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On a simple tiling of Deza and Shtogrin

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Some properties of an exceptional simple tiling by fullerenes, first described by Deza & Shtogrin [*Southeast Asian Math. Soc. Bull*. (1999), **23**, 1–11], are presented.

1. Introduction

A recent review (Delgado-Friedrichs *et al.*, 2005) of periodic nets and tilings contained the statement 'Simple tilings by polyhedra that have only five- and six-sided faces are also of special interest. It appears, though it has never been proved, that only four polyhedra (with 12, 14, 15 or 16 faces, respectively) can occur in such tilings'. This statement refers to simple tilings that are duals of the Frank–Kasper structures, but it is incorrect and has been known to be incorrect for some time. A counter-example was provided by Deza & Shtogrin (1999) and in this note we describe some properties of that structure and demonstrate that, if another counter-example exists, the net carried by the tiling must have more than seven kinds of vertex.

A *simple* polyhedron is one in which exactly three faces meet at each vertex. A *simple* tiling is a tiling by simple polyhedra in which exactly two polyhedra meet at each face, exactly three meet at each edge and exactly four meet at each vertex; their duals are tilings by tetrahedra (see *e.g.* Delgado-Friedrichs *et al.*, 2005). Simple polyhedra with only five- and six-sided faces are often (as here) referred to as *fullerenes*.

2. Enumeration of tilings by fullerenes

Systematic enumeration of tilings is best effected using Delaney–Dress symbols. In the present case, it is convenient to first enumerate all topological types of face-to-face tilings by tetrahedra in which each edge is shared by either five or six tetrahedra. The results are then dualized. Topological duals of cellular tilings (sometimes called Poincaré duals) are well defined and readily obtained in the context of Delaney–Dress symbols. Indeed, vertices, edges, faces and tiles of the original tiling correspond to tiles, faces, edges and vertices of the dual, respectively. Thus, by simply rewriting the criteria for simple tilings accordingly, the dual of a simple tiling must have tiles each composed of four triangles, three meeting at a vertex. In other words, they must be tetrahedra. For the enumeration, we adapted the general approach presented by Delgado-Friedrichs & Huson (1999). Their method consists of five steps, the first three being:

(A1) enumerate all possible equivariant polyhedra of the given topological type;

(A2) for each such equivariant polyhedron, systematically enumerate all possible identifications of pairs of faces;

(A3) for each choice of face identifications, enumerate all possible choices of degrees for each type of edge.

The remaining two steps are concerned with eliminating results that cannot be realized in Euclidean space and finding vertex coordinates. These are not modified.

For our particular application, step (A1) translates into listing all possible site symmetries of a tetrahedral tile. Step (A2), the systematic identification – or gluing – of faces, was modified so as to restrict the number of tiles (or, rather, wedges) around any edge to the numbers 1, 2, 3, 5 and 6. Any number less than 5 implies that in step (A3) a suitable rotation degree has to be assigned to the respective edge. As the number 4 does not divide 5 or 6, it is thus excluded. If an edge is already shared by five or six tiles, no rotation can be applied, as this would increase the number of tiles. As rotations of degree 5 violate the crystallographic restriction, the number 1 (which means that two adjacent faces of the same tile are glued together along the edge they share) can only result in a rotation of degree 6. In effect, step (A3) becomes trivial, while the number of face identifications to be generated in step (A2) is diminished considerably. Using these modifications, we were able to enumerate all simple tilings with only five- and six-sided tiles with up to seven kinds of vertex. In contrast, for general simple tilings, a complete enumeration has so far only been obtained for up to three kinds of vertex. As the complexity of tilings that can be enumerated in reasonable time is severely limited by combinatorial explosion, this is a significant advance.

It was found that there are precisely two tilings by fullerenes with three kinds of vertex, one with five kinds and two with seven kinds of vertex. The two tilings with three vertices and the one with five

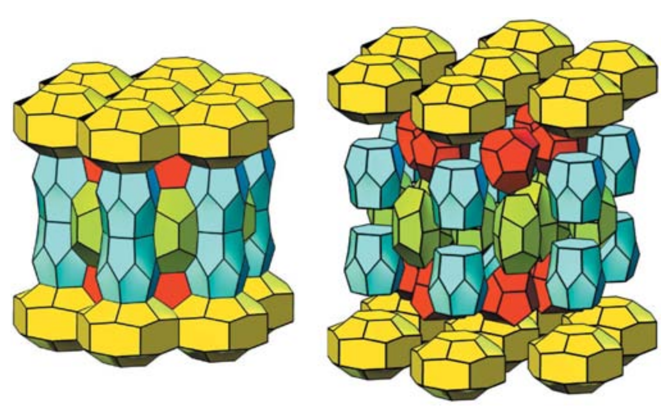

Figure 1
The Deza-Shtogrin tiling (left) shown exploded on the right.

Table 1
Coordinates for the centers of tiles and vertices (last seven rows) for an embedding of the net, **mds**, carried by the Deza-Shtogrin tiling with edges of unit length.

The first column is either the face symbol for tiles or vertex symbol for vertices. The symmetry is $P6/mmm$ with a = 3.4087, c = 8.3173.

Tile/vertex	Wyckoff	x	y	z
[$5^{12}.6^8$]	1b	0	0	1/2
[$5^{12}.6^2$]	2e	0	0	0.1665
[5^{12}]	3f	1/2	0	0
[5^{12}]	4h	1/3	2/3	0.7297
5·5·5·5·5·6	4h	1/3	2/3	0.4399
5·5·5·5·5·5	4h	1/3	2/3	0.0601
5·5·5·5·5·6	6l	0.1694	2x	0
5·5·5·5·5·6	6i	0	1/2	0.4184
5·5·5·5·5·5	12n	0	0.3533	0.2154
5·5·5·5·5·6	12n	0	0.2934	0.3331
5·5·5·5·5·5	12o	0.1862	2x	0.1196

vertices are known as clathrates I, II and III (O'Keeffe *et al.*, 1998) and in our database of nets (http://okeeffe-ws1.la.asu.edu/RCSR/home.htm) have symbols **mep**, **mtn** and **zra-d**, respectively. **mtn** is the dual of the cubic Frank–Kasper phase $MgCu_2$. A structure closely related to $MgCu_2$ is that of $MgZn_2$ [they are related as cubic and hexagonal closest packing – see O'Keeffe & Hyde (1996)] and one of the structures with seven kinds of vertex is the dual of this. We symbolize the net carried by that tiling as **mgz-x-d**. These four structures are of course well known as tilings by fullerenes with 12, 14, 15 and/or 16 faces. The second tiling with seven kinds of vertex is the Deza–Shtogrin structure, which includes a tile with 20 faces and which we now describe.

3. The Deza–Shtogrin tiling

The Deza–Shtogrin tiling is illustrated in Fig. 1. It is made up of dodecahedra, [5^{12}], tetrakaidecahedra, [$5^{12}.6^2$], and icosahedra, [$5^{12}.6^8$], in the ratio 7:2:1 and has symmetry $P6/mmm$. The icosahedron, which has 36 vertices, is familiarly known as the elongated hexagonal barrel (O'Keeffe & Hyde, 1996).

The net, to which we assign symbol **mds**, carried by the tiling permits an embedding with edges of equal length and corresponding to the shortest distances between vertices. Coordinates for a minimum density configuration subject to those constraints are given in Table 1.

The tilings dual to the Frank–Kasper structures all have average face size in the range 5.100 to 5.111 (*e.g.* O'Keeffe, 1999). On the other hand, the Deza–Shtogrin structure has average face size 56/11 = 5.091, *i.e.* is richer in pentagons.

The dual of the Deza–Shtogrin structure does not appear to correspond to a known intermetallic structure, but we note that the familiar $CaCu_5$ structure is related. The structure dual to $CaCu_5$, considered as a tiling of tetrahedra, is the tiling corresponding to the net of the zeolite DOH. This simple tiling also contains elongated hexagonal barrels but in addition contains tiles with quadrangular faces.

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