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C_{72} to C_{100} fullerenes: combinatorial types and symmetries

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The symmetry point-group statistics for all combinatorially different C_{72} to C_{100} fullerenes with free 5-gonal facets only are suggested in the paper for the first time. The shapes with automorphism group orders not less than 3 are drawn in Schlegel diagrams.

1. Introduction

The C_{20} to C_{60} fullerenes (5770 in total) were systematically enumerated and characterized by the symmetry point groups in Voytekhovsky & Stepenshchikov (2001). Their Schlegel diagrams were published in Voytekhovsky & Stepenshchikov (2002*b*). Except for the well studied C_{60} ($\bar{3}\bar{5}m$) shape, they are known to be unstable as carbon clusters. The C_{50} to C_{70} fullerenes with no triplets of adjacent 5-gonal facets were published in Voytekhovsky & Stepenshchikov (2002*a*). Among them, the C_{70} ($\overline{10}m2$) shape only is stable. Here, we contribute the symmetry point-group statistics for all the C_{72} to C_{100} fullerenes with free 5-gonal facets only. A general idea is to look for potentially stable shapes among them.

2. Theoretical background

As stated by Kroto (1987), the minimum number of adjacent 5-gonal facets and maximum symmetry point group contribute to a fullerene's stability. Schmalz *et al.* (1988) proved that two C_{50} ($\overline{10}m2$ and 32) are the simplest shapes with no triplets of adjacent 5-gonal facets. The well known C_{60} ($\bar{3}\bar{5}m$) and C_{70} ($\overline{10}m2$) are the simplest fullerenes with free 5-gonal facets only. Our computer calculations up to $n = 100$ confirm the widespread but unproved statement that, for any even $n \geq 70$, a fullerene C_n of this type exists (Voytekhovsky & Stepenshchikov, 2002*a*). Hence, our idea is to search for potentially stable shapes possessing maximum symmetry among previously generated fullerenes with minimum number of adjacent 5-gonal facets.

As in previous cases, we generated the fullerenes as their Schlegel diagrams. This is justified by the Steinitz (every 3-connected planar graph can be realized as a polyhedron) and Mani (every combinatorial automorphism of a polyhedron is affinely realizable) theorems. A general idea of our algorithm is to surround the first 6-gonal facet by other 5- and 6-gonal facets (*i.e.* to build the first corona) numbered clockwise. Then, the same procedure is repeated for the facet with sequence number two and iterated in turn for the facet with the smallest sequence number having an incomplete corona. At each step, only three facets meet at each vertex because, by definition, any fullerene is a simple polyhedron. The 5- and 6-gonal facets are added to a diagram in accordance with all previously generated possible (6, ...) sequences. The total number of 5-gonal facets equals 12 as was proved for such polyhedra (Voytekhovsky & Stepenshchikov, 2001). The last facet should automatically be the basal one of the Schlegel diagram if the above sequence leads to a fullerene. For a given total number of facets, the generating procedure is stopped in the following cases: (*a*) a fullerene is built in accordance with the given (6, ...) sequence, (*b*) a fullerene is not built if the allowed facets are already exhausted, and (*c*) at some step, the next facet could not be 5- or 6-gonal. Afterwards, the combinatorially equivalent shapes are eliminated. For all the remaining fullerenes, the automorphism and symmetry point groups are calculated.

3. Results and discussion

The numbers of C_{72} to C_{100} fullerenes with free 5-gonal facets only (total 1265) were announced in Voytekhovsky & Stepenshchikov (2002*a*) for the first time. Their symmetry point-group statistics are as follows.

$\mathbf{C_{72}}$ (total 1): $\overline{12}m2$; $\mathbf{C_{74}}$ (1): $\bar{6}m2$; $\mathbf{C_{76}}$ (2): 222, $\bar{4}3m$; $\mathbf{C_{78}}$ (5): $mm2$ – 2, $\bar{6}m2$ – 2, 32 – 1; $\mathbf{C_{80}}$ (7): $mm2$ – 2, 222 – 1, 32 – 1, $\bar{3}\bar{5}m$ – 1, $\overline{10}m2$ – 1, $\bar{5}m$ – 1; $\mathbf{C_{82}}$ (9): 2 – 3, m – 3, $3m$ – 2, $mm2$ – 1; $\mathbf{C_{84}}$ (24): 2 – 5, m – 5, 222 – 4, $mm2$ – 4, $\bar{4}2m$ – 2, 1 – 1, $\bar{3}m$ – 1, $\bar{4}3m$ – 1, $6/mmm$ – 1; $\mathbf{C_{86}}$ (19): 1 – 6, 2 – 6, m – 3, $mm2$ – 2, 3 – 1, 32 – 1; $\mathbf{C_{88}}$ (35): 1 – 11, m – 11, 2 – 7, $mm2$ – 3, 222 – 2, 23 – 1; $\mathbf{C_{90}}$ (46): 1 – 16, 2 – 16, $mm2$ – 7, m – 6, $\overline{10}m2$ – 1; $\mathbf{C_{92}}$ (86): 1 – 38, 2 – 26, m – 8, 32 – 5, 222 – 4, $mm2$ – 2, 3 – 1, mmm – 1, 23 – 1; $\mathbf{C_{94}}$ (134): 1 – 89, 2 – 26, m – 13, 3 – 3, $mm2$ – 2, $3m$ – 1; $\mathbf{C_{96}}$ (187): 1 – 108, 2 – 43, m – 14, 222 – 8, $mm2$ – 3, 32 – 3, $\overline{12}m2$ – 2, $3m$ – 1, mmm – 1, $\bar{4}2m$ – 1, $\bar{3}m$ – 1, $\bar{6}m2$ – 1, $6/mmm$ – 1; $\mathbf{C_{98}}$ (259): 1 – 169, 2 – 49, m – 30, $mm2$ – 5, 3 – 3, 32 – 3; $\mathbf{C_{100}}$ (450): 1 – 336, 2 – 62, m – 31, 222 – 9, $mm2$ – 5, 3 – 3, $\bar{4}2m$ – 1, 52 – 1, 23 – 1, $\bar{5}m$ – 1.

The fullerenes with automorphism group orders not less than 3 are drawn in Schlegel diagrams in Fig. 1 and enumerated below. Their symmetry point groups are in parentheses.

$\mathbf{C_{72}}$: 1 ($\overline{12}m2$); $\mathbf{C_{74}}$: 2 ($\bar{6}m2$); $\mathbf{C_{76}}$: 3 (222), 4 ($\bar{4}3m$); $\mathbf{C_{78}}$: 5–6 ($mm2$), 7 (32), 8–9 ($\bar{6}m2$); $\mathbf{C_{80}}$: 10 (222), 11–12 ($mm2$), 13 (32), 14 ($\bar{3}\bar{5}m$), 15 ($\overline{10}m2$), 16 ($\bar{5}$m); $\mathbf{C_{82}}$: 17 ($mm2$), 18–19 ($3m$); $\mathbf{C_{84}}$: 20–23 (222), 24–27 ($mm2$), 28–29 ($\bar{4}2m$), 30 ($\bar{3}m$), 31 ($\bar{4}3m$), 32 ($6/mmm$); $\mathbf{C_{86}}$: 33 (3), 34–35 ($mm2$), 36 (32); $\mathbf{C_{88}}$: 37–38 (222), 39–41 ($mm2$), 42 (23); $\mathbf{C_{90}}$: 43–49 ($mm2$), 50 ($\overline{10}m2$); $\mathbf{C_{92}}$: 51 (3), 52–55 (222), 56–57 ($mm2$), 58–62 (32), 63 (mmm), 64 (23); $\mathbf{C_{94}}$: 65–67 (3), 68–69 ($mm2$), 70 ($3m$); $\mathbf{C_{96}}$: 71–78 (222), 79–81 ($mm2$), 82–84 (32), 85 ($3m$), 86 (mmm), 87 ($\bar{4}2m$), 88 ($\bar{3}m$), 89 ($\bar{6}m2$), 90–91 ($\overline{12}m2$), 92 ($6/mmm$); $\mathbf{C_{98}}$: 93–95 (3), 96–100 ($mm2$), 101–103 (32); $\mathbf{C_{100}}$: 104–106 (3), 107–115 (222), 116–120 ($mm2$), 121 ($\bar{4}2m$), 122 (52), 123 (23), 124 ($\bar{5}m$).

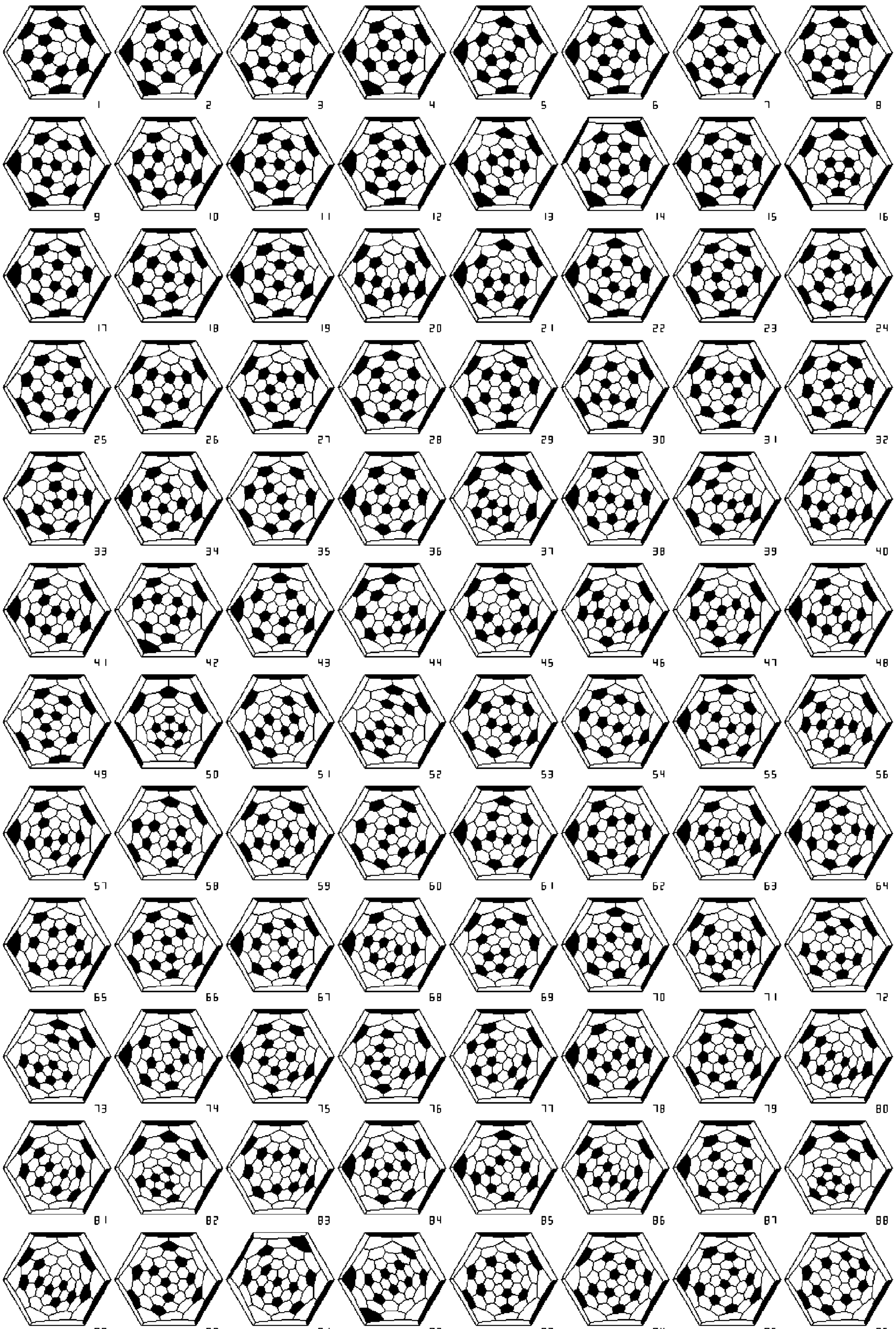

Figure 1
The most symmetrical C_{72} to C_{100} fullerenes. See text for symmetry point groups. The 5-gonal facets are filled in and emphasize the defects of a graphite-like net forming a fullerene.

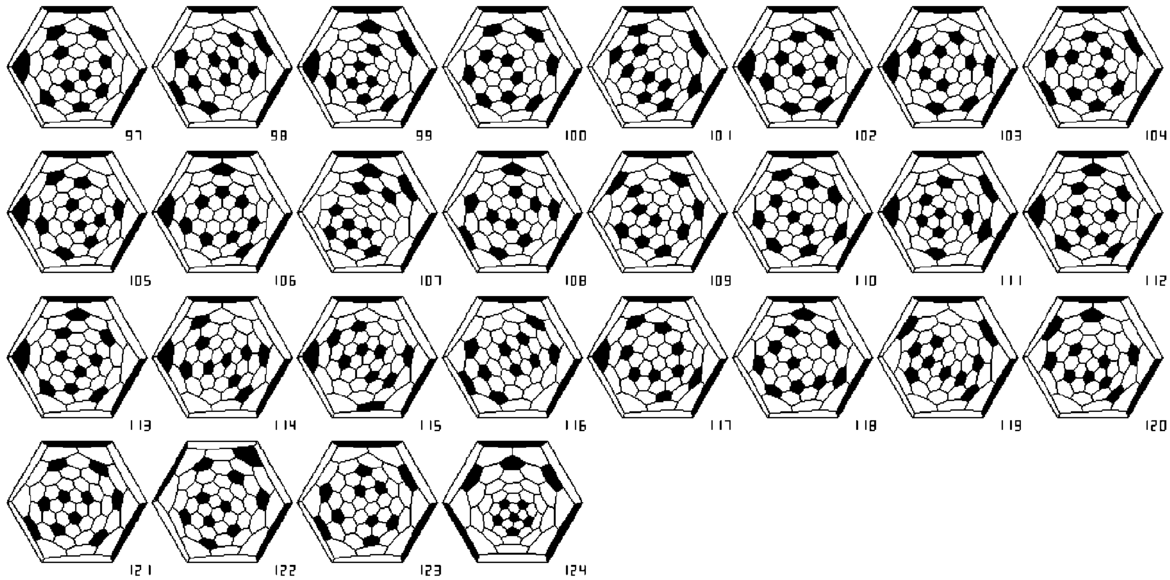

Figure 1 (continued)

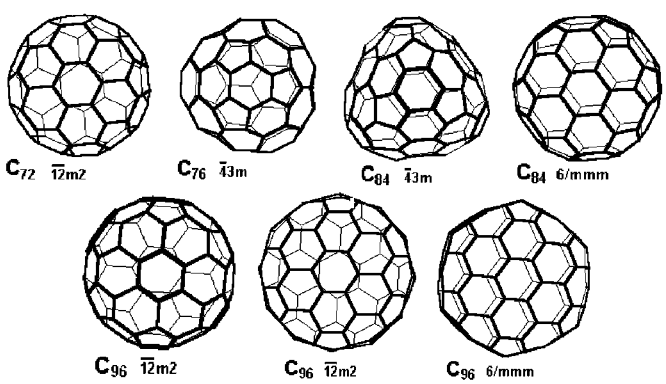

Figure 2
The fullerenes of automorphism group order 24. For any shape, the main symmetry axis is orthogonal to the plane of projection and goes through the central facet.

It follows from the above statistics that combinatorially trivial shapes (of 1 symmetry point group) prevail among the fullerenes even with free 5-gonal facets only. Considering them from the point of maximum symmetry, one may find C_{80} ($\bar{3}\bar{5}m$) as the absolutely optimum shape of the variety under consideration. Besides, the following 7 fullerenes of automorphism group order 24 may be considered as stable shapes in physical experiments: C_{72} ($\overline{12}m2$), C_{76} ($\bar{4}3m$), C_{84} ($\bar{4}3m$), C_{84} ($6/mmm$), C_{96} ($\overline{12}m2$) – 2 isomers, and C_{96} ($6/mmm$). They are given in Fig. 2.

4. Conclusions

Up to now, the full variety of C_{20} to C_{100} fullerenes has been generated and characterized by the numbers of adjacent 5-gonal facets and symmetry point groups. From the point of the two criteria given by Kroto, the most stable shapes are predicted. As usual, they are of icosahedral ($\bar{3}\bar{5}m$) symmetry. Hence, the following step should be a special study of such fullerenes.

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