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Non-periodic Central Space Filling with Icosahedral Symmetry using Copies of Seven Elementary Cells

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Abstract

It is shown that copies of seven elementary cells suffice to fill any region of Euclidean three-dimensional space. The seven elementary cells have four basic convex polyhedral shapes and three of them appear in two different sizes. The space filling is non-periodic, has a central point, and preserves the full icosahedral group.

1. Introduction

An ideal crystal exhibits a characteristic discrete repetition pattern of elementary cells which fill the three-dimensional Euclidean space $\mathbb{E}^3$. This pattern is best described by giving the space group of symmetry operations which generate the pattern. According to the standard definition, any space group is a discrete subgroup of the Euclidean group which contains a non-trivial discrete translation subgroup. This translation group generates in a crystal a periodic structure. From this periodic structure one can derive the well-known proposition that the only discrete rotational symmetries of a crystal are given by two-, three-, four-, and sixfold axes.

Non-periodic but repetitive patterns have been considered before for the Euclidean space $\mathbb{E}^2$. Goldberg (1955) gave examples of tessellations with one elementary cell and a unique center and called them central tessellations. Penrose (1974) constructed from two elementary cells various tessellations of $\mathbb{E}^2$. In particular, he found tessellations which have the symmetry group $\mathscr{C}_{5v}$ and a central point and therefore are non-periodic.

The repetitive space filling constructed in this paper for $\mathbb{E}^3$ exhibits the icosahedral symmetry group $\mathscr{I}_h$. Because of the fivefold rotation axes contained in $\mathscr{I}_h$, the pattern is central and non-periodic.

A fundamental role in what follows is played by the number

$$\varphi = \tfrac{1}{2}(1 + \sqrt{5}).$$

This number is the basic quantity in the golden section

$$a/b = b/(a + b)$$

with the solution

$$b/a = \varphi.$$

It governs the proportions of the pentagon, Fig. 1. For the pentagon $p(L)$ of edge length L, the distance between two vertices separated by a third one is φL. For the occurrence of the number φ in the dodecahedron and icosahedron see § 2.

The paper is organized as follows. In § 2, the dodecahedron and the icosahedron are used to cover by star extension central regions of $\mathbb{E}^3$. In § 3, elementary cells of four shapes are defined and described. In § 4, cells with the same proportions, but with their linear dimensions increased by powers of φ, are composed from elementary ones. On the basis of these results, the possibility of space filling is demonstrated in § 5. Supplementary results are given in § 6.

2. Star extension of the dodecahedron and the icosahedron

Denote a regular pentagon of edge length L in the plane $\mathbb{E}^2$ by $p(L)$. Extending the edge lines to their five intersections one gets the star pentagon or pentagram. These five intersections mark the vertices of a pentagon $p(\varphi^2 L)$ with the same center but vertex directions through the midpoints of the edges of $p(L)$. Call this construction of $p(\varphi^2 L)$ from $p(L)$ a star extension. Note that the star extension proceeds in steps of two generations of pentagons. Generations are introduced in definition 4.4.

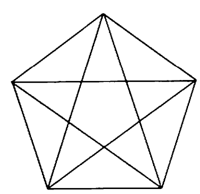

Fig. 1. Star extension of the pentagon. When the edges of the small pentagon are extended up to their intersections, they yield the pentagram. These intersections mark the five vertices of a larger pentagon whose edge length has increased by a factor φ^2. The two types of triangles inside $p(\varphi^2 L)$ have the three edge lengths $L, \varphi L, \varphi L$ and $\varphi^2 L, \varphi L, \varphi L$, respectively.

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A similar construction applies in three-space $\mathbb{E}^3$. Start with a regular dodecahedron of edge length L, which will be denoted as $d(L)$. The extended edges of $d(L)$ intersect at twelve points which mark the vertices of the star dodecahedron (Fig. 2) and, at the same time, the vertices of an icosahedron. This star extension or stellation of the dodecahedron was first described by Kepler (1619). Restricting the attention to the extended edges of a single face pentagon $p(L)$, one easily concludes that the edges of this icosahedron have the length $\varphi^2 L$. Denote this icosahedron as $i(\varphi^2 L)$. Extending now the edges of this icosahedron to their intersections, one obtains the star icosahedron $i(\varphi^2 L)$ and, at the same time, marks the vertices of a new dodecahedron. This dodecahedron is found to have the same center and orientation of faces as $d(L)$ but the edge length $\varphi^3 L$, it is denoted as $d(\varphi^3 L)$. Call the processes just described the star extensions of $d(L)$ into $i(\varphi^2 L)$, of $i(\varphi^2 L)$ into $d(\varphi^3 L)$ and of $d(L)$ into $d(\varphi^3 L)$. The star extension of d goes in steps of three generations. Clearly the star extension may be repeated n times to cover a central region of $\mathbb{E}^3$ of arbitrary size, Fig. 3. This process of covering $\mathbb{E}^3$ is of course not repetitive since it involves a scaling of the initial cells in powers of φ. Repetitive space filling requires that there be a finite set of cells which may be composed without holes and without intersections to cover arbitrary parts of Euclidean $\mathbb{E}^3$.

3. Elementary cells

In the planar star extension of the pentagon $p(L)$, there appear two triangles whose three edges have the lengths L, φL, φL and $\varphi^2 L$, φL, φL respectively. Pentagons and triangles of this type may be used as faces of cells in $\mathbb{E}^3$. Besides the dodecahedron, three such cells will be introduced, denoted by Greek names and abbreviated by their first letters, Fig. 4. The smallest edge length will in most cases be used to define the size of a cell.

3.1. *Definition: the dodecahedron* $d(L)$

Twelve pentagonal faces $p(L)$ form the dodecahedron. The symmetry group of $d(L)$ is the full icosahedral group with twofold, threefold and fivefold rotation axes. There are five mirror planes through the center and through one vertex and the opposite midpoint of an edge for any face pentagon. The full symmetry group of the dodecahedron is denoted as $\mathcal{I}_h$. Its elements are described with definitions 4.1–4.3.

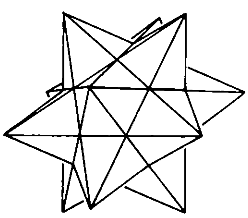

Fig. 2. Star extension of the dodecahedron. The star dodecahedron is obtained by extending the edge lines up to their intersections. The 12 intersections mark the vertices of the icosahedron.

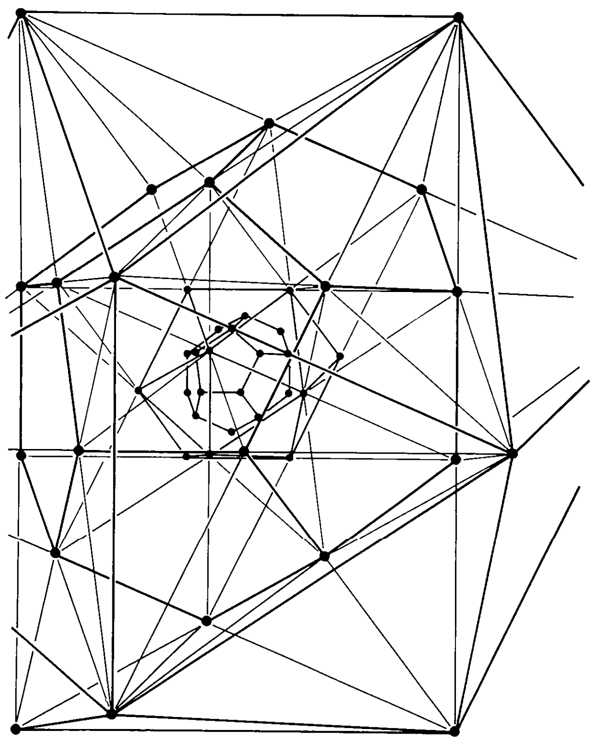

Fig. 3. Star extension of the dodecahedron and icosahedron. By extending the edge lines and marking their intersections, one obtains in $\mathbb{E}^3$ the star extensions from the dodecahedron $d(L)$ to the icosahedron $i(\varphi^2 L)$, from $i(\varphi^2 L)$ to $d(\varphi^3 L)$ and from $d(\varphi^3 L)$ to $i(\varphi^5 L)$, shown in part only. The vertices of these polyhedra are marked by filled circles; extensions of edges are shown except for $d(L)$.

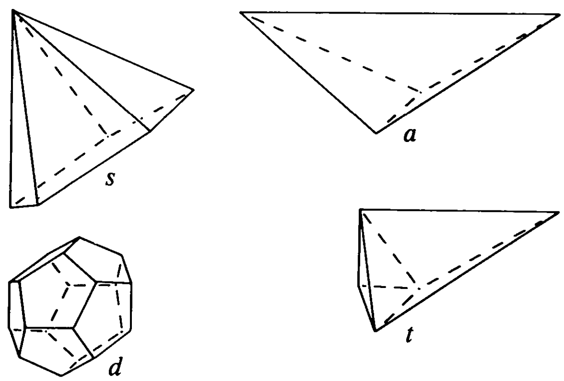

Fig. 4. Elementary cells. The four shapes of the elementary cells, dodecahedron d, *skene* s, *aetos* a and *tristomos* t, in axonometric projection. The sizes correspond to $d(L)$, $s(\varphi^2 L)$, $a(\varphi^2 L)$, $t(\varphi^2 L)$. Visible and invisible edges are drawn as solid and broken lines respectively.

3.2. *Definition: the skene (tent) $s(L)$*

Five triangles of edge length L, φL, φL form a regular five-sided pyramid $s(L)$ on a pentagon base $p(L)$. The symmetry group of $s(L)$ is $\mathscr{C}_{5v}$. It contains a fivefold rotation axis C_5 and five mirror planes containing this axis and a pentagon vertex. The name of the cell is derived from its outer shape.

3.3. *Definition: the aetos (eagle) $a(L)$*

Two triangles of edge length L, φL, φL joined at their bases, and two triangles of edge length $\varphi^2 L$, φL, φL joined at their bases are combined into a tetrahedron $a(L)$. The symmetry group of $a(L)$ is $\mathscr{C}_{2v}$. The twofold axis C_2 passes through the midpoints of the smallest and largest edge. The two mirror planes contain this axis and one of these two edges respectively. The name is suggested by the shape of $a(L)$ when the largest edge points upwards.

3.4. *Definition: the tristomos (three-edged) $t(L)$*

Three triangles of edge length L, φL, φL and three triangles of edge length L, $\varphi^{-1} L$, $\varphi^{-1} L$ form two regular three-sided pyramids on a triangular base of edge length L, L, L. These two pyramids are connected at their bases into the convex cell $t(L)$. In the case of $t(L)$ we prefer to use the base edge, not the shortest edge, for reference. The symmetry group of $t(L)$ is clearly $\mathscr{C}_{3v}$.

All four cells defined so far are convex. They arise in a natural way in the composition which leads from $d(L)$ to its star extension $d(\varphi^3 L)$, as will be shown in the next section. Some of their metrical properties are summarized in Table 2.

4. Composite cells and their generations

For the process of repetitive space filling, it will be necessary to build composite cells out of elementary ones. First, it proves convenient to introduce a notation for the faces, vertices and edges of the dodecahedron and icosahedron as well as for their symmetry operations.

4.1. *Definition: faces of the dodecahedron, vertices of the icosahedron*

Start with one pentagonal face of $d(L)$ denoted by 1. Label the five faces which have an edge common with 1 counter-clockwise as 2, 3, 4, 5, 6. For opposite faces of $d(L)$ choose numbers which add up to 13. The same set of 12 numbers 1, 2, ..., 12 applies to the vertices of the icosahedron and yields the directions of the six fivefold rotation axes C_5 through the center.

4.2. *Definition: edges of the dodecahedron and icosahedron*

For the dodecahedron, denote the common edge of two neighboring faces i, j by $i|j$. The corresponding edge of the icosahedron between the vertices i, j is denoted as i–j. The 15 twofold rotation axes C_2 of the icosahedral group pass through the center and the midpoints of these edges. The mirror planes contain one axis C_2 and one dodecahedral or one icosahedral edge.

4.3. *Definition: vertices of the dodecahedron, faces of the icosahedron*

For the dodecahedron, denote the vertex of three neighboring faces i, j, k by $i \cdot j \cdot k$. The same triple denotes a face of the icosahedron and one of the ten threefold rotation axes C_3.

The next step in the analysis will be a systematic study of composite cells according to generations as given in definition 4.4.

4.4. *Definition: sequence of generations of a cell*

A sequence of n generations of a cell y is a set of cells with the same angles and length proportions between all pairs of edges but with the reference edge length $\varphi^i L$, $\varphi^{i+1} L$, ..., $\varphi^{i+n} L$. The members of generations are denoted as $y(\varphi^i L), y(\varphi^{i+1} L), \ldots, y(\varphi^{i+n} L)$.

The following selection of elementary cells will be used in the remaining sections of this paper.

4.5. *Definition: the set of seven cells $d(L)$, $s(L)$, $a(L)$, $t(\varphi^2 L)$, $d(\varphi L)$, $s(\varphi L)$, $a(\varphi L)$ will be called elementary in what follows*

If necessary, these seven cells will be denoted as $y_i(\varphi^{q_i} L)$ according to Table 1.

Note that the set of seven elementary cells involves four shapes d, s, a, t but two generations of d, s and a. Turn now to the building of composite cells. The objective will be to buld higher generations of the cells d, s, a and t from elementary ones. It will be seen that the step from one generation to the next depends on the number of the generation. In line with the star extension, the composition will be shown to have a period of three, not of one generation(s). First of all a composite cell *laros* is introduced as a useful tool.

4.6. *The generations of the laros (sea-gull)*

1. Generation $l(\varphi^2 L)$, Figs. 5, 6: cover the faces 1, 5, 7, 9 of $d(L)$, enumerated according to definition 4.1,

Table 1. *The seven elementary cells written in the form $y_i(\varphi^{q_i} L)$*

i	1	2	3	4	5	6	7
y_i	d	s	a	t	d	s	a
q_i	0	0	0	2	1	1	1

with four $s(L)$. Insert one $a(L)$ with its smallest edge coincident with the dodecahedral edge 1|5 to complete $l(\varphi^2 L)$. Its smallest edge has length $\varphi^2 L$, its largest $\varphi^3 L$. The edge of length $\varphi^3 L$ perpendicular and opposite to the smallest one will be called the counter-edge of l. The symmetry group of $l(\varphi^2 L)$ is $\mathscr{C}_{2v}$. The name is derived from the shape of the cell when its edge 1|5 points upwards.

2. Generation $l(\varphi^3 L)$: the composition of generation 1 is repeated with the second elementary generation $d(\varphi L)$, $s(\varphi L)$, and $a(\varphi L)$.

3. Generation $l(\varphi^4 L)$: not required.

4. Generation $l(\varphi^5 L)$: the composition of generation 1 is repeated with $d(\varphi^3 L)$, $s(\varphi^3 L)$, $a(\varphi^3 L)$. These composite cells are constructed below.

4.7. *The generations of the dodecahedron*

1. Generation $d(L)$: elementary.

2. Generation $d(\varphi L)$: elementary.

3. Generation $d(\varphi^2 L)$: its construction is not needed, but a similar composite cell is constructed in relation to $s(\varphi^4 L)$.

4. Generation $d(\varphi^3 L)$, Fig. 7: this cell appears in the star extension from $d(L)$. All elementary cells except $d(\varphi L)$ will be needed to compose $d(\varphi^3 L)$. Cover the 12 faces of $d(L)$ with 12 $s(L)$ to obtain the star dodecahedron based on $d(L)$. Attach to each of the 30 dodecahedral edges one $a(L)$ with a coincident edge of length L and its largest edge connecting the outer vertices of two $s(L)$. The latter edges coincide with the edges of the icosahedron $i(\varphi^2 L)$ obtained by star extension. The icosahedron is complete except for a three-sided pyramidal hole on each of its faces; it is denoted as $i_-(\varphi^2 L)$. The hole is a regular three-sided pyramid whose sides are triangles of edge length $\varphi^2 L$, φL, φL. Now insert 20 *tristomoi* $t(\varphi^2 L)$ into these holes to obtain the star icosahedron based on $i(\varphi^2 L)$. Two *tristomoi* with a common edge of length $\varphi^2 L$ have an outer vertex distance $\varphi^3 L$; all these vertices together mark the 20 vertices of $d(\varphi^3 L)$. The composite cell $l(\varphi^2 L)$ constructed above is now fitted in between pairs of *tristomoi* with a common edge. The common edge belongs to $i(\varphi^2 L)$ and has the symbol j–k. The smallest edge of $l(\varphi^2 L)$ of length $\varphi^2 L$ coincides with j–k; its counter-edge of length $\varphi^3 L$ coincides with edge $j|k$ of

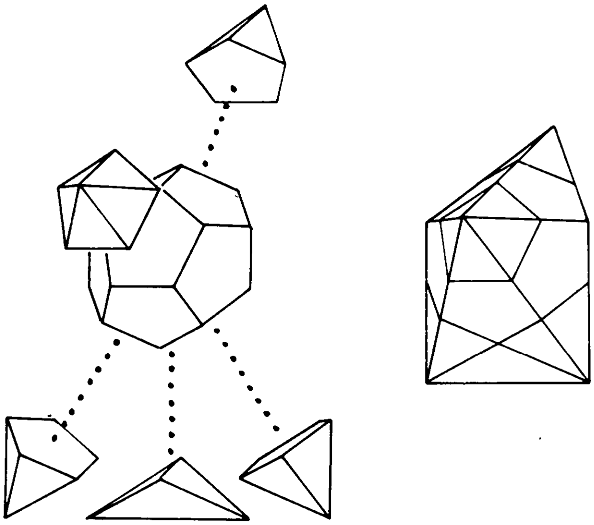

Fig. 5. Composite cell *laros*. The composite cell *laros* $l(\varphi^2 L)$ is obtained by covering $d(L)$ with four $s(L)$ and one $a(L)$ as indicated.

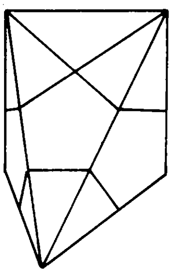

Fig. 6. Composite cell *laros*.

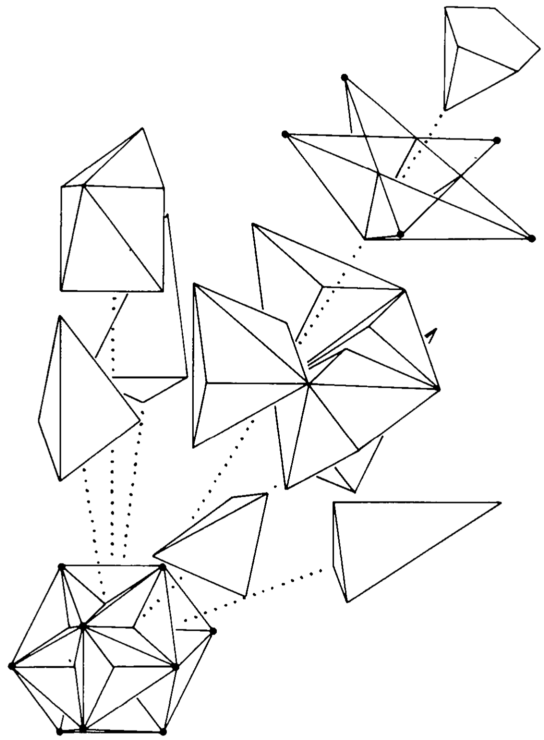

Fig. 7. Composite cell $d(\varphi^3 L)$. The steps in building one face of $d(\varphi^3 L)$ from one face of $d(L)$ are indicated, starting from the icosahedron $i_-(\varphi^2 L)$ described in the text and shown to the left in the lower part of the figure. To build the face of $d(\varphi^3 L)$, the five $t(\varphi^2 L)$ must be moved along the C_3 axes into the tetrahedral holes. One $l(\varphi^2 L)$ must be shifted back to form a ring of five $l(\varphi^2 L)$ which is moved along the C_5 axis into the intervals between the $t(\varphi^2 L)$. The hole in the face of $d(\varphi^3 L)$ has a pentagram base, it is filled by a ring of five $a(\varphi L)$ and one $s(\varphi L)$, moved along the C_5 axis. Vertices of $i_-(\varphi^2 L)$ and of $d(\varphi^3 L)$ are marked by filled circles.

$d(\varphi^3 L)$. The five *laroi* $l(\varphi^2 L)$ whose counter-edges form a pentagon $p(\varphi^3 L)$ yield with one face a part of the pentagonal face of $d(\varphi^3 L)$ but leave a pyramidal hole. The base of this hole is the star pentagon based on $p(\varphi L)$; its innermost vertex is a vertex of the embedded $i(\varphi^2 L)$. If five *aetoi* $a(\varphi L)$ are attached to the five triangular faces of one $s(\varphi L)$, this construction fills the hole up to the face of $d(\varphi^3 L)$. The same procedure is used on all faces to complete $d(\varphi^3 L)$. The composition just described and the relative positions of the six elementary cells will be referred to as standard composition and standard positions respectively.

5. Generation $d(\varphi^4 L)$: the same composition as for generation 4 applies. The required cells $d(\varphi L)$, $s(\varphi L)$, and $a(\varphi L)$ are elementary; the composite cells $t(\varphi^3 L)$, $s(\varphi^2 L)$ and $a^1(\varphi^2 L)$ are independently constructed below.

The elementary cells used in the composition of $d(\varphi^3 L)$ have intrinsic symmetry operations like rotation axes and mirror planes. In the construction all rotation axes and mirror planes of $d(\varphi^3 L)$ match corresponding symmetry operations of the elementary cells in their standard position within $d(\varphi^3 L)$. Some elementary cells like $d(\varphi L)$ and $a(\varphi L)$ have higher symmetry than the ones which are required at their position.

4.8. *The generations of the skene*

1. Generation $s(L)$: elementary.
2. Generation $s(\varphi L)$: elementary.
3. Generations $s(\varphi^2 L)$, Fig. 8: cover the faces 1, 7, 8, 9, 10, 11 of $d(L)$ with six $s(L)$. Insert on the dodecahedral edges 7|8, 8|9, 9|10, 10|11, 11|7 five $a(L)$ in standard positions. This cell is a composite subcell of $d(\varphi^3 L)$.
4. Generation $s(\varphi^3 L)$: repeat the composition of $s(\varphi^2 L)$ with the next generation $d(\varphi L)$, $s(\varphi L)$ and $a(\varphi L)$ of elementary cells.
5. Generation $s(\varphi^4 L)$: since $d(\varphi^2 L)$ is not available as an elementary or composite cell, a new procedure is required. This procedure is based in part on the standard composition from $d(L)$ to $d(\varphi^3 L)$ between two faces with the same number. The pentagonal face $p(L)$ of $d(L)$ is covered by $s(L)$. Five $a(L)$ are attached to the triangular sides of $s(L)$. Five $t(\varphi^2 L)$ are inserted into their standard position and are joined in pairs by five $l(\varphi^2 L)$. One $s(\varphi L)$ and five $a(\varphi L)$ complete the composition up to the pentagonal face $p(\varphi^3 L)$ of $d(\varphi^3 L)$; compare with Fig. 7. This face is now covered by the composite $s(\varphi^3 L)$ as required in the construction of the star dodecahedron based on $d(\varphi^3 L)$. The outer shape (not the internal composition) of the composite cell constructed so far is that of $d(\varphi^2 L)$ but with face 1 covered by $s(\varphi^2 L)$. There are five pentagonal faces $p(\varphi^2 L)$ surrounding the pentagonal face $p(\varphi^2 L)$ in the plane of the dodecahedral $p(L)$. Cover these five faces with five $s(\varphi^2 L)$ and insert five $a(\varphi^2 L)$ at their common edges to obtain $s(\varphi^4 L)$. Use the second alternative $a^2(\varphi^2 L)$ for the composition of $a(\varphi^2 L)$ to preserve the correct mirror planes of the symmetry group $\mathscr{C}_{5v}$. The composition of $s(\varphi^4 L)$ then exhibits the symmetry group $\mathscr{C}_{5v}$.

4.9. *The generations of the aetos*

1. Generation $a(L)$: elementary.
2. Generation $a(\varphi L)$: elementary. This cell could be composed out of $s(L)$ and $a(L)$. Enumerate the five triangular faces of $s(L)$ as 2, 3, 4, 5, 6. Attach two $a(L)$ to faces 2 and 4 in standard positions. With respect to its composition, this construction, shown in Fig. 9, has lower symmetry and therefore is not suited for the following construction.
3. Generation $a(\varphi^2 L)$: start with $t(\varphi^2 L)$ and attach two $a(L)$ to two triangular faces of the smaller type. Attach $s(L)$ with faces 2, 3 to the two $a(L)$ in standard positions and attach another $a(L)$ to the face 5 of $s(L)$ to obtain $a(\varphi^2 L)$. With respect to its constituents, this composite cell $a^1(\varphi^2 L)$ maintains only the mirror plane through the center and the largest edge. Alternatively, $a(\varphi^2 L)$ may be composed from one $s(\varphi L)$ and two $a(\varphi L)$ in the way outlined under $a(\varphi L)$. This version $a^2(\varphi^2 L)$ preserves the mirror plane through the center and the smallest edge and is needed in composing $s(\varphi^4 L)$.
4. Generation $a(\varphi^3 L)$, Figs. 9, 10: start with $l(\varphi^2 L)$ described above. Cover faces 2, 3 of the embedded $d(L)$ with two $s(L)$, insert five $a(L)$ in standard positions at the edges 1|2, 2|3, 3|1, 2|9, 3|7. Similarly, cover faces 10, 11 with two $s(L)$ and insert five $a(L)$ at the edges 5|10, 10|11, 11|5, 10|9, 11|7. Insert two $t(\varphi^2 L)$ into their standard positions at the vertices 1·2·3 and 5·10·11 to complete $a(\varphi^3 L)$ with the full symmetry group $\mathscr{C}_{2v}$.
5. Generation $a(\varphi^4 L)$: the composition of generation 4 is repeated to compose $a(\varphi^4 L)$ out of the second generation of elementary cells and the composite cells $l(\varphi^3 L)$ and $t(\varphi^3 L)$.

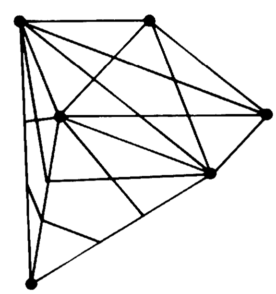

Fig. 8. Composite cell $s(\varphi^2 L)$. The composite *skene* $s(\varphi^2 L)$ is obtained from $d(L)$ by covering six faces with $s(L)$ and inserting five $a(L)$. Edges of elementary cells are drawn as solid lines, vertices of $s(\varphi^2 L)$ are marked by filled circles.

4.10. *The generations of the tristomos*

1. Generation $t(\varphi^2 L)$: elementary.

2. Generation $t(\varphi^3 L)$, Fig. 11: starting from $d(L)$, cover faces 1, 2, 3, 5, 7, 9 with six $s(L)$. Adjoin six $a(L)$ in standard positions at the edges 1|2, 2|3, 3|1, 1|5, 2|9 and 3|7. Put one $t(\varphi^2 L)$ into its standard position at the vertex 1·2·3.

3. Generation $t(\varphi^4 L)$, Fig. 11: the composition of $t(\varphi^3 L)$ can be extended along the direction 10·11·12. Cover faces 10, 11, 12 with three $s(L)$. Insert nine $a(L)$ in standard positions at the edges 10|9, 10|5, 11|5, 11|7, 12|7, 12|9 and 10|11, 11|12, 12|10. Adjoin four $t(\varphi^2 L)$ in standard positions at the vertices 5·10·11, 7·11·12, 9·12·10 and 10·11·12. At the icosahedral edges 10–11, 11–12, 12–10, attach three $l(\varphi^2 L)$ and join them in pairs by three $a(\varphi L)$. This completes the composition of $t(\varphi^4 L)$ as a composite subcell of $d(\varphi^3 L)$. An alternative procedure would be to extend the composition of $t(\varphi^3 L)$ to the next generation of elementary cells.

4. Generation $t(\varphi^5 L)$: the composition of $t(\varphi^4 L)$ described above is repeated with the elementary cells $d(\varphi L)$, $s(\varphi L)$, $a(\varphi L)$ and the composite cells $l(\varphi^3 L)$, $a(\varphi^2 L)$. As noted before, $a(\varphi^2 L)$ does not exhibit the full symmetry of $a(L)$. In the present composition, the position of $a(\varphi^2 L)$ requires only the mirror plane through the largest edge of $a(\varphi^2 L)$ as part of the symmetry group $\mathscr{C}_{3v}$ of $t(\varphi^5 L)$. This mirror plane is maintained in the composition of $a^1(\varphi^2 L)$.

The main result of this section may be summarized as follows.

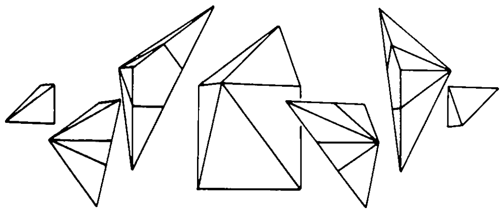

Fig. 9. Composite cell $a(\varphi^3 L)$. The composite cell $l(\varphi^2 L)$ is covered by four $s(L)$ and ten $a(L)$ to yield the cell shown in the middle part of Fig. 10. The pieces to the right and left of $l(\varphi^2 L)$ are of outer shape $a(\varphi L)$.

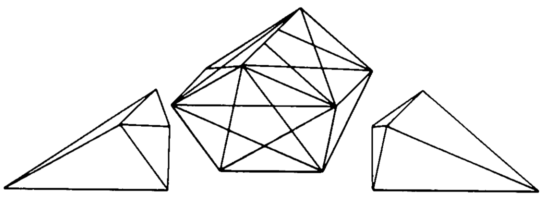

Fig. 10. Composite cell $a(\varphi^3 L)$. Insertion of two $t(\varphi^2 L)$ along the C_3 axis into the tetrahedral holes of the cell constructed according to Fig. 9 yields $a(\varphi^3 L)$.

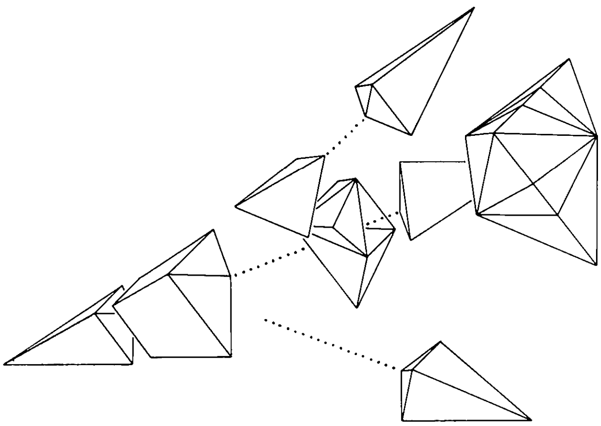

Fig. 11. Composite cells $t(\varphi^3 L)$ and $t(\varphi^4 L)$. Lower left part: partial covering of $l(\varphi^2 L)$ to the left as in Fig. 9 yields a tetrahedral hole, insertion of $t(\varphi^2 L)$ along the C_3 axis gives $t(\varphi^3 L)$. Upper right part: A combination of three $s(L)$ and nine $a(L)$, moved along the C_3 axis, covers the smaller faces of $t(\varphi^3 L)$ up to four tetrahedral holes as in $i_{-}(\varphi^2 L)$. Four $t(\varphi^2 L)$ are moved along C_3 axes into these holes. A ring of three $l(\varphi^2 L)$ with three inserted $a(\varphi L)$ is moved along the C_3 axis of $t(\varphi^3 L)$ to complete $t(\varphi^4 L)$.

4.11. *Proposition: the seven composite cells $y_i(\varphi^{q_i+3} L)$ can be composed out of the seven elementary cells $y_i(\varphi^{q_i} L)$*

The composite cells have the same central symmetry groups as the elementary ones.

Proof. The composite cells referred to are given by $d(\varphi^3 L)$, $s(\varphi^3 L)$, $a(\varphi^3 L)$, $t(\varphi^5 L)$, $d(\varphi^4 L)$, $s(\varphi^4 L)$, $a(\varphi^4 L)$. All of these composite cells are constructed with the full symmetry groups of their elementary ancestors.

Some metrical properties of plane figures and cells are listed in Table 2. In Table 3, the number of elementary cells contained in a composite cell is listed. This table allows one in principle to compute the number of elementary cells of each type which arise in the stepwise filling of central regions of $\mathbb{E}^3$.

5. Space filling with seven elementary cells and central icosahedral symmetry

The steps taken so far allow one to prove the key result of this paper given in § 5.1.

5.1. *Proposition: the seven elementary cells $d(L)$, $s(L)$, $a(L)$, $t(\varphi^2 l)$, $d(\varphi L)$, $s(\varphi L)$, $a(\varphi L)$ allow one to cover any central part of $\mathbb{E}^3$ while maintaining the full icosahedral symmetry*

They therefore allow for space filling with this symmetry.

Proof. The proof is given by induction with respect to periods of three generations of composition. Clearly $d(L)$ is elementary and covers a central region of $\mathbb{E}^3$ with icosahedral symmetry. Suppose that a dodecahedral central region $d(\varphi^{3m} L)$ of $\mathbb{E}^3$ has been covered by the repetition of the seven elementary cells, and that at the same time the other cells $s(\varphi^{3m}L)$, $a(\varphi^{3m}L)$, $t(\varphi^{3m+2}L)$, $d(\varphi^{3m+1}L)$, $s(\varphi^{3m+1}L)$, $a(\varphi^{3m+1}L)$ have been constructed from the elementary cells. This set of composite cells may be denoted as $y_i(\varphi^{3m+q_i}L)$ according to definition 4.5. Define now $L' = \varphi^{3m}L$. It was shown in proposition 4.11 that the generation $y_i(\varphi^{q_i+3}L')$ of seven composite cells can be composed out of the seven elementary cells $y_i(\varphi^{q_i}L')$. The proof applies regardless of the elementarity of the latter cells. Hence it follows from proposition 4.11 that the composite cells $y_i(\varphi^{3m+q_i+3}L)$ can be constructed from the cells $y_i(\varphi^{3m+q_i}L)$. This completes the proof of proposition 5.1 by induction. The conservation of central icosahedral symmetry is again assured by the application of proposition 4.11.

Table 2. *Metrical properties of figures in $\mathbb{E}^2$ and cells in $\mathbb{E}^3$*

Pentagon $p(L)$	
Edge length	L
Distance center–vertex	$L\varphi/(\varphi^2+1)^{1/2}$
Distance center–midpoint edge	$L\varphi^2/[2(\varphi^2+1)^{1/2}]$
Surface	$L^2\, 5\varphi^2/[4(\varphi^2+1)^{1/2}]$
Dodecahedron $d(L)$	
Edge length	L
Distance center–vertex	$L\sqrt{3}\varphi/2$
Distance center–midpoint edge	$L\varphi^2/2$
Distance center–midpoint face	$L\varphi^3/[2(\varphi^2+1)^{1/2}]$
Volume	$L^3\, 5\varphi^5/[2(\varphi^2+1)]$
Icosahedron $i(L)$	
Edge length	L
Distance center–vertex	$L[(\varphi^2+1)^{1/2}/2]$
Distance center–midpoint edge	$L\varphi/2$
Distance center–midpoint face	$L\varphi^2/(2\sqrt{3})$
Volume	$L^3\, 5\varphi^2/6$
Skene $s(L)$	
Edge length	L, φL
Height	$L\varphi^2/(\varphi^2+1)^{1/2}$
Volume	$L^3\, 5\varphi^4/[12(\varphi^2+1)]$
Aetos $a(L)$	
Edge length	L, φL, $\varphi^2 L$
Volume	$L^3\,\varphi^3/12$
Tristomos $t(\varphi^2 L)$	
Edge length	φL, $\varphi^2 L$, $\varphi^3 L$
Added height	$L\sqrt{3}\varphi^2$
Volume	$L^3\,\varphi^6/4$

Table 3. *The number of elementary cells in the construction of composite cells*

	Composite	Elementary						
		$d(L)$	$s(L)$	$a(L)$	$t(\varphi^2 L)$	$d(\varphi L)$	$s(\varphi L)$	$a(\varphi L)$
l	$l(\varphi^2 L)$	1	4	1				
	$l(\varphi^3 L)$					1	4	1
d	$d(\varphi^3 L)$	31	132	60	20		12	60
	$d(\varphi^4 L)$	32	252	360	80	31	132	60
s	$s(\varphi^2 L)$	1	6	5				
	$s(\varphi^3 L)$					1	6	5
	$s(\varphi^4 L)$	10	51	35	5	1	12	20
a	$a^1(\varphi^2 L)$		1	3	1			
	$a^2(\varphi^2 L)$						1	2
	$a(\varphi^3 L)$	1	8	11	2			
	$a(\varphi^4 L)$	2	12	12	2	1	8	11
t	$t(\varphi^3 L)$	1	6	6	1			
	$t(\varphi^4 L)$	4	21	18	5			3
	$t(\varphi^5 L)$	8	48	51	12	3	15	15

6. Notes and supplementary results

A few remarks and comments are added here to stimulate further research on the subject.

6.1. *The elementary cells*

There is a good deal of arbitrariness in the choice of elementary cells. The present selection is characterized by having only four shapes but admitting two different generations. It is believed that other (and perhaps fewer) elementary cells may be constructed from the present ones. Physicists have got used to the experience that seemingly elementary particles turn out to be composite.

6.2. *Irregular space filling*

The present paper concentrates on space filling with full icosahedral symmetry. Once the symmetry requirement is relaxed, many other ways of space filling may be derived from the present one. The generations of elementary cells provide examples of space filling with subgroups $\mathscr{C}_{5v}$, $\mathscr{C}_{3v}$ and $\mathscr{C}_{2v}$ of the icosahedral group. Besides, the number of elementary cells may be reduced. For example, the cell $a(\varphi L)$ may then be constructed from two $a(L)$ and one $s(L)$.

6.3. *The dodecahedron*

The question arises if the dodecahedron should be an elementary cell or, alternatively, should be built from other elementary cells. It is indeed possible to construct a dodecahedron from the elementary cells t and s, without using another dodecahedron.

6.4. *Proposition: composition of the dodecahedron d from t and s, Fig.* 12

Mark the midpoints of the edges of $d(2L)$. The inscribed pentagon on each face of $d(2L)$ has the edge length $\frac{1}{2}\varphi \times 2L = \varphi L$. The distance from a midpoint of an edge to the center of $d(2L)$ is $\varphi^2 L$. Hence, the pyramids with the inscribed pentagon $p(\varphi L)$ as base and the center of $d(2L)$ as top vertex are of the type $s(\varphi L)$. The midpoints of three edges of $d(2L)$ with a common vertex have, relative to each other, the distance φL. The three-pyramid with the base triangle spanned by these three midpoints and the vertex at the center of $d(2L)$ is part of $t(\varphi L)$. The three-pyramid formed by the same three points and the corresponding vertex of $d(2L)$ forms the second part of $t(\varphi L)$. Hence $d(2L)$ is composed of 20 $t(\varphi L)$ and 12 $s(\varphi L)$.

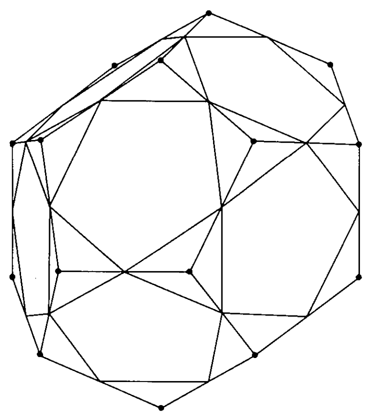

Fig. 12. Composition of the dodecahedron from *skene* and *tristomos*. When the midpoints of the edges of $d(2L)$ are connected with the center, these lines and the edge lines of the dodecahedron yield a decomposition of $d(2L)$ into 20 $t(\varphi l)$ with axes along the C_3 axes of $d(2L)$, and 12 $s(\varphi l)$ with axes along the C_5 axes of $d(2L)$. This composite cell falls outside the generations defined in § 4 but yields an alternative form of space filling.

This dodecahedron, because of the scaling factor 2, belongs to a new branch of possible generations. It was shown in proposition 5.1 that the cells s and t can be extended in periods of three generations. It follows that the composition according to proposition 6.4 can be used to yield an alternative way of space filling with icosahedral symmetry, based on the same set of elementary cells.

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References

GOLDBERG, M. (1955). *Scr. Math.* **21**, 253–260.
KEPLER, J. (1619). *Harmonices Mundi Libri V, Liber* II, p. 79. In *Gesammelte Werke*, Vol. VI (1940), edited by M. CASPAR. Munich: Verlag C. H. Beck.
PENROSE, R. (1974). *J. Inst. Math. Its Appl.* **10**, 266–271, as quoted in *Sci. Am.* (1977), **236**, January, pp. 110–121.

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The Analysis of Powder Diffraction Data

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Abstract

A comparison has been carried out between the results of analyses of several sets of neutron powder diffraction data using three different methods: the Rietveld method [Rietveld (1967). *Acta Cryst.* **22**, 151–152; (1969) *J. Appl. Cryst.* **2**, 65–71], a modification of the Rietveld method to include off-diagonal terms in the weight matrix [Clarke & Rollett (1982). *Acta Cryst.* Submitted] and the SCRAP method, which involves the estimation of observed Bragg intensities [Cooper, Rouse & Sakata (1981). *Z. Kristallogr.* **157**, 101–117]. Two simulations have also been carried out to demonstrate the way in which the results can differ in more extreme cases. This study has confirmed that the values of the estimated standard deviations given by the Rietveld method are not reliable and that, of the methods considered, only the SCRAP method will in general give reliable values for the estimated standard deviations of the structural parameters.

Introduction

An analysis of the Rietveld profile refinement method (Rietveld, 1967, 1969) by Sakata & Cooper (1979) showed how the results obtained by this method differ from those given by a conventional integrated intensity method and indicated that the values given for the e.s.d.'s (estimated standard deviations) of the refined parameters are unreliable. New methods for the refinement of powder diffraction data have subsequently been developed which will give more reliable values using two quite different approaches to the problem.

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