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New Types of Space-Filling Polyhedra with Fourteen Faces

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Abstract

A study of the staggered packing of identical hexagonal prisms leading to four-connected periodic structures with polyhedral cells of fourteen faces has been undertaken. Special attention was given to those packings that lead to periodic structures with two polyhedra per lattice point, and such that the two polyhedra are related by a pure rotation and/or enantiomorphism. The general solution for packings of this type was obtained and the topology of the intervening polyhedra was determined. It is shown that polyhedra with eight hexagonal faces and six square faces, topologically isomorphic to the truncated octahedron, can be packed with or without a rotation. The polyhedra which can be packed with the respective enantiomorphs (with or without rotation) have four square faces, four pentagonal faces and six hexagonal faces. Each type of packing is compatible with Bravais lattices of any category and each topological solution is compatible with a range of convex shapes.

1. Introduction

In the course of an investigation on the cellular structure of cork (see, for example, Gibson, Easterling & Ashby, 1981) we decided to study in detail the distinct possibilities of packing identical hexagonal prisms in a staggered way, so that the resulting four-connected structure can be described in terms of polyhedral cells, each with 14 faces (36 edges and 24 vertices). This number of faces results because a new edge, and therefore a new face, appears in the lateral faces of each prism owing to contacts with the six prisms that are laterally adjacent to it; the extra edges are shared by the basal faces of the adjacent prisms. The polyhedral cells are connected in such a way that three meet at an edge and four at a vertex. The structure is therefore tetravalent, as are many structures in crystallography (Wells, 1977), materials science (Smith, 1964) and biology (Dormer, 1980).

There are, of course, infinitely many solutions to the problem of packing identical hexagonal prisms, even if solutions are restricted to being periodic. Furthermore, for each topological solution (*i.e.* topological types of polyhedra that enter into the packing), there are infinitely many geometrical solutions since, for example, the prisms need not be straight and their bases need not be regular hexagons. The polyhedra in such 3D packings have 180° dihedral angles between six pairs of faces, but again the structure can be deformed so as to produce normal convex polyhedra with planar faces and with dihedral angles smaller than 180°. This possibility will be discussed in more detail in the final section.

A well known example of this type of packing (Dormer, 1980) is the one in which all cells are topologically isomorphic to the truncated octahedron, with six square faces and eight hexagonal faces. This packing results when the levels of the bases of the six prisms adjacent to any prism (relative to the base of the central prism) are 1/3, 2/3, 1/3, 2/3, 1/3, 2/3 in units of the height of the prisms.

In this article we describe results obtained in the course of an investigation of periodic packings of hexagonal prisms leading to structures with one or two polyhedra per lattice point. In the latter case, only solutions for which the two polyhedra are related by a rotation and/or enantiomorphism were considered.

For packings with one polyhedron per lattice point the only solution obtained corresponds to the truncated octahedron (six square faces and eight hexagonal faces). It was found, however, that there are metrical versions of this polyhedron that fill space when packed with one rotation. This result is new. Two other types of polyhedra with 14 faces (squares, pentagons and hexagons) are known that fill space with one rotation (Williams, 1968), but these are not obtained as solutions for the packing of prisms.

The tetradecahedra that fill space when packed in enantiomorphic pairs (with or without rotation) can be of two types: one is isomorphic to the truncated octahedron and the other has four quadrangular, four pentagonal and six hexagonal faces. We are not aware of other examples of enantiomorphic pairs which fill space when packed together.

The general form of the lattice vector basis compatible with each type of packing is derived, from which the Bravais type of lattice can be determined. It is concluded that all types of packing can be arranged in any type of Bravais lattice.

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2. Generation of packings

In the packings that will be studied it is possible to identify columns of polyhedra, each column comprising all prisms that are base adjacent. If H is the height of the prisms, measured parallel to the axis of the columns (z axis), the levels (z coordinates) of the bases of the prisms in a given column differ from each other by integral multiples of H. Therefore, if one level is known, all others can be identified. The levels of the prisms adjacent to a central prism are in an interval of amplitude H. The level of any prism can be taken as zero and the levels of the adjacent prisms taken in the interval 0, H or 0, $-H$. When this is done we say that the level of the central cell is reduced to zero. In the following we shall take the height of the prisms as unity.

The simplest way of generating packings is to use a three-connected planar network of identical hexagons to represent a section parallel to the bases of the prisms and inscribe in each hexagon a number defining the levels in the corresponding column, in such a way that two adjacent hexagons have levels not differing by an integer. In a periodic packing the levels must be arranged periodically. Fig. 1 shows an example of a periodic packing of prisms with five prisms per lattice point. The centres of the prisms $ABCD$ in a unit cell of the net of hexagons define a base of a parallelepipedic unit cell of the 3D lattice. The other, parallel, base is defined by the centres of the adjacent prisms in the same column as A, B, C and D. The hexagons in Fig. 1 are regular but any other net of identical hexagons could be used.

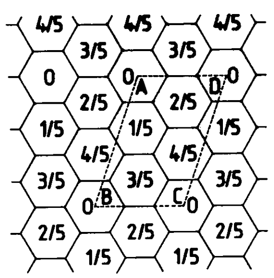
3. Topological types of individual polyhedra

The topological type of each prismatic cell can easily be inferred from the levels of the six prisms that are adjacent to it. It is straightforward to show that there are only seven topologically distinct possibilities which are enumerated in Fig. 2. The graphs in this figure represent the six lateral faces of a prismatic cell with indication of the levels of the bases of the adjacent cells. The dashed lines indicate the levels in the extreme lateral faces; this helps in the identification of the polygonalities of the resulting faces. The bases of the cells are of course hexagonal in all cases. The face content set of each cell is indicated in Fig. 2 using the usual convention of writing as a subscript the number of faces of each polygonality.

The intervening polygonalities of faces are 4, 5 and 6, the average polygonality being 5·143 in all cases. The seven polyhedra of Fig. 2 are among the 59 tetradecahedra with polygonalities between four and six, identified by Hucher & Grolier (1977), but all are non-isomorphic to the tetradecahedra identified by Williams (1968) as space fillers with one rotation.

Types I and II of Fig. 2 are those that enter in the periodic packings to be described below. Type I is of course isomorphic to the truncated octahedron. Its point symmetry in the regular hexagonal straight prismatic version is at most $\bar{3}m$, but its shape can be altered to produce a regular polyhedron with point symmetry $m\bar{3}m$; type II has a maximum point symmetry 222, which is also the maximum symmetry in the 'prismatic' version. The Schlegel representation of this polyhedron is shown at the bottom of Fig. 2.

By reducing to zero the level of a particular prismatic cell in a 3D packing it is straightforward to identify its topological type and also to conclude



LEVEL	TYPE
0	V
1/5	I
2/5	III
3/5	III
4/5	I

Fig. 1. A periodic packing of hexagonal prisms with five cells per lattice point. The numbers are the levels of the prisms, each of which has unit length. The topological types (Fig. 2) of each of the five polyhedra in a period are indicated. $ABCD$ defines a unit cell.

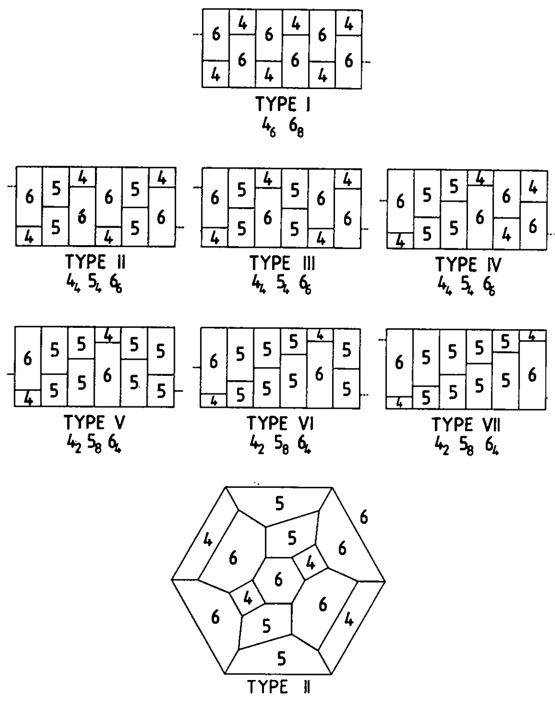


Fig. 2. The seven topological types of polyhedra that result from the staggered packing of hexagonal prisms. The graphs show the six lateral faces of the prisms with the extra edge due to contact with adjacent prisms. The exact levels of the extra edges are not relevant except for their positions relative to the levels in adjacent lateral faces. Also shown is the Schlegel representation of a type II polyhedron.

whether or not two cells are identical (identical reduced levels, in the same order). The types of polyhedra that enter in the packing of Fig. 1 were identified in this way and are indicated in that figure.

4. Simple periodic packings

In addition to operation *I* (identity) that relates two identical cells, we shall consider two other operations. The operation *R* rotates a cell by 180° about an axis parallel to the bases, changing the reduced level, α, of a particular adjacent cell into $(-\alpha)$. The levels α and $-\alpha$ (or $1-\alpha$) will be termed complementary. A rotated cell therefore has reduced levels which are complementary to those of the original cell and in reverse order. The operation *E* transforms a cell into its enantiomorph, which has the same reduced levels but in reverse order. Finally, the operation $ER = RE$ can be defined which changes the reduced levels to their complementaries in the same order. Fig. 3 summarizes the operations defined, showing the transformations of the reduced levels.*

The packings that will be discussed are those with one or two polyhedra per lattice point and such that, in the latter case, the two polyhedra are related by *E*, *R* or *RE*. We shall denote these packings by *I* (one polyhedron per lattice point) and by *E*, *R* and *RE* (two polyhedra per lattice point).

The general solution for the packings of each type is obtained as follows. A central cell is taken with the six reduced levels of adjacent cells as unknowns. For each adjacent cell the level of the cell and of three adjacent cells are defined in terms of those unknowns. The level of each adjacent cell is reduced to zero and the reduced levels are matched to those of the reference cell according to the type of packing that is being searched. All combinations have to be considered.

Two main conclusions have been drawn from this systematic analysis. The first is that all possible packings with two polyhedra per lattice point have the cells of each type in parallel alternating rows of the hexagonal network, as shown in Fig. 4(*b*) for the *RE* packing. The second conclusion is that all packings can be derived, as particular cases, from the *RE* packing. The general solution is the one shown in Figs. 4(*a*), (*d*), while Fig. 4(*c*) shows the reduced levels of cells $(-\alpha)$ and $(\beta-\alpha)$ of Fig. 4(*a*) leading to the conclusion that those cells can be related by *I* and *ER*, respectively, to the central cell of Fig. 4(*a*).

For the particular values of the levels, shown in Table 1, there are degeneracies which correspond to the other packings. If $E = I \neq R$, that is, if there is not an enantiomorph, the packing is *R*. Fig. 5(*a*) shows the solutions for this case. If $R = I \neq E$ the

* It is possible to construct a periodic three-connected network with a pair of non-regular hexagons per lattice point, the two hexagons being related by a rotation (but not with pairs of enantiomorphic hexagons!). This suggests that hexagonal prisms of two types, related by a 180° rotation about the axis of a prism, can be packed to fill space. It can be shown, however, that such packing cannot be four-connected.

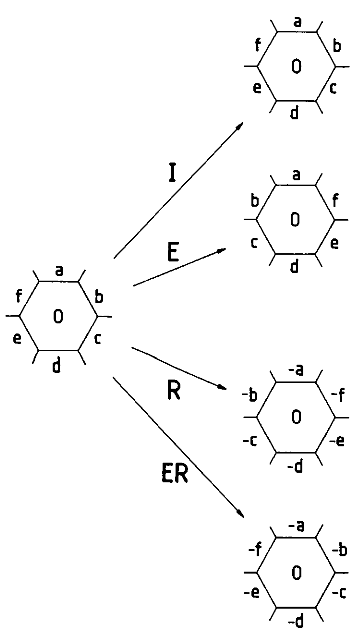


Fig. 3. Effect of operations *I*, *E*, *R* and *ER* on the reduced levels of a cell (the numbers *a* to *f* are in the interval 0, 1).

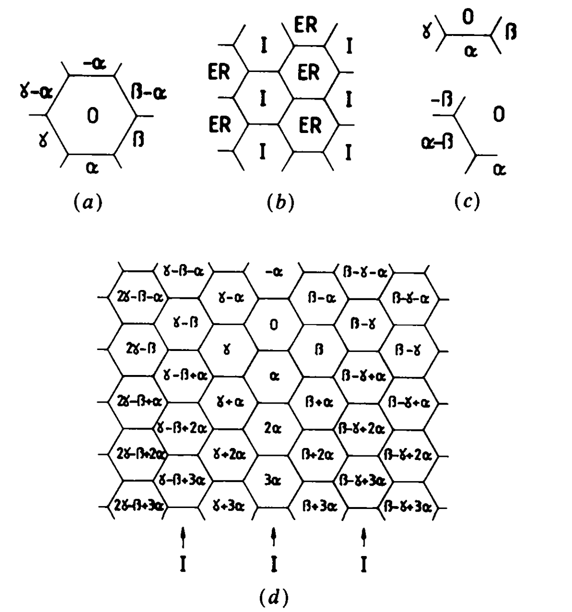


Fig. 4. (*a*) The general solution for periodic packings with at most two polyhedra per lattice point. Except for the degenerate cases indicated in Table 1, this solution leads to an *ER* packing with the *I* and *ER* types arranged as in (*b*). Reduction to zero of the levels of cells $(-\alpha)$ and $(\beta-\alpha)$ is shown in (*c*) indicating that these cells are respectively *I* and *ER* related to the cell shown in (*a*). A portion of the structure is shown in (*d*) with indication of the levels of the various cells. The topological types of polyhedra are indicated in Table 1.

packing is E, as shown in Fig. 5(b). Finally, if $R=E$, equivalent to $RE=I$, the packing is I (Fig. 5c).

The topological types were identified in each case and are indicated in Table 1. Only types I and II of Fig. 2 occur. In I and R packings the polyhedra are of type I, while in E packings the polyhedra are of type II. There are ER packings with each of these two types of polyhedra.

5. Bravais lattices of periodic packings

The hexagonal net obtained by sectioning the packings by a plane parallel to the bases of the prisms can be defined by two vectors $\mathbf{o}_1$ and $\mathbf{o}_2$ which form a primitive unit cell, as in Fig. 6(a). The planar lattice formed by the projections, on that plane, of the centres of I cells is defined by $\mathbf{o}_1$, $\mathbf{o}_2$ for I packings and by $\mathbf{o}_1$, $2\mathbf{o}_2$ for the other packings, $\mathbf{o}_1$ being taken in the direction of adjacent I cells (Fig. 6b). If a third vector $\mathbf{o}_3$ is introduced along the z axis, of length equal to the height of the prisms, the lattices are defined in each case by a vector basis $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$ given by

$$\begin{aligned} \mathbf{e}_1 &= \mathbf{o}_1 + \alpha\mathbf{o}_3 \\ \mathbf{e}_2 &= n\mathbf{o}_2 + \xi\mathbf{o}_3 \\ \mathbf{e}_3 &= \mathbf{o}_3 \end{aligned} \tag{1}$$

with the following values of n and ξ ($cf.$ Fig. 4d):

I packings: $n=1$; $\xi=\beta$;

other packings: $n=2$; $\zeta=\beta-\gamma+\alpha$.

There are no restrictions on the choice of the three non-coplanar vectors $\mathbf{o}_1$, $\mathbf{o}_2$, $\mathbf{o}_3$. In particular, $\mathbf{o}_1$, $\mathbf{o}_2$ may be chosen to define any type of planar lattice. If this lattice is not rectangular or quadrangular, the hexagons can be taken as the Wigner–Seitz cells of the lattice, as in Fig. 7(a). A net of hexagons with a quadrangular or rectangular lattice can also be constructed, as in the example of Fig. 7(b). There is also no restriction to the values of α and ξ in (1), except those indicated in Table 1 for particular types of

Table 1. *Topological types of space fillers in various packings*

Packing type	Conditions (Fig. 4a)	Topological type of polyhedra
R	$E=I$; $\beta=\gamma$ or $\beta=2\alpha$; $\alpha+\gamma=1$	I
E	$R=I$; $\alpha=1/2$; $\gamma=-\beta$ or $\beta=\alpha/2$; $\gamma=(1+\alpha)/2$	II
I	$E=R$; $\beta+\gamma-\alpha=0$	I
	$E=R=I$; $\beta=\gamma=(1+\alpha)/2$	I
ER	All other cases ($0<\alpha, \beta, \gamma<1$); $\beta, \gamma \gtrless \alpha$	I
	α between β and γ	II

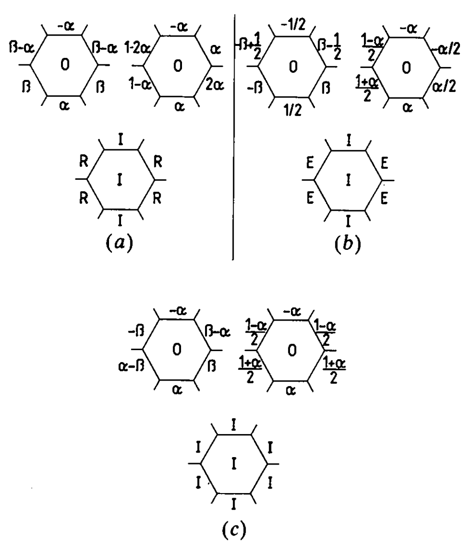


Fig. 5. For particular values of the levels α, β, γ in Fig. 4(a), the ER packing degenerates into R, E and I packings as shown respectively in (a), (b) and (c). The topological types of the polyhedra are indicated in Table 1.

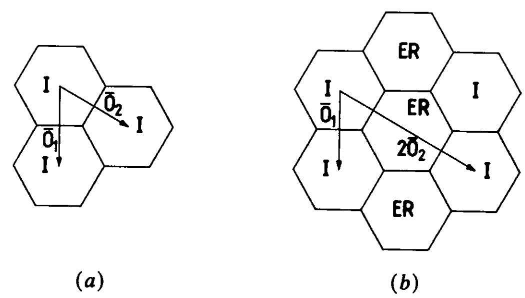


Fig. 6. Definition of the vectors $\mathbf{o}_1$ and $\mathbf{o}_2$ that enter into vector bases for the 3D periodic structures.

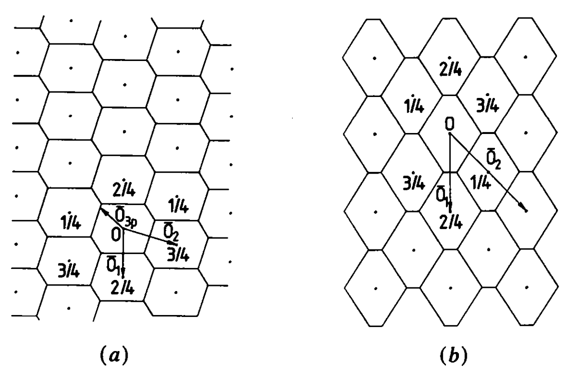


Fig. 7. (a) An I packing with a simple cubic lattice, with indication of the vectors $\mathbf{o}_1$, $\mathbf{o}_2$ and $\mathbf{o}_3$ (projection on the plane of the bases shown) used in the definition of a vector basis of the cubic lattice. (b) An E packing with a body-centred tetragonal lattice. $\mathbf{o}_3$ is perpendicular to the plane of the bases.

packing. In particular, they can be irrational, in which case the plane parallel to the bases of the prisms is not a lattice plane.

For given ($\mathbf{o}_1\mathbf{o}_2\mathbf{o}_3$) and α, ξ, the basis ($\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3$) can be determined and from it the type of Bravais lattice can be identified (for example, using the method of reduced cells). Conversely, given a vector basis ($\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3$) defining any type of Bravais lattice, there are always solutions for ($\mathbf{o}_1\mathbf{o}_2\mathbf{o}_3$) and α, ξ compatible with each type of packing.

Fig. 7(a) shows an I packing with a simple cubic lattice, in which $\mathbf{o}_1=\mathbf{u}_1-1/2\mathbf{u}_3$; $\mathbf{o}_2=\mathbf{u}_2-3/4\mathbf{u}_3$; $\mathbf{o}_3=\mathbf{u}_3$, where $\mathbf{u}_1$, $\mathbf{u}_2$, $\mathbf{u}_3$ define a cubic unit cell. The angle of $\mathbf{o}_3$ with the normal to the plane of the bases is 42·03°. Fig. 7(b) shows an E packing with a body-centred tetragonal lattice; the lattice of hexagons is quadrangular and $\mathbf{o}_3$ is perpendicular to the plane of the bases (straight prisms).

6. The shape of space fillers

The polyhedra considered so far were derived from prisms by introducing additional edges and faces, and therefore have dihedral angles of 180° between pairs of lateral faces. This geometric feature is of course not essential and completely convex space-filling polyhedra can be derived from the 'prismatic' polyhedra. For example, the regular truncated octahedron can be obtained by a suitable deformation of the topologically isomorphic I packing of prisms described above. In general, a 'prismatic' packing in which, as we have seen, the prisms need not be straight or regular, may be deformed into another space-filling packing of the same periodicity and topological type, provided the deformation is the same at lattice equivalent points. Furthermore, this deformation preserves the type of packing, in the sense that an E packing, for example, remains an E packing upon deformation.

We have used this procedure to obtain a model of an E packing consisting of truly convex polyhedra with planar faces. The complete description of this polyhedron will not be given since it is not specially relevant, but we show in Fig. 8 a perspective line diagram of the polyhedron obtained (point group 222).

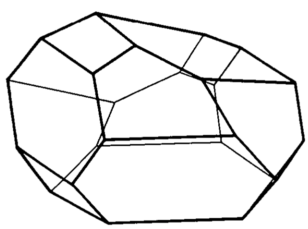


Fig. 8. Perspective view of a type II polyhedron that fills space with its enantiomorph.

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SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible.*

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A peak interpolation formula for Fourier map interpretation. By F. PAVELČÍK, *Department of Analytical Chemistry, Faculty of Pharmacy, Komensky University, CS* 832 32 *Bratislava, Czechoslovakia*

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Abstract

A weighted 19-point parabolic interpolation formula applicable to computer interpretation of Fourier maps is derived.

In the course of programming and testing a peak-picking routine for automatic interpretation of Patterson, superposition and symmetry maps (Pavelčík, 1986), we found that in some cases, where peak shapes are poor, the peak interpolation formula due to Rollett (1965) gave some corrections greater than half of the grid spacing. Instead of using a simple three-point parabolic 1D interpolation a weighted 19-point 3D parabolic interpolation was derived. The peak coordinates are given by minimizing the sum

$$\sum_{i=1}^{27} w_i\left[F_i-\left(A_0+\sum_{j=1}^{3}A_jx_j+\sum_{j=1}^{3}AA_jx_j^2\right)\right]^2,$$

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