Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Received 25 January 2002
Accepted 11 March 2002

On the spectrum of fullerenes

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The most symmetrical C_{50} to C_{70} fullerenes with minimum numbers of pairs of adjacent pentagonal facets are considered in this paper. Like the well known C_{60} ($\bar{3}\bar{5}m$) and C_{70} ($\overline{10}m2$) fullerenes with no adjacent pentagonal facets, they appear to be stable in physical experiments and cause the visible peaks in mass spectra of carbon clusters produced by laser vaporization of carbon.

1. Introduction

The first mass spectra of carbon clusters produced by laser vaporization of carbon with identification of the two main peaks as C_{60} and C_{70} polyhedral molecules named as fullerenes were published by Kroto *et al.* (1985) and Curl & Smalley (1988). This result was awarded with the Nobel Prize in 1996. But the series of additional peaks diminished in relative intensity compared with C_{60} and C_{70} and related to C_{50} – C_{90} fullerenes can also be seen in the same spectra, especially at initial stages of clustering. Our idea is to identify these peaks by taking into account some combinatorial criteria related to the fullerene's stability.

2. Theoretical background

As argued by Kroto (1987), the fullerenes in which all pentagonal facets are completely surrounded by hexagonal ones are stable. The fullerenes in which the pentagons contact each other in twos are likely to be less stable while those with triplets of adjacent pentagons are unstable. At the same time, the fullerenes become more stable with increasing symmetry. So, the minimum numbers of adjacent pentagonal facets and as high symmetry as possible evenly disperse the strain resulting from the bond-angle deformation and make the structures more stable.

The truncated icosahedron C_{60} ($\bar{3}\bar{5}\mathbf{m}$) was found to be the simplest fullerene with no adjacent pentagonal facets (Schmalz *et al.*, 1988). The next one is C_{70} ($\overline{10}\mathbf{m2}$) (Voytekhovsky, 2001). It is often mentioned without proof that, for any even $n > 70$, a fullerene C_n of the same type exists. Our computer calculations up to $n = 100$ confirm this statement with a rapidly growing variety of such fullerenes. Schmalz *et al.* (1988) also proved that two C_{50} ($\overline{10}\mathbf{m2}$ and **32**) are the simplest fullerenes with no triplets of adjacent pentagonal facets. Hence, what we investigate in this paper are all C_{50} to C_{70} fullerenes with pairs of adjacent pentagonal facets.

We generate the polyhedra as their Schlegel projections by the Fedorov recurrence algorithm. This approach is obviously justified by two well known theorems:

1. Every 3-connected planar graph can be realized as a 3-polyhedron

and

2. Every combinatorial automorphism of a 3-polyhedron is affinely realizable.

That is, there exists for each Schlegel diagram a 3-space realization of a polyhedron such that its edge graph is isomorphic to the Schlegel diagram while its symmetry point group is isomorphic to the automorphism group of the Schlegel diagram.

3. Results and discussion

A full variety of C_{20} to C_{60} fullerenes was previously generated and discussed in Voytekhovsky & Stepenshchikov (2001). We extract all C_{50} to C_{60} fullerenes with pairs of adjacent pentagons from the above data. They are shown in Fig. 1. All C_{62} to C_{70} fullerenes of this type were specially generated in the same way for this contribution. As their quantity rapidly grows, only fullerenes with automorphism group orders not less than 3 are shown in Fig. 2. Their symmetry point groups (bold letters) and numbers of pairs of adjacent pentagons are in parentheses as follows.

C_{50} (Fig. 1): 1 (**32**, 6), 2 ($\overline{10}\mathbf{m2}$, 5); C_{52}: 3 (**23**, 6); C_{54}: 4 (**2**, 6), 5 (**32**, 6); C_{56}: 6 (**1**, 5), 7, 9, 10 (**2**, 5), 8, 11 (**2**, 6), 12, 13 (**222**, 6), 14 (**222**, 4), 15 (**mm2**, 4), 16 (**mm2**, 6), 17 (**32**, 6), 18 ($\bar{3}\mathbf{m}$, 6); C_{58}: 19, 20, 22, 23, 25 (**1**, 5), 21 (**1**, 6), 24 (**1**, 4), 26, 29, 31 (**2**, 6), 27, 30 (**2**, 5), 28 (**2**, 4), 32 (**m**, 4), 33, 34 (**m**, 5), 35 (**3**, 6), 36 (**3m**, 3); C_{60}: 37, 40, 43 (**1**, 4), 38, 39, 41, 42, 44–47 (**1**, 5), 48–50, 52, 59–62 (**2**, 5), 51, 53, 56, 57 (**2**, 4), 54 (**2**, 3), 55, 58 (**2**, 6), 63 (**m**, 3), 64 (**m**, 5), 65 (**m**, 4), 66, 68 (**222**, 6), 67 (**222**, 4), 69 (**mm2**, 2), 70 (**32**, 3), 71 (**32**, 6), 72 (**mmm**, 4), 73, 74 ($\bar{4}\mathbf{2m}$, 4), 75 ($\bar{4}\mathbf{2m}$, 6), 76 (**52**, 5), 77 (**6/mmm**, 6); C_{62} (Fig. 2): 1–3 (**32**, 6), 4 ($\bar{6}\mathbf{m2}$, 6); C_{64}: 5 (**3**, 6), 6 (**222**, 2), 7–9 (**222**, 4), 10 (**222**, 6), 11 ($\bar{4}\mathbf{2m}$, 4); C_{66}: 12, 13, 15, 16, 18 (**mm2**, 4), 14 (**mm2**, 2), 17 (**mm2**, 5), 19 (**32**, 6); C_{68}: 20 (**3**, 3), 21 (**3**, 6), 22 (**222**, 2), 23–27 (**222**, 4), 28–30 (**222**, 6), 31 (**mm2**, 2), 32 (**mm2**, 4), 33 (**2/m**, 4), 34, 35 (**32**, 3), 36, 37 (**32**, 6), 38 ($\bar{3}$, 6), 39 ($\bar{4}\mathbf{3m}$, 6); C_{70}: 40–42 (**3**, 3), 43 (**3**, 6), 44 (**mm2**, 4), 45, 46 (**mm2**, 3), 47 (**mm2**, 5), 48 (**mm2**, 6), 49, 50 (**3m**, 3).

Considering fullerenes from the point of maximum symmetry (see automorphism group orders in Fig. 3) and minimum number of pairs of adjacent pentagons, one may find the absolutely optimum shapes for the following classes: C_{50} (Fig. 1): 2 ($\overline{10}\mathbf{m2}$, 5); C_{52}: 3 (**23**, 6); C_{54}: 5 (**32**, 6); C_{58}: 36 (**3m**, 3) and C_{62} (Fig. 2): 4 ($\bar{6}\mathbf{m2}$, 6). For other classes, the situation is not so clear because the symmetry grows together with the number of pairs of adjacent pentagons in the following rows: C_{56} (Fig. 1): 14 (**222**, 4), 15 (**mm2**, 4), 17 (**32**, 6), 18 ($\bar{3}\mathbf{m}$, 6); C_{60}: 69 (**mm2**, 2), 70 (**32**, 3), 72 (**mmm**, 4), 73, 74 ($\bar{4}\mathbf{2m}$, 4), 76 (**52**, 5), 77 (**6/mmm**, 6); C_{64} (Fig. 2): 6 (**222**, 2), 11 ($\bar{4}\mathbf{2m}$, 4); C_{66}: 14 (**mm2**, 2), 19

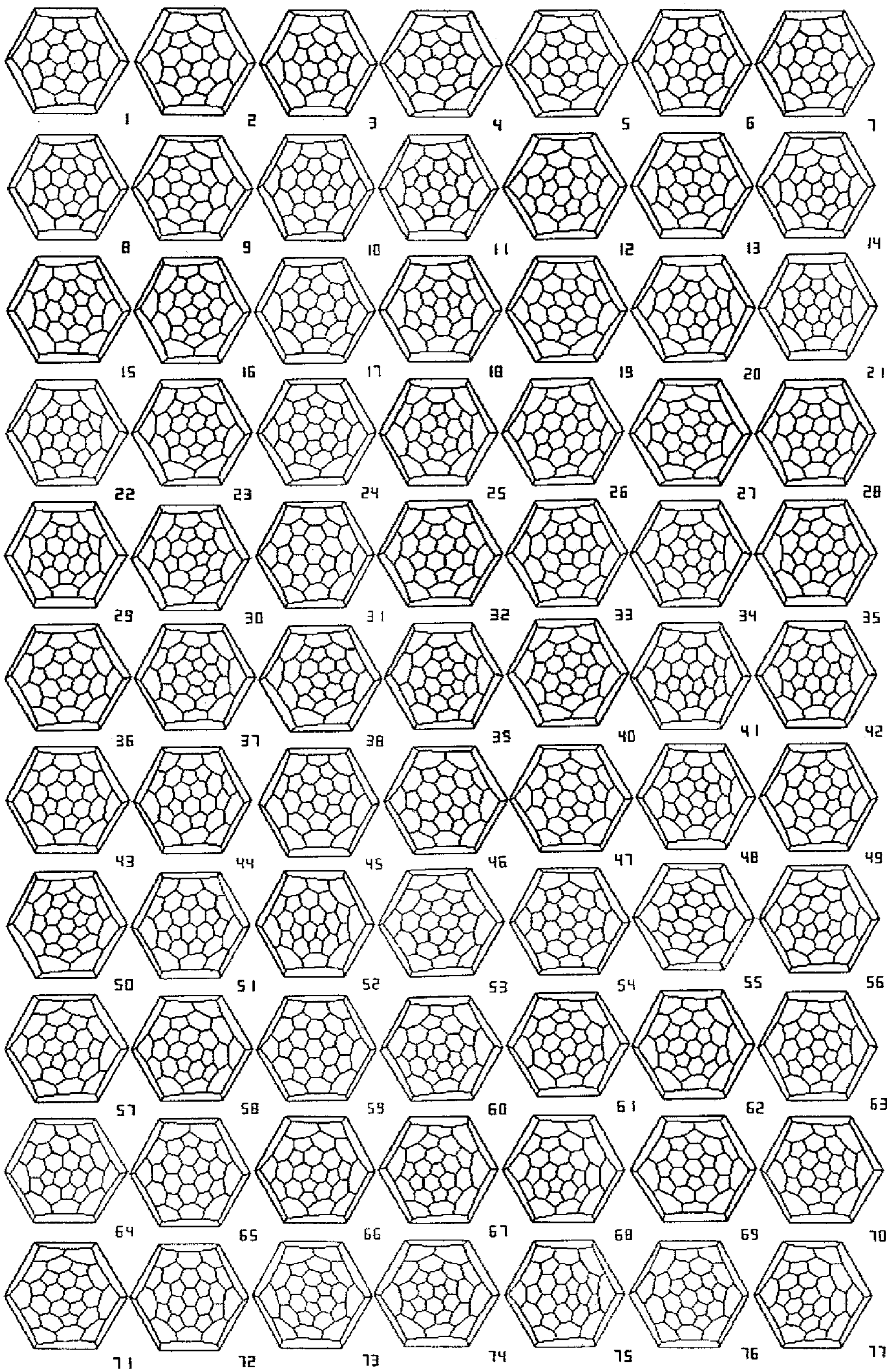

Figure 1
C_{50} to C_{60} fullerenes with pairs of adjacent pentagonal facets.

(**32**, 6) and C_{68}: 22 (**222**, 2), 31 (**mm2**, 2), 34, 35 (**32**, 3), 39 ($\bar{\mathbf{4}}\mathbf{3m}$, 6). In the case of C_{70}, two combinatorially different fullerenes have the same characteristics: 49, 50 (**3m**, 3). As the fullerenes C_{60} and C_{70} with no pairs of adjacent pentagons and very high symmetry ($\bar{\mathbf{3}}\bar{\mathbf{5}}\mathbf{m}$ and $\overline{\mathbf{10}}\mathbf{m2}$, respectively) cause the dominant peaks in the mass spectra of carbon clusters, only the above-mentioned C_{56}, C_{64}, C_{66} and C_{68} shapes should be compared by more subtle criteria.

4. Conclusions

The combinatorial criteria by Kroto (1987) allow us to predict stable C_{50}, C_{52}, C_{54}, C_{58}, C_{60}, C_{62} and C_{70} fullerenes. More subtle calculations should be done to compare C_{56} (4), C_{64} (2), C_{66} (2) and C_{68} (4) shapes.

As for the optimum C_n fullerenes with $n > 70$, they have no adjacent pentagonal facets. Our preliminary computer calculations for $n = 72$ to 100 show their great variety: 1, 1, 2, 5, 7, 9, 24, 19, 35, 46, 86, 134, 187, 259 and 450, respectively. Their combinatorial types and symmetry point groups will be reported in our following papers.

We acknowledge great benefit from the highly skilled comments made by Professor Emeritus André Authier and the unknown referee.

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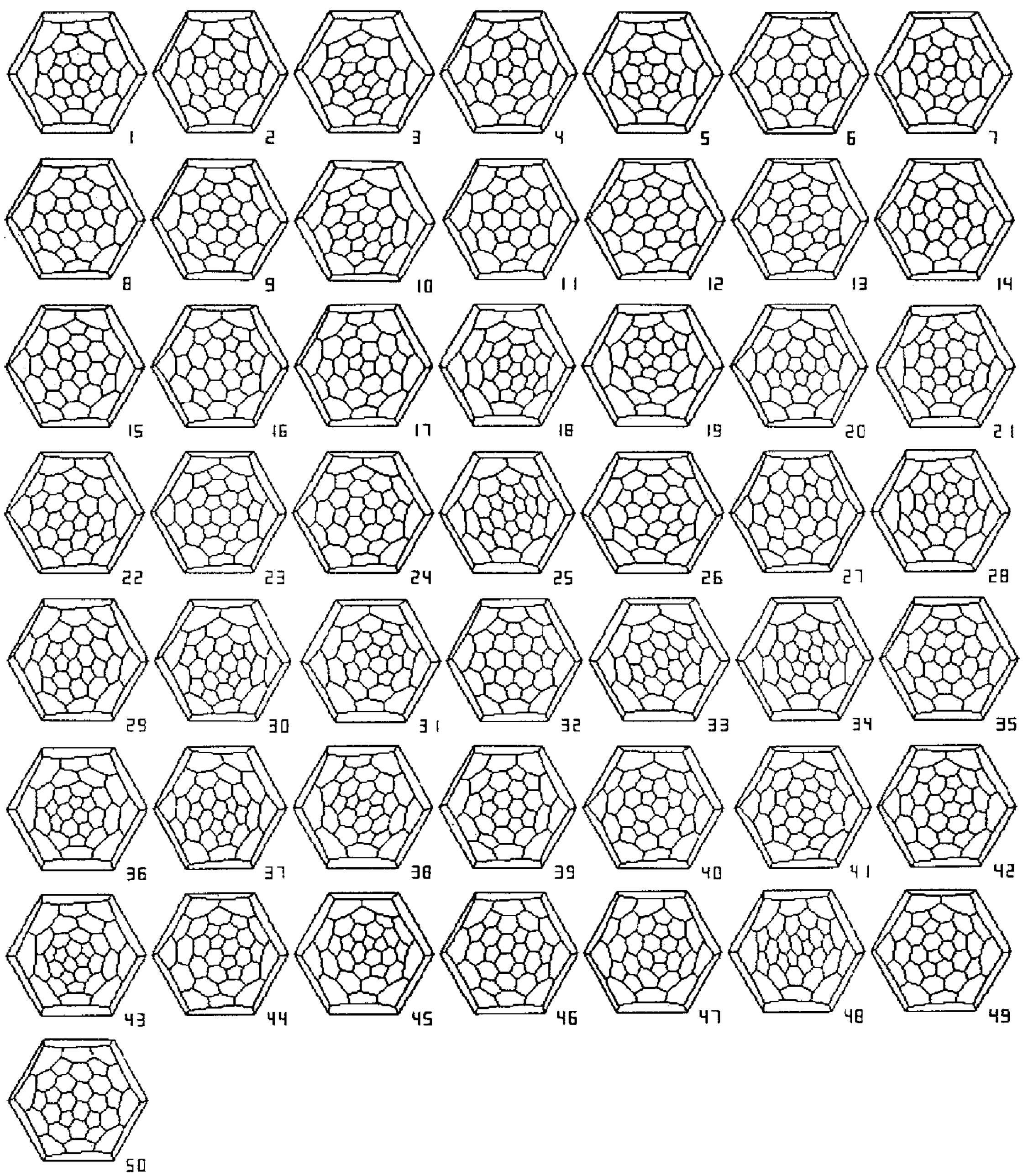

Figure 2
C_{62} to C_{70} fullerenes with pairs of adjacent pentagonal facets and automorphism group orders not less than three.

a.g.o.	s.p.g.	C_{50}	C_{52}	C_{54}	C_{56}	C_{58}	C_{60}	C_{62}	C_{64}	C_{66}	C_{68}	C_{70}	Total
1	1				1	7	11	30	80	123	256	421	929
2	2			1	5	6	15	16	32	37	72	66	250
	m					3	3	1	10	9	10	22	58
3	3					1			1		2	4	8
4	222				3		3		5		9		20
	mm2				2		1			7	2	5	17
	2/m										1		1
6	32	1		1	1		2	3		1	4		13
	3m					1						2	3
	-3										1		1
8	-42m						3		1				4
	mmm						1						1
10	52						1						1
12	23		1										1
	-3m				1								1
	-6m2							1					1
20	-10m2	1											1
24	6/mmm						1						1
	-43m										1		1
Total		2	1	2	13	18	41	51	129	177	358	520	1312

Figure 3
Automorphism group orders (a.g.o.) and symmetry point groups (s.p.g) of C_{50} to C_{70} fullerenes with pairs of adjacent pentagonal facets.

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