

New examples of generalized fullerenes

M. Deza and M. I. Shtogrin

A *fullerene* is a simple (3-valent) polyhedron whose faces are pentagons and hexagons, and therefore the number of pentagons is 12. Only 4 fullerenes have no adjacent hexagons. These are the dodecahedron F_{20} , the hexagonal barrel F_{24} (whose two hexagons are separated by two belts of pentagons), the fullerene F_{26} (which is unique with 26 vertices), and a fullerene F_{28} (one of the two with 28 vertices). They have, respectively, 0, 2, 3, and 4 non-adjacent hexagons, 20, 24, 26, and 28 vertices, and are called *Frank–Kasper fullerenes*, abbreviated as FK-fullerenes. The *elongated barrel* F_{36} is obtained from F_{24} by adding a belt of 6 hexagons between the belts of pentagons. The *elongated dodecahedron* F_{30} is obtained from F_{20} by adding a belt of 5 hexagons. The *twisted dodecahedron* F'_{20} (a related simple polyhedron with a triple axis but not a fullerene) has a belt of alternating three hexagons and three squares, and the remaining 6 faces are pentagons.

An \mathbb{R}^3 -*fullerene* (space fullerene) is defined as a simple (that is, 4-valent) normal tiling of \mathbb{R}^3 into fullerenes. An \mathbb{R}^3 -fullerene is said to be *crystalline* if its symmetry group is crystallographic — has translations in three non-coplanar directions. FK- \mathbb{R}^3 -fullerenes (or *Frank–Kasper phases*) are crystalline \mathbb{R}^3 -fullerenes whose cells are FK-fullerenes (all 4, or some of them) (see [1]–[3]). Exactly 24 FK-phases are known as metallic alloys. It was observed in [2], [3] that the proportions of the cells F_{20} , F_{24} , F_{26} , F_{28} in each of the 24 cases are linear combinations of the proportions for the basic examples A_{15} , C_{15} , and Z with proportions $2 : 6 : 0 : 0$, $16 : 0 : 0 : 8$, $3 : 2 : 2 : 0$. However, in 2008 Delgado-Friedrichs, Deza, and Dutour found all the FK- \mathbb{R}^3 -fullerenes with at most 16 cells in the fundamental domain. Three of them, with proportions $3 : 4 : 2 : 0$, $7 : 4 : 2 : 2$, $6 : 6 : 4 : 0$, are counterexamples to a general conjecture that was unsolved at that time.

The only known crystalline \mathbb{R}^3 -fullerene that is not an FK- \mathbb{R}^3 -fullerene was constructed in [4]. It was considered in detail later in [5] as the *Deza–Shtogrin tiling*. We call it the DS- \mathbb{R}^3 -fullerene. It consists of F_{20} , F_{24} , F_{36} in the proportion $7 : 2 : 1$ and has symmetry group $P6/mmm$. All the crystalline \mathbb{R}^3 -fullerenes with at most 7 orbits of vertices are A_{15} , C_{15} , Z , C_{14} , and the DS- \mathbb{R}^3 -fullerene, which have, respectively, 3, 3, 5, 7, and 7 orbits (see [5]). The DS- \mathbb{R}^3 -fullerene turned out to be the best among the known ones in the sense of the average number of sides of its faces, $56/11$, the nearest to the unattainable minimum 5.

The tiling with the group $P6/mmm$ corresponding to the clathrate H is closely related to \mathbb{R}^3 -fullerenes. The fundamental domain of this tiling has 34 vertices (water molecules), which form cells F_{20} , F'_{20} , F_{36} in the proportion $3 : 2 : 1$ (see [6]). *Clathrates* are crystalline solid substances based on crystalline water (they are similar to ice) in which non-polar molecules (usually, gases) are trapped inside cells of water molecules with hydrogen bonds. The basic clathrates of type I (A_{15} in the crystallographic terminology; they have group $Pm\bar{3}n$) and of type II (C_{15} in the crystallographic terminology; they have group $Fd\bar{3}m$) correspond to the FK- \mathbb{R}^3 -fullerenes A_{15} and C_{15} . The crystalline FK- \mathbb{R}^3 -fullerene C_{14} has group $P6_3/mmc$, whose fundamental domain consists of eight F_{20} and four F_{28} .

This research was supported by the Russian Foundation for Basic Research (grant no. 08-01-90102-Мол), the Programme “Leading Scientific Schools” (grant no. HIII-4182.2006.1), and the State Programme for Basic Research of the Mathematics Division of the Russian Academy of Sciences “Modern Problems of Theoretical Mathematics”.

AMS 2000 *Mathematics Subject Classification*. Primary 52C22; Secondary 05B45, 51M20, 92E10.

DOI 10.1070/RM2009v064n01ABEH004598.

In essence, C_{14} is a hexagonal version of C_{15} , with the same proportion $2 : 0 : 0 : 1$ but with 12 cells in the fundamental domain of the group $P6_3/mmc$. The fullerenes F_{28} form the diamond structure in C_{15} , and the hexagonal diamond (lonsdaleite) structure in C_{14} .

Below we construct infinitely many non-crystalline \mathbb{R}^3 -fullerenes from any crystalline \mathbb{R}^3 -fullerene with an axis of order 6 and with planes of mirror symmetry along the axis. This method of constructing \mathbb{R}^3 -fullerenes is a three-dimensional analogue of the method for producing \mathbb{R}^2 -fullerenes presented below.

A *generalized fullerene* (more precisely, an \mathbb{M}^n -fullerene; see [4]) is a simple tiling of a manifold \mathbb{M}^n of any dimension n (closed or unbounded) whose two-dimensional faces are pentagons and hexagons. An ordinary fullerene is an \mathbb{S}^2 -fullerene. A generalized \mathbb{P}^2 -fullerene, where \mathbb{P}^2 is the projective plane, has 6 pentagons.

We now present a method for constructing \mathbb{R}^2 -fullerenes homeomorphic to the plane that have at most 6 pentagons. Let us consider the standard tiling of the plane \mathbb{R}^2 into hexagons and choose the centre of one of the hexagons as the vertex of an angle $\pi/3$ whose boundary rays are directed along axes of mirror symmetry. We perform the following operation: we remove the interior of the angle $\pi/3$ and identify the boundary rays by a rotation through $\pi/3$. After this operation, some halves of hexagons are removed together with the interior of the angle, while the other halves are glued together into whole hexagons. Only one hexagon, at whose centre we chose the vertex of the angle $\pi/3$, becomes a pentagon after one sixth of it is removed. As a result, we obtain a simple normal tiling of the plane into hexagons and one pentagon. This simplest \mathbb{R}^2 -fullerene has group $5m$. In this \mathbb{R}^2 -fullerene any hexagon can again be replaced by a pentagon in exactly the same fashion. For that, we must remove an angle $\pi/3$ with vertex at the centre of a hexagon that does not contain the pentagon that we already have. Thus we obtain infinitely many \mathbb{R}^2 -fullerenes with two pentagons. The group of each of these \mathbb{R}^2 -fullerenes is $2m$ or 2 . This operation can be repeated six times, since six pairwise disjoint angles $\pi/3$ can be removed from the tiling of the Euclidean plane into hexagons, but not more, which follows from the equality $6 \cdot \pi/3 = 2\pi$.

The DS- \mathbb{R}^3 -fullerene has group $P6/mmm$. Let us construct a dihedral angle $\pi/3$ formed by planes of mirror symmetry. We perform the following operation: we remove the interior of the angle and identify the faces (by rotation through $\pi/3$). After this operation, some halves of fullerenes are removed, and other halves are glued together into whole fullerenes. Only those fullerenes that are pierced by the edge of the dihedral angle $\pi/3$ turn into different fullerenes after the removal of one sixth from each of them: F_{36} into F_{30} and F_{24} into F_{20} . The result is a simple normal tiling of the space \mathbb{R}^3 into fullerenes F_{36} , F_{30} , F_{24} , and F_{20} . This is a new \mathbb{R}^3 -fullerene. Its symmetry group is no longer crystallographic but a rod group, $p5/mmm$, with one translational period. In the new \mathbb{R}^3 -fullerene, along an arbitrary local axis of order 6 we can again replace F_{36} by F_{30} and F_{24} by F_{20} . For that, we remove a dihedral angle $\pi/3$ with edge along a local axis of order 6 whose interior does not contain the new fullerene F_{30} . We thus obtain infinitely many \mathbb{R}^3 -fullerenes with two local rod groups with axis of order 5. Each has rod group $pmmm$ or $p2/m11$. The operation can be repeated six times. This is the three-dimensional analogue in question.

Theorem. *This procedure produces \mathbb{R}^3 -fullerenes from all the others with group $P6/mmm$.*

Bibliography

- [1] F. C. Frank and J. S. Kasper, *Acta Crystallogr.* **11**, Part 3 (1958), 184–190; **12**, Part 7 (1959), 483–499.
- [2] Я. П. Ярмолюк, П. И. Крипякевич, *Кристаллография* **19** (1974), 539–545; English transl., Ya. P. Yarmolyuk and P. I. Kripyakevich, *Sov. Phys. Crystallogr.* **19** (1974), 334–337.

- [3] D. P. Shoemaker and B. Shoemaker, *Acta Crystallogr. Sect. B* **42**, Part 1 (1986), 3–11.
- [4] M. Deza and M. Shtogrin, *Southeast Asian Bull. Math.* **23**:1 (1999), 9–18.
- [5] O. Delgado-Friedrichs and M. O’Keeffe, *Acta Crystallogr. Sect. A* **62**:3 (2006), 228–229.
- [6] E. D. Sloan, Jr., *Clathrate hydrates of natural gases*, Dekker, New York 1998.

M. Deza

École Normale Supérieure, Paris; JAIST, Japan

E-mail: Michel.Deza@ens.fr

Presented by V. M. Buchstaber

Accepted 07/DEC/08

Translated by E. I. KHUKHRO

M. I. Shtogrin

Steklov Mathematical Institute,

Russian Academy of Sciences

E-mail: stogrin@mi.ras.ru