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ORIGINAL RESEARCH

Space fullerenes: computer search for new Frank–Kasper structures II

Mathieu Dutour Sikirić · Michel Deza

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Abstract A *Frank–Kasper* structure is a 3-periodic tiling of the Euclidean space E^3 by tetrahedra such that the vertex figure of any vertex belongs to four specified fullerenes with, respectively, 12, 14, 15, and 16 faces. Frank–Kasper structures occur in the crystallography of metallic alloys, clathrates, zeolites, and in geometrical optimization. 27 such physical structures are known. In Dutour et ai. (Acta Crystallogr A 66:637–639, 2010) we obtained, by computer enumeration, all 84 such structures with up to 20 cells in a reduced fundamental domain; 13 among them were known physical structures. In the present follow-up study, we managed, by improving the computation, to get all 37 new structures with 21 cells in a reduced fundamental domain. Those structures are described, using six invariants: group, the size of fundamental domain, mean coordination number $\bar{f}$, fraction sequence, cell orbits and major skeleton. We found pairs of distinct structures having all six invariants equal. So, we devised a new invariant, *zigzag vector,* and computed it for all 135 structures known from now; all have this invariant different. New bounds for $\bar{f}$ and new directions (computational perspectives, number of Kekule structures, space octahedrites, space cubites) are also discussed.

Keywords Frank–Kasper structures · Enumeration · E^3-tilings

M. Dutour Sikirić
Institute Rudjer Bosković, 10000 Zagreb, Croatia
e-mail: mdsikir@irb.hr

M. Deza (✉)
Ecole Normale Superieure, 75005 Paris, France
e-mail: Michel.Deza@ens.fr

Introduction

A *tiling* is a partition of Euclidean 3-space E^3 into *tiles,* i.e., interiors of *cages* (generalized polyhedra with, possibly, vertices of degree two, topologically equivalent to a sphere). Faces of tiles have vertices and edges but are not necessarily contained in an affine plane. A tiling is *face-to-face* if each face belongs to exactly two tiles; it is *normal* if the intersection of any two cages is a face, edge, point or $\emptyset$. A tiling is *simple* if four tiles meet at each vertex. So, the skeleton graph of a simple tiling is 4-regular. A tiling is 3-*periodic* (or *crystallographic)* if its automorphism group contains translations in three non-coplanar directions.

A (geometric) *fullerene* [1] F_n is a polyhedron with n, all of degree three, vertices and only 5- and 6-gonal faces. So, $p_5 = 12$ and $p_6 = \frac{n}{2} - 10$ for the number of faces. F_n exist for any even $n \geq 20$, except 22. The number of n-vertex fullerenes is 1, 0, 1, 1, 2 for $n = 20, 22, 24, 26, 28$.

The *Frank–Kasper polyhedra* are all (four) fullerenes with *isolated hexagons:* unique ones F_{20}, F_{24}, F_{26}, and one of two F_{28}, with maximal symmetry I_h, D_{6d}, D_{3h}, T_d, respectively (see Fig. 1). Crystallographers usually consider their duals as the *coordination polyhedra* with vertices of degree six being possible *disclinations* of the local icosahedral order. These duals are called *Frank–Kasper deltahedra* and denoted by $Z_{12}, Z_{14}, Z_{15}, Z_{16}$ or *X, R, Q, P*, respectively.

A *space fullerene* is a normal face-to-face simple tiling of E^3 by any fullerenes (possibly, non-congruent and with curved faces). A *Frank–Kasper space fullerene* or, for short, *FK space fullerene* is a 3-periodic space fullerene, where any tile is isomorphic to one of four *Frank–Kasper* polyhedra.

In crystal chemistry, usually are considered their duals, introduced in [2, 3] and called since *Frank–Kasper*

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structures or *Frank–Kasper phases, t.c.p.* (tetrahedrally or topologically close-packed) structures with coordination numbers 12, 14, 15, 16. Then vertices correspond to atoms and edges correspond to atomic bonds. Terms *t.c.p.* and *Frank–Kasper phase* are preferred usually in crystallography and material science, respectively.

In [4], the first 3-periodic space fullerene, which is not FK, was given. This *DS space fullerene* is a tiling of E^3 by F_{20}, F_{24} and its elongation $F_{36}(D_{6h})$ in proportion 7:2:1. In [5], an infinite number of (1-periodic only) space fullerenes (having tiles F_{20}, F_{24}, F_{30}, F_{36} with maximal symmetry I_h, D_{6d}, D_{5h}, D_{6h}, respectively) is constructed from any infinite non-periodic *plane fullerene,* i.e., a 3-regular normal plane partition with 5- and 6-gonal faces only.

In [6] (see also the Reticular Chemistry Structure Resource—RCSR-database), besides DS space fullerene named *mds,* seven other 3-periodic space fullerenes, which are not FK, are given (Table 1). So, five new putative tiles, in addition to four *Frank–Kasper* ones and $F_{36}(D_{6h})$. They are all possible ones with at most 11 vertex orbits. See Fig. 1 for the Schlegel diagrams of the newly occurring tiles.

Note that the composition of odg, given above, differ from the erroneous one given in [6] (Fig. 2). Note also that in all known [4] 4-regular tilings of the 4-sphere S^3 by fullerenes, the putative tiles were among seven ones: four *Frank–Kasper* fullerenes and $F_{30}(D_{5h})$, $F_{32}(D_{3h})$, $F_{36}(D_{6h})$.

FK space fullerenes occur in:

1. 27 known *t.c.p.* (ordered tetrahedrally close-packed phases) of *metallic alloys,* where cells are atoms.
2. *Clathrates* (compounds with one component, atomic or molecular, enclosed in framework of another), including
   - *clathrate hydrates,* where cells are solutes cavities, vertices are H_2O, edges are hydrogen bonds;

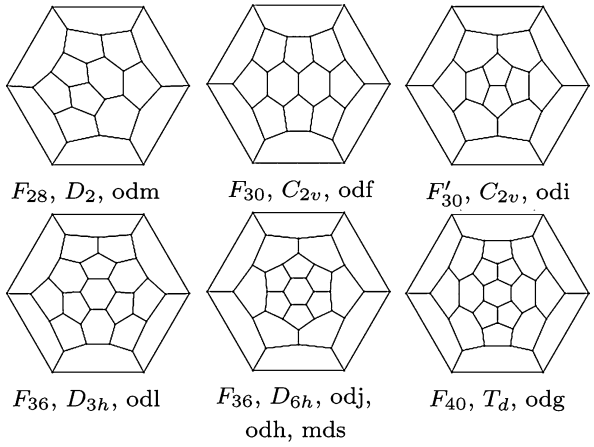

Fig. 2 The six non-FK fullerenes occurring as tiles in [6]

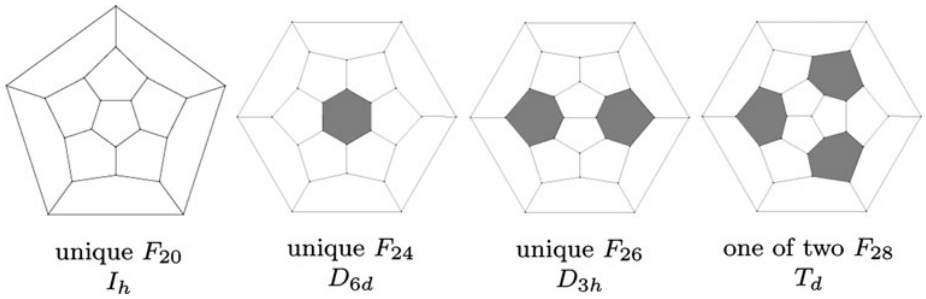

Fig. 1 The four fullerenes with isolated hexagons

Table 1 DS space fullerene and seven space fullerenes from [6]

Name DS = mds	Group *P6/mmm*	Nr υ-orbit 7	f.d. 10	f 13.20	Composition $7F_{20} + 2F_{24} + F_{36}(D_{3h})$	Zigzag vector 11^{12}, 30^{18}
odf	$Im\bar{3}$	9	23	13.30	$17F_{20} + 6F_{30}(C_{2v})$	30^{20}, 160^{6}
odg	$P\bar{4}3m$	10	21	13.26	$12F_{20} + 7F_{24} + F_{28}(T_d) + F_{40}(T_d)$	8^{12}, 27^{8}, 33^{12}, 60^{12}
odh	*P6/mmm*	10	20	13.40	$9F_{20} + 10F_{24} + F_{36}(D_{6h})$	11^{24}, 36^{4}, 78^{2}, 90^{6}, 132^{2}
odi	$P4_2/nmc$	11	18	13.3	$6F_{20} + F_{24} + 2F'_{30}(C_{2v})$	8^{4}, 24^{4}, 28^{8}, 30^{8}, 33^{8}, 46^{8}
odj	*P6/mmm*	11	17	13.29	$10F_{20} + 4F_{24} + 2F_{26} + F_{36}(D_{6h})$	30^{12}, 46^{6}, 52^{6}, 102^{2}
odl	$P6_3/mcm$	11	30	13.3	$8F_{20} + 6F_{24} + F_{36}(D_{3h})$	27^{12}, 30^{16}, 48^{2}, 52^{6}, 96^{2}, 318^{2}
odm	$R\bar{3}c$	11	20	13.40	$6F_{20} + F_{24} + 3F_{28}(D_2)$	3^{2}, 11^{18}, 19^{12}, 25^{6}, 36^{6}, 105^{2}, 180^{2}

For each such non-FK space fullerene, we give the space group, the number of vertex orbits, the number of cells in a fundamental domain, the average coordination number, and the composition

- *clathrasils* (silicate materials with clathrate structure);
- *zeolites* (hydrated microporous aluminosilicate minerals), where vertices are tetrahedra SiO_4 or $SiAlO_4$, cells are H_2O, edges are oxygen bridges.

3. *Soap froths* (foams, liquid crystals).
4. An affine version of A_{15} gives, a better solution to Kelvin's problem see [7] for details.

See [8] for updated table of all 27 known physical FK space fullerenes, with their invariants and explanations.

The enumeration techniques

In [8], the first computer enumeration of FK space fullerenes was implemented and the results were tabulated. The enumeration method consists of enumerating oriented manifolds formed by a number of cells. The method is to add cells one-by-one in a tree search algorithm. For each new cell added, the set of possibilities is considered itself in a tree search; so we have a double tree search. This standard approach [9] makes relatively small memory usage and can be parallelized very easily [10]; it is the basic technique of combinatorial enumeration. The resulting objects are then checked for isomorphism. After that, it is checked whether the obtained oriented manifolds admit Euclidean universal covering or not. Finally, the universal coverings are checked for isomorphism. The fundamental domain under translation contains $n = 21$ k cells with k belonging to $\{1, 2, 3, 4, 6\}$. This is because the size of the point group of a 3-dimensional *Bieberbach groups,* i.e., fixed point free groups, having only rotations, belongs to $\{1, 2, 3, 4, 6\}$. See [8] for more details on the relation between the enumeration procedure and Bieberbach groups.

The key computational bottleneck is in computing the initial list of manifolds. This can take months of computations in some cases, while the next steps are much faster. Thus there is a general interest in improving the speed of the combinatorial enumeration part of the problem. Unfortunately, all known methods for enumerating such manifolds are quite inefficient. Moreover, there is some ground to believe that general efficient enumeration procedure are not possible ($P = NP$ questions).

Thus our focus was on improving the enumeration procedure. The enumeration procedure works by adding cells one by one in all possible ways. The algorithm keeps track of all the connected components of the boundary. It selects one of the maximal size and finds the possible other connected components to which it can be attached. So, we have a double tree search being done for the enumeration which explains, in a way, the slowness of the enumeration.

Part of the effort went into improving the existing C program. By doing this, we managed a 2.5-fold improvement. Apart from that, speed improvement can come from two sources. One possibility is proving some theoretical results on the possible final structures. Any such result can give a potential pruning method for the tree search. A typical example of such strategy is given in [11]. In [8], many conjectures that had been stated over the years on the structure of FK space fullerenes, had been proved wrong. Thus it seems that FK space fullerenes have few or no obvious algebraic structure that would have helped in their enumeration.

So, we used the second possibility to use the symmetries of the space fullerenes in order to reduce the time of the enumeration. We want to be able to detect if a branch in the tree search has already been covered in the enumeration without having to store the enumeration itself. The technique is to generate all possible reorderings and kill a branch if there is a reordering that makes it lexicographically higher. Using a *breadth first search*, one can index the vertices of the structure uniquely by starting from one vertex and one direction. So, the possible reorderings are actually exactly the directed edges of the structure. So, for every cell of the structure, we store the list of directed edges and, for each of them, check whether they can yield a symmetry reduction or not. At the end of the process, only the directed edges, for which we cannot prove that they give a reduction in the branching, are left. Since the ordering is lexicographic, those directed edges have to be all equivalent and since they define the structure uniquely, they also index the elements of the rotation symmetry group of the structure. So, the symmetry reduction is done in a polynomial time, which is expected, since for cell-complexes, everything is determined by one single flag. In general, symmetry reduction does not always yield speed up because the cost of symmetry might offset the cost of treating the branch anyway. But in our case, the symmetry reduction is cheap and thus one does not face this problem. We find out that, whenever we used this symmetry reduction method, we got a speedup.

One problem of this approach is that after the whole enumeration is finished, many structures have a universal cover which is not the Euclidean plane. They correspond instead to one of seven other *Thurston geometries* [12]. So, quite often we get several hundreds manifolds and no periodic structures. This is a major limitation and we believe that this sort of exhaustive enumeration has reached here its limits. For the enumeration up to 21 cells in the reduced domain we found 834 manifolds up to oriented equivalence, 545 up to equivalence. Of those, 299 are Euclidean and after testing equivalence of tilings, this gave $84 + 37 = 121$ distinct tilings.

One possible replacement could be iterative generation scheme, that is from a given space fullerene rules for

generating new space fullerenes. If this could be done (see [13] for fullerenes), then we would be able to generate easily millions of possible structures.

Up to isometric equivalence, there are [14] exactly ten *flat* (i.e., locally isometric to E^3) compact manifolds: the quotients T^3/F of 3-torus by F, where $\mathcal{F} \subset SL(3,Z)$ is the cyclic group of order 1,2,3,4,6 or $Z_2 \times Z_2$. There is exactly one orientable manifold for each such F and two non-orientable ones with $F = Z_2$ and two with $Z_2 \times Z_2$. Nine of the ten flat spaces can be obtained as torus T^2 or Klein bottle K^2 bundles over the circle S^1. The direct products $T^2 \times S^1 = T^3$ and non-orientable one $K^2 \times S^1$ are among them. The other seven bundles are twisted products. It will be interesting to find out to which of six above oriented flat manifolds relates each of 84 + 37 obtained FK space fullerenes. Moreover, is a space fullerene can come from one of 4 above non-oriented manifolds?

Finally, a new challenge to practical crystallography and chemistry is to check the existence of physical compounds having one of new geometrical structures.

Invariants and statistics for obtained structures

Especially important among 27 known physical FK structures are space fullerenes $A15$, $C15$ and Z. They correspond to clathrate hydrates of type I, II and IV. Their *fraction sequences* (4-vectors $x = (x_{20}, x_{24}, x_{26}, x_{28})$ representing proportion of four FK fullerenes in the fundamental domain) are $\upsilon_{A15} = (1, 3, 0, 0)$, $\upsilon_{C15} = (2, 0, 0, 1)$, and $\upsilon_Z = (3, 2, 2, 0)$. Clearly, any 4-vector x is a linear combination $a_0\upsilon_{120} + a_1\upsilon_{A15} + a_2\upsilon_Z + a_3\upsilon_{C15}$, where $\upsilon_{120} = (1, 0, 0, 0)$. In these terms, long-standing conjecture, *Yarmolyuk–Kripyakevich rule* ([15, 16], for example) means that a_0 should be 0. We obtained in [8] the first (five) counterexamples to this conjecture. One of them (Nr. 58 of Table 3 and Fig. 7 in [8]) is presented as structure odk in [6]. The present computation produced six new counterexamples; see Table 4 and Fig. 8. Note that structures 2, 3 (as well as of structures 5, 6), given in this Table, differ only by their group.

The *major skeleton Maj* ($\mathcal{F}$) of a space fullerene $\mathcal{F}$ is a graph with the vertices being all non-dodecahedral tiles of $\mathcal{F}$ and an edge between vertices if the corresponding cells share a 6-gonal face. Major skeletons are given in the last column of our Tables as partial fractions (x_{24}; x_{26}; x_{28}) of the connected components, together with the number of components of this type if finite. If a Z is put as prefix, then there exists a translation vector υ of the space group, such that all translations give distinct components of the major skeleton. If a Z/pZ is put as prefix, then there is a translation of vector υ of the space group such that the translations by $0, \upsilon, \ldots, (p-1)\upsilon$ are all distinct but the translation under $p\upsilon$ is a symmetry of this component of the major skeleton.

Contrary to the situation with all known physical FK structures and to implicit hypothesis in [2, 3], we found examples of different structures with isomorphic major skeletons, whenever the reduced fundamental domain contains $N = 19$, 20 or 21 cells and the fraction sequence is not among known physical ones. In the Table 3 of [8], structures 3, 4 with fraction (11, 2, 2, 4), differ only by their cell orbits. Structures 19, 21, 24–26 with fraction (10, 4, 4, 2), as well as 41–45 with fraction (10, 5, 2, 3), have the same major skeletons. Structures 25, 26, as well as 44, 45 have all six invariants of the table the same. Similar examples appear in Table 2 of 26 structure of the present study. Structures 19, 21 differ only by the group, while 6, 9 differ only by their major skeleton. Structures 7, 8 (as well as 15, 16) have all six invariants of the table the same.

The *average coordination number* $\bar{f}$ of a space fullerene is the mean number of faces per cell in its fundamental domain. Clearly,

$$12 < \bar{f} = \frac{12x_{20} + 14x_{24} + 15x_{26} + 16x_{28}}{x_{20} + x_{24} + x_{26} + x_{28}} < 16 \qquad (1)$$

for any FK space fullerene. Clearly also, Yarmolyuk–Kripyakevich rule, when it holds, implies $6x_{20} - 2x_{24} - 7x_{26} - 12x_{28} = 0$ and so, $13.(3) \le \bar{f} \le 13.5$ with equalities on left and right side for and only for *Laves structures* (having fraction sequence (2, 0, 0, 1)) and $A15$, respectively.

33 among 37 obtained new structures have the same $\bar{f} = \frac{94}{7} \approx 13.428$, as FK space fullerene Z with fraction sequence (3, 2, 2, 0). Five of them are, moreover, *Z-like,* i.e., have the same fraction; cf. Table 3. But in Table 4, structure 1 has $\bar{f} = 13.(3)$, i.e., it is the first, other than Laves structures, FK space fullerene with this minimal $\bar{f}$. Structures 4–6 of Table 4 with fraction sequence (5, 10, 6, 0) have $\bar{f} = \frac{290}{21} \approx 13{,}810$. So, the problem is to find the maximal and minimal $\bar{f}$ over all FK space fullerenes violating Yarmolyuk–Kripyakevich rule.

It is also interesting to find minimal $\bar{f}$ over all (not only FK) space fullerenes; such structures could be energetically competitive with diamond. As now, the best is the DS space fullerene with $\bar{f} = 13.2$.

Note that for all 27 known physical structures and (84−13) + 37 = 108 new structures found by us, it holds.

$$x_{20} \ge \max\left\{1, \frac{1}{3}x_{24}, \frac{5}{6}x_{26}, 2x_{28}\right\}. \qquad (2)$$

In fact, $x_{20} = \frac{5}{6}x_{26}$ holds only for the structures 4–6 in Table 4.

So, one expect to have relatively many dodecahedra in the fundamental domain of a space fullerene. Several other

Table 2 FK space fullerenes with 21 cells in the reduced fundamental domain, with new fraction sequence respecting Yarmolyuk–Kripyakevich rule

No.	Group	f.d.	f	Fraction	Cell orbits	Major skeleton
1	$Pmc2_1$	42	13.428	(9, 7, 4, 1)	$(18_2^5{}_{,4}{}^2, 14_2^5{}_{,4}, 8_2^4, 2_2)$	2(3, 4, 1), $2Z^2$(2, 0, 0), Z^2(4, 0, 0)
2	$Pmc2_1$	42	13.428	(9, 7, 4, 1)	$(18_2^5{}_{,4}{}^2, 14_2^5{}_{,4}, 8_2^4, 2_2)$	(10, 8, 2), $2Z^2$(2, 0, 0)
3	$P6_4$	63	13.428	(9, 7, 4, 1)	$(27_3^3{}_{,6}{}^3, 21_3^3{}_{,6}{}^2, 12_3^2{}_{,6}, 3_3)$	(15, 6, 3), $3Z$(0, 2, 0), $3Z^2$(2, 0, 0)
4	$Amm2$	42 × 2	13.428	(9, 7, 4, 1)	$(36_4^3{}_{,8}{}^3, 28_{4,8}{}^3, 16_4^4, 4_4)$	(2, 8, 2), $6Z^2$(2, 0, 0)
5	$Cmm2$	42 × 2	13.428	(9, 7, 4, 1)	$(36_{4,8}{}^4, 28_{4,8}{}^3, 16_4^2{}_{,8}, 4_4)$	Z(0, 4, 0), $Z/2Z$(10, 4, 2), $2Z^2$(2, 0, 0)
6	$Cmc2_1$	84 × 2	13.428	(9, 7, 4, 1)	$(72_{16}{}^2{}_{,8}{}^5, 56_{16,8}{}^5, 32_8^4, 8_8)$	2(10, 4, 2), $2Z$(0, 4, 0), $4Z^2$(2, 0, 0)
7	$Cmc2_1$	84 × 2	13.428	(9, 7, 4, 1)	$(72_{16,8}{}^7, 56_{16}{}^2{}_{,8}{}^3, 32_8^4, 8_8)$	(12, 16, 4), $8Z^2$(2, 0, 0)
8	$Cmc2_1$	84 × 2	13.428	(9, 7, 4, 1)	$(72_{16,8}{}^7, 56_{16}{}^2{}_{,8}{}^3, 32_8^4, 8_8)$	(12, 16, 4), $8Z^2$(2, 0, 0)
9	$Cmc2_1$	84 × 2	13.428	(9, 7, 4, 1)	$(72_{16}{}^2{}_{,8}{}^5, 56_{16,8}{}^5, 32_8^4, 8_8)$	$Z/3Z$(20, 16, 4), $4Z^2$(2, 0, 0)
10	$P1_2/m1$	21	13.428	(9, 8, 2, 2)	$(9_1^3{}_{,2,4}, 8_2^4, 2_2, 2_2)$	$Z/3Z$(6, 2, 2), Z^2(2, 0, 0)
11	$Pnnm$	42	13.428	(9, 8, 2, 2)	$(18_{2,4}{}^2{}_{,8}, 16_4^4, 4_4, 4_4)$	$Z/3Z$(12, 4, 4), $2Z^2$(2, 0, 0)
12	$Pmma$	42	13.428	(9, 8, 2, 2)	$(18_2^3{}_{,4,8}, 16_4^4, 4_4, 4_4)$	$Z/3Z$(12, 4, 4), $2Z^2$(2, 0, 0)
13	$Pmmn$	42	13.428	(9, 8, 2, 2)	$(18_2^3{}_{,4}{}^3, 16_4^4, 4_4, 4_4)$	(4, 4, 4), $2Z^2$(2, 0, 0), $2Z^2$(4, 0, 0)
14	$Pmn2_1$	42	13.428	(9, 8, 2, 2)	$(18_2^7{}_{,4}, 16_2^4{}_{,4}{}^2, 4_2^2, 4_2^2)$	(8, 4, 4), $4Z^2$(2, 0, 0)
15	$Pmc2_1$	42	13.428	(9, 8, 2, 2)	$(18_2^5{}_{,4}{}^2, 16_2^6{}_{,4}, 4_2^2, 4_2^2)$	2(4, 2, 2), $2Z^2$(2, 0, 0), Z^2(4, 0, 0)
16	$Pmc2_1$	42	13.428	(9, 8, 2, 2)	$(18_2^5{}_{,4}{}^2, 16_2^6{}_{,4}, 4_2^2, 4_2^2)$	2(4, 2, 2), $2Z^2$(2, 0, 0), Z^2(4, 0, 0)
17	$P3_121$	63	13.428	(9, 8, 2, 2)	$(27_{3,6}{}^4, 24_6^4, 6_6, 6_6)$	(12, 6, 6), $6Z^2$(2,0,0)
18	$Cmmm$	42 × 2	13.428	(9, 8, 2, 2)	$(36_{16,4,8}{}^2, 32_{16,8}{}^2, 8_8, 8_8)$	(4, 4, 4), $6Z^2$(2,0,0)
19	$C2/m$	42 × 2	13.428	(9, 8, 2, 2)	$(36_{16,4,8}{}^2, 32_8^4, 8_8, 8_8)$	$Z/3Z$(12, 4, 4), $2Z^2$(2, 0, 0)
20	$C2/m$	42 × 2	13.428	(9, 8, 2, 2)	$(36_{4,8}{}^4, 32_{16,8}{}^2, 8_8, 8_8)$	(8, 4, 4), $4Z^2$(2, 0, 0)
21	$Imm2$	42 × 2	13.428	(9, 8, 2, 2)	$(36_{16,4,8}{}^2, 32_8^4, 8_8, 8_8)$	$Z/3Z$(12, 4, 4), $2Z^2$(2, 0, 0)
22	$P6_122$	126	13.428	(9, 8, 2, 2)	$(54_{12}{}^3{}_{,6}{}^3, 48_{12}{}^4, 12_{12}, 12_{12})$	(24, 12, 12), $12Z^2$(2, 0, 0)
23	$Cmca$	84 × 2	13.428	(9, 8, 2, 2)	$(72_{16}{}^2{}_{,32,8}, 64_{16}{}^4, 16_{16}, 16_{16})$	$Z/3Z$(24, 8, 8), $4Z^2$(2, 0, 0)
24	$Cmca$	84 × 2	13.428	(9, 8, 2, 2)	$(72_{16}{}^4{}_{,8}, 64_{16}{}^2{}_{,32}, 16_{16}, 16_{16})$	(16, 8, 8), $8Z^2$(2, 0, 0)
25	$Cmc2_1$	84 × 2	13.428	(9, 8, 2, 2)	$(72_{16,8}{}^7, 64_{16}{}^2{}_{,8}{}^4, 16_8^2, 16_8^2)$	(16, 8, 8), $8Z^2$(2, 0, 0)
26	$Cmc2_1$	84 × 2	13.428	(9, 8, 2, 2)	$(72_{16}{}^2{}_{,8}{}^5, 64_{16,8}{}^6, 16_8^2, 16_8^2)$	(24, 8, 8), $4Z^2$(2, 0, 0)

For each such FK space fullerene we give the space group, the number of cells in a fundamental domain, the average coordination number, the fraction sequence, the partition of cells into orbits and a description of the major skeleton

Table 3 FK space fullerenes with 21 cells in the reduced fundamental domain, with physical fraction sequence (of Z)

No.	Group	f.d.	f	Fraction	Cell orbits	Major skeleton
1	$Pmmn$	42	13.428	(3, 2, 2, 0)	$(18_{2,4}{}^2{}_{,8}, 12_2^2{}_{,4}{}^2, 12_2^4{}_{,4}, 0)$	Z(0, 4, 0), $2Z$(2, 4, 0), $2Z^2$(4, 0, 0)
2	$P2_12_12$	42	13.428	(3, 2, 2, 0)	$(18_{2,4}{}^4, 12_2^2{}_{,4}{}^2, 12_2^4{}_{,4}{}^2, 0)$	Z(0, 4, 0), $2Z/2Z$(6, 4, 0)
3	$C2/m$	42 × 2	13.428	(3, 2, 2, 0)	$(36_{16,4,8}{}^2, 24_8^3, 24_8^3, 0)$	$2Z$(2, 4, 0), Z(8, 4, 0)
4	$Cmca$	84 × 2	13.428	(3, 2, 2, 0)	$(72_{16}{}^2{}_{,32,8}, 48_{16}{}^3, 48_{16}{}^3, 0)$	$2Z$(12, 12, 0)
5	$Cmcm$	84 × 2	13.428	(3, 2, 2, 0)	$(72_{16,32,8}{}^3, 48_{16,8}{}^4, 48_{16}{}^2{}_{,8}{}^2, 0)$	$4Z$(0, 4, 0), $2Z$(8, 4, 0), $2Z^2$(4, 0, 0)

For each such FK space fullerene we give the space group, the number of cells in a fundamental domain, the average coordination number, the fraction sequence, the partition of cells into orbits and a description of the major skeleton

conjectures seems likely: one that any fullerene is realized as a cell in a space fullerene. Another one is existence of a sequence of F_{24}'s giving a cycle in the major skeleton of some space fullerene; this is excluded in [2, 3] but we see no reason for their non-existence.

Any space fullerene contains at least two types of cells, because otherwise existed a regular E^3-tiling by some fullerene with tetrahedral vertex-stars. But such S^3-tiling by dodecahedra exists: it is the regular 4-polytope 120-cell. We expect that dodecahedra are always among tiles of any space fullerene. Maybe techniques from Diagram Geometry (as in [17]) could help to prove it. Non-simple normal face-to-face E^3-tilings by dodecahedra exist; cf. [18].

Enumeration and partial, say, classification of space fullerenes having only two type of cells, one of them Dodecahedron, requires new techniques. For example, are such structures with cells F_{26} are possible? Is $A15$ unique such structure with fraction (1, 3, 0, 0)?

Table 4 FK space fullerenes with 21 cells in the reduced fundamental domain, with fraction sequence breaking Yarmolyuk–Kripyakevich rule

No.	Group	f.d.	f	Fraction	Cell orbits	Major skeleton
1	$P6_3/mcm$	42	13.333	(10, 8, 0, 3)	($20_{12,2,6}$, $16_{2,4}$, 0, 6_6)	$Z/3Z(12, 0, 6)$, $2Z^2(2, 0, 0)$
2	$P4_12_12$	84	13.428	(11, 4, 2, 4)	($44_{4,8}{}^5$, $16_8{}^2$, 8_8, $16_8{}^2$)	$4Z(4, 2, 4)$
3	$P4_32_12$	84	13.428	(11, 4, 2, 4)	($44_{4,8}{}^5$, $16_8{}^2$, 8_8, $16_8{}^2$)	$4Z(4, 2, 4)$
4	$P4_2/m$	42	13.810	(5, 10, 6, 0)	($10_{2,8}$, $20_4{}^3{}_8$, $12_{4,8}$, 0)	$4Z(1, 2, 0)$, $2Z^2(2, 0, 0)$, $2Z^2(6, 2, 0)$
5	$P4_3$	84	13.810	(5, 10, 6, 0)	($20_4{}^5$, $40_4{}^{10}$, $24_4{}^6$, 0)	$8Z(1, 2, 0)$, $4Z^2(2, 0, 0)$, $4Z^2(6, 2, 0)$
6	$P4_1$	84	13.810	(5, 10, 6, 0)	($20_4{}^5$, $40_4{}^{10}$, $24_4{}^6$, 0)	$8Z(1, 2, 0)$, $4Z^2(2, 0, 0)$, $4Z^2(6, 2, 0)$

For each such FK space fullerene we give the space group, the number of cells in a fundamental domain, the average coordination number, the fraction sequence, the partition of cells into orbits and a description of the major skeleton

Zigzag structure of space fullerenes

If we have a cell-complex C of dimension 3, then a *flag* is a list $f = (F_0, F_1, F_2, F_3)$ with F_0 being a vertex, F_1 an edge, F_2 a face, F_3 a cell and $F_0 \subset F_1 \subset F_2 \subset F_3$.

Table 5 Zigzag vectors of physical space fullerenes from Table 1 of [8]

No.	Phase	Zigzag vector
1	C_{14}	11^{12}, 30^{14}, 132^2
2	C_{15}	8^6, 30^{12}
3	C_{36}	30^{24}, 63^4, 84^2, 246^2
4	6-layers	30^{36}, 96^2, 117^4, 354^2
5	8-layers	30^{48}, 126^4, 160^6, 180^2
6	9-layers	30^{18}, 132^2, 210^2
7	10-layers	30^{60}, 52^6, 198^2, 393^4
8	Mg_4Zn_7	19^4,30^{18}, 109^2, 161^2, 1294^2
9	X	19^{12},30^{24}, 33^8, 457^4, 500^4
10	T	27^8,35^{12},73^{12}, 74^{12}, 186^8, 204^8
11	C	11^{16},30^{12}, 93^2,182^2,309^2
12	K_7Cs_6	30^{24},216^2,312^2
13	$p\sigma$	11^{12},14^4,30^{12}, 307^4
14	μ	11^6,19^6,30^{12}, 174^2
15	M	11^8,30^{16}, 120^8,253^8
16	R	11^{24},105^2,271^6,762^2
17	K	11^{19}, 14, 16, 27, 33^2,35, 46, 62, 87, 195, 275, 281, 293^2, 353, 677, 839
18	Z	8^{12},11^{12},30^6,36^2
19	P	11^8,30^8,36^8,403^8
20	δ	11^{20}, 16^8, 19^8, 27^8, 33^4, 52^4, 262^2, 292^4, 546^2
21	ν	27^4, 30^8, 36^{18}, 49^4, 70^8, 74^{12}, 92^4, 172^4, 184^2, 188^2, 322^2, 325^4
22	J_{comp}	8^{12}, 19^4, 30^4, 36^8, 112^2, 177^4
23	F_{comp}	19^{24},36^{14}, 90^6, 100^6, 180^2, 198^2, 360^2
24	K_{comp}	19^{12}, 27^4, 36^{22}, 82^4, 117^4, 122^2, 134^2, 164^2, 202^2, 344^2, 350^2, 542^2
25	H_{comp}	8^8, 11^4, 30^2, 36^6, 324^2
26	σ	11^8, 19^8, 36^8, 82^8, 220^4
27	A_{15}	8^{12}, 30^8, 36^6

A *flag operator* σ_i is an operation that sends a flag f to the unique flag $\sigma_i(f)$ that differs from f in position i. The *moving operator* m is the composition operator defined by.

$$m(f) = \sigma_0(\sigma_1(\sigma_2(\sigma_3(f))))). \quad (3)$$

A *zigzag* is a finite or infinite sequence $(f_i)_{i\in I}$ of flags, such that $f_{i+1} = m(f_i)$; if the zigzag is finite of length N, then $I = \{1, \ldots, N\}$ and $i + 1$ is interpreted modulo N. So, if I is infinite, then necessarily $I = Z$. The notion of zigzag was introduced in a chemical setting in [19] and the above formalism is exposed in [20].

In the case of space fullerenes, we have an adequate cell complex on which to build zigzags. Let us denote by $L = Z\upsilon_1 + Z\upsilon_2 + Z\upsilon_3$ the crystallographic translation group. Up to L, there is only a finite number of flags; so, if we start from a given flag f_0 and apply the operator m, then we get a sequence of flags f_1, …, f_{l-1} with $l > 0$ and then $f_l = f_0 + \upsilon$ with υ being some translation vector in L. It may happen that $\upsilon = 0$, in which case the zigzag is finite. We do not know a single case of this phenomenon but we have no reason to believe that it does not occur. Hence, to the set of zigzags z_1, …, z_M we associate the number l, which is a kind of length under periodicity and vector υ. We write a *zigzag vector* $l_1^{m_1}, l_2^{m_2}, \ldots, l_r^{m_r}$, which indicates that there are m_i zigzags of length l_i. We list the zigzag vectors in Tables 5, 6,7, 8, 9 and 10.

Table 6 Zigzag vectors of space fullerenes from Table 2 of [8]

No.	Zigzag vector
1	8^8, 11^8, 30^{10}, 36^2, 182^2
2	11^{20}, 30^4, 36^4, 104^4, 219^4
3	8^{10}, 11^{16}, 30^8, 33^4, 166^2
4	8^{16}, 11^{16}, 14^2, 16^4, 22^4, 30^8, 96^4, 406^2
5	11^8, 16^4, 30^8, 36^4, 292^2, 400^2
6	8^8, 11^4, 19^8, 22^4, 27^8, 30^4, 33^4, 36^4
7	8^{12}, 11^{10}, 19^6, 27^6, 33^2, 63^2, 66^2, 248^2, 309^2
8	8^2, 11^4, 19^4, 22^4, 27^4, 30^{12}, 33^4, 36^4, 57^4, 70^4, 222^2
9	11^8, 27^4, 30^4, 33^4, 36^4, 236^2, 428^2
10	8^{16}, 11^4, 14^2, 19^8, 27^8, 33^4, 46^2, 49^4, 686^2, 740^2
11	8^{12}, 30^4, 36^8, 79^8, 188^2

Table 7 Zigzag vectors of space fullerenes from Table 3 of [8]

No.	Zigzag vector
1	16^8, 19^8,30^{12}, 46^8, 60^4,336^4
2	19^6, 30^{18}, 33^6, 222^2
3	30^{36}, 96^2, 102^2, 150^2,408^2
4	30^{36}, 132^2, 624^2
5	8^{12}, 30^{10}, 36^2, 92^4,115^4
6	11^8,30^4, 36^2, 118^2,156^2, 234^2
7	16^8, 30^8, 36^4, 52^4, 60^4, 408^4
8	11^{16}, 30^{10}, 36^4, 106^2, 328^2, 552^2
9	27^6, 30^{18}, 57^6, 126^2
10	19^{12}, 30^6, 33^3, 52^3, 71^3, 237, 279, 633, 696,1167
11	19^8,2 4^4, 30^8, 36^4, 90^2, 267^4, 356^2
12	11^{12}, 19^4, 30^{18}, 33^4, 192^2, 332^4
13	8^{20},30^{16}, 36^4, 52^2,87^8, 150^4
14	8^{12}, 30^{12}, 33^8, 36^4,252^2
15	11^{14}, 30^6, 36^2, 38^4, 93^2, 312^2
16	30^{36}, 102^2, 117^4, 492^2
17	8^{12}, 30^8, 36^4, 444^2
18	8^4, 11^8, 30^{10}, 47^4, 114^4, 152^2
19	11^8, 30^{12}, 36^4, 41^4, 74^2, 100^4,140^2,144^8
20	8^8, 22^4, 30^{24}, 33^4, 84^4, 126^4, 223^4
21	11^8, 30^{16}, 36^4, 52^4, 90^4, 364^4
22	11^8, 19^2, 27^4, 30^8, 33^8, 36^2, 41^2, 46^2, 62^4, 68^2
23	11^8, 14^4, 30^{12}, 41^8, 476^4
24	11^{16}, 24^4, 30^8, 36^4, 90^2, 93^4, 134^2, 137^4, 178^4
25	11^8, 22^8, 30^8, 36^4, 38^4, 484^4
26	11^{16}, 30^{10}, 36^4, 71^4, 916^2
27	30^{24}, 324^2
28	8^{12}, 11^{12}, 30^{24}, 78, 84^7, 114^2, 122^6, 162^4, 168, 238^3
29	11^{12}, 14^6, 57^3, 84^3, 99, 108, 141, 276, 378, 403^3, 618, 636
30	8^4, 11^4, 14^4, 19^4, 27^4, 30^8, 84^4, 238^2
31	16^8, 19^8, 30^4, 36^8, 60^4,137^4,315^4
32	11^{20},30^4, 36^8, 402^2, 652^2
33	11^4, 14^2, 24^4, 27^8, 30^8, 33^4, 36^4, 46^4, 90^2, 111^4, 257^4
34	8^6, 11^4, 30^4, 36^2, 130^2, 204^2, 208^2
35	8^{12}, 30^{12}, 36^4, 194^4, 226^2,454^2
36	11^4, 16^4, 19^4, 30^{10}, 36^8, 103^4, 168^4, 440^2
37	16^8, 27^8, 30^8, 36^4, 60^4, 200^2, 684^2
38	8^2,11^4, 22^4, 30^{20}, 33^4, 256^4, 416^2
39	8, 11^6, 13^2, 19^4, 27^4, 30^{13}, 33^2, 38^4, 47^2, 80^2, 106^2, 174^2,228, 230, 286^2
40	8^{12}, 19^8, 30^8, 33^4, 36^4, 68^4, 166^2
41	11^4,14^2, 19^4, 30^8, 33^4, 36^4, 38^4, 41^4, 49^4, 65^4, 115^4, 420^2
42	8^2, 11^8, 19^4,30^{16}, 36^4, 52^2, 95^4, 362^4
43	11^8, 19^4, 30^8, 33^4, 36^4, 41^4, 68^4, 73^4, 126^4, 206^4
44	8^6, 11^4, 19^4, 27^4,30^{12}, 36^4, 68^4, 842^2
45	8^2, 11^4, 30^8, 33^4, 36^4, 38^4, 52^4, 68^4, 764^2
46	8^{20}, 30^{12}, 36^8, 52^2, 177^8
47	8^{10}, 11^8, 30^8, 46^4, 64^2, 108^4, 588^2

Table 7 continued

No.	Zigzag vector
48	8^{20}, 30^{12}, 36^8, 117^8, 292^2
49	8^{10},11^{12}, 14^2, 22^4, 63^4, 64, 68^2, 188^2, 200,318^2, 336
50	8^8, 11^{12}, 30^4, 36^2, 80^2, 206^2
51	8^8, 30^8, 36^4, 358^2, 378^2
52	11^8, 16^4, 30^4, 36^8, 100^2, 115^4, 350^2
53	8^{20}, 30^8, 36^{12}, 68^2, 188^2, 564^2
54	8^{20}, 30^8, 36^{12}, 52^2, 324^2, 444^2
55	5^{16}, 30^{48}, 52^2, 326^4, 600^2
56	8^{20}, 30^4, 36^{16}, 46^8, 696^2
57	5^8, 30^{24}, 52^4, 96^8, 118^4
58	5^8, 30^{16}, 33^8, 58^8
59	5^8, 11^8, 19^8, 30^{16}, 33^8, 58^4, 72^4, 238^4
60	5^{24}, 30^{42}, 84^6, 96, 98^3, 102, 131^6, 194^3

Table 8 Zigzag vectors of space fullerenes from Table 2

No.	Zigzag vector
1	11^4, 16^4, 19^4, 30^8, 33^4, 36^8, 38^4, 46^4, 302^2, 548^2
2	16^4, 22^4, 30^8, 36^4, 586^4
3	8^{12}, 11^{12}, 30^{18}, 36^6, 52^6, 84, 90^6, 120^2, 334^3, 386^3
4	8^{24}, 30^{12}, 33^8, 36^{12}, 38^4, 54^4, 60^4, 66^4, 190′
5	16^4, 19^8, 22^4, 30^{12}, 36^4, 104^2, 180^2,376^4
6	11^8, 30^{16}, 33^8, 36^8, 41^8, 54^4, 68^4, 956^4
7	11^{16}, 30^8, 33^8, 36^{16}, 38^8, 41^8, 111^8, 126^4, 162^4,178^4, 280^4
8	8^4,11^{24}, 30^{16}, 36^{16}, 38^4, 44^4, 54^{12}, 123^8, 132^8, 348^4
9	11^{16}, 30^{16}, 36^8, 44^4, 120^4,136^4,180^4, 362^8
10	8^6, 22^4, 30^8, 33^4, 36^2, 150^2, 280^2
11	8^{12}, 30^{24}, 33^8, 36^4, 52^4, 362^4
12	8^{12}, 30^{16}, 33^8, 36^4, 71^4, 78^2, 84^2,161^8
13	16^8, 19^8, 30^8, 36^{12}, 71^4, 411^4
14	8^2,11^4, 30^4, 36^8, 38^4, 60^4, 76^4, 251^4, 356^2
15	11^4, 16^4, 30^{10}, 36^8, 224^4, 644^2
16	11^4,16^4, 30^8, 33^4, 36^8, 98^4, 430^4
17	8^{12},11^{12}, 30^{12}, 36^{12}, 90^{12}, 387, 537, 573, 723
18	8^{24}, 30^{16}, 36^{12}, 60^8, 324^4
19	16^8, 22^8,30^8, 36^4, 548^4
20	16^4, 19^4, 22^4, 30^8, 36^8, 158^4,180^4, 193^4
21	8^{12}, 27^{12}, 30^{16}, 33^{20}, 36^4, 38^4, 52^4, 204^4
22	8^{24}, 11^{24}, 30^{24}, 36^{24}, 84, 87^2, 90^{24}, 96^2, 108^2, 126, 197^6, 498^2, 732, 738
23	16^{16}, 22^{16}, 24^4, 30^{32}, 36^8, 226^8, 500^4
24	16^8, 22^8, 30^{16}, 36^{16}, 73^8, 106^8, 180^8, 191^8
25	11^{16}, 30^8, 36^{16}, 38^8, 41^8, 44^4, 136^4, 427^8
26	14^4, 27^8, 30^{16}, 36^8, 38^4, 54^8, 90^8, 116^4, 738^4

This new invariant, zigzag vector, looks to be very sensitive: all space fullerenes, known from now, have it different. The simplest zigzag vectors, (8^6, 30^{12}), (30^{24},

Table 9 Zigzag vectors of space fullerenes from Table 3

No.	Zigzag vector
1	16^8, 30^{12}, 36^8, 81^8, 136^4, 228^4
2	8^4, 11^2, 19^{10}, 27^2, 33^2, 52^2, 66^2, 137^2, 220^2, 317^2, 466^2
3	16^{12}, 22^{12}, 30^{12}, 65^8, 83^4, 144^4, 159^4
4	16^{24}, 22^{32}, 30^{24}, 80^8, 180^8, 234^8
5	16^8, 30^{24}, 36^8, 60^8, 124^8, 182^8, 212^8

Table 10 Zigzag vectors of space fullerenes from Table 4

No.	Zigzag vector
1	30^{24}, 36^4, 41^{12}, 192^2, 558^2
2	5^{16}, 30^{72}, 74^2, 77^4, 112^4, 502^2, 806^2
3	5^{16}, 30^{72}, 134^4, 3 06^4, 44 0^4
4	5^{12}, 8^8, 15^8, 23^4, 36^4, 70^4, 81^4, 103^4, 121^4, 249^4
5	5^{24}, 8^{16}, 15^{16}, 23^8, 36^8, 58^2, 68, 70^8, 81^8, 152, 324, 434^2, 444^4, 480
6	5^{24}, 8^{16}, 15^{16}, 23^8, 36^8, 70^8, 81^8, 196^2, 375^4, 440, 446^2, 560

324^2) and (11^{12}, 30^{18}), (30^{20}, 160^6) have *C*15, structure 27 from Table 7 and non-FK space fullerenes DS and odf. The most complicated zigzag vector, 136 zigzags of 14 different sizes, have structure 22 from Table 10.

Crystallographic realizability and perfect matching considerations

A *perfect matching* (or *Kekulé structure,* in chemical terms) in a graph *G* is a set of edges *E* such that every vertex belong to exactly one edge of *E*. Perfect matchings are a classical tool used to evaluate the chemical realizability of a fullerene graph *G* [21]. They might be of interest for space fullerenes also but we have to qualify how they could be used. First of all, the *skeleton Skel* ($\mathcal{F}$) of a space fullerene $\mathcal{F}$ is the graph with vertices being the cells of $\mathcal{F}$ with two cells being adjacent if they share a face; cf. major skeleton above. If $\mathcal{F}$ is periodic over three non-coplanar directions υ_1, υ_2 and υ_3 defining a lattice *L*, then we can consider the number of perfect matchings of the quotient *Skel*(*F*)/*L*. Let us assume for simplicity, that *Skel* ($\mathcal{F}$)/*L* has an even number of vertices. Then it is likely that for any sublattice L' of L of index d the number $n_{\mathrm{per}\ f}(\mathcal{F}, L')$ of perfect matchings of *Skel* ($\mathcal{F}$)/L' is asymptotic to.

$$\alpha^d \tag{4}$$

for some constant α. Since the number of perfect matchings of a graph with υ vertices of degree at most k is bounded by k^{υ}, we have the inequality $\alpha \leq k_0$, where k_0 is the maximal number of faces over all cells. The skeleton of the dual tessellation, or, in other words, *dual skeleton* is a 4-regular graph and one may expect the same asymptotic behavior

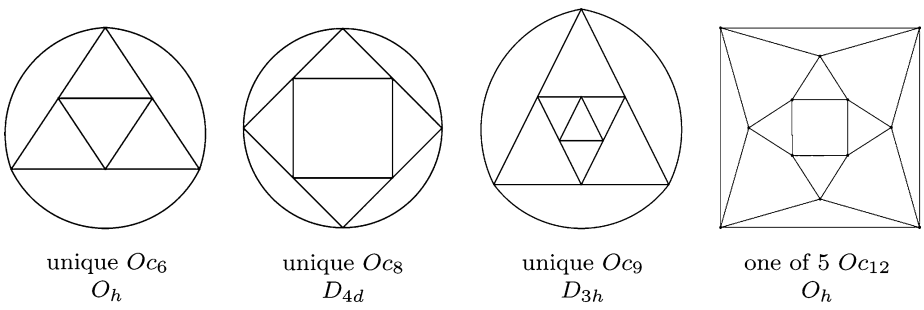

Fig. 3 The four octahedrites with isolated 4-gons

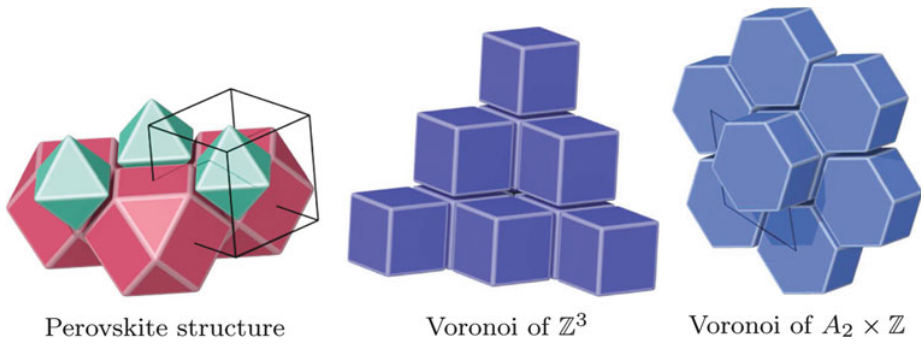

Fig. 4 Three of 28 uniform E^3-tilings: perovskite structure and two space cubites

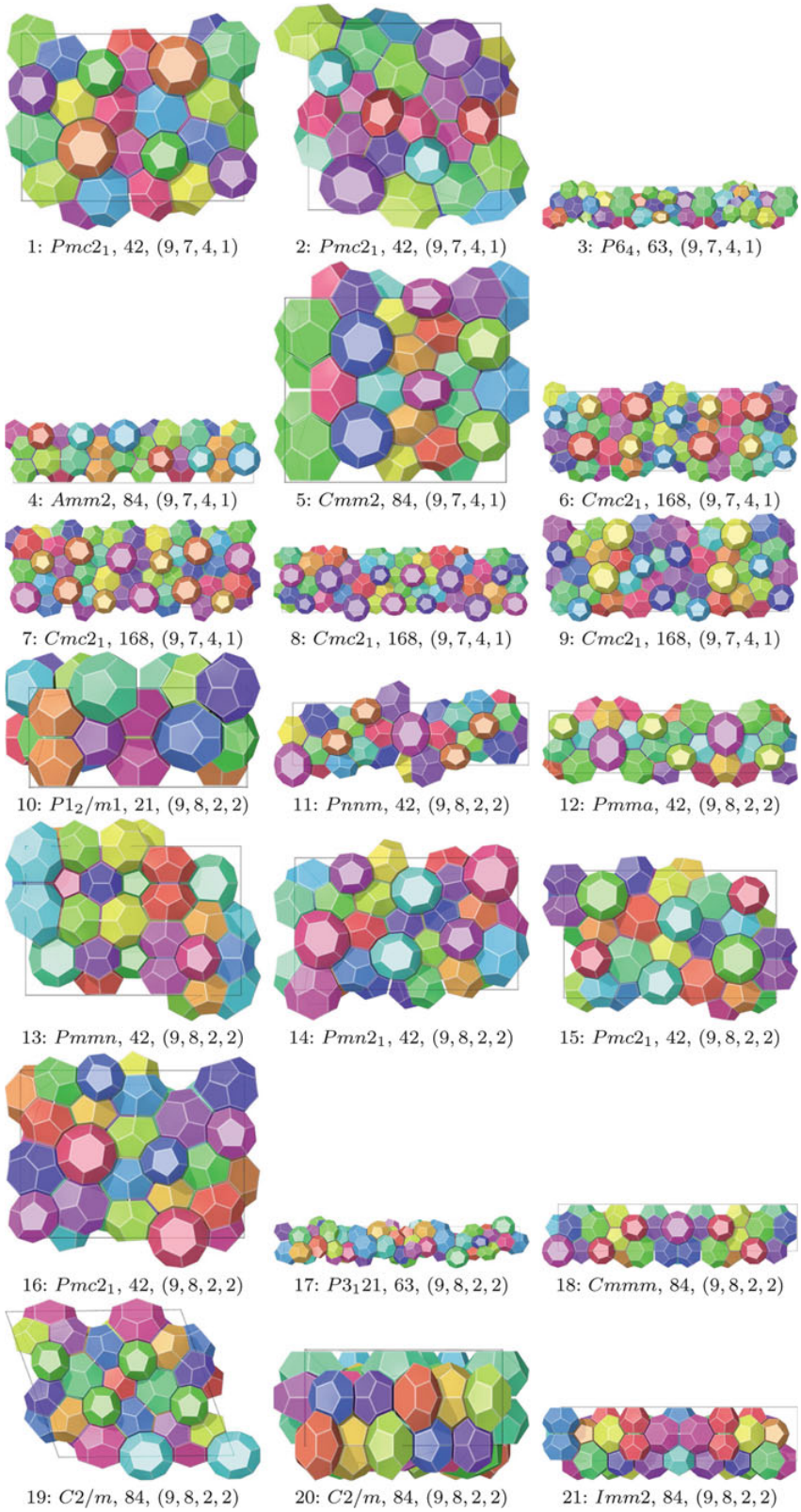

Fig. 5 FK space fullerenes with 21 cells in the reduced fundamental domain, with new fraction sequence respecting Yarmolyuk–Kripyakevich rule (*first part*)

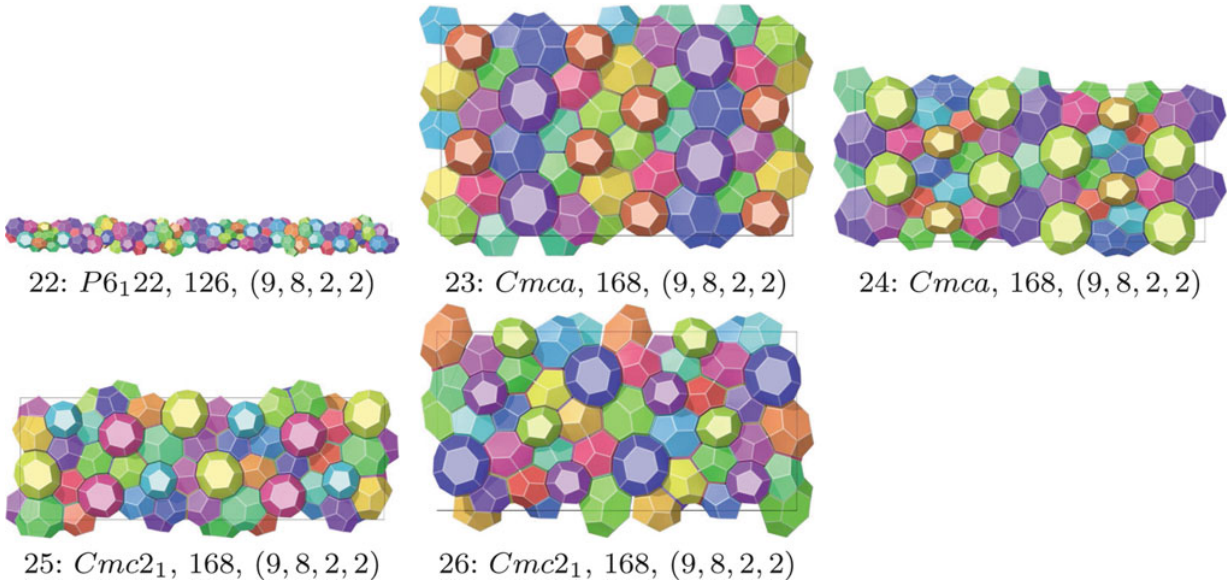

Fig. 6 Space fullerenes with 21 cells in the reduced fundamental domain, with new fraction respecting Yarmolyuk–Kripyakevich rule (*second part*)

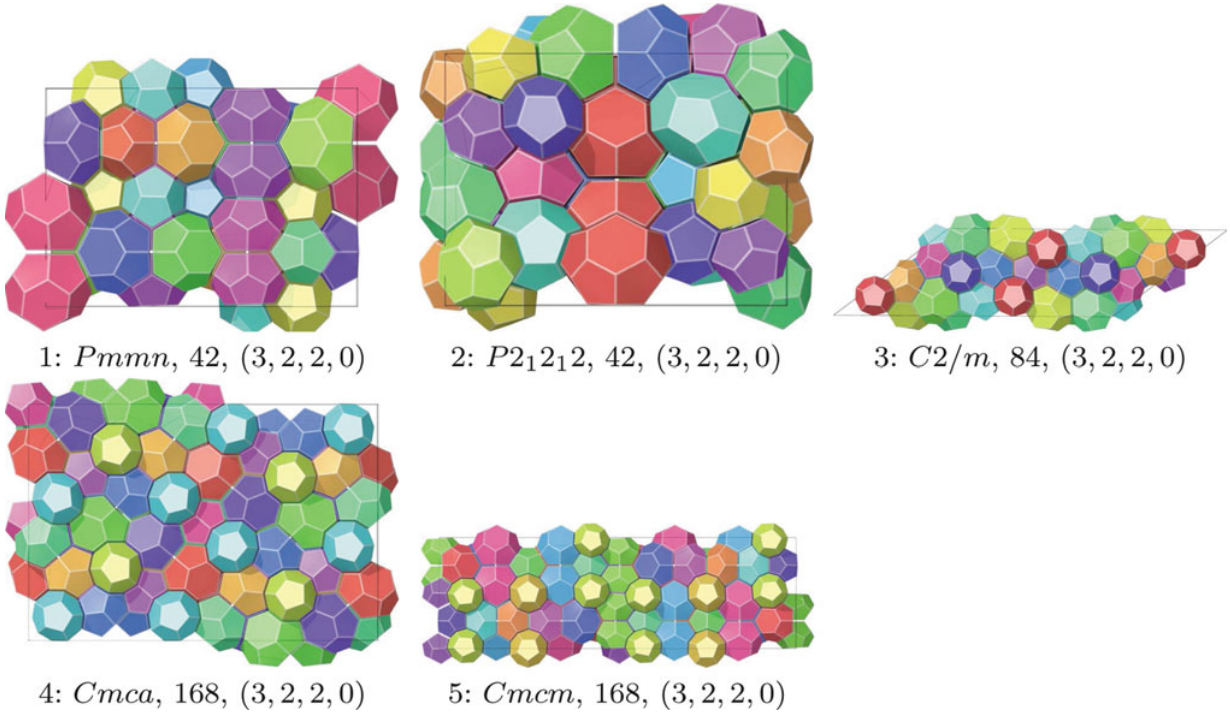

Fig. 7 FK space fullerenes with 21 cells in the reduced fundamental domain, with physical fraction sequence (of Z)

with a constant $\alpha \leq 4$. Another possible construction is the *medial graph construction Med* $(\mathcal{F})$ where vertices of *Med* $(\mathcal{F})$ are edges of F with two edges being adjacent if they have a common vertex and are contained in a common face. A perfect matching in *Med* $(\mathcal{F})$ corresponds to an assignment of hydrogen bonds in a clathrate structure; so, the enumeration of perfect matchings of *Med* $(\mathcal{F})/L$ gives the number of L-periodic assignments of hydrogen bonds.

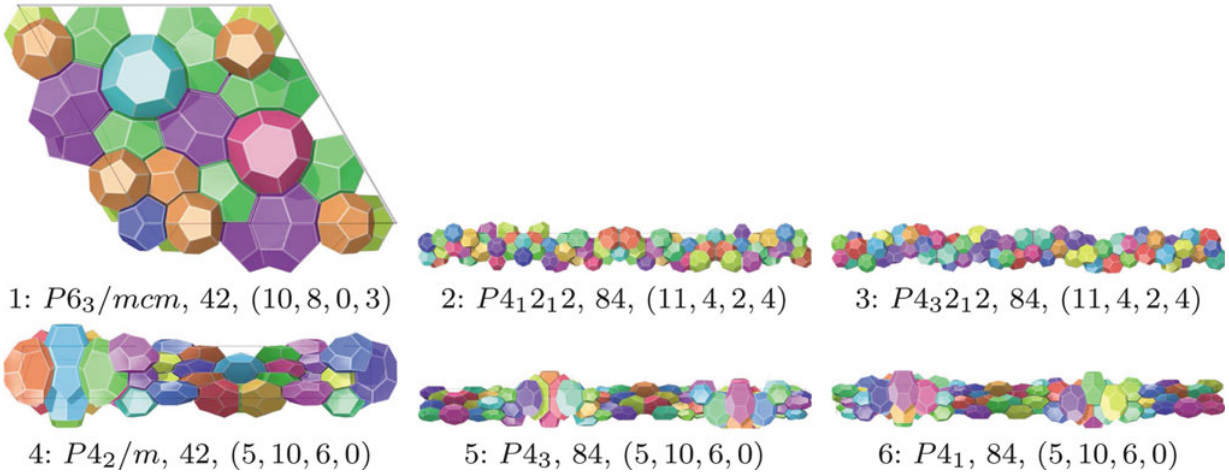

Fig. 8 FK space fullerenes with 21 cells in the reduced fundamental domain, with fraction sequence breaking Yarmolyuk–Kripyakevich rule

Again, we can expect the same asymptotic behavior with $\alpha \leq 6$ since *Med* $(\mathcal{F})$ is 6-regular.

We designed a very fast program for enumerating perfect matchings under symmetry. As a consequence, we can derive in 0.01 s the 158 orbits of perfect matchings of Buckminsterfullerene $F_{60}(I_h)$ [22]. Unfortunately, we found out that the program cannot be applied to the space fullerene case, because the number of perfect matchings is extremely high even for simple structures. A more realistic study would have been to study numerically the crystallographic realizability of the structures, but again there are so many possibilities for choosing atoms for each cells, that an exhaustive search is infeasible.

Space octahedrites and cubites

Similarly to fullerenes, an *octahedrite* O_{C_n} is a polyhedron with n, all of degree 4, vertices and only 3-gonal and 4-gonal faces. So, $p_3 = 8$ and $p_4 = n - 6$ for the number of faces. O_{C_n} exist for all $n \geq 6$, except 7. The *FK octahedrites* are all (four) octahedrites with isolated 4-gons: Octahedron ($APrism_3$), $APrism_4$, doubled $APrism_3$ and cuboctahedron (Fig. 3).

A *space octahedrite* is a normal face-to-face 6-regular (moreover, with octahedral vertex-stars) partition of E^3 by octahedrites. A *FK space octahedrite* is a such 3-periodic partition by FK octahedrites only. The only known 3-periodic space octahedrite is the FK one, which is such tiling by octahedron and cuboctahedron only, in proportion 1:1, representing physical crystal *perovskite structure* (see Fig. 4). It is an analog of prominent physical FK space fullerenes, Laves structures, which are similar E^3-tilings by smallest and largest FK fullerene only. It is one of 28 *uniform* (vertex-transitive and with Archimedean tiles) E^3-tilings and the Delaunay tiling of *J-complex* (mineral perovskite structure).

The *fraction sequence* (x_6, x_8, x_9, x_{12}) of a given FK space octahedrite is the 4-vector representing the proportion (x_6:x_8:x_9:x_{12}) of 6-, 8-, 9- and 12-vertex FK octahedrites in its fundamental domain. The *average coordination number* of such space octahedrite is the number (Figs. 5, 6, 7, 8).

$$\bar{f} = \frac{8x_6 + (8x_8 + 2x_8) + (8x_9 + 3x_9) + (8x_{12} + 6x_{12})}{x_6 + x_8 + x_9 + x_{12}}. \tag{5}$$

Clearly, $8 < \bar{f} < 14$ since extremal fraction sequences (1, 0, 0, 0) and (0, 0, 0, 1) are impossible. The perovskite structure has the fraction sequence (1, 0, 0, 1) and so, its $\bar{f}$ **is** $11 = \frac{8+14}{2}$.

The *major skeleton* of a space octahedrite is the graph having as vertices all non-octahedral tiles, two of them being connected by an edge if they are adjacent on a 4-gonal face. The major skeleton of the perovskite is the graph Z^3.

The general chemical formula for perovskite compounds is ABX_3 where A and B are two cations (the A-atoms are larger), and X is an anion that bonds to both. The most abundant solid phase in the Earth, is such distorted structure of *magnesium silicate* $MgSiO_3$.

Analogic *space cubites* are normal face-to-face, with bipyramidal stars, tilings of E^3 by *cubites,* i.e. 3-regular polyhedra with only 4- and 6-gonal faces. *FK space cubites* are such 3-periodic tilings by Cube ($Prism_4$) and $Prism_6$ only (any other cubite has adjacent 6-gons). Examples are such 6- and 5-regular tilings by Cube and by $Prism_6$: Voronoi tilings of lattices Z^3 and $A_2 \times Z$ with stars $Prism_4^*$

(octahedron) and *Prism* $^{*}_{3}$, respectively. They are uniform E^3-tilings.

Examples of non-Euclidean analogs of space fullerenes, octahedrites and cubites are tilings of 3-sphere S^3 by Dodecahedron (120-cell), by Octahedron (24-cell) and of hyperbolic 3-space H^3 by F_{24} *(Löbell space)*.

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