

Regular Polytopes, Root Lattices, and Quasicrystals*

R. Bruce King

Department of Chemistry, University of Georgia, Athens, Georgia 30602, USA
(E-mail: rbking@sunchem.chem.uga.edu.)

RECEIVED APRIL 1, 2003; REVISED JULY 8, 2003; ACCEPTED JULY 10, 2003

Key words
polytopes
root lattices
quasicrystals
icosahedron

The icosahedral quasicrystals of five-fold symmetry in two, three, and four dimensions are related to the corresponding regular polytopes exhibiting five-fold symmetry, namely the regular pentagon (H_2 reflection group), the regular icosahedron $\{3,5\}$ (H_3 reflection group), and the regular four-dimensional polytope $\{3,3,5\}$ (H_4 reflection group). These quasicrystals exhibiting five-fold symmetry can be generated by projections from indecomposable root lattices with twice the number of dimensions, namely $A_4 \rightarrow H_2$, $D_6 \rightarrow H_3$, $E_8 \rightarrow H_4$. Because of the subgroup relationships $H_2 \subset H_3 \subset H_4$, study of the projection $E_8 \rightarrow H_4$ provides information on all of the possible icosahedral quasicrystals. Similar projections from other indecomposable root lattices can generate quasicrystals of other symmetries. Four-dimensional root lattices are sufficient for projections to two-dimensional quasicrystals of eight-fold and twelve-fold symmetries. However, root lattices of at least six-dimensions (e.g., the A_6 lattice) are required to generate two-dimensional quasicrystals of seven-fold symmetry. This might account for the absence of seven-fold symmetry in experimentally observed quasicrystals.

INTRODUCTION

The symmetries that cannot be exhibited by true crystal lattices include five-fold, eight-fold, and twelve-fold symmetry. For this reason crystallographers were startled by the discovery by Shechtman and coworkers¹ that rapidly solidified aluminum-manganese alloys of approximate composition Al_6Mn gave electron diffraction patterns having apparently sharp spots and five-fold symmetry axes. Subsequent work² led to the discovery of a number of related alloys, particularly aluminum-rich alloys, exhibiting five-fold and other crystallographically forbidden symmetries. These materials are now called quasicrystals.^{3,4,5,6} Such quasicrystals are seen to represent a new type of incommensurate crystal structure whose Fourier transform consists of a δ function as for periodic crystals

but with point symmetries incompatible with traditional crystallography. More specifically, ordered solid state quasicrystalline structures with five-fold symmetry exhibit quasiperiodicity in two dimensions and periodicity in the third.

Quasicrystals are seen to exhibit lower order than true crystals but a higher order than truly amorphous materials. The order in icosahedral quasicrystals, *i.e.*, quasicrystals exhibiting five-fold symmetry, can formally be described in six-dimensional hyperspace in which the atoms are three-dimensional subspaces. The actual icosahedral quasicrystal structures are then three-dimensional projections of this six-dimensional hyperspace.^{7,8,9}

The use of such projection models to describe quasicrystal structures requires an understanding of higher dimensional crystal lattices from which such projections to

* This paper is dedicated to Nenad Trinajstić in recognition of his pioneering contributions to mathematical chemistry.

two or three dimensions can be made. The simplest such higher dimensional lattices are the primitive hypercubic lattices Z^n , which are generated from all integral linear combinations of unit vectors along n orthogonal Cartesian axes. However, in many cases more complicated higher dimensional lattices are required, such as various types of centered hypercubic lattices. These higher dimensional lattices correspond to the root lattices, which are generated from all integral linear combinations of the vectors (roots) of so-called root systems.^{10,11} These root systems form a certain class of vector stars with specific allowed symmetries, lengths, and angles.^{10,11,12} Such root systems arise in different contexts such as crystallographic finite reflection groups^{10,12} or finite-dimensional semi-simple Lie algebras.¹¹ The connection between root lattices and quasicrystals was first presented in a short letter by Baake, Joseph, Kramer, and Schlottmann¹³ with particular attention to two-dimensional quasilattices having rotational symmetries of orders 5, 8, 10, and 12.

This paper extends this connection between root lattices and quasicrystals to the important three-dimensional case of icosahedral quasicrystals with a more detailed survey of the key areas of mathematics involved in this connection. In addition the existence of root lattices is related to the existence of regular polytopes in higher dimensional spaces, which is also examined in this paper.

REGULAR POLYTOPES FROM REGULAR TESSELLATIONS

The term polytope generalizes the two-dimensional concept of polygon and the three-dimensional concept of polyhedron to any number of dimensions.¹⁴ Thus an

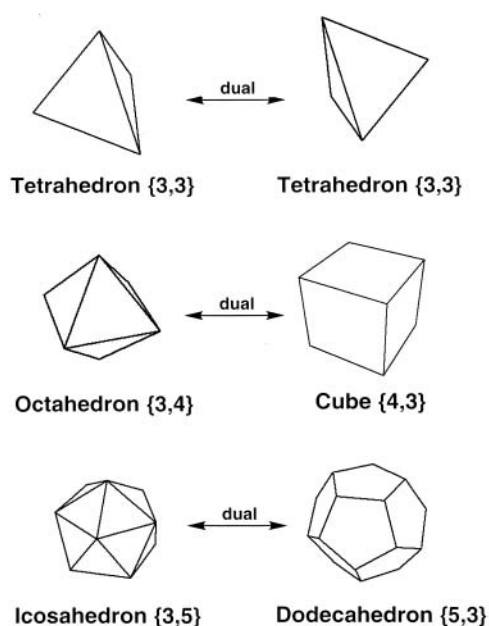


Figure 1. The five regular »Platonic« polyhedra showing their Schäfli symbols and the dual pairs. Note that the tetrahedron is self-dual.

TABLE I. Properties of the regular (Platonic) polyhedra

Polyhedron	Face type	Vertex degrees	Number of edges	Number of faces	Number of vertices
Tetrahedron {3,3}	Triangle	3	6	4	4
Octahedron {3,4}	Triangle	4	12	8	6
Cube {4,3}	Square	3	12	6	8
Icosahedron {3,5}	Triangle	5	30	20	12
Dodecahedron {5,3}	Pentagon	3	30	12	20

n -dimensional polytope is a connected set («complex») of facets of each dimension less than n where the 0-dimensional facets are called vertices, the 1-dimensional facets are called edges, the 2-dimensional facets are called faces, the 3-dimensional facets are called cells, *etc.* Such a polytope is a regular polytope when the component facets of each dimension are identical regular polytopes and all facets of each dimension are equivalent (*i.e.*, transitive as discussed below). In two-dimensions the regular polytopes are the infinite number of regular polygons whereas in three dimensions the regular polytopes are the five regular »Platonic« polyhedra (Figure 1 and Table I).

The concept of a tessellation is useful for generating regular polytopes of low dimension as well as related lattices. In this connection, embedding a network of polygons into a surface can be described as a tiling or tessellation of the surface.¹⁵ In a formal sense a tiling or tessellation of a surface is a countable family of closed sets $T = \{T_1, T_2, \dots\}$ which cover the surface without gaps or overlaps. More explicitly, the union of the sets T_1, T_2, \dots (which are known as the tiles of T) is the whole surface and the interiors of the sets T_i are pairwise disjoint. In the tessellations of interest in this paper, the tiles are the polygons, which, in the case of tessellations corresponding to polyhedra, are the faces of the polyhedra. Tessellations can be described in terms of their flags, where a flag is a triple (V, E, F) consisting of a vertex V , and edge E , and a face F which are mutually incident. A tiling T is called regular if its symmetry group $G(T)$ is transitive on the flags of T . A regular tessellation consisting of q regular p -gons at each vertex can be described by the so-called Schäfli notation $\{p, q\}$. The Schäfli notation can be generalized to higher dimensions in the obvious way.

First consider regular tessellations in the Euclidean plane, *i.e.*, a flat surface of zero curvature. In the Euclidean plane, the angle of a regular p -gon, $\{p\}$, is $(1 - 2/p)\pi$; hence q equal $\{p\}$'s (of any size) will fit together around a common vertex if this angle is equal to $2\pi/q$, leading to the relationship

$$(p - 2)(q - 2) = 4 \quad (1)$$

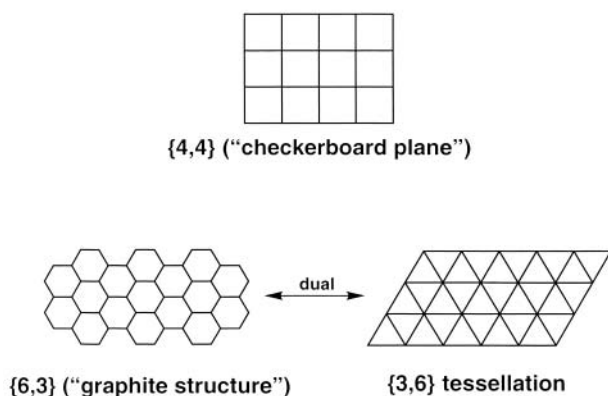


Figure 2. The three regular tessellations of the plane, namely the self-dual $\{4,4\}$ checkerboard tessellation and the $\{6,3\} \leftrightarrow \{3,6\}$ dual pair.

There are only three integral solutions of equation (1), which lead to the three regular tessellations of the plane $\{4,4\}$, $\{6,3\}$, and $\{3,6\}$ depicted in Figure 2. The tessellation $\{6,3\}$ is familiar in chemistry as the structure of graphite whereas the tessellation $\{4,4\}$ corresponds to the checkerboard.

Now consider the regular tessellations of the sphere that correspond to the regular polyhedra (Figure 1). The angle of a regular spherical polygon $\{p\}$ is greater than $(1 - 2/p)\pi$ and gradually increases from this value to π when the circumradius increases from 0 to $\pi/2$. Thus if

$$(p - 2)(q - 2) < 4 \quad (2)$$

the size of $\{p\}$ can be adjusted so that its angle is exactly $2\pi/q$; then q such $\{p\}$'s will fit together around a common vertex leading to the regular spherical tessellations $\{2,q\}$, $\{p,2\}$, $\{3,3\}$, $\{3,4\}$, $\{4,3\}$, $\{3,5\}$, and $\{5,3\}$. The tessellation $\{2,q\}$, formed by q lunes (*i.e.*, spherical polygons with two vertices and two edges) joining two antipodal points, is called the q -gonal hosohedron.¹⁶ The tessellation $\{p,2\}$, formed by two p -gons, each covering a hemisphere, is called the p -gonal dihedron, since it has two faces. The remaining five regular spherical tessellations correspond to the five regular polyhedra (Figure 1 and Table I).

The concept of duality is important in the study of polyhedra as well as higher dimensional polytopes. In three dimensions a given polyhedron P can be converted into its dual P^* by locating the vertices of P^* above the centers of the faces of P and the centers of the faces of P^* above the vertices of P . Two vertices in the dual P^* are connected by an edge when the corresponding faces in P share an edge. The process of dualization has the following properties:

(i) The numbers of vertices (v and v^*), edges (e and e^*), and faces (f and f^*) in a pair of dual polyhedra P and P^* satisfy the relationships $v^* = f$, $e = e^*$, $f = v^*$.

(ii) Dual polyhedra have the same symmetry elements and thus belong to the same symmetry point group.

(iii) Dualization of the dual of a polyhedron leads to the original polyhedron.

(iv) The degrees of the vertices of the polyhedron correspond to the number of edges in the corresponding face polygons of its dual. Thus the duals of the deltahedra are trivalent polyhedra, *i.e.*, polyhedra in which all vertices are of degree 3.

(v) The dual of a regular polyhedron $\{p,q\}$ in the Schafli notation is $\{q,p\}$.

The dual pairs for the Platonic polyhedra consist of the cube/octahedron and dodecahedron/icosahedron (Figure 1). The tetrahedron is self-dual, *i.e.*, the dual of a tetrahedron is another tetrahedron. Also the concept of duality can be extended from standard polyhedra embedded in the surface of a sphere to polygonal networks embedded in surfaces of non-zero genus. In this connection the author has studied the Dyck and Klein tessellations of genus 3 surfaces with octagons and heptagons, respectively.^{17,18,19,20,21} Such Platonic tessellations and their duals are of interest in connection with possible structures of zeolite-like carbon and boron nitride allotropes with negative curvature.

Now consider regular polytopes of higher dimension ($n \geq 3$). In any dimension there are always the following three regular polytopes:

(i) The simplex α_n with a Schafli symbol of the type $\{3, \dots, 3\}$ analogous to the tetrahedron in three dimensions;

(ii) The cross polytope β_n with a Schafli symbol of the type $\{3, \dots, 4\}$ analogous to the octahedron in three dimensions;

(iii) The hypercube or measure polytope γ_n with a Schafli symbol of the type $\{4, \dots, 3\}$ analogous to the cube in three dimensions.²²

The cross polytope β_n and the corresponding hypercube γ_n for any given value of n are mutually dual similar to the cube and octahedron in three dimensions.

In five or more dimensions the three polytopes α_n , β_n , and γ_n are the only possible regular polytopes.^{22,23} However, in four dimensions there are the following six regular polytopes (Figure 3):

(i) The simplex α_4 or $\{3,3,3\}$ with 5 vertices, 10 edges, 10 triangular faces, and 5 tetrahedral cells with an automorphism group (*i.e.*, a four-dimensional symmetry point group) of order $5! = 120$. Each vertex is of degree 4. This polytope is derived from embedding the complete graph K_5 into four-dimensional space and is self-dual.

(ii) The cross polytope β_4 or $\{3,3,4\}$ with 8 vertices, 24 edges, 32 triangular faces, and 16 tetrahedral cells. The 8 vertices of $\{3,3,4\}$ are located along the four Cartesian axes with coordinates of the type $(\pm x_i, 0, 0, 0)$ where $0 < i \leq 4$. The 24 edges of $\{3,3,4\}$ connect each vertex

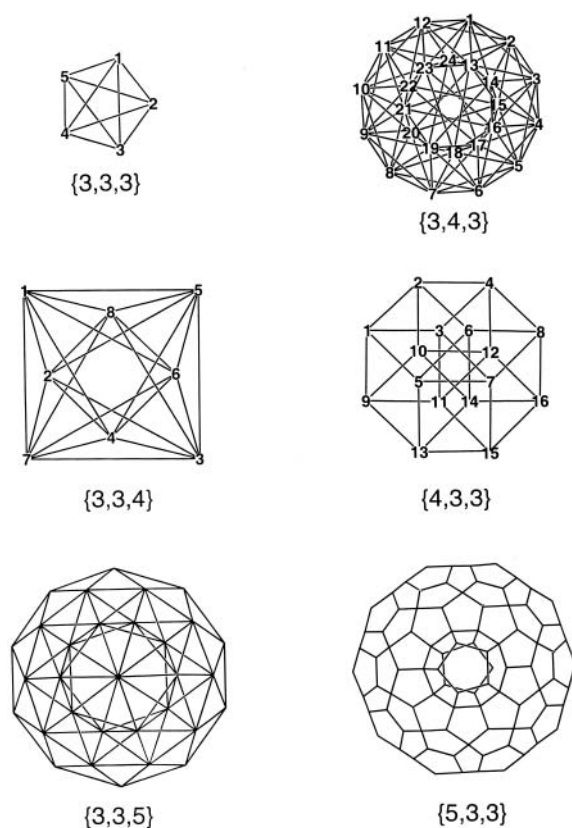


Figure 3. Projections of the six regular four-dimensional polytopes and their Schläfli symbols. For clarity only the »front« portions of the large $\{3,3,5\}$ and $\{5,3,3\}$ polytopes are shown.

with every other vertex except for its antipode on the same axis so that each vertex is of degree 6.

(iii) The hypercube or tesseract γ_4 or $\{4,3,3\}$ with 16 vertices, 32 edges, 24 square faces, and 8 cubic cells. Each vertex is of degree 4.

(iv) The self-dual $\{3,4,3\}$ polytope with 24 vertices, 96 edges, 96 triangular faces, and 24 octahedral cells with an automorphism group of order $3 \cdot 2^4 \cdot 4! = 1152$. Each vertex is of degree 8. This polytope is obtained by truncating the vertices of the $\{3,3,4\}$ cross polytope β_4 so that both the vertex figures and truncated cells coincidentally become congruent regular octahedra. There are no regular polytopes analogues to the $\{3,4,3\}$ polytope in either three dimensions or more than four dimensions.

(v) The $\{3,3,5\}$ polytope with 120 vertices, 720 edges, 1200 triangular faces, and 600 tetrahedral cells. Each vertex is of degree 12. This polytope may be regarded as the four-dimensional analogue of the three-dimensional icosahedron (Figure 1).

(vi) The $\{5,3,3\}$ polytope with 600 vertices, 1200 edges, 720 pentagonal faces, and 120 dodecahedral cells. Each vertex is of degree 4. This polytope may be regarded as the four-dimensional analogue of the three-dimensional regular dodecahedron.

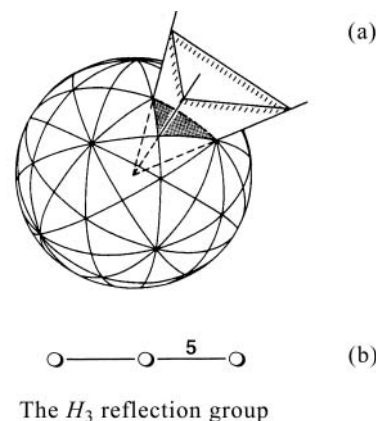


Figure 4. (a) Generation of the H_3 reflection group ($\approx I_h$ point group); (b) The Coxeter-Dynkin diagram for the H_3 reflection group.

The cross polytope $\{3,3,4\}$ and the hypercube $\{4,3,3\}$ form a dual pair having an automorphism group of order $2^4 \cdot 4 = 384$. Similarly the $\{3,3,5\}$ and $\{5,3,3\}$ polytopes form a dual pair with an automorphism group of order $120^2 = 14400$.

Of particular interest in connection with the theory of icosahedral quasicrystals to be discussed in this paper is the fact that the regular icosahedron has a four-dimensional analogue, namely the $\{3,3,5\}$ polytope, but no regular polytope analogues beyond four dimensions.

ROOT LATTICES FROM REFLECTION GROUPS

In order to provide a clearer geometric picture, this paper derives root lattices from reflection groups¹⁰ rather than from Lie groups.¹¹ In this connection consider a kaleidoscope whose three mirrors (or walls) cut the sphere in a spherical triangle having angles $\pi/2$, $\pi/3$, and $\pi/5$ (Figure 4a). The reflections in these walls generate a group of order 120 called the H_3 reflection group. The whole surface of the sphere is divided into 120 triangles, one for each group element. In this specific example the H_3 reflection group is isomorphic to the icosahedral point group I_h .

The group H_3 is an example of a finite or spherical reflection group. Such groups are called irreducible if they cannot be generated by direct products of smaller irreducible groups. In general, such irreducible reflection groups are generated by reflections in the walls of a spherical simplex, all of whose dihedral angles are submultiples of π . The infinite cone bounded by the reflecting walls or hyperplanes (*i.e.*, the kaleidoscope) is a fundamental region of the reflection group. If R_i is the reflection in the i th wall of the fundamental region, a set of generating relations for the corresponding reflection group can be generated by the following set of defining relations:

$$R_i^2 = (R_i R_j)^{p_{ij}} = 1 \quad (i, j = 1, \dots, n) \quad (1)$$

In Eq. (1) π/p_{ij} is the angle between the i th and j th walls. Coxeter has proven that every finite group with a set of defining relations of this form is a reflection group. Such reflection groups can be described by a Coxeter-Dynkin diagram, which has one vertex for each wall with two vertices being joined by a line labeled with the exponents p in the defining relations (Eq. 1). Certain abbreviations are customarily used for lines labelled with small values of p , as shown in Figure 5a. The Coxeter-Dynkin diagram for the reflection group H_3 is given in Figure 4b.

Finite reflection groups can be classified into crystallographic and non-crystallographic reflection groups. In the crystallographic reflection groups, the values of p can only have the values 2, 3, 4, and 6, since only such reflection groups are associated with crystal lattices. The Coxeter-Dynkin diagrams for the only finite indecomposable non-crystallographic reflection groups are given in Figure 5b. The groups with two vertices in their Coxeter-Dynkin diagrams correspond to the symmetries of the regular polygons $\{p\}$ as two-dimensional point groups. The group H_3 as noted above (Figure 4) corresponds to the symmetry point group I_h of the regular icosahedron $\{3,5\}$ or its dual, namely the regular dodecahedron $\{5,3\}$ (Figure 1). Similarly the group H_4 corresponds to the four-dimensional symmetry point group of the regular four-dimensional polytope $\{3,3,5\}$ or its dual $\{5,3,3\}$ (Figure 3).

The crystallographic reflection groups each correspond to a so-called root lattice. In this connection each reflecting hyperplane is specified by a vector perpendicular to it, which is called a root vector or simply a root. The root vectors perpendicular to the walls of the fundamental region are called the fundamental roots for the group whereas the entire set of root vectors is called a root system. The entire root system arises from all images of the fundamental roots under the actions of the group. The root system generates a lattice called the root lattice and the fundamental roots form an integral basis for the root lattice.

The above procedure defines a lattice Λ from the root system. Conversely, given a lattice Λ , a root (vector) for Λ can be defined as a vector $r \in \Lambda$ for which the associated reflection

$$x \rightarrow x - 2 \frac{x \cdot r}{r \cdot r} r \tag{2}$$

is a symmetry of Λ . If Λ is integral and unimodular, the roots correspond to the vectors of norm 1 or 2 in Λ , which are called the short and long roots, respectively. The roots corresponding to the walls of any one fundamental region are a set of fundamental roots for the lattice Λ . If Λ is not a root lattice, the fundamental roots in general are not a basis for Λ .

Table II lists all of the indecomposable finite root systems, which necessarily correspond to all of the indecomposable crystallographic finite reflection groups. The first column is the usual designation for the root system. These designations use early letters of the alphabet with subscripts corresponding to the dimension of the corresponding lattice. The second column lists the lattice corresponding to the root system in question. If all of the roots are of the same length, then the lattice is the same as that of the root system. However, if the root

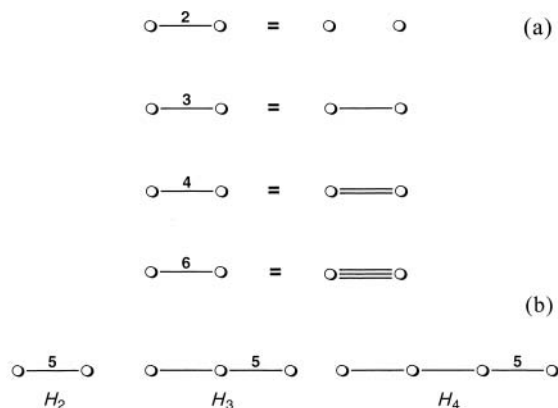


Figure 5. (a) Abbreviations used in Coxeter-Dynkin diagrams; (b) The Coxeter-Dynkin diagrams for the only finite indecomposable non-crystallographic reflection groups, namely H_2 , H_3 , and H_4 .

TABLE II. The indecomposable finite root systems

Root system	Lattice	Number of root vectors	Construction
A_n	A_n	$n(n+1)$	Projection of $e_i - e_j$ ($i, j = 1$ to $n-1$) into n -space
B_n	Z^n	$2n^2$	$\{\pm e_i, \pm e_i \pm e_j\}$ where ($i, j = 1$ to n)
C_n	D_n	$2n^2$	$\{\pm 2e_i, \pm e_i \pm e_j\}$ where ($i, j = 1$ to n)
D_n	D_n	$2n(n-1)$	$\{\pm e_i \pm e_j\}$ where ($i, j = 1$ to n)
G_2	A_2	12	$\{(1,0), (\frac{3}{2}, \frac{\sqrt{3}}{2})\}$ and six-fold rotations of these points
F_4	D_4	48	$B_4 \oplus \{ \frac{1}{2}(\pm e_1 \pm e_2 \pm e_3 \pm e_4) \}$
E_6	E_6	72	$A_5 \oplus \{ \pm \sqrt{2}e_7, \frac{1}{2}(\pm e_1 \pm e_2 \pm e_3 \pm e_4 \pm e_5 \pm e_6) \pm e_7 / \sqrt{2} \}$ with 3+3-
E_7	E_7	126	$A_7 \oplus \{ \frac{1}{2}(\pm e_1 \pm e_2 \pm e_3 \pm e_4 \pm e_5 \pm e_6 \pm e_7 \pm e_8) \}$ with 4+4-
E_8	E_8	240	$D_8 \oplus \{ \frac{1}{2}(\pm e_1 \pm e_2 \pm e_3 \pm e_4 \pm e_5 \pm e_6 \pm e_7 \pm e_8) \}$ with even # +

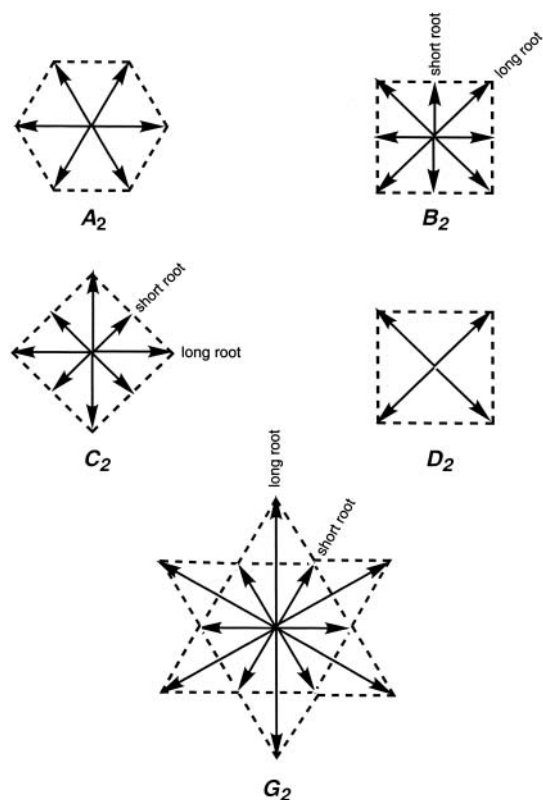


Figure 6. Diagrams of the fundamental roots for the two-dimensional root lattices A_2 , B_2 , C_2 , D_2 , and G_2 .

system has both short and long roots of different lengths, then the corresponding lattice is that of another root system where all of the roots are of the same length. In this connection the designation Z^n is the primitive n -dimensional (hyper)cubic lattice generated by points where all of the coordinates are integers. Figure 6 shows the fundamental roots for the readily visualized two-dimensional lattices A_2 , B_2 , C_2 , D_2 , and G_2 .

From Table II and the examples in Figure 6 the root systems A_n , D_n , and E_n are seen to have all roots of the same length whereas the root systems B_n , C_n , G_2 , and F_4 have roots of two different lengths. Thus although all of the root systems in Table II are indecomposable, the root systems A_n , D_n , and E_n are in a sense more »fundamental« or »basic« than the others and are sufficient to model crystallographic and quasicrystallographic lattices.

CRYSTALLOGRAPHIC LATTICES FROM ROOT LATTICES

The D_n root lattices generate cubic and hypercubic crystallographic lattices. Thus for a D_n root lattice the root vectors are the vectors $\pm e_i \pm e_j$ ($i, j = 1, 2, \dots, n$), where e_i is the unit vector along coordinate i . There are $2n(n-1)$ such vectors. The root lattice D_2 corresponds to the $\{4,4\}$ planar checkerboard tessellation (Figure 2a). The fundamental roots of the D_3 lattice are located at the edge midpoints

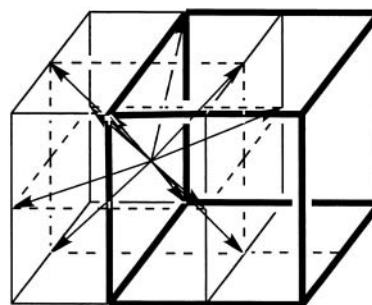


Figure 7. Relationship between the fundamental roots of the D_3 lattice (i.e., the edge midpoints of the cube with the edges in light solid lines) and the face-centered cubic lattice with a unit cell indicated by a cube with edges in bold solid lines.

of a cube with the origin as its center (the »left« cube indicated in light solid lines in Figure 7). The corresponding three-dimensional lattice is the face-centered cubic lattice with the »right« cube in bold solid lines in Figure 7 as a unit cell.

The A_n root lattices are generated by a projection method which is related to the projection method used to generate quasicrystalline lattices from higher dimensional crystalline lattices discussed later in this paper. Thus the root vectors for A_n can be constructed by taking $n+1$ mutually orthogonal unit vectors. These vectors are then used to form all possible $n(n+1)$ root vectors of the form $e_i - e_j$ ($i, j = 1, 2, \dots, n+1$) in an $(n+1)$ -dimensional space and then projecting them onto a suitable n -dimensional subspace. In the case of the A_2 lattice (Figure 6) the fundamental root vectors are located at the vertices of a cube and the projection is on a plane perpendicular to a C_3 axis of the cube (Figure 8). The resulting projection (after ignoring the two vertices of the cube projecting onto the origin) leads to the two-dimensional hexagonal lattice $\{6,3\}$ (Figure 2) similar to the structure of graphite.

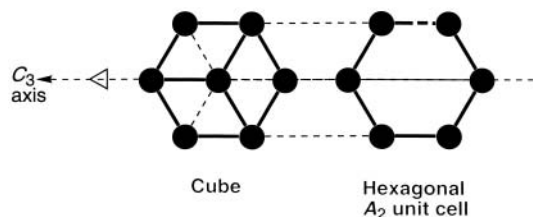


Figure 8. Generation of the A_2 root lattice (the planar $\{6,3\}$ hexagonal lattice in Figure 2b) by a projection from the vertices of a cube on a plane perpendicular to the C_3 axis of the cube.

The A_3 root lattice can be generated from the 16 vertices of the tesseract $\{4,3,3\}$ (Figure 3) by a similar projection procedure from four to three dimensions. The unit cell of the resulting root lattice is defined by 12 points after ignoring the four points projecting to the origin. In fact the A_3 root lattice is identical to the D_3 root lattice and thus also corresponds to the face-centered cubic lattice.

QUASICRYSTALLOGRAPHIC LATTICES FROM PROJECTIONS OF CRYSTALLOGRAPHIC ROOT LATTICES

The icosahedral quasicrystals have quasilattices derived from the finite non-crystallographic reflection groups H_2 , H_3 , and H_4 , all of which have five-fold symmetry and form the subgroup sequence $H_2 \subset H_3 \subset H_4$.^{24,25} The two-dimensional reflection group H_2 contains the symmetries of the regular pentagon and is of order 20. This quasilattice, which corresponds to Penrose tiling,²⁶ can be generated by a suitable projection into two dimensions of the four-dimensional root lattice from the crystallographic reflection group A_4 , also of order $n(n+1) = (4)(5) = 20$ for $n = 4$. Similarly, the three-dimensional group H_3 contains the 120 symmetries of the regular icosahedron as indicated by the operations in the point group I_h . The corresponding three-dimensional quasilattice can be generated by a suitable projection of the six-dimensional root lattice from the crystallographic reflection group D_6 into three dimensions.^{7,8} Note that the D_6 reflection group has $2n(n-1) = 2(6)(5) = 60$ root vectors corresponding to the order of the icosahedral pure rotation group I , which is a subgroup of index 2 in the full icosahedral group I_h . Finally, the four-dimensional group H_4 contains the symmetries of the four-dimensional polytope $\{3,3,5\}$ or its dual $\{5,3,3\}$. The corresponding four-dimensional quasilattice can be generated by a suitable projection of the eight-dimensional root lattice from the crystallographic reflection group E_8 into four dimensions.²⁷ Note that the E_8 reflection group has 240 root vectors, which is a factor of the 14,400 operations in the symmetry group of the $\{3,3,5\}$ polytope.

This analysis indicates that all of the possible icosahedral quasilattices, namely the quasilattices derived from the non-crystallographic finite reflection groups H_2 , H_3 , and H_4 , can be obtained by a suitable projection from a root lattice in exactly twice the number of dimensions (Table II). This appears to relate to the fact that the operations of period five in the icosahedral quasicrystals (*i.e.*, C_5) generate the irrational »golden ratio« $\tau = (1 + \sqrt{5})/2$. Thus for an icosahedral quasilattice of n dimensions, n coordinates from the overlying $2n$ -dimensional lattice are required to generate the rational points of the quasilattice and another n coordinates are required to generate the quasilattice points containing the irrationality τ .

Two-dimensional quasilattices with periods other than five can also be generated from projections of higher dimensional root lattices into two dimensions. Thus, the four-dimensional root lattice D_4 with $2n(n-1) = 24$ root vectors for $n = 4$ can be used to generate a quasiperiodic pattern of either octagonal (8-fold) or dodecagonal (12-fold) symmetry depending on the projection used.¹³ Dodecagonal quasicrystals can also be generated by projection from the F_4 root lattice with 48 root vectors.²⁸ In all cases the unique rotational symmetry of the quasilattice is a factor of the number of root vectors in the higher dimensional

root lattice used for the projection model. This observation can be used to determine the minimum number of dimensions required for a crystallographic lattice to generate a quasicrystal lattice with a given rotational symmetry.

To illustrate this point, consider the problem of using the projection method to generate a two-dimensional quasilattice with seven-fold symmetry, a symmetry that has not been observed experimentally in known quasicrystals. In this connection the lowest dimensional root lattices containing numbers of root vectors that are multiples of seven are the six-dimensional root lattices A_6 with $(6)(7) = 42$ root vectors and E_6 with 126 root vectors. Thus the generation of a two-dimensional quasilattice with seven-fold symmetry requires projection from a six-dimensional root lattice¹³ in contrast to a two-dimensional quasilattice with five-fold symmetry (H_2) where projection from the four-dimensional A_4 root lattice is sufficient.

Acknowledgment. – I am indebted to the National Science Foundation for partial support of this project under Grant CHE-0209857.

REFERENCES

1. D. Shechtman, I. Blech, D. Gratias, and J. W. Cahn, *Phys. Rev. Lett.* **53** (1984) 1951.
2. D. Shechtman and I. A. Blech, *Metall. Trans. A* **16** (1985) 105.
3. D. Levine and P. J. Steinhardt, *Phys. Rev. Lett.* **53** (1984) 2477.
4. D. Levine and P. J. Steinhardt, *Phys. Rev. B* **34** (1986) 596.
5. C. Janot, *Quasicrystals: a Primer*, Clarendon Press, Oxford, UK, 1994.
6. D. DiVincenzo and P. J. Steinhardt (Eds.), *Quasicrystals: the State of the Art*, World Scientific Publishers, Singapore, 1999.
7. P. Bak, *Scri. Metall.* **20** (1986) 1199.
8. R. K. Mandal and S. Lele, *Phys. Rev. Lett.* **62** (1989) 2695.
9. M. Senechal, *Quasicrystals and Geometry*, Cambridge University Press, Cambridge, UK, 1995.
10. J. H. Conway and N. J. A. Sloane, *Sphere Packings, Lattices, and Groups*, Springer, New York, 1999, Chapter 4.
11. B. J. Wybourne, *Classical Groups for Physicists*, Wiley-Interscience, New York, 1974.
12. H. M. S. Coxeter, *Ann. Math.* **35** (1934) 588.
13. M. Baake, D. Joseph, P. Kramer, and M. Schlottmann, *J. Phys. A. Math. Gen.* **23** (1990) L1037.
14. B. Grünbaum, *Convex Polytopes*, Interscience Publishers, New York, 1967.
15. B. Grünbaum, and G. C. Shephard, *Tilings and Patterns: An Introduction*, Freeman, New York, 1989.
16. H. S. M. Coxeter and W. O. J. Moser, *Generators and Relations for Discrete Groups*, Springer-Verlag, Berlin, 1972.
17. R. B. King, *J. Phys. Chem.* **100** (1996) 15096.
18. R. B. King, *J. Chem. Inf. Comput. Sci.* **38** (1998) 180.
19. R. B. King, *Croat. Chim. Acta* **73** (2000) 993.
20. R. B. King, *Croat. Chim. Acta* **75** (2002) 447.
21. R. B. King, *J. Mol. Struct.* **656** (2003) 119.
22. H. S. M. Coxeter, *Regular Polytopes*, 2nd ed., MacMillan, New York, 1963, Chapters 7 and 8.

23. H. S. M. Coxeter, *Regular Complex Polytopes*, 2nd ed., Cambridge University Press, Cambridge, UK, 1991, Chapter 4.
24. O. P. Shcherbak, *Russ. Math. Surv.* **43** (1988) 149.
25. M. Baake and R. V. Moody, *Can. J. Math.* **51** (1999) 1258.
26. R. Penrose, *Bull. Inst. Math. Appl.* **10** (1974) 266.
27. J. F. Sadoc and R. Mosseri, *J. Phys. A. Math. Gen.* **26** (1993) 1789.
28. J. Morita and K. Sakamoto, *Commun. Algebra* **28** (2000) 255.

SAŽETAK

Pravilni politopi, rešetke s korijenskim vektorima i kvazikristali

R. Bruce King

Ikozaedrijski kvazikristali peterostuke simetrije u dvije, tri i četiri dimenzije povezani su s odgovarajućim pravilnim politopima koji posjeduju peterostruku simetriju: pravilni pentagon (H_2 grupa refleksije), pravilni ikozaedar $\{3,5\}$ (H_3 grupa refleksije) i pravilni četverodimenzionalni politop $\{3,3,5\}$ (H_4 grupa refleksije). Kvazikristali, koji posjeduju peterostruku simetriju mogu se generirati pomoću projiciranja iz rešetaka s korijenskim vektorima (root lattices) s dvostrukim brojem dimenzija: $A_4 \rightarrow H_2$, $D_6 \rightarrow H_3$ i $E_8 \rightarrow H_4$. Zbog odnosa grupa $H_2 \subset H_3 \subset H_4$, projiciranje $E_8 \rightarrow H_4$ daje podatke o svim mogućim ikozaedrijskim kvazikristalima. Slično projiciranje iz drugih rešetaka s korijenskim vektorima može poslužiti za generiranje kvazikristala različitih simetrija. Četverodimenzionalne rešetke s korijenskim vektorima dovoljne su za projiciranje na dvodimenzionalne kvazikristale osmerostruke i dvanaesterostruke simetrije. Međutim, generiranje dvodimenzionalnih kvazikristala sedmerostruke simetrije zahtjeva rešetke s korijenskim vektorima od najmanje šest dimenzija. To je možda razlog zašto pripremljeni kvazikristali ne posjeduju sedmerostruku simetriju.