MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **66** (2011) 285-292

ISSN 0340 - 6253

Remarks on Fowler–Manolopoulos Predictor of Fullerene Stability[1]

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(Received October 27, 2010)

Abstract

We present a relation between the Fowler-Manolopoulos predictor of fullerene stability, defined as the standard deviation of the hexagon neighbor indices, and the counts of a few simple fullerene substructures made up jointly from pentagons and hexagons. This result extends the previous approach of Ju et al. [*MATCH Commun. Math. Comput. Chem.* **64** (2010) 419–424] that was applicable to isolated pentagon fullerenes only.

1 Introduction

A fullerene is a molecule made up of n carbon atoms, whose molecular graph is a cubic, planar graph consisting of 12 pentagonal and $\frac{n}{2} - 10$ hexagonal faces. It was very early observed that pentagon adjacencies influence the stability of fullerenes [1, 2], leading to the rule that the isolated pentagon (IP) fullerenes are more stable from those that contain adjacent pentagons. However, besides dividing fullerenes into two groups of more stable (IP fullerenes) and less stable (non-IP fullerenes), this rule does not distinguish stabilities of fullerenes within the same group. The number of other predictors of fullerene stability

[1]This work was supported by the research program P1-0285 of the Slovenian Agency for Research and the research grant 144015G of the Serbian Ministry of Science and Environmental Protection.

have been proposed in the literature, among which the Kekulé counts [3], the Wiener index [4, 5], the independence number [6, 7], the bipartivity [8] and the Fowler-Manolopoulos predictor [9, 10, 11].

Recently, Ju et al. [12] presented a relationship between the Fowler-Manolopoulos predictor and a particular hexagon structure counts, in order to provide a graphical explanation for the predictor. However, their discussion is valid for isolated pentagon fullerenes only, and our task here is to extend this type of relationship to all fullerenes.

2 Main result

The neighbor index of a hexagon in a fullerene is the number of other hexagons adjacent to it [13]. Let h_k be the number of hexagons in a fullerene with neighbor index k, $k = 0, \ldots, 6$. Fowler and Manolopoulos introduce the standard deviation σ_h of the neighbor index distribution as a predictor of fullerene stability [9]. That is,

$$\sigma_h = \sqrt{\langle k^2 \rangle - \langle k \rangle^2},$$

where

$$\langle k \rangle = \sum_k k h_k \Big/ \sum_k h_k$$

and

$$\langle k^2 \rangle = \sum_k k^2 h_k / \sum_k h_k.$$

Ju et al. [12] expressed σ_h for IP fullerenes in terms of the number of vertices n and the number w of pairs of nonadjacent hexagon edges shared with two other hexagons (see Fig. 1):

$$\sigma_h = \sqrt{18 + \frac{4w - 600}{n - 20} - \left(6 - \frac{120}{n - 20}\right)^2}.$$

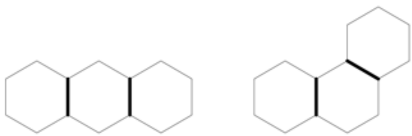

Figure 1: Structures that contribute to the number of pairs of nonadjacent hexagon edges shared with two other hexagons.

However, as the stability of fullerenes appears to depend on the distribution of pentagons, we find it more convenient to relate σ_h to the numbers of structures formed jointly from hexagons and pentagons. Further, since each structure contains at least one pentagon, and the whole fullerene contains just 12 pentagons, it is much easier to count such structures which are localized in pentagon neighborhoods, than to enumerate w, whose structures are spread all over the fullerene.

In particular, we express σ_h in an arbitrary fullerene by the following structure counts: the number a of edges common to a pentagon and a hexagon; the number b of vertices common to a pentagon and two hexagons; and the number c of pairs of hexagon edges belonging to neighboring, mutually nonadjacent hexagon and pentagon (see Fig. 2).

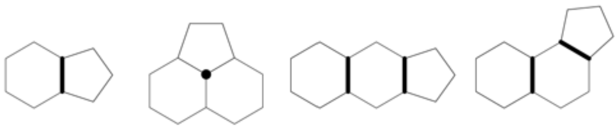

Figure 2: Structures that contribute to the a, b and c counts.

Theorem 1 *For an arbitrary fullerene F holds*

$$\sum_k k h_k = 3(n-20) - a, \tag{1}$$

$$\sum_k k^2 h_k = 18(n-20) - (6a + 2b + c), \tag{2}$$

$$\sigma_h = \sqrt{\frac{12a - 4b - 2c}{n-20} - \frac{4a^2}{(n-20)^2}}. \tag{3}$$

Proof. Each hexagon in F has one of 13 different neighborhood types depicted in Fig. 3. Here h_k for $k \in \{0,1,5,6\}$, or $h_{k,j}$ for $k \in \{2,3,4\}$, denote the number of hexagons with corresponding neighborhood type. Note that $h_k = h_{k,1} + h_{k,2} + h_{k,3}$ for $k \in \{2,3,4\}$. In table below we give the a, b and c counts produced by each neighborhood type:

	h_0	h_1	$h_{2,1}$	$h_{2,2}$	$h_{2,3}$	$h_{3,1}$	$h_{3,2}$	$h_{3,3}$	$h_{4,1}$	$h_{4,2}$	$h_{4,3}$	h_5	h_6
a	6	5	4	4	4	3	3	3	2	2	2	1	0
b	0	2	2	4	4	2	4	6	2	4	4	2	0
c	0	3	6	4	4	7	5	3	6	4	4	3	0

If we sum these counts over all hexagons in F, then each a and c structure is counted once, while each b structure is counted twice. Hence

$$\begin{aligned}
6h_0 + 5h_1 + 4(h_{2,1} + h_{2,2} + h_{2,3}) + 3(h_{3,1} + h_{3,2} + h_{3,3}) + 2(h_{4,1} + h_{4,2} + h_{4,3}) + h_5 &= a, \\
2h_1 + 2h_{2,1} + 4h_{2,2} + 4h_{2,3} + 2h_{3,1} + 4h_{3,2} + 6h_{3,3} + 2h_{4,1} + 4h_{4,2} + 4h_{4,3} + 2h_5 &= 2b, \\
3h_1 + 6h_{2,1} + 4h_{2,2} + 4h_{2,3} + 7h_{3,1} + 5h_{3,2} + 3h_{3,3} + 6h_{4,1} + 4h_{4,2} + 4h_{4,3} + 3h_5 &= c.
\end{aligned}$$

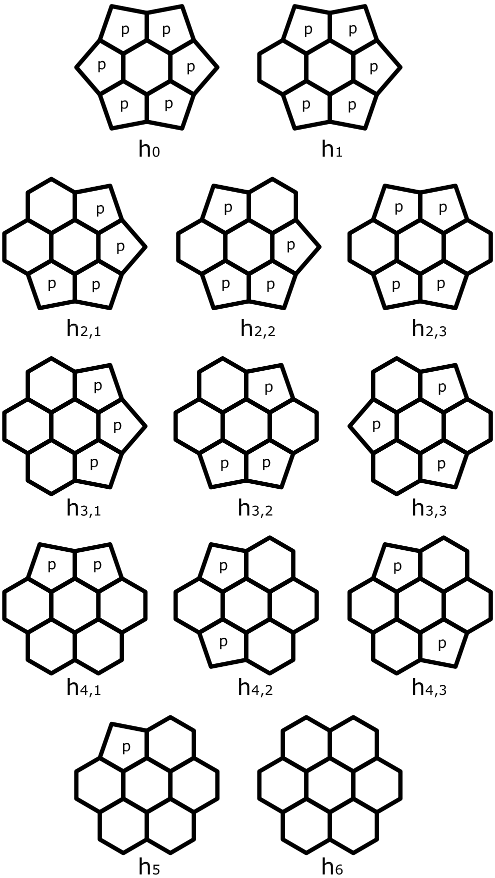

Figure 3: Possible neighborhoods of a hexagon in a fullerene.

Then

$$\begin{aligned}
& \sum_k k h_k \\
= \quad & 6(h_0 + h_1 + h_{2,1} + h_{2,2} + h_{2,3} + h_{3,1} + h_{3,2} + h_{3,3} + h_{4,1} + h_{4,2} + h_{4,3} + h_5 + h_6) \\
- \quad & (6h_0 + 5h_1 + 4(h_{2,1} + h_{2,2} + h_{2,3}) + 3(h_{3,1} + h_{3,2} + h_{3,3}) + 2(h_{4,1} + h_{4,2} + h_{4,3}) + h_5) \\
= \quad & 6\left(\frac{n}{2} - 10\right) - a = 3(n-20) - a
\end{aligned}$$

and

$$\sum_k k^2 h_k$$

$$
\begin{aligned}
&= 36(h_0 + h_1 + h_{2,1} + h_{2,2} + h_{2,3} + h_{3,1} + h_{3,2} + h_{3,3} + h_{4,1} + h_{4,2} + h_{4,3} + h_5 + h_6) \\
&- 6\,(6h_0 + 5h_1 + 4(h_{2,1} + h_{2,2} + h_{2,3}) + 3(h_{3,1} + h_{3,2} + h_{3,3}) + 2(h_{4,1} + h_{4,2} + h_{4,3}) + h_5) \\
&- (2h_1 + 2h_{2,1} + 4h_{2,2} + 4h_{2,3} + 2h_{3,1} + 4h_{3,2} + 6h_{3,3} + 2h_{4,1} + 4h_{4,2} + 4h_{4,3} + 2h_5) \\
&- (3h_1 + 6h_{2,1} + 4h_{2,2} + 4h_{2,3} + 7h_{3,1} + 5h_{3,2} + 3h_{3,3} + 6h_{4,1} + 4h_{4,2} + 4h_{4,3} + 3h_5) \\
&= 36\left(\frac{n}{2} - 10\right) - 6a - 2b - c = 18(n-20) - (6a + 2b + c).
\end{aligned}
$$

Finally,

$$
\begin{aligned}
\sigma_h &= \sqrt{\frac{\sum_k k^2 h_k}{\sum_k h_k} - \left(\frac{\sum_k k h_k}{\sum_k h_k}\right)^2} \\
&= \sqrt{\frac{18(n-20) - (6a+2b+c)}{n/2 - 10} - \left(\frac{3(n-20) - a}{n/2 - 10}\right)^2} \\
&= \sqrt{\frac{12a - 4b - 2c}{n-20} - \frac{4a^2}{(n-20)^2}}. \qquad \blacksquare
\end{aligned}
$$

3 On the behaviour of σ_h and $\langle k^2 \rangle$

Among IP fullerenes, the a and b counts are constant and equal to 60 each. Thus, among IP fullerenes both σ_h and $\langle k^2 \rangle$ depend on the c count only:

$$
\begin{aligned}
\sigma_h &= \sqrt{\frac{480 - 2c}{n-20} - \frac{14400}{(n-20)^2}}, \\
\langle k^2 \rangle &= 36 - \frac{960 + 2c}{n - 20}.
\end{aligned}
$$

Each pair of pentagons at distance two from each other in an IP fullerene reduces the c count by two of four, depending on whether the two pentagons have one or two hexagons as common neighbors. Thus, σ_h and $\langle k^2 \rangle$ clearly favorize those IP fullerenes with smaller number of pairs of pentagons at distance two.

The maximum count of c structures is 180, obtained when every two pentagons in a fullerene are at distance at least three from each other. Such fullerenes have smallest $\sigma_h = \sqrt{\frac{120}{n-20} - \frac{14400}{(n-20)^2}}$ and smallest $\langle k^2 \rangle = 36 - \frac{1320}{n-20}$, and they should represent most stable IP fullerenes. However, note that σ_h and $\langle k^2 \rangle$ do not distinguish such fullerenes from each other, and have no implications on their geometry.

On the other hand, a relatively small value of $c = 100$ structures is obtained for tubular IP fullerenes having two caps as shown in Fig. 4, which have larger values $\sigma_h = \sqrt{\frac{280}{n-20} - \frac{14400}{(n-20)^2}}$ and $\langle k^2 \rangle = 36 - \frac{1160}{n-20}$.

The predictive behaviour of σ_h and $\langle k^2 \rangle$ becomes quite different when pentagons are allowed to be adjacent. A tubular fullerene with two caps as shown in Fig. 5 has two pairs of adjacent pentagons, and thus $a = 56$, $b = 56$ and $c = 168$. Clearly, $\sigma_h =$

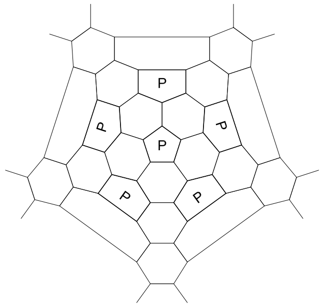

Figure 4: A cap of an IP tubular fullerene with $c = 100$.

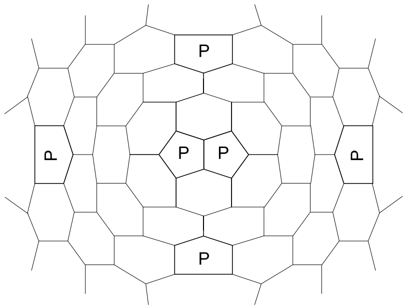

Figure 5: A cap of a non-IP tubular fullerene with $a = b = 56$ and $c = 168$.

$\sqrt{\frac{112}{n-20} - \frac{12544}{(n-20)^2}}$ and $\langle k^2 \rangle = 36 - \frac{1232}{n-20}$. Thus, its second moment lies between the two IP fullerenes mentioned above.

Another tubular fullerene with two caps as shown in Fig. 6 has six pairs of adjacent pentagons, and thus $a = 48$, $b = 48$ and $c = 132$. Clearly, $\sigma_h = \sqrt{\frac{120}{n-20} - \frac{9216}{(n-20)^2}}$ and $\langle k^2 \rangle = 36 - \frac{1032}{n-20}$. Thus, its σ_h lies between the two IP fullerenes above for $n \geq 53$.

Altogether, the ranges of σ_h values for IP and non-IP fullerenes have nonempty overlap, meaning that σ_h cannot separate IP from non-IP fullerenes. The same observation holds the ranges of $\langle k^2 \rangle$ values. Moreover, non-IP fullerenes usually have smaller σ_h value from IP fullerenes, clearly prohibiting us from extending the expectation that smaller σ_h yields more stable fullerene from IP fullerenes to all fullerenes.

To conclude, Theorem 1 shows that the Fowler-Manolopoulos predictor depends only on the configuration of 12 pentagons and their second neighborhoods in a fullerene. The number of such configurations is certainly finite and, in principle, it would be possible to enumerate them all and rank them according to values of σ_h and $\langle k^2 \rangle$ they produce. This

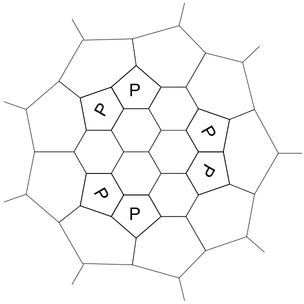

Figure 6: A cap of a non-IP tubular fullerene with $a = b = 48$ and $c = 132$.

ranking could be used to elaborate the correlation between σ_h, $\langle k^2 \rangle$ and fullerene stability in more detail, and we leave it as an interesting problem for future research, especially in the light of above remarks.

Acknowledgement. The author is indebted to anonymous referee for constructive remarks and for pointing out the references [10, 11].

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