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A theorem on the fullerenes with no adjacent pentagons

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The theorem that a fullerene C_n with any even $n \geq 70$ and no adjacent pentagons exists is proved.

1. Introduction

As stated by Kroto (1987), an absence of adjacent pentagons correlates with a fullerene's stability. The well known C_{60} $(\bar{3}\bar{5}m)$ and C_{70} $(\overline{10}m2)$ are the simplest fullerenes with this property (Schmalz *et al.*, 1988). There are unique C_{72} and C_{74} fullerenes with no adjacent pentagons (Fig. 1). Our computations up to $n = 100$ confirm that their varieties rapidly increase with n (Voytekhovsky & Stepenshchikov, 2002, 2003). Here, we prove that, for any even $n \geq 70$, a fullerene C_n of this type exists.

2. General idea

Fig. 2 shows a series of fullerenes resulting from C_{60} $(\bar{3}\bar{5}m)$ by inserting a belt of five hexagons around a fivefold symmetry axis with a right cap rotated at each step. The series can be continued to infinity; however, there are gaps in it. Our general idea is to find some initial C_n fullerenes of sequential even n to generate an endless series covering, in total, any even $n \geq 70$.

As any fullerene is a simple polyhedron, *i.e.* only three edges meet at each vertex, then

$$n = 2f - 4,$$

where f is the total number of facets. Let us insert N additional facets into the initial fullerene at every step of the generating procedure; then

$$n' = 2(f + N) - 4$$

and

$$n' - n = 2N.$$

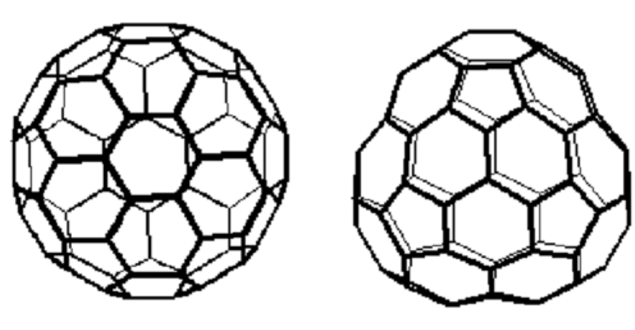

Figure 1
The unique C_{72} $(\overline{12}m2)$ and C_{74} $(\bar{6}m2)$ fullerenes with no adjacent pentagons.

As n is even, it follows from the latter that we need precisely N initial fullerenes and an appropriate series to fill the gaps.

3. Lemma and corollary

Let us consider any closed contour built from the edges of a fullerene (Fig. 3). The question is how many pentagons and hexagons do we need to fill it up if only three edges meet at each vertex? In accordance with the following lemma, a contour significantly affects the result:

Lemma. Let $e_{\rm in}$ and $e_{\rm out}$ be the numbers of edges touching a contour from inside and outside, respectively. Then, the number f_5 of pentagons inside a contour equals $6 + e_{\rm in} - e_{\rm out}$, regardless of the number f_6 of hexagons.

(Do not take f_5 for the total number of pentagons of a fullerene, which is known to equal 12.)

To prove this, let us consider the filling of a contour as a planar graph with the total numbers f of facets, v of vertices and e of edges, respectively, where

$$\begin{aligned} f &= f_5 + f_6, \\ 3v &= 5f_5 + 6f_6 + (e_{\rm in} + 2e_{\rm out}), \\ 2e &= 5f_5 + 6f_6 + (e_{\rm in} + e_{\rm out}). \end{aligned}$$

The terms in parentheses correctly account for the contributions of the facets touching a contour. Then, from the Euler equation

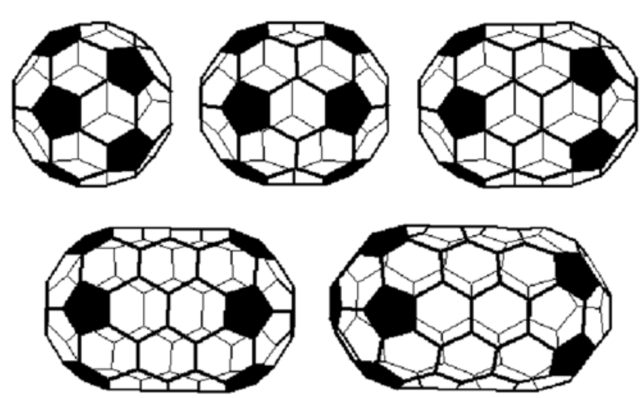

Figure 2
A series of fullerenes resulting from C_{60} $(\bar{3}\bar{5}m)$: C_{70} $(\overline{10}m2)$, C_{80} $(\bar{5}m)$, C_{90} $(\overline{10}m2)$, C_{100} $(\bar{5}m)$.

$$f + v = e + 1,$$

where 1 is used instead of 2 because we consider the inner facets of a graph only, we immediately obtain

$$f_5 = 6 + e_{\rm in} - e_{\rm out}$$

with no restrictions on f_6. The lemma is proved.

Now, let us surround a contour with a corona of hexagons. For its new outer contour, we have

$$f_5 = 6 + e'_{\rm in} - e'_{\rm out}.$$

But, $e'_{\rm in} = e_{\rm out}$. Hence

$$e'_{\rm out} = e_{\rm out} + (6 - f_5).$$

That is, the following corollary is obtained:

Corollary. The number of facets in the sequential coronas will increase if $f_5 < 6$, decrease if $f_5 > 6$, or be the same if $f_5 = 6$.

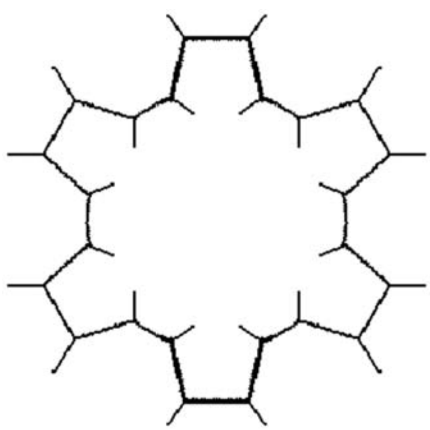

Figure 3
A contour with outer and inner edges.

The latter case leads to the series of elongated fullerenes named tubulenes (Fig. 2).

4. Theorem

Fig. 3 shows a special regular 'gear' contour for which $e_{\rm in} = e_{\rm out} = 12$. Our next idea is to use it to construct six initial fullerenes, each one from two caps bounded by the same 'gears'. Four conditions let us fill up the 'gears' with pentagons and hexagons (Fig. 4): (i) it follows from the above lemma that $f_5 = 6$, *i.e.* we use precisely six pentagons; (ii) three edges only meet at each vertex because any fullerene is a simple polyhedron; (iii) there are no adjacent pentagons because we are interested in this type of fullerene only; and (iv) at least one pentagon is at the contour, otherwise we can delete 12 hexagons touching it and obtain a contour of the same type.

The next step is to construct the fullerenes from two caps, avoiding adjacent pentagons. The cases of interest are (the numbers correlate with Fig. 4): C_{76} = 4 + 4; C_{78} = 4 + 5 and 5 + 8; C_{80} = 3 + 4, 4 + 6, 5 + 5 and 6 + 8; C_{82} = 3 + 5 and 5 + 6; C_{84} = 2 + 4, 2 + 8, 3 + 3, 3 + 6 and 6 + 6; C_{86} = 2 + 5 and 2 + 7. Finally, one can take any set of initial fullerenes $C_{76}, \ldots, C_{86}$ from the above list to generate the endless series of tubulenes. This is possible because it follows from the above lemma that $e'_{\rm out} = e_{\rm out} = 12$. As the unique C_{70}, C_{72} and C_{74} fullerenes with no adjacent pentagons have already been found, the following theorem is proved:

Theorem. For any even $n \geq 70$, a fullerene C_n with no adjacent pentagons exists.

5. Conclusions

The above lemma allows us to test whether any graphite tube can be closed as a tubulene or not. At the same time, the theorem shows the way to classify all the tubulenes C_n with respect to the total number n of vertices, and the type and mutual orientation of both caps.

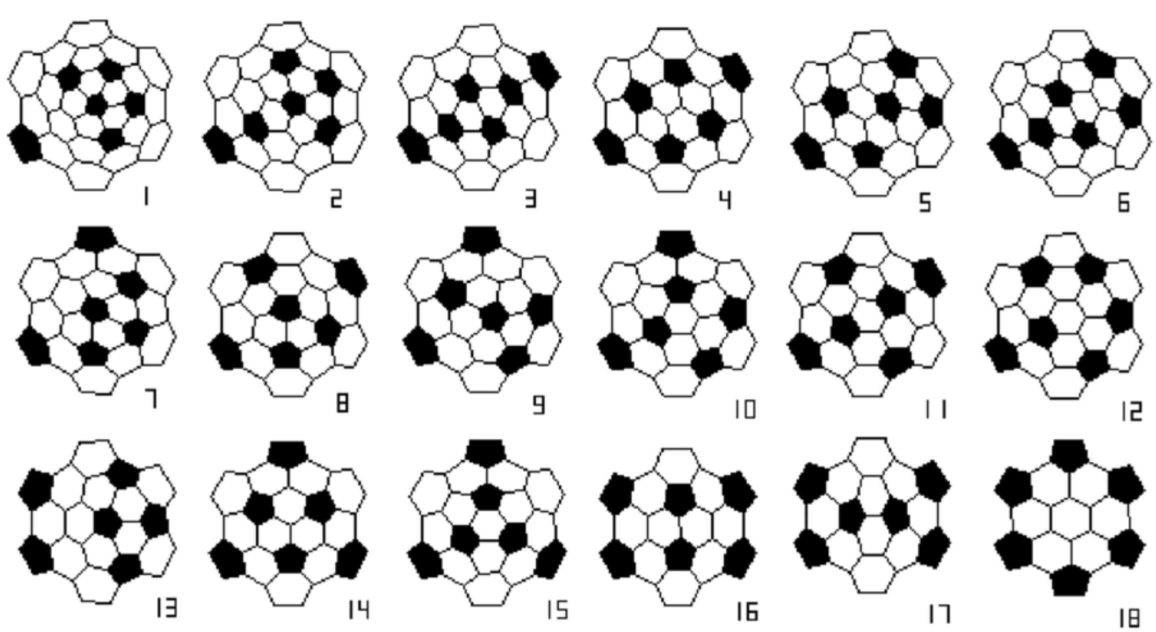

Figure 4
All the ways to fill up the 'gear' with pentagons (black) and hexagons.

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References

Kroto, H. W. (1987). *Nature (London)*, **329**, 529–531.
Schmalz, T. G., Seitz, W. A., Klein, D. J. & Hite, G. E. (1988). *J. Am. Chem. Soc.* **110**, 1113–1127.
Voytekhovsky, Y. L. & Stepenshchikov, D. G. (2002). *Acta Cryst.* A**58**, 295–298.
Voytekhovsky, Y. L. & Stepenshchikov, D. G. (2003). *Acta Cryst.* A**59**, 283–285.