axes should give a precession photograph with two mirror planes normal to each other, but all other twofold axes of the quasicrystal should give photographs with no plane at all.

Sixth, the stereographic projection of the symmetry elements observed in this quasicrystal by Mai, Tao, Zeng & Zhang (1988) clearly indicates the consistency of the threefold and twofold axes with the threefold and fourfold axes of a cube respectively.

So a model of a quasicrystal structure including the hypothesis of the special sort of quasicrystal containing the translationally symmetrical subgroup of atoms was supported by experimental facts.

Attention has been concentrated in this paper on an explanation of quasicrystal structures taking into consideration the principles of CCMAI. But as a result one can make a conclusion about the efficiency of the CCMAI as a common theoretical background for both crystals and quasicrystals.

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The Icosahedral Point Groups

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Abstract

Basic group-theoretical properties of the icosahedral point groups are derived. Here are given the permutations of the vertices of an icosahedron under the action of the elements of the icosahedral point groups, the icosahedral point groups' multiplication tables, subgroups, sets of conjugate subgroups, centralizers and normalizers of arbitrary subsets and coset and double coset decompositions.

1. Introduction

Basic group-theoretical properties of the 32 crystallographic point groups have been tabulated by Janovec, Dvorakova, Wike & Litvin (1989). Here, we extend that work to the icosahedral point groups. Icosahedral point groups have been of interest in connection with the vibrational (Boyle & Parker, 1980) and electronic properties (Boyle, 1972) of icosahedral molecules. Much work has been done on the coupling coefficients of the icosahedral groups, see for example Golding (1973), Boyle & Ozgo (1973), Pooler (1980) and Fowler & Ceulemans (1985). The representations of the icosahedral group have been studied by Backhouse & Gard (1974) and polynomial invariants by Cummins & Patera (1988). Additional interest in the icosahedral groups stems from the icosahedral symmetry of biological macromolecules (Litvin, 1975) and the discovery of quasicrystals (Shechtman, Blech, Gratias & Cahn, 1984; see also Nelson, 1986).

In § 2 we define the icosahedral groups in terms of the symmetry of an icosahedron inscribed in a cube. In § 3 we give the permutations of the vertices of the icosahedron under the action of the elements of the icosahedral point groups, the icosahedral point groups' multiplication tables, subgroups, sets of conjugate subgroups, centralizers and normalizers of arbitrary subsets, and coset and double coset decompositions.

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Table 1. *The Cartesian coordinates of the vertices of the icosahedron shown in Fig.* 1

The ratio $v/u = \tau - 1$, where τ is the golden ratio (1/2) [sqr(5) + 1].

Vertex no.	Coordinates		
1	v	0	u
2	$-v$	0	u
3	0	u	v
4	u	v	0
5	u	$-v$	0
6	0	$-u$	v
7	$-u$	v	0
8	0	u	$-v$
9	v	0	$-u$
10	0	$-u$	$-v$
11	$-u$	$-v$	0
12	$-v$	0	$-u$

2. The icosahedral point groups

One can inscribe an icosahedron in a cube whose vertices are given in a Cartesian coordinate system by $(\pm u, \pm u, \pm u)$. The vertices of the inscribed icosahedron are given by (Longuet-Higgins & Roberts, 1955)

$$(\pm u, \pm v, 0); \quad (0, \pm u, \pm v); \quad (\pm v, 0, \pm u); \quad (1)$$

where $v/u = (1/2)[\text{sqr}(5) - 1] = \tau - 1$, and $\tau =$ the golden ratio $= (1/2)[\text{sqr}(5) + 1]$. We index the twelve vertices of the icosahedron in Table 1 and show a diagram of the icosahedron inscribed in a cube in Fig. 1. This indexing scheme follows that of Muetterties & Wright (1967) and Boyle & Parker (1980) where in the latter the values of the coordinates are given by taking $u = \tau/2$ and $v = 1/2$.

For the elements of the icosahedral groups we use the standard International [Schoenflies] notation with additional notations to represent uniquely the group elements. These additional notations consist of indices of the vertices of the icosahedron in Fig. 1. A rotation of 180° about an axis passing through the center of the icosahedron and the middle of the edge of the icosahedron which connects the ith and jth vertices is denoted by $2(ij)$ $[C_2(ij)]$. i and j are the indices of two vertices of the icosahedron which are permuted under the action of this rotation.

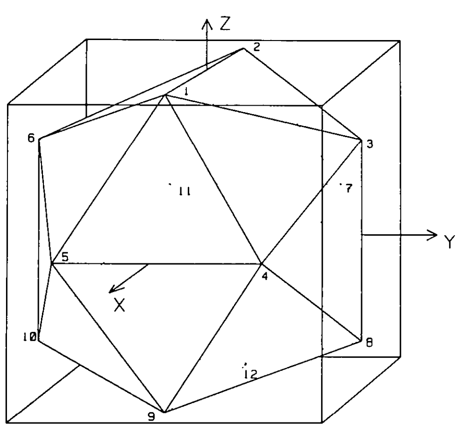

Fig. 1. An icosahedron inscribed in a cube. The numbering scheme of the vertices is that given by Boyle & Parker (1980).

Table 2. *The permutations of the vertices of the icosahedron in Fig.* 1 *induced by a set of generators of the icosahedral group* $2/M\bar{3}\bar{5}$

Generator	Permutation
2 (1 2)	(1, 2) (3, 6) (4, 11) (5, 7) (8, 10) (9, 12)
3 (1 4 3)	(1, 4, 3) (2, 5, 8) (6, 9, 7) (10, 12, 11)
5 (1-12)	(1) (12) (2, 6, 5, 4, 3) (7, 11, 10, 9, 8)
$\bar{1}$	(1, 12) (2, 9) (3, 10) (4, 11) (5, 7) (6, 8)

A rotation of 120° about an axis passing through the center of the icosahedron and the center of the triangular face whose vertices are indexed by i, j and k is denoted by $3(ijk)$ $[C_3(ijk)]$. Looking at the center of the icosahedron from the center of the triangular face, the rotation $3(ijk)$ $[C_3(ijk)]$ is a counter-clockwise rotation which induces the permutation (i, j, k) of the three vertices of the triangular face.

A rotation of 72° about an axis passing through the center of the icosahedron and the two vertices indexed by i and j is denoted by $5(i-j)$ $[C_5(i-j)]$. Looking at the center of the icosahedron from the ith vertex, the rotation $5(i-j)$ $[C_5(i-j)]$ is a counter-clockwise rotation. i and j are the indices of the two vertices of the icosahedron which are invariant under the action of this rotation.

The icosahedral group 235 $[I]$ contains sixty elements, all proper rotations which leave the icosahedron invariant. A set of generators of this group is the elements 2(1 2) $[C_2(1\,2)]$, 3(1 4 3) $[C_3(1\,4\,3)]$ and 5(1-12) $[C_5(1\text{-}12)]$.

The icosahedral group $2/M\bar{3}\bar{5}$ $[I_h]$ contains 120 elements, all proper and improper rotations which leave the icosahedron invariant. This group is the direct product of the icosahedral group 235 $[I]$ and the group consisting of the identity and spatial inversion.

3. Group-theoretical properties

The following group-theoretical properties of the icosahedral groups have been calculated.*

* A computer program on disk for IBM compatible computers entitled *The Icosahedral Point Groups* is available as SUP53561 (1 diskette) through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. This program gives all the group-theoretical information on the icosahedral groups listed in § 3 of this paper. This includes the permutation of the vertices of an icosahedron under the action of the group elements, the icosahedral point groups' multiplication tables, subgroups, sets of conjugate subgroups, centralizers and normalizers of arbitrary subsets and coset and double coset decompositions.

Table 3. *Conjugate subgroups of the subgroup* 2(4 5) 2(3 8) 2(1 2) *in the icosahedral group* 235 *and the corresponding conjugating elements*

Subgroup:	2(4 5) 2(3 8) 2(1 2)
Conjugating elements:	1, 2(4 5), 2(3 8), 2(1 2), 3(1 4 3), 3^2(1 4 3), 3(2 3 7), 3^2(2 3 7), 3(1 6 5), 3^2(1 6 5), 3(4 9 8), 3^2(4 9 8)
Conjugate subgroup:	2(2 7) 2(3 4) 2(1 6)
Conjugating elements:	5(1–12), 5^3(4–11), 2(5 10), 3^2(1 2 6), 2(1 3), 5^4(3–10), 5^2(2–9), 3(4 5 9), 2(1 5), 5^4(5–7), 3(3 4 8), 5^2(6-8)
Conjugate subgroup:	2(1 5) 2(2 3) 2(4 8)
Conjugating elements:	5^2(1–12), 3^2(3 4 8), 2(2 7), 5^4(6–8), 3^2(1 3 2), 5(5–7), 2(2 6), 5^2(4–11), 3^2(1 5 4), 5(2–9), 5^2(3–10), 2(5 6)
Conjugate subgroup:	2(5 10) 2(2 6) 2(1 4)
Conjugating elements:	5^3(1–12), 3^2(3 8 7), 2(4 9), 5(3–10), 5^4(2–9), 3(1 5 4), 5^3(6–8), 2(3 4), 5^4(4–11), 3(1 2 6), 2(2 3), 5^3(5–7)
Conjugate subgroup:	2(1 3) 2(5 6) 2(4 9)
Conjugating elements:	5^4(1–12), 5^2(5–7), 2(4 8), 3(1 3 2), 5(4–11), 2(1 4), 3(3 8 7), 5^3(3–10), 5(6–8), 2(1 6), 5^3(2–9), 3^2(4 5 9)

3.1. *Symbols*

The symbols for the icosahedral point groups and their elements are given in both International and Schoenflies notation.

3.2. *Permutation of the vertices of an icosahedron*

The transformation of position vectors under the action of group elements is given symbolically by $R' = gR$, where R is a position vector, g is an element of the group G, and R' is the position vector into which R is transformed under the action of the group element g. In terms of the components of the position vectors

$$R_i' = D(g)_{ij}R_j \tag{2}$$

where the matrix $D(g)$ is the matrix of the vector representation of the group G corresponding to the element g.

A set of generators for the icosahedral group $2/M\bar{3}\bar{5}$ [I_h] and the corresponding matrices $D(g)$ are

$$\begin{aligned} D[2(1\,2)] &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ D[3(1\,4\,3)] &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \\ D[5(1\text{–}12)] &= \begin{pmatrix} 0{\cdot}5 & -0{\cdot}5\tau & 0{\cdot}5/\tau \\ 0{\cdot}5\tau & 0{\cdot}5/\tau & -0{\cdot}5 \\ 0{\cdot}5/\tau & 0{\cdot}5 & 0{\cdot}5\tau \end{pmatrix} \\ D[\bar{1}] &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \end{aligned} \tag{3}$$

A set of generators for the icosahedral group 235 [I] and corresponding matrices $D(g)$ are those given in (3) excluding $g = \bar{1}$.

The elements of the icosahedral groups induce permutations of the vertices of the icosahedron shown in Fig. 1. We give the matrices $D(g)$ for all elements of the icosahedral groups and the corresponding permutations of the vertices of the icosahedron. The permutations of the twelve vertices of the icosahedron induced by the generators given in (3) are given in Table 2.

3.3. *Multiplication tables*

The multiplication tables of the icosahedral point groups are given. The product of any two elements can also be calculated.

3.4. *Subgroups*

The symbols and elements are given for each of the 58 subgroups of the icosahedral group 235 [I] and the 163 subgroups of the icosahedral group $2/M\bar{3}\bar{5}$ [I_h].

3.5. *Conjugate subgroups*

For a given group G and subgroup S of G, a subgroup S' is a conjugate subgroup of S in G if there exists an element g of G such that $gSg^{-1} = S'$. The element g is called a conjugating element of S'. For each icosahedral point group G and subgroup S of G, one can calculate the conjugate subgroups S' and the conjugating elements of each conjugate subgroup. An example of this is given in Table 3.

3.6. *Centralizers*

For a given group G and subset B of elements in G, the centralizer C of the subset B in G is the subgroup of all elements g of G which commute with all elements b of the subset B, *i.e.* if $gbg^{-1} = b$ for all elements of B. For each icosahedral point group G one can calculate the centralizer C of an arbitrary subset B of G. For example, the centralizer of the subset {2(4 8), M(2 3)} in the icosahedral point group $2/M\bar{3}\bar{5}$ is the subgroup M(1 5)M(2 3)M(4 8).

3.7. *Normalizers*

For a given group G and subset B of elements in G, the normalizer N of the subset B in G is the subgroup of all elements g of G such that $gBg^{-1} = B$, where gBg^{-1} denotes the subset of elements gbg^{-1} of G for all elements b of the subset B. For each icosa-

Table 4. *The left coset and double coset decomposition of the subgroup* 2(1 3) 2(5 6) 2(4 9) *in the icosahedral group* 235

1	2(1 3)	2(5 6)	2(4 9)
2(4 5)	5^3(6-8)	3(1 3 2)	5^4(3-10)
5^2(6-8)	2(2 7)	5^4(1-12)	3(1 4 3)
3^2(1 3 2)	5(1-12)	2(4 8)	5^3(5-7)
5(3-10)	3^2(1 4 3)	5^2(5-7)	2(2 6)
2(3 8)	3^2(4 5 9)	5^4(2-9)	5^2(1-12)
3(4 5 9)	2(1 6)	5^2(3-10)	5^4(4-11)
5(2-9)	5^3(3-10)	2(1 5)	3(4 9 8)
5^3(1-12)	5(4-11)	3^2(4 9 8)	2(5 10)
2(1 2)	5(5-7)	5^3(4-11)	3(3 8 7)
5^4(5-7)	2(3 4)	3(1 6 5)	5^3(2-9)
5^2(4-11)	3^2(1 6 5)	2(2 3)	5(6-8)
3^2(3 8 7)	5^2(2-9)	5^4(6-8)	2(1 4)
3(2 3 7)	3^2(3 4 8)	3(1 5 4)	3^2(1 2 6)
3^2(2 3 7)	3(1 2 6)	3(3 4 8)	3^2(1 5 4)

hedral point group one can calculate the normalizer N of an arbitrary subset B of G. For example, the normalizer of the subset {2(4 8), 2(2 6)} in the icosahedral point group $2/M\bar{3}\bar{5}$ is the subgroup $2(1\,3)/M$.

3.8. *Coset and double coset decompositions*

For a given group G and subgroup S, one can write the left coset decomposition of G with respect to S:

$$G = S + g_2S + g_3S + \ldots + g_nS. \quad (4)$$

g_iS denotes the subset of elements of G found by multiplying each element of the subgroup S from the left by the element g_i. Each set of elements g_iS of G, for $i = 1, 2, \ldots, n$, is called a left coset of G with respect to S, and the elements $g_1 = 1, g_2, \ldots, g_n$ are called the coset representatives.

For a given group G and subgroup S of G, one can write the double coset decomposition of G with respect to S:

$$G = S + Sg_2S + Sg_3S + \ldots + Sg_mS. \quad (5)$$

Sg_iS denotes the subset of distinct elements of G found by multiplying each element of the subset g_iS from the left by every element of the subgroup S. Each set of elements Sg_iS of G, for $i = 1, 2, \ldots, m$, is called a double coset of G with respect to S, and the elements $g_i = 1, g_2, \ldots, g_m$ are called double coset representatives. Each double coset of G with respect to S is made up of a set of left cosets of G with respect to S.

The double cosets Sg_iS and $S(g_l)^{-1}S$ are either identical or disjoint. If identical, then the double coset Sg_iS is called an *ambivalent* double coset and, if disjoint, the two double cosets are called *complementary* double cosets (Janovec, 1972).

For a given icosahedral point group G and subgroup S of G, one can calculate the left coset decomposition of G with respect to S and the double coset decomposition of G with respect to S. The listing of the left coset decomposition of the point group G with respect to S is given within the listing of the double coset decomposition of the point group G with respect to S. In listing the double coset decomposition of G with respect to S one obtains a list where in each row are the elements of each left coset of the left coset decomposition of G with respect to S. The left cosets which make up a single double coset are grouped together. Between each set of left cosets which make up a single double coset is a dashed line -----, except in the case of the members of a pair of complementary double cosets where a dotted line ····· is used to separate them. An example of such a double coset decomposition is given in Table 4.

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