

Partition of π -Electrons Among the Faces of Fullerene Graphs and Possible Applications to Fullerene Stability

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Abstract

We apply the concepts of importance and redundancy to compute and analyze the partition of π -electrons among faces of nanotubical fullerenes. We also discuss the deviation from uniform distribution as a potential predictor of fullerene stability.

1 Introduction

In this paper we consider the π -electron content in faces of several classes of fullerene graphs and its deviations from the uniform distribution. There are several ways to define and compute the average π -electron content of a ring of carbon atoms. Here we use the edge-based approach employed in several recent papers [1–3, 12, 16–21, 27–29], where it was applied to various benzenoid and coronoid species. The method relies on the Pauling bond order, and hence requires counting Kekulé structures in the considered clusters. We extend this line of research to three-dimensional structures, first by deriving explicit formulas for the Pauling bond order of edges in nanotubical carbon clusters, and then by deriving explicit formulas for the average π -electron content of faces in such structures. From these formulas we then obtain the deviation of the so computed π -electron content from

the uniform distribution, in which an atom shared by k rings contributes $1/k$ electrons to each ring. We show that there is a net migration of electrons among various regions of considered clusters and we determine the patterns of such migrations.

Besides obtaining analytical results for narrow nanotubes with sufficiently high symmetry, we have also computed the average π -electron content of all faces of fullerene graphs for several numbers of atoms for which stable isomers were experimentally verified. Our results indicate that some local aspects of π -electron distribution might be relevant for fullerene stability.

2 Preliminaries

In this section we introduce basic concepts needed for our task. We model the carbon clusters by their graphs, in which vertices represent carbon atoms, and edges represent the bonds between them. All clusters considered in this paper are represented by graphs that are finite, simple and connected; in addition, all of them are 3-regular and 3-connected. We refer the reader to any classical monograph on graph theory (such as, e.g., [33]) for definitions of those and related concepts.

2.1 Importance, redundancy, and Pauling bond order

A **matching** M in a graph G is a collection of edges of G such that no two edges from M share a vertex. If each vertex of G is incident with an edge of M , the matching M is called **perfect**. The number of perfect matchings of G is usually denoted by $K(G)$. It follows easily from a classical result of Petersen that all graphs considered in this paper have at least one perfect matchings. Perfect matchings figure prominently in both the mathematical and in the chemical literature, where they are usually called **Kekulé structures**. For a comprehensive treatment of matchings we refer the reader to [24].

Let e be an edge of G . The **importance** $\iota(e)$ of e is defined as the number of perfect matchings in G that contain e . A closely related concept has been long known in chemistry under the name of Pauling bond order: The **Pauling bond order** $p(e)$ of an edge e is obtained by dividing its importance by the total number of perfect matchings in G , $p(e) = \iota(e)/K(G)$. Another closely related concept is **redundancy** of an edge. Its is defined as the number of perfect matchings in G that do not contain e , and denoted by $\rho(e)$. Since the set of all perfect matchings in G can be partitioned to those matchings

that contain e and to those that do not contain e , we have $\iota(e) + \rho(e) = K(G)$, for any edge e of G . If the edge e connects vertices u and v in G , we can write [7]

$$\iota(e) = K(G - u - v), \quad \rho(e) = K(G - e).$$

For any vertex $u \in V(G)$ we have

$$K(G) = \sum_{e=uv} \iota(e),$$

where we sum over all edges of G incident with u .

2.2 π -electron distribution

In the clusters considered here, each carbon atom is adjacent to three other carbon atoms. This leaves one π -electron per carbon atom for forming carbon-carbon double bonds. Since in our clusters no carbon atom can participate in more than one double bond, any pattern of double bonds obviously forms a Kekulé structure that is mathematically represented by a perfect matching.

While the number of π -electrons that participate in Kekulé structures is equal to the number of atoms in the compound, the pattern of their distribution among the bonds is described by the distribution of Pauling bond orders [18]. Since that quantity can be thought of as a measure of the π -electron content of a given bond, we can also use it to measure the π -electron content of rings of carbon clusters.

Let G be a planar graph with a perfect matching, and H one of its faces. We denote the boundary of H (i.e., the set of all edges incident with H) by ∂H . Let M be a perfect matching of G . Each edge from ∂H participating in M represents a double bond and hence carries two electrons. As the edge is shared between two faces, each of them gets one of its electrons. Under such scheme, the total number of electrons given to H by M is obtained by counting edges from ∂H in M . The **total π -electron content** of H , $\pi(H)$, is obtained by summing such contributions over all perfect matchings of G . The **average π -electron content** of a face H , $\bar{\pi}(H)$, is then obtained by dividing its total π -electron content by the number of perfect matchings in G . Hence, $\bar{\pi}(H) = \frac{\pi(H)}{K(G)}$.

By double counting of edges, one can obtain a simple expression for the total π -electron content of a face in terms of importances of edges from ∂H .

Theorem A

$$\pi(H) = \sum_{e \in \partial H} \iota(e).$$

By dividing the above expression by $K(G)$ we obtain a formula for $\bar{\pi}(H)$ equivalent to formula (1) of reference [18]. However, we find formula from Theorem A more convenient for computations that follow.

A similar formula, in which U denotes the unbounded face of G ,

$$\pi(H) = \sum_{e \in \partial H} \iota(e) + \sum_{e \in \partial H \cap \partial U} \iota(e)$$

was employed in ref. [12] for computing the π -electron content of rings of a class of benzenoid compounds known as benzenoid parallelograms. The difference arises from the fact that the unbounded face of a planar graph representing a benzenoid parallelogram does not belong to the parallelogram. Hence the pairs of electrons in double bonds lying on ∂U are not shared and must be counted twice in bounded faces that share them with U .

There are also other ways to define the π -electron content of a face of G . The simplest one is to assume that an atom (i.e., a vertex) shared by k rings gives $1/k$ of its π -electron to each ring. Since all atoms in our clusters are shared by exactly three rings, this method gives the same number of electrons to all faces of the same size in G , hence it is very coarse. In spite of that, it could be used as kind of baseline for comparisons with other, more sophisticated, distributions. As it is atom-based, we denote the so constructed π -electron content of a ring H by $\pi_a(H)$. The difference between $\bar{\pi}(H)$ and $\pi_a(H)$ is called the **π -electron excess** of a face H of G and denoted by $\varepsilon_\pi(H)$. Hence, $\varepsilon_\pi(H) = \bar{\pi}(H) - \pi_a(H)$.

In the next section we compute $\bar{\pi}(H)$ and $\varepsilon_\pi(H)$ for all faces of narrow nanotubical fullerenes. A similar problem was considered in ref. [3], where the authors looked at the distribution of π -electrons in trivalent regular and semi-regular polyhedra (three Platonic and seven Archimedean polyhedra). In order to obtain the distributions, they first construct all perfect matchings and then compute their contributions to particular faces and the corresponding averages. Here we employ much faster approach following from Theorem A.

3 Nanotubical fullerenes

Fullerene graphs are 3-connected, cubic planar graphs with only pentagonal and hexagonal faces. Due to Euler's formula, the number of pentagonal faces in a fullerene graph is always twelve. If the pentagons are grouped into two more or less compact patches, we

obtain a class of tubular fullerene graphs called nanotubes. In nanotubes, two pentagon-containing caps are separated by a number of layers of hexagons. When the caps are hemi-dodecahedral, we obtain the narrowest possible nanotube in which the caps are separated by certain number of belts composed of 5 hexagons. Such nanotubes exist for any number of vertices $m = 10p$, where $p \geq 2$. For $p = 2$ we get the dodecahedron as a special case of nanotube without hexagonal faces. We refer the reader on ref. [14] for background information on fullerenes.

In the rest of this section we denote by T_n the narrow nanotube in which two hemi-dodecahedral caps are separated by n belts of 5 hexagons. The two pentagons adjacent only to other pentagons are called polar pentagons; one of them is the northern, the other the southern polar pentagon. We denote the polar pentagonal edges with a , and radial edges with b . As before, $K(T_n)$ denotes the number of perfect matchings in T_n . We denote

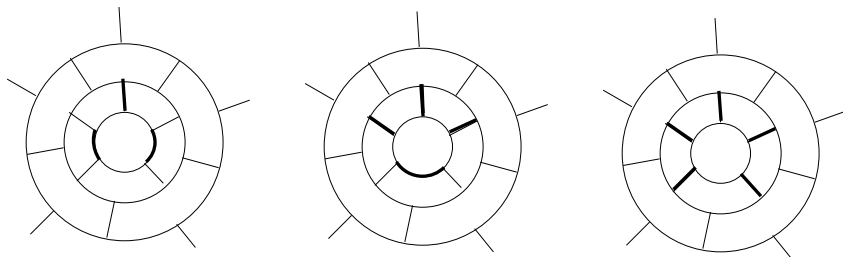


Figure 1. $K_i(T_n)$ number of perfect matchings in T_n involving i radial edges.

by $K_i(T_n)$ the number of perfect matchings in T_n including i radial edges incident with the northern polar pentagon. Because of the parity, it must be $i = 1, 3$ or 5 . It follows

$$K(T_n) = K_1(T_n) + K_3(T_n) + K_5(T_n).$$

It is immediately clear that $K_5(T_n) = 1$: The five radial edges incident with the northern polar pentagon force the five radial edges shared by five hexagons in the first hexagonal belt, they in turn force next five radial edges, and so on, all the way to the southern polar pentagon. Hence, $K_5(T_n) = 1$.

Next in the order of difficulty is computing $K_1(T_n)$. Look at a perfect matching containing one radial edge incident with the northern polar pentagon. It saturates exactly one vertex on the first circle parallel with the polar pentagon. There are five different ways to saturate the remaining four vertices on this circle. Each of them uses exactly one

radial edge from the next layer of hexagons, and the whole situation shifts one step toward south, again all the way to the southern polar pentagon. Hence, in each perfect matching counted by $K_1(T_n)$ there is exactly one out of five radial edges from each hexagonal belt and exactly one radial edge incident with a polar hexagon. That gives $K_1(T_n) = 5^{n+2}$.

The case $K_3(T_n)$ is the most complicated. Look at the northernmost belt of T_n . Any three edges contained in a perfect matching counted by $K_3(T_n)$ must saturate consecutive vertices on the northern polar pentagon. Denote by T'_n the open (on the northern side) nanotube that remains when we delete the polar pentagon and any three radial edges incident with it that participate in a perfect matching. Here the parameter n counts the intact hexagonal belts. By T''_n we denote a similar nanotube, the one that remains when three non-consecutive edges from a hexagonal belt participate in a perfect matching. Again, n counts intact hexagonal belts. Graphs T'_n and T''_n are shown in Fig. 2. If a perfect

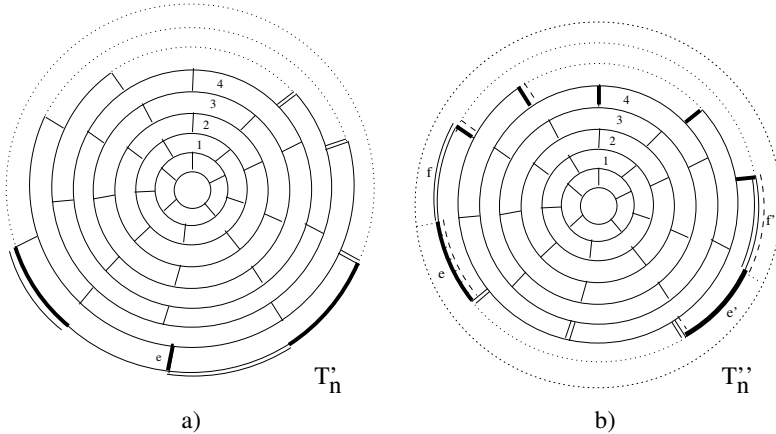


Figure 2. $K_3(T_n)$ number of perfect matchings in T_n involving 3 radial edges.

matching in T'_n contains the edge denoted by e in Fig. 2a, then it forces the two bold edges on the outer circle, leaving graph T''_n . If e is not contained in a perfect matching, then its end-vertex on the outer circle must be saturated by one of the two remaining edges. If it is saturated with the edge on the right, denoted by a double line, then the other edges denoted by double lines are forced, and the remaining graphs is T'_{n-1} . By symmetry, the left edge does the same. Hence,

$$K(T'_n) = 2K(T'_{n-1}) + K(T''_n).$$

Let us now look at T''_n . Each perfect matching in T''_n contains one and exactly one of pairs $\{e, e'\}$, $\{e, f'\}$, $\{e', f\}$ and $\{f, f'\}$. The pair $\{e, e'\}$ forces all bold edges, leaving the graph T'_{n-2} . The pair $\{f, f'\}$ forces the edges denoted by double lines, leaving T''_{n-1} . Finally, $\{e, f'\}$ (and then, by symmetry, $\{e', f\}$) forces the edges denoted by dashed lines, leaving again T''_{n-1} . Hence,

$$K(T''_n) = K(T'_{n-2}) + 3K(T''_{n-1}).$$

Denote now $K(T'_n) = t'_n$, $K(T''_n) = t''_n$. We have a system of linear recurrences

$$\begin{aligned} t'_n &= 2t'_{n-1} + t''_n \\ t''_n &= t'_{n-2} + 3t''_{n-1}. \end{aligned}$$

By expressing t''_n from the first relation and plugging it into second, we obtain a linear two-term recurrence with constant coefficients for t'_n ,

$$t'_n = 5t'_{n-1} + 5t'_{n-2}$$

with the initial conditions $t'_0 = 50$, $t'_1 = 175$. This recurrence has the explicit solution

$$t'_n = 5 \left[(5 - 2\sqrt{5}) \left(\frac{5 - \sqrt{5}}{2} \right)^n + (5 + 2\sqrt{5}) \left(\frac{5 + \sqrt{5}}{2} \right)^n \right].$$

This can be further simplified by noting that

$$5(5 - 2\sqrt{5}) = \left(\frac{5 - \sqrt{5}}{2} \right)^3, \quad 5(5 + 2\sqrt{5}) = \left(\frac{5 + \sqrt{5}}{2} \right)^3,$$

finally yielding

$$t'_n = \left(\frac{5 - \sqrt{5}}{2} \right)^{n+3} + \left(\frac{5 + \sqrt{5}}{2} \right)^{n+3}.$$

Since there are five different ways to have three edges incident with a polar pentagon in a perfect matching, we finally obtain

$$K_3(T_n) = 5t'_{n-3} = 5 \left[\left(\frac{5 - \sqrt{5}}{2} \right)^n + \left(\frac{5 + \sqrt{5}}{2} \right)^n \right].$$

From this we readily obtain the importance of a radial edge as

$$\begin{aligned} \iota_n(r) &= \frac{1}{5}K_1(T_n) + \frac{3}{5}K_3(T_n) + 1 \\ &= 5^{n+1} + 3 \left[\left(\frac{5 - \sqrt{5}}{2} \right)^n + \left(\frac{5 + \sqrt{5}}{2} \right)^n \right] + 1. \end{aligned}$$

The importance of non-radial edges is now given by

$$\iota_n(b) = 2 \cdot 5^{n+1} + \left(\frac{5 - \sqrt{5}}{2}\right)^n + \left(\frac{5 + \sqrt{5}}{2}\right)^n,$$

and the total number of perfect matchings in T_n is given as

$$K(T_n) = 5^{n+2} + 5 \left[\left(\frac{5 - \sqrt{5}}{2}\right)^n + \left(\frac{5 + \sqrt{5}}{2}\right)^n \right] + 1.$$

This result was reported in [30] and also in [26] along with some other results on the number of perfect matchings in various types of nanotubes.

It follows immediately that the number of π -electrons given to hexagonal faces is equal to $\frac{2\iota_n(r) + 4\iota_n(b)}{\iota_n(r) + 2\iota_n(b)} = 2$, independent of n . The number of π -electrons in polar pentagons tends to 2 with increasing n , while the number of electrons in non-polar pentagons approaches the value of $\frac{8}{5} = 1.6$. We see that the hexagonal faces obtain the same number of π -electrons as under the uniform distribution, while the polar pentagons acquire some electrons at the expense of their non-polar pentagonal neighbors. Their excess is, however, rather small, as the whole net migration includes $2/3$ of one electron for long nanotubes. That does not appear very surprising, given rather large degree of similarity among the hexagonal faces. We have wondered whether similar patterns are observed also for wider nanotubes and for general fullerenes.

We have performed some preliminary computations for another class of narrow nanotubes, with two caps in which one hexagon is surrounded with six pentagons and those caps are connected by a number of belts of six hexagons. It turns out that, again, the non-polar hexagons are given 2 electrons each. For other fullerenes we were unable to obtain explicit formulas, but we found the emerging patterns nevertheless very interesting.

4 Fullerene stability

There are many more possible fullerene structures than there are observed fullerene species. Many graph-theoretic invariants have been tested, with mixed results, as possible predictors and selectors of stable isomers. We mention here the number of pentagon-pentagon adjacencies, the independence number [13,15], the bipartite edge frustration [11] and bipartivity [8], the smallest eigenvalue [10], the separator [9], and many others [22,32]. See a nice review in ref. [23]. In any case, it became clear very soon that the number of perfect matchings is not very useful as a predictor of fullerene stability: The most stable

isomer of C_{60} , the one with full icosahedral symmetry group known also as the buckminsterfullerene, has 12500 perfect matchings, while the narrow nanotube on 60 atoms, considered to be the least stable isomer, has 16501 perfect matchings. This stands in marked contrast to the benzenoid case, where the number of perfect matchings is strongly correlated with their stability [6]. However, our results indicate that there still might be a relationship, though a more subtle one, between perfect matchings and stability.

In the rest of this section $C_n : m(S)$ denotes the fullerene isomer on n atoms that appears with number m in spiral algorithm of ref. [14] and has the symmetry group S . For example, the buckminsterfullerene is $C_{60} : 1812(I_h)$, while the narrow nanotube on 60 atoms is $C_{60} : 1(D_{5h})$.

In the previous section we have found that the total number of electrons in each hexagon of a narrow nanotube is equal to 2, the same as under uniform distribution. Since there are $\frac{n}{2} - 10$ hexagonal faces, this leaves 20 electrons that are awarded to pentagonal faces, independent on the number of vertices. On the other hand, in ref. [3] it was reported that each of 20 hexagons in the buckminsterfullerene receives $\frac{54}{25}$ electrons, and each of 12 pentagons only $\frac{35}{25}$ electrons. Hence the total number of electrons given to all pentagons in buckminsterfullerene is only 16.8. Motivated by this observation, we have performed computations for all 1812 isomers of C_{60} and found out that the total number of electrons in pentagons remains between those two extreme values. Moreover, the extremal values are achieved only on one isomer each.

Let G be a fullerene graph on n vertices. As before, we denote $\bar{\pi}_6(G) = \frac{1}{n/2-10} \sum_H \pi(H)$ and $\bar{\pi}_5(G) = \frac{1}{12} \sum_P \pi(P)$. In this notation, our observation about the total number of π -electron assigned to hexagonal faces can be compactly stated.

Observation

$$\bar{\pi}_6(C_{60} : 1(D_{5h})) < \bar{\pi}_6(C_{60} : p) < \bar{\pi}_6(C_{60} : 1812(I_h)).$$

We have done computations also for all 8192 isomers of C_{70} and observed the same pattern. It seemed as if the more stable isomers have more of their π -electrons assigned to hexagonal faces. Hence we formulated the following

Hypothesis

$$\bar{\pi}_6(C_n : p) > \bar{\pi}_6(C_n : q) \implies C_n : p \text{ is more stable than } C_n : q.$$

In order to empirically test the hypothesis, we have computed the amount of π -electrons assigned to hexagonal faces for all fullerene isomers with isolated pentagons

on 76, 78, 80, 82 and 84 vertices, as well as for all fullerene isomers on 32, 36 and 40 vertices. We have then taken eleven experimentally verified isolated pentagon isomers and examined how were they ranked by our criterion among all isomers on the same number of vertices. The considered isomers were $C_{60} : 1(I_h)$, $C_{70} : 1(D_{5h})$, $C_{76} : 1(D_2)$, $C_{78} : 1(D_3)$, $C_{78} : 2(C_{2v})$, $C_{78} : 3(C_{2v})$, $C_{80} : 1(D_{5d}), 2(D_2)$, $C_{82} : 3(C_2)$, $C_{84} : 22(D_2)$, $C_{84} : 23(D_{2d})$ [25]. (Here the numbers denote the order in which the isomer appears in spiral algorithm among all IP isomers on the given number of vertices.) In addition, we considered isomers $C_{32} : 6(D_3)$ [5], $C_{36} : 15(D_{6h})$ and $C_{40} : 38(D_2)$, $C_{40} : 39(D_{5d})$ indicated by energy calculations as the most stable non-IP isomers on 32, 36 and 40 vertices. In a way of comparison, we have also looked at the rank given to the same isomers by their bipartivity, a well-performing indicator of stability. The results are shown in Table 1.

Table 1. Ranking of most stable isomers by bipartivity $\beta(C_n)$ and by the number of π -electrons in hexagons $\bar{\pi}_6(C_n)$.

n	Isomer no.	$\beta(C_n)$	$\bar{\pi}_6(C_n)$
60	1	1	1
	1	1	1
	1	2	1
78	1	4	3
	2	3	2
	3	2	4
80	1	1	1
	2	2	2
82	3	7	3
84	22	3	16
	23	4	15
32	6	1	1
36	15	6	15
40	38	2	2
	39	1	1

One can see that two indicators have rather similar performances, with some exceptions: $\bar{\pi}_6(C_n)$ is better than bipartivity for isomers with 82 atoms, while bipartivity outperforms $\bar{\pi}_6(C_n)$ on isomers with 84 and 36 vertices. Hence, the amount of π -electrons assigned to hexagons is not itself sensitive enough to accurately predict stable isomers. Nevertheless, we believe that by closer analysis of local aspects of π -electron distributions we might be able to identify some structural properties indicative of greater stability. In this direction we have investigated various extremal and statistical properties of the

distribution, such as, e.g., the spread of values assigned to faces of different types. The results are not conclusive, but we find them promising.

5 Concluding remarks

In this paper we have computed the patterns of partition of π -electrons among faces of several classes of fullerene graphs. In particular, we have obtained explicit formulas for narrow fullerene nanotubes. We have also computed the number of π -electrons assigned to pentagons and hexagons for large number of fullerene isomers and investigated its potential as a predictor of fullerene stability. The results are not completely satisfactory, but we believe that potentially useful information is contained in local patterns of those distributions.

The methods used here could be adapted to work also for other interesting classes of polyhedral clusters, such as, e.g., the prisms, m -barrels and m -generalized fullerenes considered in ref. [4]. Also, in spite of lot of work done on them, there are still many classes of benzenoid and coronoid compounds that have not been investigated.

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