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C_{20} to C_{60} fullerenes: combinatorial types and symmetries

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A figure giving the point groups for all combinatorially non-isomorphic C_{20} to C_{60} fullerenes (5770 in common) is contributed. The fullerenes of 6 to 120 automorphism group orders (80 in common) are drawn in the Shlegel projections and characterized by the point groups.

1. Introduction

There is no doubt that the laboratory synthesis (Curl & Smalley, 1988) and subsequent findings of stable C_{60} clusters in rocks (Zeidenberg *et al.*, 1996) are the most impressive events in carbon crystallography and mineralogy for the last 15 years. The fullerenes of less than 60 atoms are known to be unstable and registered in physical experiments in a minor amount, with those of 20–36 atoms forming a 'restricted zone' (Helden *et al.*, 1993). But just these types of fullerene-like crystalline pores were identified in many clathrate compounds over the last 50 years (Ripmeester & Ratcliffe, 1998). Hence, our idea is to systematically generate the series of fullerenes up to the well known C_{60} shape.

2. Characterization of fullerenes

We define fullerenes as simple (three edges meet at each vertex) polyhedra, with only pentagonal and hexagonal facets allowed. Let f_5 and f_6 be the numbers of pentagonal and hexagonal facets and f, e and v be the numbers of facets, edges and vertices of any fullerene. Then,

$$f_5 + f_6 = f, \quad 5f_5 + 6f_6 = 2e \quad \text{and} \quad f_5 = 6f - 2e.$$

At the same time,

$$f - e + v = 2, \quad 2e = 3v \quad \text{and} \quad 6f - 2e = 12.$$

Hence,

$$f_5 = 12, \quad f = 12 + f_6 \quad \text{with} \quad f_6 \geq 0.$$

It follows from the above that

$$v = 2f - 4 \geq 20 \quad \text{and} \quad f_6 = f - 12 = v/2 - 10.$$

Thus, any fullerene may be characterized by the vertex C_v and facet $5_{12}6_{v/2-10}$ notations. We use the latter in the generating algorithm. Most of the above equations are due to Euler. They are provided here for the readers' convenience.

3. Generating algorithm

We construct a fullerene in the Shlegel projection in the following way. A general idea is to take the first facet and surround it by other facets numbered clockwise. Then, the same procedure should be repeated with the facets numbered as 2, 3 *etc*. As the fullerenes are simple polyhedra, only three facets meet at each vertex. The last facet should be the basal one of the Shlegel projection.

In the simplest case of fullerene 5_{12}, we begin with a pentagonal facet and build the only possible projection (Fig. 1, No. 1). For fullerene $5_{12}6_1$, we begin with the hexagonal facet and try to build the projection. This procedure does not lead to a fullerene. For fullerenes $5_{12}6_n$ with $n > 1$, we also begin with a hexagonal facet. But, in this case, to check all the variants, we previously enumerate the (6, ...) sequences with any permutations of $n - 1$ sixes in $n + 11$ dotted positions. Then we generate the facets in the above procedure in accord with them. For example, the (6, 5, ..., 5, 6) sequence leads to the only fullerene $5_{12}6_2$ (No. 2). The generating procedure is stopped in three cases: (*a*) a fullerene is built in accord with a given sequence; (*b*) a fullerene is not built if the given facets are already exhausted; (*c*) at some step, the next facet would not be pentagonal or hexagonal.

The duplicated fullerenes of the same combinatorial type for a given $5_{12}6_n$ formula should be eliminated. To do this, we use their adjacency matrices for arbitrary initial numbering of the vertices. Two fullerenes belong to the same combinatorial type if and only if their adjacency matrices are reducible to each other by the symmetrical permutations of rows and columns. Afterwards, we calculate the automorphism group order of a given fullerene as the number of different vertex reindexings that save its adjacency matrix.

4. Results and discussion

The series of C_{20} to C_{60} fullerenes was found to consist of 5770 representatives. They are characterized by the automorphism group orders and point groups in Fig. 2. As in a general case (Voytekhovsky, 2001), they mostly belong to 1, 2 and m classes. For given v, the variety of C_v fullerenes slightly drops as an automorphism group order increases. Simultaneously, their physical stability is known to increase (Curl & Smalley, 1988; Helden *et al.*, 1993). The fullerenes of 6 to 120 automorphism group orders are in Fig. 1:

C_{20}: 1 ($\bar{3}\bar{5}m$); C_{24}: 2 ($\overline{12}m2$); C_{26}: 3 ($\bar{6}m2$); C_{28}: 4 ($\bar{4}3m$); C_{30}: 5 ($\overline{10}m2$); C_{32}: 6 (32), 7 ($\bar{3}m$), 8 ($\bar{6}m2$); C_{34}: 9 ($3m$); C_{36}: 10, 11 ($\bar{4}2m$), 12 ($\bar{6}m2$), 13 ($6/mmm$); C_{38}: 14 (32), 15 ($3m$), 16 ($\bar{6}m2$); C_{40}: 17 ($3m$), 18 (mmm), 19, 20 ($\bar{5}m$), 21 ($\bar{4}3m$); C_{42}: 22 (32); C_{44}: 23, 24 (32), 25 (23), 26–28 ($\bar{3}m$), 29, 30 ($\bar{6}m2$); C_{48}: 31 (32), 32, 33 (mmm), 34, 35 ($\overline{12}m2$); C_{50}: 36, 37 (32), 38 ($3m$), 39 ($\bar{6}m2$), 40, 41 ($\overline{10}m2$); C_{52}: 42, 43 ($3m$), 44, 45 (mmm), 46–50 ($\bar{4}2m$), 51 (23); C_{54}: 52 (32), 53 ($\bar{6}m2$); C_{56}: 54–59

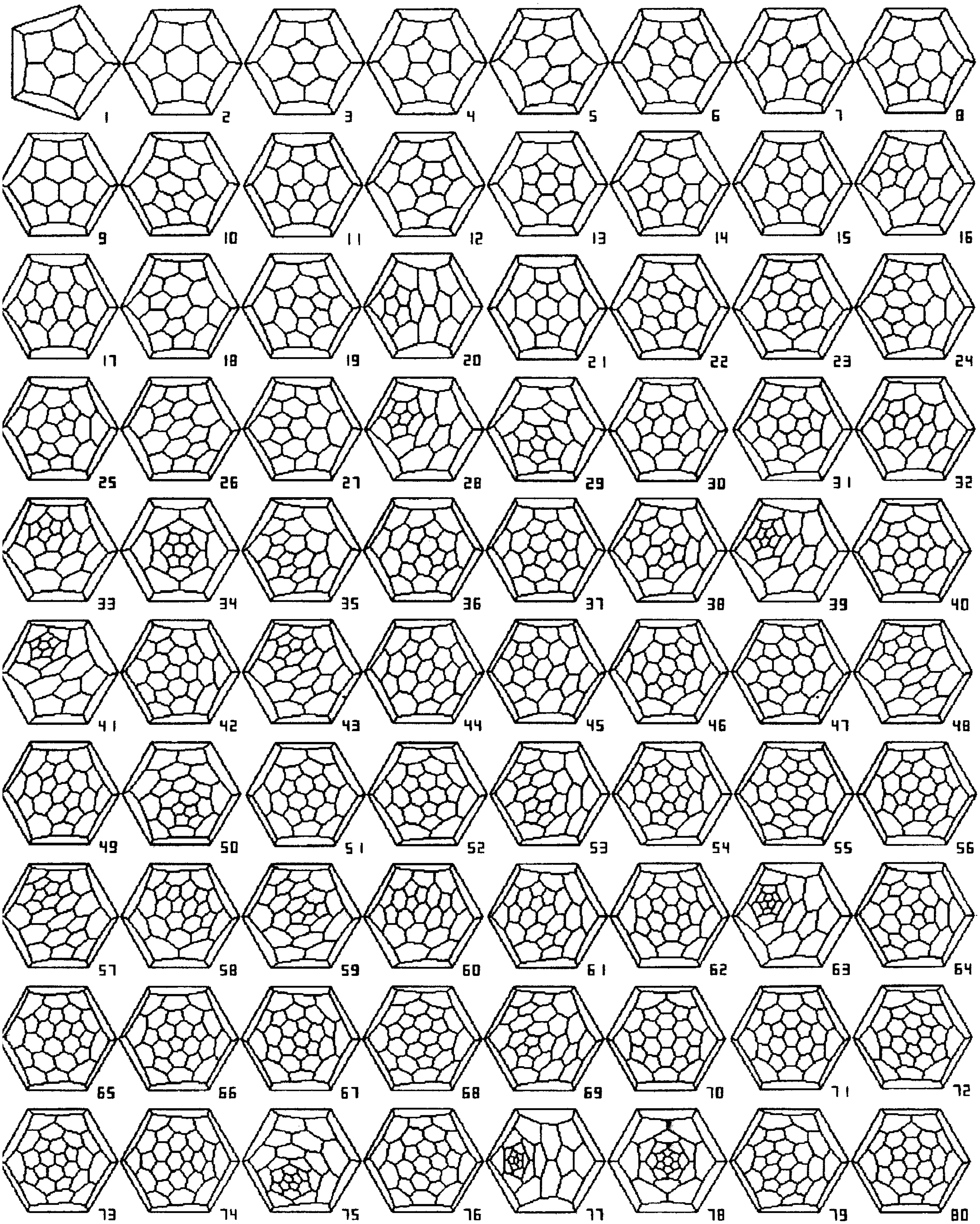

Figure 1
C_{20} to C_{60} fullerenes of 6 to 120 automorphism group orders in the Shlegel projections. See text for the point groups.

a.g.o.	p.g.	20	24	26	28	30	32	34	36	38	40	42	44	46	48	50	52	54	56	58	60	Σ
1	1								2	7	8	23	42	69	117	195	307	470	700	1037	1508	4485
2	-1																		1			1
	2						2	3	4	5	14	11	22	22	52	37	78	62	135	98	189	734
	m							2	2		7	6	7	19	16	25	26	38	49	58	67	322
3	3										1			2		2	3		3	4		15
4	-4												1								2	3
	222				1		1		2		3		6		5		9		10		19	56
	2/m														1		1		2		4	8
	mm2					2			1	2	2	4	3	4	3	6	3	8	13	6	9	66
6	32						1			1		1	2		1	2		1	6		3	18
	3m							1		1	1					1	2			2	1	9
8	mmm										1				2		2		1		1	7
	-42m								2								5		1		4	12
10	52																				1	1
12	23												1				1					2
	-3m						1						3						2			6
	-6m2			1			1		1	1			2			1		1				8
20	-5m										2										1	3
	-10m2					1										2						3
24	6/mmm								1												2	3
	-43m				1						1								1			3
	-12m2		1												2							3
120	-3-5m	1																			1	2
Σ		1	1	1	2	3	6	6	15	17	40	45	89	116	199	271	437	580	924	1205	1812	5770

Notes: a.g.o. - automorphism group orders, p.g. - point groups.

Figure 2
Point-group statistics for C_{20} to C_{60} fullerenes

(32), 60 (*mmm*), 61 ($\bar{4}2m$), 62, 63 ($\bar{3}m$), 64 ($\bar{4}3m$); C_{58}: 65, 66 (3*m*); C_{60}: 67–69 (32), 70 (3*m*), 71 (*mmm*), 72–75 ($\bar{4}2m$), 76 (52), 77 ($\bar{5}m$), 78, 79 (6/*mmm*), 80 ($\bar{3}\bar{5}m$).

Except for the famous No. 80 shape, Nos. 34, 35, 40, 41, 64 and 77–79 appear to be the most probable fullerenes in physical experiments. They are far from the 'restricted zone' and can be realized as shapes of rather high symmetry.

Except for Nos. 1, 2, 5, 19, 20, 34, 35, 40, 41, 76, 77 and 80, most of the C_{20} to C_{60} fullerenes are of crystalline symmetry. Hence, they may be considered as probable structural units of various crystalline (*e.g.* clathrate) compounds.

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