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The Fedorov algorithm revised

Yury L. Voytekhovsky†

Laboratory for Mathematical Investigations in Crystallography, Mineralogy and Petrography, Kola Branch of Petrozavodsk State University, Russia, and Laboratory for Platinum Group Elements Ore Genesis, Geological Institute of the Kola Science Centre, Russian Academy of Sciences, Russia. Correspondence e-mail: voyt@geoksc.apatity.ru

All the simple 12- to 20-hedra with no triangular and quadrilateral facets (118 in common) are calculated in the Schlegel projections. Among them, all the fullerenes with 20 to 36 vertices (35 in common) are found. Thus, the γ operation is eliminated from the Fedorov algorithm up to a 21-hedra generating procedure.

1. Introduction

The Fedorov (1893) recurrence algorithm appears to be the most suitable tool to generate a full polyhedral variety. Nowadays, the exact numbers of 4- to 12-hedra and simple (only three edges meet at each vertex) 13-hedra are declared (Engel, 1994). The main defect of the algorithm is a large amount of duplicated shapes which are to be eliminated. Fedorov himself noted that some simplifications of the algorithm were urgently required.

The well known Euler theorem states that there are no polyhedra without triangular, quadrilateral and pentagonal facets simultaneously. The Fedorov idea was to find the operations to generate all kinds of polyhedra. They are as follows: α, β and γ are to obtain simple $(n+1)$-hedra from simple n-hedra ($n \geq 4$), while the reduction operation (we denote it ω) is to find non-simple $(n+1)$-hedra from the previously generated simple $(n+1)$-hedra. More precisely, α cuts any vertex with a new triangular facet resulting, β cuts any edge with a new quadrilateral facet resulting and γ generates a new pentagonal facet. Fedorov (1893, p. 251) explains the latter as follows. Let k_1, k_2 and k_3 be adjacent edges of a simple polyhedron, k_1' and k_1'' be adjacent to k_1, and k_2' and k_2'' adjacent to k_2. Then, γ cuts k_1', k_1'', k_2', k_2'' and k_3. Finally, ω reduces any edge (*i.e.* joins two adjacent vertices) if no triangular facets meet at it.

All the above operations are obligatory in the algorithm. However, to optimize it, α is to generate any polyhedron with, at least, one triangular facet, β with no triangular and, at least, one quadrilateral facet, γ with no triangular and quadrilateral and, at least, one pentagonal facet. In the latter case, a polyhedron should have not less than 12 pentagonal facets (see below). That is why γ was used by Fedorov to generate a dodecahedron only. It was not needed to obtain simple 13-hedra (Voytekhovsky *et al.*, 2000). Hence, our idea is to independently generate a series of simple polyhedra without triangular and quadrilateral facets to postpone the first application of γ as far as possible.

2. Polyhedra characterization

Let f_i be the number of i lateral facets while f, e and v are the numbers of facets, edges and vertices of any simple polyhedron with $f_3 = f_4 = 0$, respectively. Then

$$f = f_5 + f_6 + \ldots, \quad 2e = 5f_5 + 6f_6 + \ldots .$$

Hence,

$$f_5 = (6f - 2e) + f_7 + 2f_8 + 3f_9 + \ldots .$$

At the same time,

$$f - e + v = 2, \quad 2e = 3v.$$

Hence,

$$6f - 2e = 12.$$

Finally,

$$f_5 = 12 + f_7 + 2f_8 + 3f_9 + \ldots$$

and

$$f = 12 + f_6 + 2f_7 + 3f_8 + 4f_9 + \ldots . \quad (1)$$

The diophantine equation (1) was found to have 67 solutions for f = 12–20 and an obvious restriction $f_i \geq 0$. For any solution, all the possible polyhedra were built into the Schlegel projections. The general way to build a polyhedron was to fill in the chosen (basal) facet with other facet projections. As the resulting Shlegel projection is required to save the symmetry of a polyhedron, the most expedient way is to choose a unique facet, if any, as the basal one. For example, in the case of $5_{13}6_4 7_1$ polyhedra, the only heptagonal facet was taken as the basal one. In the case of a $5_{14}6_4 7_2$ polyhedra, a heptagonal facet was taken as the basal one. In most cases, a basal facet has the greatest number of edges. However, in the case of a $5_{15}6_1 7_3$ polyhedron, only the hexagonal facet should be taken as the basal one to save the $3m$ symmetry of the polyhedron.

Generally, there is no algorithm that fills in the chosen basal facet with other facet projections. To do this, one should use various combinatorial methods. For example, in the simple case of the $5_{18}9_2$ polyhedron, we choose a nonagonal facet as the basal one. Afterwards, we try to fill it in with other facet projections in the assumption that two nonagonal facets are in contact with each other. This leads to nothing. Hence, the basal facet should be surrounded by nine pentagonal facets. Next, we assume that another nonagonal facet is in contact with them in any position. This also leads to nothing. Finally, we build one more ring of pentagonal facets with a nonagonal one

† Correspondence address: 14 Fersman Street, 184209 Apatity, Russia.

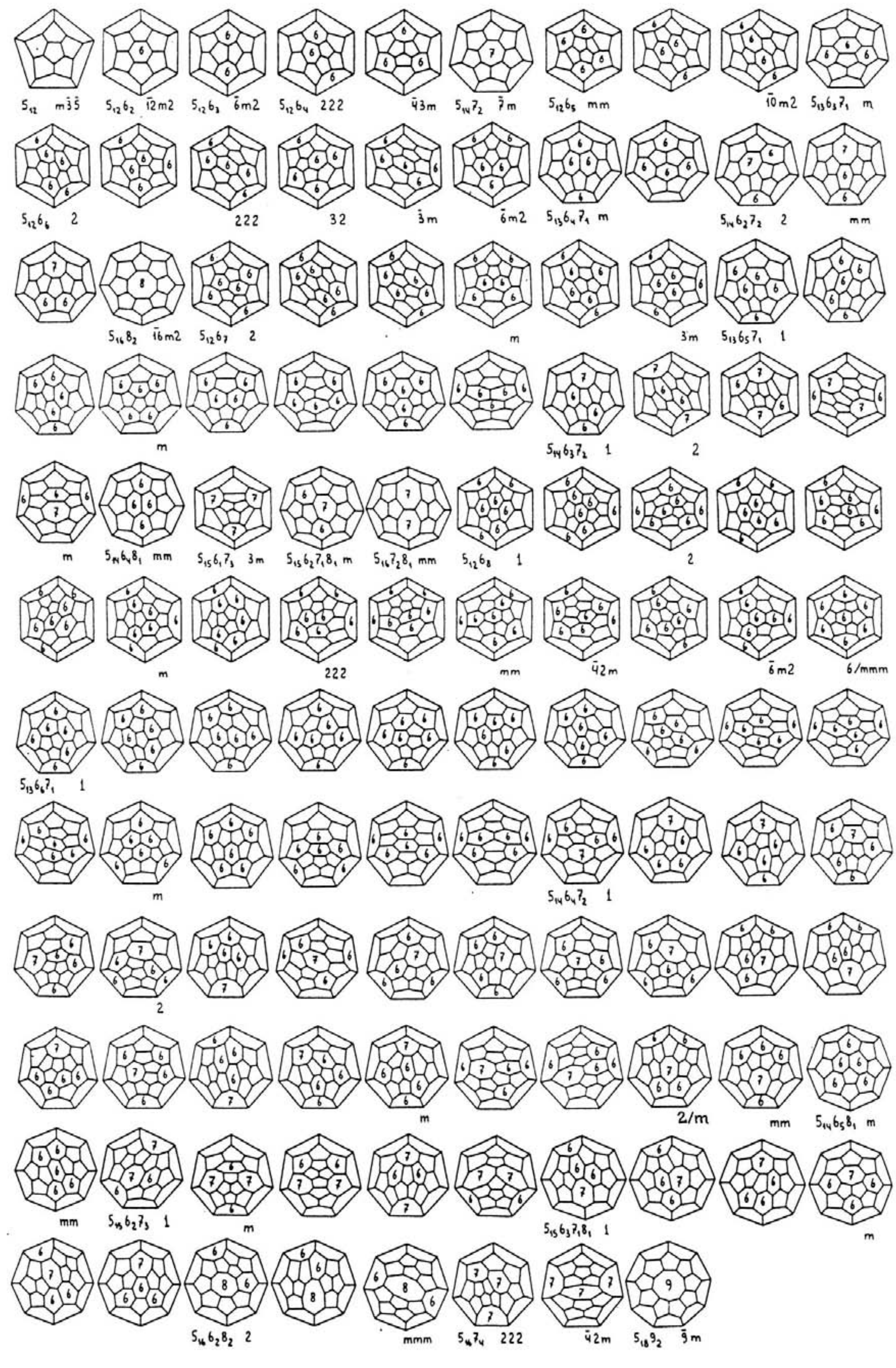

Figure 1
All simple 12- to 20-hedra without triangular and quadrilateral facets in the Schlegel projections. The facet symbols and symmetry point groups are given for the first representatives in the series only, 6- to 9-lateral facets are marked with numbers.

Table 1
The number (n) of polyhedra, if any, related to the diophantine equation (1) solutions.

f	f_5	f_6	f_7	f_8	f_9	n
12	12					1
14	12	2				1
15	12	3				1
16	12	4				2
	14		2			1
17	12	5				3
	13	3	1			1
	12	6				6
18	13	4	1			2
	14	2	2			3
	16			2		1
	12	7				6
	13	5	1			8
	14	3	2			5
19	14	4		1		1
	15	1	3			1
	15	2	1	1		1
	16		2	1		1
	12	8				15
	13	6	1			16
	14	4	2			23
	14	5		1		2
20	15	2	3			5
	15	3	1	1		6
	16		4			2
	16	2		2		3
	18				2	1

in the centre. This extremely routine procedure was made for all equation (1) solutions and has resulted in 118 polyhedra (Fig. 1). Their numbers, if any, are given in Table 1.

It follows from the latter that a simple f-hedron with $f_3 = f_4 = 0$ never has i-lateral facets if $f < 2i + 2$. However, we neither have proof nor counter-argument to this conjecture. When proven, it could help in further searching for the polyhedra under discussion.

The class of calculated polyhedra contains 35 fullerenes, *i.e.* simple polyhedra with pentagonal and hexagonal facets only. This important class of polyhedral molecules was specially studied by us (in collaboration with Dmitry G. Stepenshchikov). The symmetry point groups for all 20- to 60-vertex fullerenes (5770 in common) will be reported in our next paper.

3. Conclusions

All simple 12- to 20-hedra with no triangular and quadrilateral facets are calculated. Among them, all fullerenes with 20–36 vertices are found. Thus, the γ operation is eliminated from the Fedorov recurrence algorithm up to a 21-hedra generating procedure. This significantly reduces the computer time when searching even for simple 14- and 15-hedra.

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