superspaces,* respectively). This connection between a quasicrystal and a higher-dimensional crystal is the basis of the projection method which has been widely used for the construction and description of quasicrystalline structures (see [1] and Refs. therein). The concept of superspace and superlattices is older than quasicrystals. It has been used to describe incommensurate structures, such as TTF-TCNQ [2, 3, 4].

The association of quasicrystals to higher-dimensional crystals opens a way to the application of crystallographic concepts to quasicrystals. In this work we describe the principles of the extension of crystallographic methods to quasicrystals (« quasicrystallography »). We first illustrate these ideas with the discussion of N-fold rotational symmetries in 2 dimensions, and then give a detailed application to *icosahedral quasicrystals* which have been discovered in 1984 by Schechtman *et al.* [5]. Icosahedral quasicrystals can be associated with a Bravais lattice

(*) *Present and permanent address.*

whose dimension is at least 6 (a group theoretical proof is given in Sect. 3). In this article we derive a complete classification of all 6-dimensional periodic structures with icosahedral symmetry, i.e. we calculate all 6-dimensional icosahedrally symmetric Bravais lattice types, point groups, and space groups. Such a classification is useful for the interpretation of experimental data (diffraction experiments), but also valuable in itself. Some of the main results can be found in [6].

The paper is organized as follows. In the next section we describe the general principles for the extension of crystallography to quasicrystals and apply them to *2-dimensional N-fold rotational symmetries*. The application to icosahedral symmetry follows in section 3 where we also describe the two icosahedral point groups. In section 4 the icosahedral Bravais lattices in 6 dimensions are classified. It is shown that there are only 3 inequivalent Bravais lattices types. Section 5 contains some general remarks about space groups and a detailed discussion of the problem of *space group equivalence,* followed by the calculation of the space groups. Like in ordinary 3-dimensional crystallography nonsymmorphic space group symmetries lead to extinctions of Bragg peaks. These extinctions are calculated systematically in section 6.

Some of the problems treated in this article have been addressed before by other authors. While there are some incorrect statements about the number of possible Bravais lattices [7, 8], Janssen [9] gives the correct lattices but offers no proof that no more exist. Recently several proofs have been given [10-12] which are somewhat different from the one presented in section 4. It should be mentioned that Plesken and Hanrath [13] earlier presented a complete classification of all six-dimensional Bravais lattice types, finding a total number of 826. However, their analysis, based on integral representation theory of finite groups, relies on extensive computer calculations, whereas our treatment, which is restricted to the icosahedral point groups, needs only elementary group theory and can be done analytically.

A classification of space groups has been given by Janssen [9]. His results do not completely agree with ours : He finds 16 space groups instead of our 11. This discrepancy requires a careful discussion of the question of space group equivalence. If, besides coordinate shifts and point group elements, only the inversion is taken as an equivalence transformation (as in 3-dimensional crystallography), we end up with exactly the 16 space groups of Janssen. However, we will show that some of these space groups are equivalent *via* the so-called quasidilatations (« inflation-deflation transformations »). In contrast to the involved algorithm used by Janssen [9] our calculation uses only simple linear algebra.

2. Extension of crystallography to quasicrystals ; 2-dimensional quasicrystalline symmetries.

In this section we describe the general ideas for extending crystallographic methods to quasicrystals and apply them to the simple case of plane noncrystallographic symmetries, i.e. N-fold symmetries with $N = 5$ or $N \geq 7$.

2.1 GENERAL PRINCIPLES. — The basic step is the connection of a quasicrystal to a higher-dimensional crystal. This is the key idea of the projection method which has been widely used for the description of quasicrystals (see [1] and references therein). In order to allow for a rigorous mathematical treatment let us specify this idea in terms of group theory : A d-dimensional ($d = 1, 2$ or 3) quasicrystal is said to have point symmetry group G, if its Fourier transform has point symmetry group G. However, G is not compatible with a d-dimensional Bravais lattice, at it would be for ordinary crystals. We therefore look for a D-dimensional ($D > d$) representation $\mathfrak{D}_D$ of G which can be viewed as the point group of some D-dimensional Bravais lattice $\mathfrak{L}$ (here and in the following the lower index of a representation always denotes its dimension). Such a representation has to satisfy two important conditions :

(i) The characters of $\mathfrak{D}_D$ are integers.

(ii) $\mathfrak{D}_D$ contains the standard representation $\mathfrak{D}_d^S$ of G, which is given by all $d \times d$-matrices of orthogonal transformations leaving the quasicrystal diffraction pattern invariant (hence $\mathfrak{D}_D$ is reducible).

The first restriction follows from the requirement that $\mathfrak{D}_D$ is the point group of a Bravais lattice $\mathfrak{L}$. Consider the matrices of $\mathfrak{D}_D$ written in a basis of $\mathfrak{L}$. Since $\mathfrak{L}$ is invariant under all elements of $\mathfrak{D}_D$, all lattice vectors are transformed into lattice vectors. Consequently, all entries of the $\mathfrak{D}_D$-matrices are integers and hence the characters of $\mathfrak{D}_D$ as well. The meaning of the second condition becomes clear by formulating the projection method in the above group theoretical terms. If $\mathfrak{D}_D$ satisfies condition (ii), then this representation has a d-dimensional invariant subspace $E_\parallel^d$ corresponding to the standard representation $\mathfrak{D}_d^S$. It is this subspace onto which a « strip » of $\mathfrak{L}$ is projected [7, 14]. $E_\parallel^d$ is called the *physical subspace.* The structure factor of the resulting d-dimensional quasiperiodic structure has exactly point group symmetry G or $\mathfrak{D}_d^S$ respectively. This is easily seen by considering the method for the Fourier transformation of quasiperiodic structures by means of the projection formalism [14].

In the following a representation of a point group G that satisfies the condition (i) and (ii) will be called a *crystallographic representation* of G. In most cases we are interested in dimensions as low as possible, just for the sake of mathematical simplicity. The crystallographic representation of G with minimal dimension will be called the *minimal crystallographic representation* of G. For a d-dimensional crystal with point group G, the minimal crystallographic representation has dimension d, for a d-dimensional quasicrystal this dimension is larger than d.

Given a (noncrystallographic) point group G, the « construction of the crystallography of G » can now simply be described as follows : Find the minimal crystallographic representation $\mathfrak{D}_D$ of G and then classify all D-dimensional periodic structures with point group $\mathfrak{D}_D$. In the following sections we will carry out this program for the icosahedral point groups. Before doing so we briefly sketch the application of the above theory to another important class of quasicrystalline symmetries, namely to

2.2 2-DIMENSIONAL NONCRYSTALLOGRAPHIC SYMMETRIES.— In 2 dimensions the noncrystallographic point groups are just the symmetry groups G_N of the regular N-gons with $N = 5$ and $N \geq 7$. In the rest of this section we outline the construction of the minimal crystallographic representations of the groups G_N. We first restrict our attention to the *cyclic groups* $C_N \subset G_N$. C_N is the group of all proper rotations that leave the regular N-gon invariant :

$$C_N = \{\mathbf{E}, \mathbf{R}_{(N)}, \mathbf{R}_{(N)}^2, \ldots, \mathbf{R}_{(N)}^{N-1}\} . \quad (2.1)$$

Here $\mathbf{E}$ is the identity and $\mathbf{R}_{(N)}$ the $\frac{2\pi}{N}$-rotation around the origin. The standard representation of C_N is

$$\mathfrak{D}_2^S(N) : \left\{ \mathbf{R}_{(N)}^l \to \begin{pmatrix} \cos\left(\frac{2\pi l}{N}\right) & -\sin\left(\frac{2\pi l}{N}\right) \\ \sin\left(\frac{2\pi l}{N}\right) & \cos\left(\frac{2\pi l}{N}\right) \end{pmatrix}, l = 0, \ldots, N-1 \right\} \quad (2.2)$$

Since C_N is an Abelian group, all its irreducible representations are 1-dimensional. They are given by

$$\mathfrak{D}_1^l(N) : \left\{ \mathbf{R}_{(N)}^m \to e^{\frac{2\pi i}{N} lm} \quad m = 0, \ldots, N-1 \right\} . \quad (2.3)$$

The standard representation $\mathfrak{D}_2^S(N)$ has the decomposition

$$\mathfrak{D}_2^S(N) = \mathfrak{D}_1^1(N) \oplus \mathfrak{D}_1^{(N-1)}(N) . \quad (2.4)$$

The characters of all irreducible representations $\mathfrak{D}_1^l(N)$ of C_N are given by the following matrix :

$$(\chi ij) = \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & c & c^2 & \cdots & c^{N-1} \\ 1 & c^2 & c^4 & \cdots & c^{2(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & c^{(N-1)} & c^{2(N-1)} & \cdots & c^{(N-1)^2} \end{pmatrix} \quad (2.5)$$

where χij is the character of the group element $\mathbf{R}_{(N)}^i$ in the representation $\mathfrak{D}_1^j(N)$ and $c = \exp\left(\frac{2\pi i}{N}\right)$.

The character table (2.5) together with (2.4) allows us at once to write down a crystallographic representation of C_N :

$$\mathfrak{D}_N \equiv \bigoplus_{l=0}^{N-1} \mathfrak{D}_1^l(N) . \quad (2.6)$$

However, $\mathfrak{D}_N$ is not the *minimal* crystallographic representation ; with the help of (2.5) it is not difficult to construct the latter. It is given by

$$\mathfrak{D}^{\min}(N) \equiv \bigoplus_{l \in \delta_N} \mathfrak{D}_1^l(N) , \quad (2.7)$$

where δ_N is the set of all integers between 1 and $N-1$, with which N has no common divisor. The dimension of $\mathfrak{D}^{\min}(N)$ is equal to the number of elements of the set δ_N. It is the so-called *Euler number or Euler function* $\varphi(N)$ [15]. If N is prime then $\varphi(N) = N - 1$.

Without proof we note that the minimal crystallographic representation of the whole symmetry group $G_N \supset C_N$ of the regular N-gon has also dimension $\varphi(N)$. We thus arrive at the result that

The minimal dimension, in which 2-dimensional N-fold rotational symmetries are compatible with Bravais lattices, is $\varphi(N)$ dimensions.

There are methods for the construction of quasiperiodic structures with arbitrary N-fold symmetry [16]. Several quasicrystals with 2-dimensional noncrystallographic symmetries have been observed to date (they are periodic in the direction perpendicular to the quasiperiodic plane) namely *octagonal* ($N = 8$) [17], *decagonal* ($N = 10$) [18, 19] and *dodecagonal* ($N = 12$) [20] quasicrystals. For all these point group symmetries the minimal dimension in which a Bravais lattice exists, is 4 : $\varphi(8) = \varphi(10) = \varphi(12) = 4$.

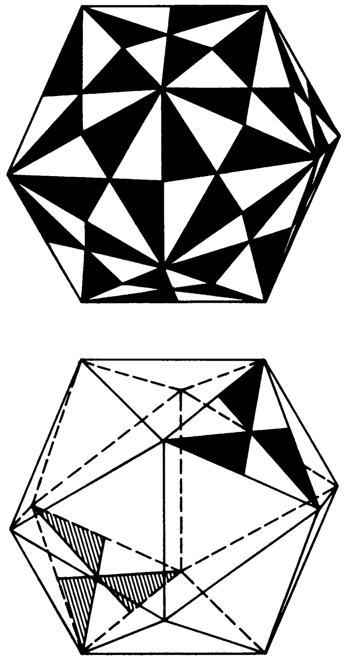
We do not go further into details of the crystallography of the point groups C_N and G_N. For $N = 5$, 8, 10, and 12 this has recently been done by Gähler [21] and a more extensive treatment for N up to 23 has been presented by Rokhsar *et al.* [22]. The latter analysis is based on a different approach and does not refer to higher-dimensional periodic structures.

3. Icosahedral symmetry : point groups and crystallographic representations.

We first discuss the point groups. There are exactly two icosahedral point groups, namely the group Y of all proper rotations leaving the icosahedron invariant (with 60 elements) and the group $Y_I = Y \times \mathbf{I}$ ($\mathbf{I}$ = inversion) of all symmetry transformations of the icosahedron (120 elements). A proof that no more icosahedral point groups exist can be found in [11]. In *Hermann-Mauguin notation* the two point groups Y and Y_I are 532 and $\overline{53}\,\frac{2}{m}$, respectively.

Symmetry groups of polyhedra can be represented nicely by painting these in various ways, thereby reducing the point group of the unpainted polyhedron (see [23], chap. 7). Figures 1a and 1b show a way of painting the icosahedron in a way that reduces the point group from Y_I to Y.

We first discuss the point group Y. It is generated by two elements, namely by the 72°-rotation $\mathbf{A}_5$ around the 5-fold symmetry axis $\hat{\mathbf{e}}_1$ and the 120°-rotation $\mathbf{A}_3$ around the 3-fold symmetry axis $\hat{\mathbf{e}}_1 + \hat{\mathbf{e}}_2 + \hat{\mathbf{e}}_3$ (see Fig. 2). The group Y has fine conjugacy classes which are represented by $\{\mathbf{E}, \mathbf{A}_5, \mathbf{A}_5^2, \mathbf{A}_3, \mathbf{A}_5\,\mathbf{A}_2\}$, respectively. The transformation $\mathbf{A}_5\,\mathbf{A}_3$ is the 180°-rotation around the 2-fold symmetry axis $\hat{\mathbf{e}}_1 + \hat{\mathbf{e}}_2$. Since Y has five conjugacy classes, it has five irreducible representations, namely a 1-dimensional, two 3-dimensional, a 4-dimensional, and a 5-dimensional representation. We denote them by $\mathcal{D}_1$, $\mathcal{D}_3$, $\mathcal{D}_{\bar{3}}$, $\mathcal{D}_4$, and $\mathcal{D}_5$. A detailed construction of these representations can be found in [24]. The standard representation is $\mathcal{D}_3$. From the character



a)

b)

Fig. 1. — (a) A painted icosahedron with point group symmetry Y (532). (b) The transparent picture elucidates the absence of an inversion centre.

table (Tab. I) it can be seen that any representation of Y satisfying condition (i) is of the form

$$n_1 \cdot \mathcal{D}_1 \oplus n_3 \cdot (\mathcal{D}_3 \oplus \mathcal{D}_{\bar{3}}) \oplus n_4 \cdot \mathcal{D}_4 \oplus n_5 \cdot \mathcal{D}_5\,, \qquad n_1, n_3, n_4, n_5 \geq 0\,. \quad (3.1)$$

The representation of minimal dimension obeying condition (ii) (i.e. the minimal crystallographic representation) is the one corresponding to $n_1 = n_4 = n_5 = 0$, $n_3 = 1$, i.e. $\mathcal{D}_3 \oplus \mathcal{D}_{\bar{3}}$. Its dimension is 6 and we will denote it by $\mathcal{D}_6$.

The explicit form of the representation $\mathcal{D}_6$ can be obtained as follows. Consider an icosahedron in

Table I. — *The characters of the representations of the two icosahedral point groups* Y *and* Y_I. *The numbers in parantheses in the top row are the numbers of elements of the corresponding conjugacy class. The table has to be read as follows : The label* $i\,(= 1, 3, \bar{3}, 4$ *or* $5)$ *in the leftmost column stands for* $\mathcal{D}_i$ *in the case of the point group* Y *(elements* $\mathbf{E}$, $\mathbf{A}_5\,\mathbf{A}_3$, $\mathbf{A}_3$, $\mathbf{A}_5$, $\mathbf{A}_5^2$*), and for* $\mathcal{D}_{i,I}$ *in the case of* Y_I. *For the representations* $\mathcal{D}'_{i,I}$, *the characters in the rightmost column have to be replaced by their negatives.*

	1 (1)	$\mathbf{A}_5\,\mathbf{A}_3$ (15)	$\mathbf{A}_3$ (20)	$\mathbf{A}_5$ (12)	$\mathbf{A}_5^2$ (12)	$\mathbf{I}$ (1)
1	1	1	1	1	1	1
3	3	− 1	0	$\frac{1}{2}(\sqrt{5}+1)$	$\frac{1}{2}(1-\sqrt{5})$	− 3
$\bar{3}$	3	− 1	0	$\frac{1}{2}(1-\sqrt{5})$	$\frac{1}{2}(\sqrt{5}+1)$	− 3
4	4	0	1	− 1	− 1	− 4
5	5	1	− 1	0	0	− 5

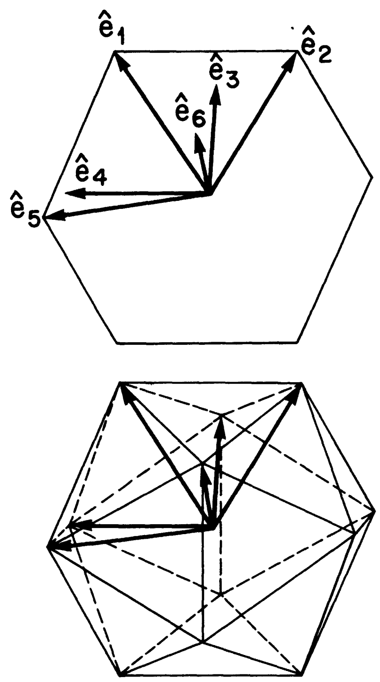


Fig. 2. — The 6 5-fold symmetry axes of the icosahedron.

R^3 with its six five-fold symmetry axes (Fig. 2). Let the six unit vectors $\{\hat{\mathbf{e}}_i\}_{i=1,\dots,6}$ be directed along these axes. The transformations of Y then act as permutations of the vectors $\hat{\mathbf{e}}_i$ (sometimes with a change of sign). These permutations can be written as 6×6-matrices ; they constitute the $\mathfrak{D}_6$-representation. We write down the explicit form of the generating set $\{\mathbf{A}_5, \mathbf{A}_3\}$ of Y :

$$\mathbf{A}_5 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \qquad (3.2a)$$

and

$$\mathbf{A}_3 = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \qquad (3.2b)$$

Furthermore we will need the matrix representing the 180°-rotation $\mathbf{A}_2 = \mathbf{A}_5^2\,\mathbf{A}_3\,\mathbf{A}_5^{-1}$ around the two-fold symmetry axis $\hat{\mathbf{e}}_1 + \hat{\mathbf{e}}_4$ (see Fig. 2) :

$$\mathbf{A}_2 = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} \qquad (3.2c)$$

Since in the following we will use only the $\mathfrak{D}_6$-representation of Y we use the same labels $\mathbf{A}_5$ and $\mathbf{A}_3$ for both the elements of Y and those of $\mathfrak{D}_6$.

For the point group Y_I we follow the same procedure. A generating set of Y_I is $\{\mathbf{A}_5, \mathbf{A}_3, \mathbf{I}\}$. The group Y_I has ten conjugacy classes and hence ten irreducible representations. On the subgroup $Y \subset Y_I$ they are identical to the representations of Y while the inversion is once represented by the 6×6-unit matrix and once by its negative. We denote the representations by $\mathfrak{D}_{i,\mathrm{I}}$ and $\mathfrak{D}'_{i,\mathrm{I}}$ respectively, where $i = 1, 3, \bar{3}, 4$ or 5 (see Tab. I). The standard representation is $\mathfrak{D}_{3,\mathrm{I}}$. The lowest-dimensional representation satisfying conditions (i) and (ii) is $\mathfrak{D}_{6,\mathrm{I}} = \mathfrak{D}_{3,\mathrm{I}} \oplus \mathfrak{D}_{\bar{3},\mathrm{I}}$.

This completes the construction of the minimal crystallographic representations of the icosahedral point groups Y and Y_I. It is the purpose of the following sections to classify all 6-dimensional periodic structures whose point group is either $\mathfrak{D}_6$ or $\mathfrak{D}_{6,\mathrm{I}}$.

Before proceeding let us mention two technical points which will be important in the following.

Scaling transformations : Let us denote by $\mathbf{P}^{\parallel}$ and $\mathbf{P}^{\perp} = \mathbf{E} - \mathbf{P}^{\parallel}$ the orthogonal projectors onto the 3-dimensional invariant subspaces $E^3_{\parallel}$ (the « physical subspace ») and $E^3_{\perp}$ of $\mathfrak{D}_6$ corresponding to $\mathfrak{D}_3$ and $\mathfrak{D}_{\bar{3}}$ respectively ; $\mathbf{P}^{\parallel}$ is given by

$$\mathbf{P}^{\parallel} = \frac{1}{\sqrt{20}} \cdot \begin{pmatrix} \sqrt{5} & 1 & 1 & 1 & 1 & 1 \\ 1 & \sqrt{5} & 1 & -1 & -1 & 1 \\ 1 & 1 & \sqrt{5} & 1 & -1 & -1 \\ 1 & -1 & 1 & \sqrt{5} & 1 & -1 \\ 1 & -1 & -1 & 1 & \sqrt{5} & 1 \\ 1 & 1 & -1 & -1 & 1 & \sqrt{5} \end{pmatrix} \qquad (3.3)$$

We introduce the *scaling transformations*

$$\mathbf{T}_{\mu\nu} = \mu \cdot \mathbf{P}^{\parallel} + \nu \cdot \mathbf{P}^{\perp} \; , \quad \mu, \nu \in \mathbb{R} \qquad (3.4)$$

($\mathbb{R}$ denotes the real numbers) which obviously commute with every single element of $\mathfrak{D}_6$:

$$\mathbf{T}_{\mu\nu}\,\mathbf{A}\mathbf{T}_{\mu\nu}^{-1} = \mathbf{A}, \quad \forall \mu, \nu \in \mathbb{R}, \; \mathbf{A} \in \mathfrak{D}_6 \,. \qquad (3.5)$$

The name « scaling transformation » should express the fact that $\mathbf{T}_{\mu\nu}$ just changes the length scales in $E^{\parallel}$ and $E^{\perp}$. Of particular importance will be the transformation with $\mu = -\nu = \sqrt{5}$:

$$\mathbf{M} = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & -1 & -1 & 1 \\ 1 & 1 & 0 & 1 & -1 & -1 \\ 1 & -1 & 1 & 0 & 1 & -1 \\ 1 & -1 & -1 & 1 & 0 & 1 \\ 1 & 1 & -1 & -1 & 1 & 0 \end{pmatrix} . \qquad (3.6)$$

In terms of $\mathbf{E}$ and $\mathbf{M}$ the scaling transformation (3.4) can be written as

$$\mathbf{T}_{\mu\nu} = \frac{1}{2}(\mu + \nu) \cdot \mathbf{E} + \frac{1}{2\sqrt{5}}(\mu - \nu) \cdot \mathbf{M} . \quad (3.7)$$

Defining relations : For the calculation of space groups the following properties of Y, or $\mathfrak{D}_6$ respectively, will be useful. Let a group G be generated by two elements a and b and the three identities

$$a^5 = b^3 = (ab)^2 = e \quad (3.8)$$

where e is the unit element of G. Then G is isomorphic to the icosahedral group Y and the isomorphism can be chosen in such a way that it transforms a into $\mathbf{A}_5$ and b into $\mathbf{A}_3$ [25]. We call the relations (3.8) the *defining relations* of the group Y. The group $\mathrm{Y_I}$ can be described in the same way : If a group G is generated by three elements a, b and c that satisfy the five identities

$$a^5 = b^3 = (ab)^2 = c^2 = e,\ ac = ca,\ bc = cb , \quad (3.9)$$

then G is isomorphic to $\mathrm{Y_I}$ and the isomorphism can be chosen such that a transforms into $\mathbf{A}_5$, b into $\mathbf{A}_3$, and c into $\mathbf{I}$.

4. Icosahedral Bravais lattices.

In this section we derive the complete list of all 6-dimensional Bravais lattices which are invariant under the group $\mathfrak{D}_6$. We call them $\mathfrak{D}_6$-*invariant* or *icosahedral Bravais lattices.* Since Bravais lattices are always inversion symmetric, the considerations in this section are independent of whether the point group is Y or $\mathrm{Y_I}$.

The definition of the *equivalence of Bravais lattices* is the standard definition used in ordinary crystallography :

Definition : Let $\mathfrak{L}$ and $\mathfrak{L}'$ be two Bravais lattices with point group G. $\mathfrak{L}$ is called *equivalent* to $\mathfrak{L}'$, if a linear transformation exists which transforms $\mathfrak{L}$ into $\mathfrak{L}'$ and commutes (not necessarily element wise) with the point group G.

In our cases all elements of $\mathfrak{D}_6$ are equivalence transformations. Since $\mathfrak{D}_6$ is reducible there is an important additional class of equivalence transformations, namely the scaling transformations $\mathbf{T}_{\mu\nu}$ defined in (3.4). [Due to (3.4), the latter do not only commute with the transformation group $\mathfrak{D}_6$ as a whole, but even with every single element of $\mathfrak{D}_6$]. If we have found some $\mathfrak{D}_6$-invariant Bravais lattice $\mathfrak{L}$ then the whole equivalence class

$$\mathrm{T}(\mathfrak{L}) = \{\mathbf{T}_{\mu\nu}\mathfrak{L} \mid \mu, \nu \in \mathbb{R}\} \quad (4.1)$$

of Bravais lattices is $\mathfrak{D}_6$-invariant. $\mathrm{T}(\mathfrak{L})$ is called a *Bravais lattice type.* We now state the main assertion of this section :

Theorem : In 6-dimensions there are three $\mathfrak{D}_6$-invariant Bravais lattice types (4.1). Each of them contains exactly one of the following three Bravais lattices :

$$\mathfrak{L}_{\mathrm{SC}} = \{(n_1, n_2, \dots, n_6) \mid n_i \in \mathbb{Z}\}, \quad (4.2a)$$

$$\mathfrak{L}_{\mathrm{FCC}} = \{(n_1, n_2, \dots, n_6) \mid\ |n_1 + n_2 + \cdots + n_6 = 0 \pmod 2\} , \quad (4.2b)$$

$$\mathfrak{L}_{\mathrm{BCC}} = \{(n_1, n_2, \dots, n_6) \mid n_i = n_j \pmod 2,\quad \forall i, j\} . \quad (4.2c)$$

In (4.2a) $\mathbb{Z}$ denotes the set of integers. ($\mathfrak{L}_{\mathrm{SC}}$, $\mathfrak{L}_{\mathrm{FCC}}$, and $\mathfrak{L}_{\mathrm{BCC}}$ are the 6-dimensional simple cubic, face-centered cubic, and body-centered cubic lattice, respectively.)

It is clear that the three lattice types (4.2a)-(4.2c) are $\mathfrak{D}_6$-invariant since they are invariant even under the much larger cubic group. What is less trivial is (a) that no further inequivalent $\mathfrak{D}_6$-invariant lattice types exist and (b) that the three lattices themselves are inequivalent.

In order to prove the theorem, we first prove an auxiliary lemma on 2-dimensional lattices :

Lemma 1 : Consider the 2-dimensional space $\mathbb{R}^2$ of pairs (x, y) and the linear transformation

$$\mathbf{Q} : \mathbb{R}^2 \mapsto \mathbb{R}^2, \quad (x, y) \to (x + y, x) . \quad (4.3)$$

If a 2-dimensional lattice $\mathfrak{L}$ is invariant under the transformation $\mathbf{Q}$ then a basis $\{\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2\}$ of $\mathfrak{L}$ exists such that $\hat{\mathbf{e}}_2 = \mathbf{Q}(\hat{\mathbf{e}}_1)$.

Proof of Lemma 1 : Consider the *pseudonorm*

$$\langle\ \rangle : \mathbb{R}^2 \mapsto \mathbb{R}, \quad \langle(x, y)\rangle = |x^2 - xy - y^2| . \quad (4.4)$$

One checks easily that $\langle\ \rangle$ is an invariant of $\mathbf{Q}$: $\langle\mathbf{Q}(\mathbf{x})\rangle = \langle\mathbf{x}\rangle\ \ \forall \mathbf{x} \in \mathrm{R}^2$. Using this invariance one gets the identity

$$\langle\mu\mathbf{E} + \nu\mathbf{Q}(\mathbf{x})\rangle = \frac{1}{4} \cdot |(2\mu + \nu)^2 - 5\nu^2| \cdot \langle\mathbf{x}\rangle , \qquad \forall \mu, \nu \in \mathbb{R}, \quad \mathbf{x} \in \mathbb{R}^2 . \quad (4.5)$$

An obvious property of the operators $\mathbf{U}_{\mu\nu} = \mu\mathbf{E} + \nu\mathbf{Q}$ is the following one : If a lattice $\mathfrak{L}$ is invariant under the action of $\mathbf{Q}$, then this is true as well for the lattice $\mathbf{U}_{\mu\nu}\mathfrak{L}$.

Consider some fixed 2-dimensional lattice $\mathfrak{L}$ and choose a nonzero lattice vector a with minimal pseudonorm $\langle\ \rangle$. Such a vector is not uniquely specified but exists since $\mathfrak{L}$ is a lattice which is invariant under $\mathbf{Q}$. Furthermore consider the vector $\mathbf{b} = \mathbf{Q}(\mathrm{a})$ and the lattice $\mathfrak{L}'$ generated by $\mathbf{a}$ and $\mathbf{b}$. We shall prove now that $\mathfrak{L}$ coincides with $\mathfrak{L}'$. Suppose this is not the case and choose a vector $\mathbf{c}$ belonging to $\mathfrak{L}$

but not to $\mathcal{L}'$ ($\mathcal{L}'$ is a sublattice of $\mathcal{L}$). Change the vector $\mathbf{c}$ by adding and subtracting $\mathbf{a}$ and $\mathbf{b}$ so that it takes the form

$$\mathbf{c} = s\mathbf{a} + t\mathbf{b} \quad (0 \leq s, t < 1) . \tag{4.6}$$

Now $\mathbf{c}$ lies inside the parallelogram with edges $\mathbf{a}$ and $\mathbf{b}$. There exists a transformation $\mathbf{U}_{\mu\nu} = \mu\mathbf{E} + \nu\mathbf{Q}$ transforming $\mathbf{a}$ into $(0, 1)$ and $\mathbf{b}$ into $(1, 0)$. The other objects are transformed as

$$\mathcal{L}' \mapsto \mathbb{Z}^2,\ \mathcal{L} \mapsto \mathcal{W} \supset \mathbb{Z}^2,\ \mathbf{c} \to (s, t),\ (0 \leq s, t < 1) . \tag{4.7}$$

The vector (s, t) belongs to $\mathcal{W}$ but not to $\mathbb{Z}^2$. Let us consider the set of points in the unit square having pseudonorm not less unity (this set is depicted in Fig. 3). The identity (3.4) implies that all nonzero vectors of $\mathcal{W}$, including (s, t), have pseudonorm not less than unity. This means that (s, t) lies inside the dashed region of the unit square (Fig. 3). Since this region occupies less than one half of the unit square, the vector $(1 - s, 1 - t)$ has pseudonorm less than unity. But this vector belongs to $\mathcal{W}$ since both $(1, 1)$ and (s, t) do. Because all nonzero vectors of $\mathcal{W}$ have pseudonorm larger than 1, this implies that $(1 - s, 1 - t) = (0, 0)$, i.e. $s = 1$, $t = 1$. This contradiction to the previous assumption (that $\mathbf{c} \notin \mathcal{L}$) proves Lemma 1. **QED.**

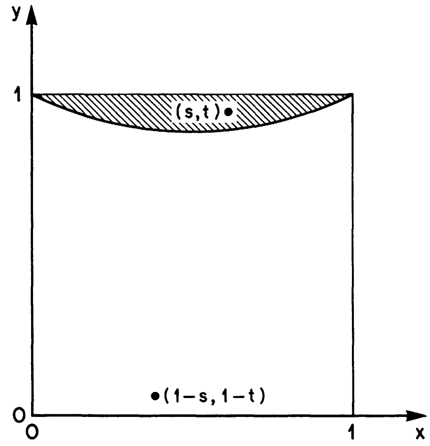


Fig. 3. — The dashed region in the unit square is the set of points (s, t) with pseudonorm not less than 1: $\langle (s, t) \rangle \geq 1$. The point with minimal y-coordinate is $\left(\frac{1}{2}, \frac{1}{4} \cdot (\sqrt{21} - 1)\right)$.

Proof of the theorem: Consider the transformation $\mathbf{A}_2$ representing the 180°-rotation around the two-fold symmetry axis $\hat{\mathbf{e}}_1 + \hat{\mathbf{e}}_4$ (see Eq. (3.2c) and Fig. 2). $\mathbf{A}_2$ has two invariant subspaces: A 2-dimensional one with eigenvalue $+1$ and a 4-dimensional one with eigenvalue -1. We denote the 2-dimensional eigenspace by V.

Y (or $\mathcal{D}_6$ respectively) has a subgroup generated by $\mathbf{A}_3$ and $\mathbf{A}_2$; it is the group of all rotational symmetries of the tetrahedron. It includes three elements of order two: $\mathbf{A}_2$, $\mathbf{A}_2' = \mathbf{A}_3^{-1}\mathbf{A}_2\mathbf{A}_3$, and $\mathbf{A}_2'' = \mathbf{A}_3^{-2}\mathbf{A}_2\mathbf{A}_3^2$. These three transformations correspond to rotations of the tetrahedron around its 2-fold axis and form a conjugacy class of the tetrahedral group. By V′ and V″ we denote the 2-dimensional eigenspaces of $\mathbf{A}_2'$ and $\mathbf{A}_2''$ with eigenvalue 1. The three subspaces V, V′ and V″ of R^6 are pairwise orthogonal, as can easily be checked. Hence R^6 is the orthogonal sum of these subspaces:

$$\mathrm{R}^6 = \mathrm{V} \oplus \mathrm{V}' \oplus \mathrm{V}'' . \tag{4.8}$$

The transformation $\mathbf{A}_3$ acts as a cyclic permutation on the three subspaces:

$$\mathrm{V} = \mathbf{A}_3(\mathrm{V}'),\ \mathrm{V}' = \mathbf{A}_3(\mathrm{V}''),\ \mathrm{V}'' = \mathbf{A}_3(\mathrm{V}) . \tag{4.9}$$

Let $\mathcal{L} \subset \mathrm{R}^6$ be a Bravais lattice which is invariant under all $\mathcal{D}_6$-transformations (an icosahedral Bravais lattice). Consider the lattice $\mathcal{M} \subset \mathrm{V}$ which is the intersection of $\mathcal{L}$ with V. This intersection is not empty since V is a rational subspace in R^6. Analogously we define $\mathcal{M}' \subset \mathrm{V}'$ and $\mathcal{M}'' \subset \mathrm{V}''$. The lattice $\mathcal{W} \equiv \mathcal{M} + \mathcal{M}' + \mathcal{M}''$ is also a sublattice of $\mathcal{L}$.

Now we note that the operator $\mathbf{P} = \frac{1}{2}(\mathbf{E} + \mathbf{A}_2)$ is a projector onto the subspace V. $\mathbf{P}$ projects $\mathcal{L}$ onto $\frac{1}{2}\mathcal{M}$. [The lattice $\alpha\mathcal{M}$, $\alpha \in \mathbb{R}$ is defined as the lattice $\mathcal{M}$, scaled by a factor of α: $\alpha\mathcal{M} = \{x \in \mathbb{R}^6 \mid \alpha^{-1}x \in \mathcal{M}\}$]. In the same way $\mathbf{P}' = \frac{1}{2}(\mathbf{E} + \mathbf{A}_2')$ and $\mathbf{P}'' = \frac{1}{2}(\mathbf{E} + \mathbf{A}_2'')$ project $\mathcal{L}$ onto $\frac{1}{2}\mathcal{M}'$ and $\frac{1}{2}\mathcal{M}''$, respectively. Since $\mathcal{M}$, $\mathcal{M}'$, and $\mathcal{M}''$ are pairwise orthogonal the operators $\mathbf{P}$, $\mathbf{P}'$, and $\mathbf{P}''$ form an orthogonal decomposition of the unit operator $\mathbf{E}$:

$$2\,\mathbf{E} = (\mathbf{E} + \mathbf{A}_2) \oplus (\mathbf{E} + \mathbf{A}_2') \oplus (\mathbf{E} + \mathbf{A}_2'') . \tag{4.10}$$

The l.h.s. of (4.10) multiplies lattice vectors of $\mathcal{L}$ by a factor of 2 while the r.h.s. projects them onto lattice vectors of $\mathcal{W}$. Conseqently, if $x \in \mathcal{L}$ then $2\,x \in \mathcal{W}$; we write $2\,\mathcal{L} \subset \mathcal{W}$. Combined with the relations obtained above this gives

$$2\,\mathcal{L} \subset \mathcal{W} \subset \mathcal{L} \quad \text{or} \quad \mathcal{W} \subset \mathcal{L} \subset \frac{1}{2}\mathcal{W} . \tag{4.11}$$

Now we construct a simple basis of $\mathcal{W}$ using equivalence transformations of the type (4.3). The vectors of the subspace V, written in the standard basis described in section 3, take the form

$$(x, 0, y, x, y, 0),\quad x, y \in \mathbb{R} . \tag{4.12}$$

Consider the operator $\mathbf{R} = 2\,\mathbf{P}\mathbf{A}_5 = (\mathbf{E} + \mathbf{A}_2)\,\mathbf{A}_5$, which transforms the subspace V onto itself. $\mathbf{R}$ preserves the lattice $\mathcal{M}$. If we write the vectors (4.12) as pairs (x, y) then the action of $\mathbf{R}$ is given by

$$\mathbf{R} : (x, y) \rightarrow (x + y, x) . \tag{4.13}$$

We are now in a position to apply Lemma 1 : There exists a vector $\mathbf{s} \in \mathcal{L}$ such that the two vectors $\mathbf{s}$ and $\mathbf{Rs}$ form a basis of $\mathcal{L}$. By applying the operator $\mathbf{A}_3$ to the basis $\{\mathbf{s}, \mathbf{Rs}\}$ we obtain a basis $\{\mathbf{A}_3\,\mathbf{s}, \mathbf{A}_3\,\mathbf{Rs}\}$ of the lattice $\mathcal{L}'$. The same procedure is applied to obtain a basis of $\mathcal{L}''$. Finally the set

$$\{\mathbf{s}, \mathbf{Rs}, \mathbf{A}_3\,\mathbf{s}, \mathbf{A}_3\,\mathbf{Rs}, \mathbf{A}_3^2\,\mathbf{s}, \mathbf{A}_3^2\,\mathbf{Rs}\} \tag{4.14}$$

forms a basis of $\mathcal{W}$. Now consider the scaling transformation $\tilde{\mathbf{T}}_{\mu\nu} = \mu\mathbf{E} + \nu\mathbf{M}$ (defined in (3.7)) with

$$\mu = \frac{y - 2x}{2(y^2 + xy - x^2)} , \quad \nu = \frac{y}{2(y^2 + xy - x^2)} . \tag{4.15}$$

$\tilde{\mathbf{T}}_{\mu\nu}$ transforms $\mathbf{s}$ into (1, 0, 0, 0, 0, 0). We let $\tilde{\mathbf{T}}_{\mu\nu}$ act on the lattices $\mathcal{L}$, $\mathcal{W}$, $\mathcal{M}$, $\mathcal{M}'$, and $\mathcal{M}''$ to obtain the new set of lattices $\tilde{\mathcal{L}}$, $\tilde{\mathcal{W}}$, $\tilde{\mathcal{M}}$, $\tilde{\mathcal{M}}'$, and $\tilde{\mathcal{M}}''$. The new « tilde set » is equivalent to the old set in the sense of (4.1). In all the following considerations we shall use the new lattices and for convenience we will drop the tilde.

The transformed basis (4.14) looks very simple :

$$\begin{aligned} \mathbf{b}_1^{\mathcal{M}} &= (1, 0, 0, 1, 0, 0), \\ \mathbf{b}_2^{\mathcal{M}} &= (0, 0, 1, 0, 1, 0), \\ \mathbf{b}_1^{\mathcal{M}'} &= (0, 1, 0, 0, 0, 1), \\ \mathbf{b}_2^{\mathcal{M}'} &= (1, 0, 0, -1, 0, 0), \\ \mathbf{b}_1^{\mathcal{M}''} &= (0, 0, 1, 0, -1, 0), \\ \mathbf{b}_2^{\mathcal{M}''} &= (0, 1, 0, 0, 0, -1) . \end{aligned} \tag{4.16}$$

Since the equivalence transformation $\tilde{\mathbf{T}}_{\mu\nu}$ does not affect the relation (4.11) between $\mathcal{W}$ and $\mathcal{L}$ we have to consider only a finite set of lattices which include $\mathcal{W}$ and are included in $\frac{1}{2}\mathcal{W}$.

In the next part of the proof we show how to simplify the analysis using the symmetry properties of the lattice $\mathcal{L}$. $\mathcal{L}$ is invariant under the whole groupe Y whereas $\mathcal{W}$ is invariant only under the tetrahedral subgroup of Y. We symmetrize $\mathcal{W}$ with respect to Y :

$$\mathcal{W}' = \mathcal{W} + \mathbf{A}_5(\mathcal{W}) + \mathbf{A}_5^2(\mathcal{W}) + \mathbf{A}_5^3(\mathcal{W}) + \mathbf{A}_5^4(\mathcal{W}) . \tag{4.17}$$

The lattice $\mathcal{W}'$ includes $\mathcal{W}$ and is included in $\mathcal{L}$ since $\mathcal{L}$ is $\mathcal{D}_6$-symmetric :

$$\mathcal{W} \subset \mathcal{W}' \subset \mathcal{L} \subset \frac{1}{2}\mathcal{W} . \tag{4.18}$$

A simple calculation shows that $\mathcal{W}'$ is identical to the face-centered cubic lattice $\mathcal{L}_{\text{FCC}}$ defined in (4.2b). By applying the symmetrization procedure (4.17) to the lattices reciprocal to those in (4.18) the « upper limit » in (4.18) can be lowered :

$$\mathcal{W} \subset \mathcal{W}' \subset \mathcal{L} \subset \mathcal{W}'' \subset \frac{1}{2}\mathcal{W} . \tag{4.19}$$

Calculation shows that $\mathcal{W}''$ is identical to the body-centered cubic lattice $\frac{1}{2}\mathcal{L}_{\text{BCC}}$ defined in (4.2c).

For the following analysis we introduce the definition the *index* $(\mathcal{L} : \mathcal{L}')$ of a sublattice $\mathcal{L}' \subset \mathcal{L}$ in the lattice $\mathcal{L}$. Every lattice is an additive Abelian group. The index $(\mathcal{L} : \mathcal{L}')$ is defined as the number of different cosets of the subgroup $\mathcal{L}' \subset \mathcal{L}$ [15].

The index $\left(\frac{1}{2}\mathcal{L}_{\text{BCC}} : \mathcal{L}_{\text{FCC}}\right)$ is equal to 4. Together with (4.19) this means that one has to take into account only three different nonzero vectors of the factor group $\mathcal{W}''/\mathcal{W}'$ as possible vectors of $\mathcal{L}$. These candidates are

$$\begin{aligned} \mathbf{p} &= (1, 0, 0, 0, 0, 0) \\ \mathbf{q} &= \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right) \\ \mathbf{r} &= \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}\right) . \end{aligned} \tag{4.20}$$

Let us discuss the possible cases. We have to consider the $\mathcal{D}_6$-invariant lattices $\mathcal{L} \supset \mathcal{L}_{\text{FCC}}$ which contain at least one of the vectors $\mathbf{p}$, $\mathbf{q}$, or $\mathbf{r}$ of (4.20). For the sake of brevity we write use the abbreviation

$$\mathcal{L}_{\text{FCC}} + \mathbf{x} \equiv \mathcal{L}_{\text{FCC}} \cup \left\{\sum_{i=1}^{6} n_i\,\mathbf{A}_{(i)}\,\mathbf{x} \,|\, n_i \in \mathbb{Z}, \mathbf{A}_{(i)} \in \mathcal{D}_6\right\} . \tag{4.21}$$

We have to consider the following three cases :

(i) $\mathcal{L} = \mathcal{L}_{\text{FCC}} + \mathbf{p}$: In this case $\mathcal{L}$ is the simple cubic lattice $\mathcal{L}_{\text{SC}}$ defined in (4.2a).

(ii) $\mathcal{L} = \mathcal{L}_{\text{FCC}} + \mathbf{q}$: This lattice is transformed into $\mathcal{L}_{\text{SC}}$ by the equivalence transformation of type (3.7), namely $\mathbf{T} = \frac{1}{2}(\mathbf{M} - \mathbf{E})$.

(iii) $\mathcal{L} = (\mathcal{L}_{\text{FCC}} + \mathbf{p}) + \mathbf{q}$: In this case $\mathcal{L} = \frac{1}{2}\mathcal{L}_{\text{BCC}}$.

Since the vector $\mathbf{p} + \mathbf{q} + \mathbf{r}$ is an $\mathcal{L}_{\text{FCC}}$ lattice vector all other possibilities are reduced to the above three. This completes the proof of the theorem. **QED.**

In order to complete the analysis of icosahedral Bravais lattices we prove

Lemma 2 : The three Bravais lattices $\mathcal{L}_{\text{SC}}$, $\mathcal{L}_{\text{FCC}}$ and $\mathcal{L}_{\text{BCC}}$ are pairwise inequivalent.

Proof of Lemma 2 : The lattices $\mathcal{L}_{\text{FCC}}$ and $\mathcal{L}_{\text{BCC}}$ are invariant under the action of the transformation $\frac{1}{2}(\mathbf{E} + \mathbf{M})$ while the lattice $\mathcal{L}_{\text{SC}}$ is not. Hence neither $\mathcal{L}_{\text{FCC}}$ nor $\mathcal{L}_{\text{BCC}}$ are equivalent to $\mathcal{L}_{\text{SC}}$.

Suppose $\mathfrak{L}_{FCC}$ and $\mathfrak{L}_{BCC}$ are equivalent. Since the indices $(\mathfrak{L}_{SC} : \mathfrak{L}_{FCC})$ and $\left(\frac{1}{2}\mathfrak{L}_{BCC} : \mathfrak{L}_{SC}\right)$ are both equal to 2, equivalence of $\mathfrak{L}_{FCC}$ and $\mathfrak{L}_{BCC}$ would imply the possibility of embedding $\mathfrak{L}_{SC}$ into itself with index 4. This in turn would mean that an equivalence transformation $\tilde{\mathbf{T}}_{\mu\nu} = \mu\mathbf{E} + \nu\mathbf{M}$ exists which (i) transforms $\mathfrak{L}_{SC}$-lattice vectors into $\mathfrak{L}_{SC}$-lattice vectors and (ii) changes the 6-dimensional volume by a factor of 4 : $\det(\tilde{\mathbf{T}}_{\mu\nu}) = 4$. We show that conditions (i) and (ii) are in contradiction. First we note that, since

$$\tilde{\mathbf{T}}_{\mu\nu}((1,0,0,0,0,0)) = (\mu, \nu, \nu, \nu, \nu, \nu) , \quad (4.22)$$

both μ and ν have to be integers. On the other hand

$$4 = \det(\tilde{\mathbf{T}}_{\mu\nu}) = (\mu^2 - 5\nu^2)^3 \quad (4.23)$$

implies $\mu^2 - 5\nu^2 = \sqrt{4}$. This contradiction proves Lemma 2. **QED.**

Before turning to the calculation of space groups we have to discuss some important symmetry properties of the three lattice types $\mathfrak{L}$, $\mathfrak{L}_{FCC}$ and $\mathfrak{L}_{BCC}$. Of course these lattices are invariant under all elements of $\mathfrak{D}_6$. In addition, however, there is a class of lattice symmetries which is due to the reducibility of $\mathfrak{D}_6$: $\mathfrak{L}_{FCC}$ and $\mathfrak{L}_{BCC}$ are both invariant under the scaling transformation (see (3.4))

$$\mathbf{Q}_1 = \mathbf{T}_{\mu=\tau, \nu=\tau-1} = \frac{1}{2} \cdot (\mathbf{E} + \mathbf{M}) , \quad (4.24)$$

where $\tau = \frac{1}{2} \cdot (1 + \sqrt{5})$ is the golden mean, $\mathbf{E}$ is the unit matrix and $\mathbf{M}$ has been defined in (3.6). The lattice $\mathfrak{L}_{SC}$ is invariant under

$$\mathbf{Q}_2 = \mathbf{T}_{\mu=\tau^3, \nu=(\tau-1)^3} = \mathbf{Q}_1^3 = 2 \cdot \mathbf{E} + \mathbf{M} \quad (4.25)$$

(but not under $\mathbf{Q}_1$). We call $\mathbf{Q}_1$ and $\mathbf{Q}_2$ quasidilatations. They have already been described by Elser [26]. They will be important for the question of space group equivalence.

5. Icosahedral space groups.

5.1 DEFINITIONS. — The detailed theory of space groups can be found in [27] ; in the following we give some definitions and remarks as far as they are of importance for the calculation of icosahedral space groups. The *space group* S of a *d*-dimensional periodic structure with Bravais lattice $\mathfrak{L}$ is defined as the group of all inhomogeneous transformations

$$(\mathbf{H}|\mathbf{h}) : \mathbf{x} \mapsto \mathbf{H}\mathbf{x} + \mathbf{h} \quad (5.1)$$

which leave the structure invariant. The shift $\mathbf{h} \in \mathbb{R}^d$ will be called the *translational part* or *non-primitive translation* of the space group element $(\mathbf{H}|\mathbf{h})$. The homogeneous part $\mathbf{H}$ is an orthogonal linear transformation, $\mathbf{H} \in \mathcal{O}(d)$. The transformations $\mathbf{H}$ alone constitute the *point group* of the structure. If it is (not) possible to transform all translations $\mathbf{h}$ to $\mathbf{0}(\bmod \mathfrak{L})$ simultaneously for all elements of S, then S is called a *(non-)symmorphic* space group.

The group structure of S is constituted by the unit element $(\mathbf{E}|\mathbf{0})$, the multiplication rule

$$(\mathbf{H}_1|\mathbf{h}_1)(\mathbf{H}_2|\mathbf{h}_2) = (\mathbf{H}_1\mathbf{H}_2|\mathbf{H}_1\mathbf{h}_2 + \mathbf{h}_1) , \quad (5.2)$$

and the inverse

$$(\mathbf{H}|\mathbf{h})^{-1} = (\mathbf{H}^{-1}|-\mathbf{H}^{-1}\mathbf{h}) . \quad (5.3)$$

The effect of an inhomogeneous coordinate transformation $(\mathbf{T}|\mathbf{t})$ on a space group element $(\mathbf{H}|\mathbf{h})$ is described by

$$(\mathbf{H}|\mathbf{h}) \mapsto (\mathbf{T}|\mathbf{t})(\mathbf{H}|\mathbf{h})(\mathbf{T}|\mathbf{t})^{-1} = = (\mathbf{T}\mathbf{H}\mathbf{T}^{-1}|\mathbf{T}[\mathbf{h} + (\mathbf{E} - \mathbf{H})\mathbf{t}]) . \quad (5.4)$$

Here $\mathbf{T} : \mathbb{R}^d \mapsto \mathbb{R}^d$ is a nonsingular transformation (i.e. $\det \mathbf{T} \neq 0$) and $\mathbf{t}$ an arbitrary parallel shift. Of course the translation $\mathbf{h} \in \mathbb{R}^3$ depends on the choice of the coordinate origin. Let $\mathrm{E}_\lambda^{\mathbf{H}}$ denote the eigenspace of the transformation $\mathbf{H}$ with eigenvalue λ :

$$\mathrm{E}_\lambda^{\mathbf{H}} = \{\mathbf{x} \in \mathbb{R}^d | \mathbf{H}\mathbf{x} = \lambda\mathbf{x}\} . \quad (5.5)$$

From (5.3) it follows that the component $\mathbf{h}_\perp$ of $\mathbf{h}$ orthogonal to $\mathrm{E}_{\lambda=1}^{\mathbf{H}}$ can be transformed to zero by an appropriate coordinate shift $(\mathbf{E}|\mathbf{t})$, whereas the component $\mathbf{h}_\parallel$ of $\mathbf{h}$ parallel to $\mathrm{E}_{\lambda=1}^{\mathbf{H}}$ is not affected by any coordinate shift and thus has an invariant meaning. In 3-dimensional crystallography, $\mathbf{h}_\parallel$ defines a *screw axis*. The latter term has a meaning only if $\mathrm{E}_{\lambda=1}^{\mathbf{H}}$ is 1-dimensional. This is not the case in 6-dimensional icosahedral crystallography where we have $\dim(\mathrm{E}_{\lambda=1}^{\mathbf{A}_5}) = \dim(\mathrm{E}_{\lambda=1}^{\mathbf{A}_3}) = \dim(\mathrm{E}_{\lambda=1}^{\mathbf{A}_2}) = 2$. This means that the term screw axis loses its meaning in 6-dimensional icosahedral crystallography.

5.2 SPACE GROUP EQUIVALENCE. — The problem of *space group equivalence* deserves special attention. Space groups are equivalent if they transform into each other by a shift of the origin and/or a change of the Bravais lattice basis [27]. In formal terms :

Definition : Let $\mathrm{S}^{(i)} = \{(\mathbf{H}_1^{(i)}|\mathbf{h}_1^{(i)}), \ldots, (\mathbf{H}_N^{(i)}|\mathbf{h}_N^{(i)})\}$, $i = 1, 2$, be two space groups belonging to the same point group and Bravais lattice. $\mathrm{S}^{(1)}$ and $\mathrm{S}^{(2)}$ are called *equivalent* if there exists an inhomogeneous transformation $(\mathbf{Z}|\mathbf{z})$, $\mathbf{Z} \in \mathrm{GL}(N, \mathbb{Z})$ (not necessarily a space group element), such that

$$(\mathbf{H}_{\mathrm{P}(l)}^{(2)}|\mathbf{h}_{\mathrm{P}(l)}^{(2)}) = (\mathbf{Z}|\mathbf{z})(\mathbf{H}_l^{(1)}|\mathbf{h}_l^{(1)})(\mathbf{Z}|\mathbf{z})^{-1} , \quad \forall l = 1, \ldots, N . \quad (5.6)$$

$GL(N, \mathbb{Z})$ is the group of non-singular $N \times N$-matrices with integer entries.
$(P(1), P(2), \ldots, P(N))$ is some permutation of $(1, 2, \ldots, N)$.

Let us compare ordinary 3-dimensional crystallography with 6-dimensional icosahedral crystallography. If a 3-dimensional space group contains the inversion $\mathbf{I}$ then the only equivalence transformations $(\mathbf{Z}|\mathbf{z})$ *are the space group elements themselves.* If the space group does not contain $\mathbf{I}$, then $\mathbf{I}$ itself can be considered as an equivalence transformation. It is well known that the number of inequivalent space groups in 3 dimensions is either 219 or 230, depending on whether $\mathbf{I}$ is considered as an equivalence transformation or not. (Two space groups that are equivalent *via* inversion are called an *enantiomorphic pair*).

For 6-dimensional icosahedral symmetry things are different. In this case there are $GL(N, \mathbb{Z})$-transformations which do not belong to the point groups $\mathfrak{D}_6$ or $\mathfrak{D}_{6,\mathrm{I}}$ but commute with all elements of these groups. These are the quasidilatations $\mathbf{Q}_1$ and $\mathbf{Q}_2$ defined in (4.24) and (4.25). According to the above definition they have to be considered as equivalence transformations. The calculations of sections 6 and 7 will show that if quasidilatations are not taken into account we arrive at exactly the 16 space groups given by Janssen [9].

5.3 DEFINING RELATIONS. — For a given Bravais lattice $\mathfrak{L}$ and a given point group $P = \{\mathbf{H}_1, \ldots, \mathbf{H}_n\}$ a space group $S = \{(\mathbf{H}_1|\mathbf{h}_1), \ldots, (\mathbf{H}_n|\mathbf{h}_n)\}$ is characterized completely by the translational parts $\mathbf{h}_i$ on a generating set of S. Generating sets are $\mathcal{G}_Y = \{(\mathbf{A}_5|\mathbf{a}_5), (\mathbf{A}_3|\mathbf{a}_3)\}$ for the point group Y and $\mathcal{G}_{Y_I} = \{(\mathbf{A}_5|\mathbf{a}_5), (\mathbf{A}_3|\mathbf{a}_3), (\mathbf{I}|\mathbf{i})\}$ for the point group Y_I. The translational parts of the elements of $\mathcal{G}_Y$ and $\mathcal{G}_{Y_I}$ are determined by the defining relations [25] of the space groups. The defining relations for the space groups belonging to the point group Y follow from (3.8). They are given by

$$(\mathbf{A}_5|\mathbf{a}_5)^5 = (\mathbf{A}_3|\mathbf{a}_3)^3 = [(\mathbf{A}_5|\mathbf{a}_5)(\mathbf{A}_3|\mathbf{a}_3)]^2 = (\mathbf{E}|\mathbf{0}). \quad (5.7)$$

For the space groups belonging to the poing group Y_I, (3.9) yields the defining relations (5.7) and in addition

$$(\mathbf{I}|\mathbf{i})^2 = (\mathbf{E}|\mathbf{0}), \quad (5.8a)$$

$$(\mathbf{A}_5|\mathbf{a}_5)(\mathbf{I}|\mathbf{i}) = (\mathbf{I}|\mathbf{i})(\mathbf{A}_5|\mathbf{a}_5), \quad (5.8b)$$

$$(\mathbf{A}_3|\mathbf{a}_3)(\mathbf{I}|\mathbf{i}) = (\mathbf{I}|\mathbf{i})(\mathbf{A}_3|\mathbf{a}_3). \quad (5.8c)$$

In the two following paragraphs we describe in detail the solution of these equations.

5.4 SPACE GROUPS CORRESPONDING TO POINT GROUP Y. — We have to calculate the non-primitive translations for the generating elements $\mathbf{A}_5$ and $\mathbf{A}_3$. They are completely fixed by the defining relations (5.7). The point group elements $\mathbf{A}$ automatically satisfy the defining relations ; we only have to worry about the *translational parts* $\mathbf{a}$. With respect to the problem of *equivalence*, the derivation will be divided into two parts : First, the effect of parallel shifts is considered, and then inversion and quasidilatations will be taken into account.

We set $\mathbf{x} = \mathbf{a}_5$ and $\mathbf{y} = \mathbf{a}_3$ (in order to reduce the number of indices). Using (5.2), (5.7) reads

$$(\mathbf{A}_5^4 + \mathbf{A}_5^3 + \mathbf{A}_5^2 + \mathbf{A}_5 + \mathbf{E})\,\mathbf{x} = \mathbf{0} \,(\mathrm{mod}\, \mathfrak{L}), \quad (5.9a)$$

$$(\mathbf{A}_3^2 + \mathbf{A}_3 + \mathbf{E})\,\mathbf{y} = \mathbf{0} \,(\mathrm{mod}\, \mathfrak{L}), \quad (5.9b)$$

$$(\mathbf{A}_5\mathbf{A}_3 + \mathbf{E})(\mathbf{A}_5\mathbf{x} + \mathbf{y}) = \mathbf{0} \,(\mathrm{mod}\, \mathfrak{L}). \quad (5.9c)$$

$\mathfrak{L}$ stands for either $\mathfrak{L}_{SC}$, $\mathfrak{L}_{FCC}$ or $\mathfrak{L}_{BCC}$; we do not yet specify it. Here and in the rest of this section, all vector equations are to be understood modulo $\mathfrak{L}$.

Equivalence by parallel shifts

The direct solution of the system (5.9) presents no principal difficulties but is somewhat tedious. It can be greatly simplified by showing that the non-primitive translation $\mathbf{y}$ can always be transformed to a Bravais lattice vector by a suitable shift of the origin. To see this, suppose we have found a solution $\mathbf{x} = (x_1, \ldots, x_6)$ and $\mathbf{y} = (y_1, \ldots, y_6)$ to (5.9). Inserting $\mathbf{y}$ into (5.9) yields

$$\begin{pmatrix} y_1 + y_2 + y_3 \\ y_1 + y_2 + y_3 \\ y_1 + y_2 + y_3 \\ y_4 - y_5 + y_6 \\ -(y_4 - y_5 + y_6) \\ y_4 - y_5 + y_6 \end{pmatrix} = 0 \,(\mathrm{mod}\, \mathfrak{L}). \quad (5.10)$$

Now consider the 2-parameter family of shifts

$$\mathbf{u}_{s,t} = \begin{pmatrix} s \\ s + y_1 + y_3 \\ s - y_2 - y_3 \\ t \\ -t - y_5 + y_6 \\ t + y_4 - y_5 \end{pmatrix}. \quad (5.11)$$

The parameters s and t will be fixed below. Using (5.4) the transformed vector $\mathbf{y}'$ can easily be calculated ; one finds

$$\begin{aligned} \mathbf{y}' &= \mathbf{y} + (\mathbf{E} - \mathbf{A}_3)\,\mathbf{u}_{s,t} = \\ &= (\mathbf{A}_3^2 + \mathbf{A}_3 + \mathbf{E})\,\mathbf{y} - 2(y_1 + y_2 + y_3)\,\hat{\mathbf{e}}_2 \\ &\quad + 2(y_4 - y_5 + y_6)\,\hat{\mathbf{e}}_5 . \end{aligned} \quad (5.12)$$

This transformed vector $\mathbf{y}'$ is a lattice vector of $\mathfrak{L}_{SC}$ as well as of $\mathfrak{L}_{FCC}$ and $\mathfrak{L}_{BCC}$. This follows at once from (5.9b) and (5.10). Without proof we note that, for $\mathfrak{L}_{SC}$ and $\mathfrak{L}_{FCC}$, $\mathbf{y}$ can always be transformed to $\mathbf{0}$ while for $\mathfrak{L}_{BCC}$ some solutions of (5.9) exist for which $\mathbf{y}$ can only be transformed to a *non zero* lattice vector.

Under the shift $\mathbf{u}_{s,t}$ the vector $\mathbf{x}$ is transformed to

$$\mathbf{x}' = \mathbf{x} + (\mathbf{E} - \mathbf{A}_5)\,\mathbf{u}_{s,t} = \begin{pmatrix} x_1 \\ x_2 + y_1 + y_3 - y_4 + y_5 + (s - t) \\ x_3 - y_1 - y_2 - 2\,y_3 \\ x_4 + y_2 + y_3 - (s - t) \\ x_5 - y_5 + y_6 - 2\,t \\ x_6 + y_4 - y_6 + 2\,t \end{pmatrix} . \tag{5.13}$$

By fixing the free parameters s and t as

$$t = -\frac{1}{2}(x_6 + y_4 - y_6) \text{ and}$$
$$s = t - (x_2 + y_1 + y_3 - y_4 + y_5)\,, \tag{5.14}$$

the second and sixth components of $\mathbf{x}'$ become zero. Hence we arrive at the following result : Without loss of generality we can restrict ourselves to solutions of (5.9) satisfying the 8 constraints

$$\mathbf{y} = \mathbf{0}(\mathrm{mod}\,\mathfrak{L})\,;\quad x_2 = x_6 = 0\,. \tag{5.15}$$

Equations (5.9) are then reduced to

$$(5.9a): \quad (5\,x_1, h, h, h, h, h) = \mathbf{0}(\mathrm{mod}\,\mathfrak{L})\,, \tag{5.16a}$$

$$(5.9c): \quad (x_1 + x_3, x_4, x_1 + x_3, x_4, 0, 0) = \mathbf{0}(\mathrm{mod}\,\mathfrak{L})\,, \tag{5.16b}$$

while (5.9b) is identically satisfied. Here, $h = x_3 + x_4 + x_5$. For all of the three Bravais lattices, equations (5.16) imply

$$5\,x_1 = m,\ x_3 + x_4 + x_5 = k,\ x_1 + x_3 = l,\ x_4 = n,\quad (k, l, m, n \in \mathbb{Z})\,, \tag{5.17}$$

or

$$\mathbf{x} = \left(\frac{m}{5}, 0, l - \frac{m}{5}, n, k - n - l + \frac{m}{5}, 0\right) . \tag{5.18}$$

This expression has to be considered for the three Bravais lattices.

(i) Simple cubic lattice $\mathfrak{L}_{SC}$: Since $k, l, m, n \in \mathbb{Z}$, we are left with

$$\mathbf{x}_m = \left(\frac{m}{5}, 0, -\frac{m}{5}, 0, \frac{m}{5}, 0\right)(\mathrm{mod}\,\mathfrak{L}_{SC})\quad m \in \{0, 1, 2, 3, 4\}\,. \tag{5.19}$$

(ii) Face-centered cubic lattice $\mathfrak{L}_{FCC}$: Equation (5.16a) implies $m + 5\,k = 0\,(\mathrm{mod}\,2)$, which is the case for $k = (2\,j + 1)\,m$, $j \in \mathbb{Z}$. Equation (5.16b) yields no additional constraints. Different choices of l and n correspond to shifts of $\mathbf{x}$ by $\mathfrak{L}_{FCC}$ lattice vectors, thus l and n are arbitrary integers. Choosing $j = 2$, $l = n = 0$, we obtain

$$\mathbf{x}_m = \left(\frac{m}{5}, 0, -\frac{m}{5}, 0, \frac{6\,m}{5}, 0\right)(\mathrm{mod}\,\mathfrak{L}_{FCC})\,,\quad m \in \{0, 1, 2, 3, 4\}\,. \tag{5.20}$$

(iii) Body-centered cubic lattice $\mathfrak{L}_{BCC}$: (5.16a) yields $m = k(\mathrm{mod}\,2)$. From (5.16b) we obtain $n = l = 0\,(\mathrm{mod}\,2)$, and therefore

$$\mathbf{x}_m = \left(\frac{m}{5}, 0, -\frac{m}{5}, 0, \frac{6\,m}{5}, 0\right)(\mathrm{mod}\,\mathfrak{L}_{BCC})\,,\quad m \in \{0, 1, 2, 3, 4\}\,. \tag{5.21}$$

By making full use of the freedom of choosing the origin we have reduced the number of inequivalent space groups to *at most 5* for every Bravais lattice. Before we turn to quasidilatations we discuss the

Equivalence by inversion (enantiomorphic pairs)

The inversion $\mathbf{I}$ does not belong to the point group Y. By (5.4), nonprimitive translations $\mathbf{a}$ change sign under the inversion $(\mathbf{I}\,|\,\mathbf{0}) : \mathbf{a} \mapsto -\mathbf{a}$. For the nonprimitive translations (5.19-21) we have $-\mathbf{x}_m = \mathbf{x}_{5-m}$ hence the space groups corresponding to $\mathbf{x}_m$ and $\mathbf{x}_{5-m}$ are *enantiomorphic pairs.* This equivalence further reduces the maximal number of inequivalent space groups : m takes only the three values $\{0, 1, 2\}$ in (5.19-21). This is exactly the set of space groups found by Janssen [9]. (Calculation shows that all differences between Janssen's results and (5.19-21) are just due to different choices of the origin and the generating set.)

Equivalence by quasidilatations

Of course we must not restrict attention to pure quasidilatations $\mathbf{Q}_1$ or $\mathbf{Q}_2$ but we eventually have to consider combined transformations of the type $(\mathbf{Q}_i\,|\,\mathbf{u})$, $i = 1, 2$.

We start with the simple cubic lattice $\mathfrak{L}_{SC}$. Under a pure quasidilatation $(\mathbf{Q}_2\,|\,\mathbf{0})$, $\mathbf{x}_m$ is transformed to

$$\mathbf{x}'_m = \mathbf{Q}_2\,\mathbf{x}_m = \left(\frac{2\,m}{5}, \frac{m}{5}, -\frac{2\,m}{5}, \frac{m}{5}, \frac{4\,m}{5}, \frac{3\,m}{5}\right), \tag{5.22}$$

which is not of the form $\mathbf{x}_m$ anymore. However, we still are free to perform a shift by $\mathbf{u}_{s,t} = (s, s, s, t, -t, t)$ without changing $\mathbf{y}$ since $\mathbf{u}_{s,t} \in \mathrm{E}^{\mathbf{A}_3}_{\lambda=1}$. We obtain

$$\begin{aligned}\mathbf{Q}_2\,\mathbf{x}_m \mapsto \mathbf{Q}_2\,\mathbf{x}_m + (\mathbf{E} - \mathbf{A}_5)\,\mathbf{u}_{s,t} &= \\ = \Big(\frac{2m}{5}, -\frac{m}{5} + s - t, -\frac{2m}{5}, \frac{m}{5} - s + t,\\ \frac{4m}{5} - 2t, \frac{3m}{5} + 2t\Big)\,. \end{aligned} \quad (5.23)$$

Choosing $t = -\frac{3m}{10}$ and $s = \frac{m}{10}$, i.e. $\mathbf{u}_{s,t} = \frac{m}{10}(1, 1, 1, 3, -3, 3)$, the vector on the r.h.s. of (5.23) becomes $\mathbf{x}_{2m}$ (mod 5). In terms of (5.5) we can write

$$(\mathbf{Q}_2|\tilde{\mathbf{u}})(\mathbf{A}_5|\mathbf{x}_m)(\mathbf{Q}_2|\tilde{\mathbf{u}})^{-1} = (\mathbf{A}_5|\mathbf{x}_{2m}(\mathrm{mod}\ 5)). \quad (5.24)$$

with $\tilde{\mathbf{u}} = \mathbf{Q}_2^{-1}\,\mathbf{u}_{s,t}$. This action has two orbits: $\{\mathbf{x}_m = 0\}$ and $\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4\}$; the first one corresponds to the symmorphic space group, he second one to all nonsymmorphic space groups. We are left with only 2 inequivalent space groups belonging to the Bravais lattice $\mathcal{L}_{\mathrm{SC}}$ and the point group Y.

The calculations for $\mathcal{L}_{\mathrm{FCC}}$ and $\mathcal{L}_{\mathrm{BCC}}$ are similar and not carried through in detail here. The quasidilatation $\mathbf{Q}_1 = \frac{1}{2} \cdot (\mathbf{E} + \mathbf{M})$ can be shown to have exactly the same effect (5.24) on the non-primitive translations $\mathbf{x}_m$ given in (5.20, 21). This leads us to the final result :

For the point group Y, there are 2 inequivalent space groups for each of the lattices $\mathcal{L}_{\mathrm{SC}}$, $\mathcal{L}_{\mathrm{FCC}}$, and $\mathcal{L}_{\mathrm{BCC}}$. They are given by (5.19-21) with $m = 0,1$ and are listed in table II.

5.5 THE SPACE GROUPS CORRESPONDING TO POING GROUP Y_{I}. — The calculations in this paragraph are very similar in spirit to those for the point group Y ; we only quote the essential steps. Setting $\mathbf{x} = \mathbf{a}_5$, $\mathbf{y} = \mathbf{a}_3$, and $\mathbf{z} = \mathbf{i}$, the defining relations (5.7, 8) become

$$(\mathbf{A}_5^4 + \mathbf{A}_5^3 + \mathbf{A}_5^2 + \mathbf{A}_5 + \mathbf{E})\,\mathbf{x} = \mathbf{0}(\mathrm{mod}\ \mathcal{L})\,, \quad (5.25a)$$
$$(\mathbf{A}_3^2 + \mathbf{A}_3 + \mathbf{E})\,\mathbf{x} = \mathbf{0}(\mathrm{mod}\ \mathcal{L})\,, \quad (5.25b)$$
$$(\mathbf{A}_5\,\mathbf{A}_3 + \mathbf{E})(\mathbf{A}_5\,\mathbf{y} + \mathbf{x}) = \mathbf{0}(\mathrm{mod}\ \mathcal{L})\,, \quad (5.25c)$$
$$\mathbf{x} + \mathbf{A}_5\,\mathbf{z} = \mathbf{z} - \mathbf{x}(\mathrm{mod}\ \mathcal{L})\,, \quad (5.25d)$$
$$\mathbf{y} + \mathbf{A}_3\,\mathbf{z} = \mathbf{z} - \mathbf{y}(\mathrm{mod}\ \mathcal{L})\,, \quad (5.25e)$$
$$2\,\mathbf{z} = \mathbf{0}(\mathrm{mod}\ \mathcal{L})\,. \quad (5.25f)$$

After a parallel shift $\mathbf{u}$ satisfying $\mathbf{z} - 2\,\mathbf{u} = \mathbf{0}(\mathrm{mod}\ \mathcal{L})$, equations (5.25d-f) are reduced to

$$2\,\mathbf{x} = \mathbf{0}(\mathrm{mod}\ \mathcal{L})\,, \quad (5.26a)$$
$$2\,\mathbf{y} = \mathbf{0}(\mathrm{mod}\ \mathcal{L})\,, \quad (5.26b)$$
$$\mathbf{z} = \mathbf{0}(\mathrm{mod}\ \mathcal{L})\,. \quad (5.26c)$$

Table II. — *The* 11 *icosahedral space groups. The table contains the translational parts of the generating sets of the point groups* Y *and* $\mathrm{Y_I}$, *namely* $\{(\mathbf{A}_5|\mathbf{a}_5), (\mathbf{A}_3|\mathbf{a}_3)\}$ *and* $\{(\mathbf{A}_5|\mathbf{a}_5), (\mathbf{A}_3|\mathbf{a}_3), (\mathbf{I}|\mathbf{i})\}$, *respectively.*

	point group Y	point group $\mathrm{Y_I}$
$\mathcal{L}_{\mathrm{SC}}$	2 space groups $\mathbf{a}_5 = \left(\frac{m}{5}, 0, -\frac{m}{5}, 0, \frac{m}{5}, 0\right)$ $\mathbf{a}_3 = \mathbf{0}$ $m \in \{0, 1\}$	2 space groups $\mathbf{a}_5 = \left(0, 0, 0, 0, \frac{m}{2}, \frac{m}{2}\right)$ $\mathbf{a}_3 = \mathbf{i} = \mathbf{0}$ $m \in \{0, 1\}$
$\mathcal{L}_{\mathrm{FCC}}$	2 space groups $\mathbf{a}_5 = \left(\frac{m}{5}, 0, -\frac{m}{5}, 0, \frac{6m}{5}, 0\right)$ $\mathbf{a}_3 = \mathbf{0}$ $m \in \{0, 1\}$	2 space groups $\mathbf{a}_5 = \left(0, 0, 0, 0, \frac{m}{2}, -\frac{m}{2}\right)$ $\mathbf{a}_3 = \mathbf{i} = \mathbf{0}$ $m \in \{0, 1\}$
$\mathcal{L}_{\mathrm{BCC}}$	2 space groups $\mathbf{a}_5 = \left(\frac{m}{5}, 0, -\frac{m}{5}, 0, \frac{6m}{5}, 0\right)$ $\mathbf{a}_3 = \mathbf{0}$ $m \in \{0, 1\}$	1 space group (only symmorphic) $\mathbf{a}_5 = \mathbf{a}_3 = \mathbf{i} = \mathbf{0}$

Equivalence by parallel shifts

Concerning space group equivalence due to parallel shifts, there is a difference to the last paragraph : In order to preserve the validity of equations (5.26), we can only apply coordinate shifts $\mathbf{u}$ satisfying $2\,\mathbf{u} = \mathbf{0} (\mathrm{mod}\, \mathcal{L})$. However, calculation shows that, similar to (6.15), we still can restrict ourselves to the solution of (5.25) satisfying

$$\mathbf{y} = \mathbf{0} (\mathrm{mod}\, \mathcal{L}) \quad \text{and} \quad \mathbf{z} = \mathbf{0} (\mathrm{mod}\, \mathcal{L}) \tag{5.27}$$

without loss of generality. Making full use of all allowed parallel shifts, as in paragraph 5.4, we arrive at a set of space groups characterized by the following non-primitive translations :

(i) Simple cubic lattice $\mathcal{L}_{\mathrm{SC}}$:

$$\mathbf{x}_m = \left(0, 0, 0, 0, \frac{m}{2}, \frac{m}{2}\right), \quad \mathbf{y} = \mathbf{0},\ \mathbf{z} = \mathbf{0},\ (\mathrm{mod}\, \mathcal{L}_{\mathrm{SC}}), \tag{5.28}$$

where $m \in \{0, 1\}$.

(ii) Face-centered cubic lattice $\mathcal{L}_{\mathrm{FCC}}$:

$$\mathbf{x}_{mn} = \left(0, \frac{m}{2}, 0, -\frac{m}{2}, \frac{n}{2}, -\frac{n}{2}\right), \quad \mathbf{y} = \mathbf{0},\ \mathbf{z} = \mathbf{0},\ (\mathrm{mod}\, \mathcal{L}_{\mathrm{FCC}}), \tag{5.29}$$

where $m \in \{0, 1\}$.

(iii) Body-centered cubic lattice $\mathcal{L}_{\mathrm{BCC}}$:

$$\mathbf{x} = \mathbf{0},\ \mathbf{y} = \mathbf{0},\ \mathbf{z} = \mathbf{0},\ (\mathrm{mod}\, \mathcal{L}_{\mathrm{BCC}}). \tag{5.30}$$

Only the symmorphic space group exists in this case.

The space groups corresponding to (5.28-30) are exactly those found by Janssen [9].

Equivalence by quasidilatations.

Quasidilatations act as follows on the above space groups. The non-primitive translation $\mathbf{x}_m = 1$ for $\mathcal{L}_{\mathrm{SC}}$ is invariant under $\mathbf{Q}_2$. For the face-centered lattice the action of $(\mathbf{Q}_1 | \mathbf{0})$ on $\mathbf{x}_{mn}$ can be described by the action on the pair (m, n) as follows :

$$(m, n) \to (m + n, m) \quad (\mathrm{mod}\, 2), \tag{5.31}$$

which has the two orbits

$$\{(0, 0)\} \quad \text{and} \quad \{(0, 1), (1, 1), (1, 0)\}. \tag{5.32}$$

For $\mathcal{L}_{\mathrm{BCC}}$, things are trivial. We are left with the following final result :

For the point group $\mathrm{Y_I}$, there are two non-equivalent space groups for the Bravais lattices $\mathcal{L}_{\mathrm{SC}}$ and $\mathcal{L}_{\mathrm{FCC}}$. The space groups of $\mathcal{L}_{\mathrm{SC}}$ are given by (5.28), the space groups of $\mathcal{L}_{\mathrm{FCC}}$ latter by (5.29) with $m = 0$, $n \in \{0, 1\}$. For the lattice $\mathcal{L}_{\mathrm{BCC}}$, only the symmorphic space group exists according to (5.30). The space groups are tabulated in table II.

We close this section with a remark concerning *space group notation.* The *Hermann-Mauguin* notation which is commonly used in 3-dimensional crystallography is inappropriate for labelling the icosahedral space groups since it relies on space group properties like *screw axes* and *glide planes.* Above, the former were shown to be inexistent in icosahedral crystallography.

6. Systematic extinctions.

We now calculate the systematic extinction of Bragg peaks due to the *nonsymmorphic space group symmetries.* The reciprocal lattices of the three Bravais lattices (4.2a-c) are

$$\mathcal{L}_{\mathrm{SC}}^{\mathrm{R}} = 2\,\pi \,.\, \mathcal{L}_{\mathrm{SC}}, \quad \mathcal{L}_{\mathrm{FCC}}^{\mathrm{R}} = \pi \,.\, \mathcal{L}_{\mathrm{BCC}}, \quad \mathcal{L}_{\mathrm{BCC}}^{\mathrm{R}} = \pi \,.\, \mathcal{L}_{\mathrm{FCC}}. \tag{6.1}$$

Table III. — *Extinctions due to nonsymmorphic space group symmetries. The extinctions given in the table for the point group* Y *all correspond to the point group element* $\mathbf{A}_5$ *(for the simple cubic Bravais lattice* $\mathcal{L}_{\mathrm{SC}}$ *this is shown explicitely in section 5.), while the extinctions for the point group* $\mathrm{Y_I}$ *all correspond to the point group elements* $\mathbf{A}_5\,\mathbf{A}_3$ *and* $\mathbf{A}_5\,\mathbf{A}_3\,\mathbf{I}$. *All other conjugacy classes of Y and* Y_I *yield no extinctions. The complete extinction pattern is obtained by acting on the tabulated extinctions with whole point group.*

	point group Y	point group $\mathrm{Y_I}$
$\mathcal{L}_{\mathrm{SC}}$	$\mathbf{k} = 2\pi \cdot (n, l, l, l, l, l)$ $n \notin 5\,\mathbb{Z}$	$\mathbf{k} = 2\pi \cdot (n_1, n_2, -n_1, -n_2, n_5, n_6)$ $n_5 - n_6$ odd
$\mathcal{L}_{\mathrm{FCC}}$	$\mathbf{k} = \pi\,(n, l, l, l, l, l)$ $n + 5\,l \notin 10\,\mathbb{Z}$	$\mathbf{k} = \pi\,(n_1, n_2, -n_1, -n_2, n_5, n_6)$ $n_5 - n_6 \notin 4\,\mathbb{Z}$
$\mathcal{L}_{\mathrm{BCC}}$	$\mathbf{k} = \pi\,(n, l, l, l, l, l)$ $n + 5\,l \notin 10\,\mathbb{Z}$	no extinctions (only symmorphic space group)

Extinctions of Bragg peaks are due to zeroes of the form factor

$$\mathcal{F}(\mathbf{k}) = \int_{\text{u.c.}} d^6 r \, \rho(\mathbf{r}) \, \mathrm{e}^{i\mathbf{kr}} , \tag{6.2}$$

where $\rho(\mathbf{r})$ is a periodic density distribution and u.c. is a unit cell. Let $\rho(\mathbf{r})$ be invariant under a space group element $(\mathbf{H}|\mathbf{h})$, i.e. $\rho(\mathbf{r}) = \rho(\mathbf{Hr} + \mathbf{h})$. In this case,

$$\mathcal{F}(\mathbf{k}) = \mathrm{e}^{i\mathbf{kh}} \cdot \mathcal{F}(\mathbf{H}^{-1}\mathbf{k}) . \tag{6.3}$$

If, for some Bragg peak position $\mathbf{k}_0$,

$$\mathcal{F}(\mathbf{k}_0) = \mathcal{F}(\mathbf{Hk}_0) \tag{64.a}$$

and

$$\mathrm{e}^{i\mathbf{k}_0 \mathbf{h}} \neq 1 , \tag{6.4b}$$

then (6.3) implies $\mathcal{F}(\mathbf{k}_0) = 0$, i.e. the peak at $\mathbf{k}_0$ is absent. Equation (6.4a) is satisfied if $\mathbf{k}_0$ is invariant under the point group element $\mathbf{H}$, i.e. if $\mathbf{k}_0$ lies in $\mathrm{E}^{\mathbf{H}}_{\lambda=1}$ [see definition (5.5)]. In this way every point group element $\mathbf{H}$ can be associated with some set of extinctions (possibly the zero set). It is easy to verify that all extinctions are obtained by calculating those corresponding to one element of each conjugacy class of the point group and then acting on these extinctions by all elements of the point group. The five conjugacy classes of the point group Y are represented by $\mathbf{E}$, $\mathbf{A}_5$, $\mathbf{A}_5^2$, $\mathbf{A}_3$, and $\mathbf{A}_5\,\mathbf{A}_3$.

The eingenspaces with eigenvalue 1 of these point group elements are :

$$\mathbf{A}_5 : (s, t, t, t, t, t) , \tag{6.5a}$$
$$\mathbf{A}_5^2 : (s, t, t, t, t, t) , \tag{6.5b}$$
$$\mathbf{A}_3 : (s, s, s, t, -t, t) , \tag{6.5c}$$
$$\mathbf{A}_5\,\mathbf{A}_3 : (s, t, s, t, 0, 0) , \tag{6.5d}$$

where $s, t \in \mathbb{R}$. The point group Y_I has ten conjugacy classes, namely those of Y and in addition five represented by $\mathbf{I}$, $\mathbf{A}_5\,\mathbf{I}$, $\mathbf{A}_5^2\,\mathbf{I}$, $\mathbf{A}_3\,\mathbf{I}$, and $\mathbf{A}_5\,\mathbf{A}_3\,\mathbf{I}$. The eigenspaces with eigenvalue $+1$ are those of (6.5a-d) and in addition

$$\mathbf{A}_5\,\mathbf{I} : \text{none} , \tag{6.6a}$$
$$\mathbf{A}_5^2\,\mathbf{I} : \text{none} , \tag{6.6b}$$
$$\mathbf{A}_3\,\mathbf{I} : \text{none} , \tag{6.6c}$$
$$\mathbf{A}_5\,\mathbf{A}_3\,\mathbf{I} : (s, t, -s, -t, u, v) , \tag{6.6d}$$

where $s, t, u, v \in \mathbb{R}$.

As an example we calculate the extinctions for the nonsymmorphic space group corresponding to the Bravais lattice $\mathfrak{L}_{\mathrm{SC}}$ and point group Y.

Conjugacy class of $\mathbf{A}_5$: Using (6.1), the Bragg peak positions lying in the eigenspace (6.5a) are given by

$$\mathbf{k}_{lm} = 2\,\pi \,.\, (l, m, m, m, m, m), \; l, m \in \mathbb{Z} . \tag{6.7}$$

Inserting the nonprimitive translations $\mathbf{a}_5$ from table II, the phase factor in (6.3) becomes

$$\mathbf{k}_{lm} \cdot \mathbf{a}_5 = 2\,\pi \cdot \left[\frac{l-m}{5} + \frac{m}{5} \right] = \frac{2\,\pi l}{5} . \tag{6.8}$$

Hence (6.4b) is satisfied if $l \neq 0 (\mathrm{mod}\, 5)$.

Conjugacy class of $\mathbf{A}_3$: Yields no additional extinctions since $\mathbf{a}_3 = 0$.

Conjugacy class of $\mathbf{A}_5\,\mathbf{A}_3$: The Bragg peaks in the eigenspace (6.5d) are at positions

$$\mathbf{k}_{lm} = 2\,\pi \cdot (l, m, l, m, 0, 0) . \tag{6.9}$$

The translation of $\mathbf{A}_5\,\mathbf{A}_3$ is equal to $\mathbf{a}_5$ and the phase factor in (6.3) becomes zero for all values of l and m. Thus this conjugacy class yields no additional extinctions.

The extinctions for the other nonsymmorphic space groups are calculated in the same manner. The results are given in table III.

7. Summary and conclusions.

We have shown how crystallographic methods can be applied to quasicrystalline symmetries by relating them to crystalline symmetries in a higher-dimensional space. Periodic structures with icosahedral symmetry exist in 6 (or more) dimensions. It turned out that surprisingly few types of such 6-dimensional structures exist. The question of space group equivalence has been shown to be important : In icosahedral crystallography there is a class of equivalence transformations which has no analogy in ordinary 3-dimensional crystallography, namely the quasidilatations. The existence of this kind of equivalence transformations is characteristic for the crystallography of noncrystallographic symmetries.

High energy electron diffraction (HEED) data are best fitted by *the simple cubic Bravais lattice* $\mathfrak{L}_{\mathrm{SC}}$ [28]. Convergent beam electron diffraction indicates that the point group is Y_I [29, 30]. Until recently, diffraction experiments were limited to HEED or powder diffraction by X-rays and neutrons due to the small grain sizes. HEED can reveal Bravais lattices but is known to be unreliable for the investigation of space groups. This is because of the importance of multiple scattering processes which can give rise to nonzero scattering amplitude at all Bragg angles. Recently, however, an X-ray diffraction study on uniformly oriented AlLiCu quasicrystals (grain size around 100 μm) has been reported [31]. The HEED result that the Bravais lattice is $\mathfrak{L}_{\mathrm{SC}}$, is confirmed. Nevertheless, significant deviations from the calculated diffraction pattern [28] are found. A careful space group analysis of these experimental data would be very interesting. Nonsymmorphic space group symmetries have been observed (by HEED) in octagonal [17] and decagonal [19, 32] quasicrystals which have been addressed in section 2.

We finally point out that a space group analysis of quasicrystal diffraction data could be important for the question whether quasiperiodic or *icosahedral glass models* [33] are more appropriate for the description of the icosahedral phase. This question is still open. If a diffraction pattern could be fitted well to one of those belonging to a non-symmorphic space group, this would strongly favour the quasiperiodic models.

Note added : After submission of this paper we became aware of an article by Rokhsar, Wright and Mermin [34], where the same problems are treated. These authors obtain exactly the same results ; however, their approach is rather different from the one presented in our article. Our method is a real space formalism. We map the d-dimensional « quasicrystallography » onto ordinary crystallography in a higherdimensional space, using the concepts of the projection method. Rokhsar *et al.* treat the problem in **k**-space, which has the physical dimensionality d. In this latter approach, which has been used for ordinary crystal symmetries as well [35], there is no conceptual difference between crystallographic and non-crystallographic point group symmetries.

Acknowledgments.

We are grateful to W. Baltensperger, T. M. Rice, C. Beeli, G. Blatter, F. Gähler, P. A. Kalugin, A. Yu. Kitayev, and H.-U. Nissen for useful discussions and to C. Beeli, G. Blatter, and H.-U. Nissen for helpful comments on the manuscript. One of us (J.R.) is deeply indebted to the Landau Institute for Theoretical Physics at Moscow for the warm hospitality during the time when this work was begun ; he thanks the USSR Academy of Sciences and the Schweizerischer Nationalfonds for financial support.

References

[1] Henley, C. L., *Solid State Comm.* **8** (1987) 59.
[2] de Wolff, P. M., *Acta Cryst. A* **30** (1974) 777.
[3] Janner, A. and Janssen, T., *Phys. Rev. B* **15** (1977) 643.
[4] Bak, P. and Janssen, T., *Phys. Rev. B* **17** (1978) 437.
[5] Shechtman, D., Blech, I., Gratias, D. and Cahn, J. W., *Phys. Rev. Lett.* **53** (1984) 1951.
[6] Rhyner, J. and Levitov, L. S., Proceedings of the 8th General Conference of the Condensed Mater Division of the European Physical Society, Budapest (1988), to be published in *Physica Scripta* (1988).
[7] Kalugin, P. A., Kitayev, A. Yu and Levitov, L. S., *J. Phys. Lett.* **46** L-601 (1985).
[8] Bak, P., *Phys. Rev. B* **32** (1985) 5764.
[9] Janssen, T., *Acta Cryst. A* **42** (1986) 261.
[10] Rokhsar, D. S., Mermin, N. D. and Wright, D. C., *Phys. Rev. B* **35** (1987) 548.
[11] Rhyner, J., Thesis, Zürich (1987), unpublished.
[12] Martinais, D., *C. R. Acad. Sci. Paris, Ser.* **305** (1987) 509.
[13] Plesken, W. and Hanrath, W., *Math. Comp.* **43** (1984) 573.
[14] Elser, V., *Acta Cryst. A* **42** (1985) 36.
[15] van der Waerden, B. L., Algebra, Springer (1960).
[16] Gähler, F. and Rhyner, J., *J. Phys. A* **19** (1986) 267.
[17] Wang, N., Chen, H. and Kuo, K. H., *Phys. Rev. Lett.* **59** (1987) 1010.
[18] Bendersky, L., *Phys. Rev. Lett.* **55** (1985) 1461.
[19] Fung, K. G., Yang, C. Y., Zhou, Y. Q., Zhao, J. G., Zhan, W. S. and Shan, B. G., *Phys. Rev. Lett.* **56** (1986) 2060.
[20] Ishimasa, T., Nissen, H.-U. and Fukano, Y., *Phys. Rev. Lett.* **55** (1985) 511.
[21] Gähler, F., preprints and Thesis, Zürich (1987), unpublished.
[22] Rokhsar, D. S., Wright, D. C. and Mermin, N. D., *Acta Cryst. A* **44** (1988) 197.
[23] Ashcroft, N. W. and Mermin, N. D., *Solid State Phys.*, Holt-Saunders, New York (1976).
[24] Speiser, A., Die Theorie der Gruppen von endlicher Ordnung, Birkhäuser, Basel (1987).
[25] Coxeter, H. S. M. and Mozer, W. O. J., Generators and Relations for Discrete Groups, Springer (1972).
[26] Elser, V., *Phys. Rev. B* **32** (1985) 4892.
[27] Janssen, T., Crystallographic Groups, North-Holland (1973).
[28] Cahn, J. W., Shechtman, D. and Gratias, D., *J. Mater. Res.* **1** (1986) 13.
[29] Bendersky, L. and Kaufman, M. J., *Philos. Mag. B* **53** (1986) L75.
[30] Cassada, W. A., Shiflet, G. J. and Poon, S. J., *Phys. Rev. Lett.* **56** (1986) 2276.
[31] Denoyer, F., Heger, G., Lambert, M., Lang, J. M. and Sainfort, P., *J. Phys. France* **48** (1987) 1357.
[32] Bendersky, L., *J. Phys. France* **47** (1986) C3-457.
[33] Stephens, P. W. and Goldman, A. M., *Phys. Rev. Lett.* **56** (1986) 1168.
[34] Rokhsar, D. S., Wright, D. C. and Mermin, N. D., *Phys. Rev. B* **37** (1988) 8145.
[35] Bienenstock, A. and Ewald, P. P., *Acta Cryst.* **15** (1962) 1253.