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COMPUTING THE WIENER INDEX OF AN INFINITE CLASS OF FULLERENES

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ABSTRACT. One the most famous topological index is the Wiener index. It represents the sum of distances of a connected graph and was widely used in correlational studies involving various physical, chemical and biological properties. This topological index was introduced in 1947 by one of the pioneer of this area Harold Wiener. In the present paper, we compute the Wiener index of an infinite class of fullerenes.

Key Words: *Wiener index, Fullerene graphs, Distance matrix*.

INTRODUCTION

Throughout this paper all graphs considered are simple and connected. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The distance $d_G(x, y)$ between two vertices x and y of V(G) is defined as the length of any shortest path in G connecting x and y. The distance number or Wiener index is a topological invariant widely used in studies of structure-property and structure-activity. In the last decades it has been also studied by pure mathematics, see [1 – 5].

The Wiener index was first defined by Wiener to obtain the sum of distances between carbon atoms in saturated hydrocarbons [6] but, Hosoya reformulated the Wiener index respect to the distances between any pair of vertices:

$$W(G) = \sum_{u,v\in V(G)} d_G(u,v).$$

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Some physical properties, such as the boiling point, are related to the geometric structure of the molecules. The first investigations of the Wiener index were made by Harold Wiener in 1947 who realized that there are correlations between the boiling points of paraffin and the structure of the molecules.

The main goal of this paper is to compute the Wiener index of a new infinite class of fullerene graphs, $C_{20n + 60}$. The first member of this class is the well-known IPR fullerene C_{60} with icosahedral symmetry group. Here, our notation is standard and mainly taken from standard books of graph theory [7]. We encourage reader to references [8 - 12] for more details about the concept of Wiener index.

RESULTS AND DISCUSSION

Fullerene graphs are mathematical models of fullerenes, polyhedral molecules made of carbon atoms whose faces are pentagons and hexagons. A fullerene is a planar, 3-regular and 3-connected graph that has only pentagonal and hexagonal faces. Such graphs on n vertices exist for all even $n \geq 24$ and for $n = 20$. By Euler's theorem, one can prove that the number of pentagons and hexagons in a fullerene molecule C_n are 12 and $n/2 - 10$, respectively. The first fullerene discovered by Robert Curl, Harold Kroto and Richard Smalley was buckminsterfullerene C_{60}, [13, 14].

In this section by solving a recursive sequence we determine the Wiener index of a class of fullerene graphs with exactly $20n + 60$ ($n = 0, 1, 2,..$) vertices. Clearly, they have $10n + 90$ edges. We denote this class of fullerenes by $C_{20n + 60}$. The first member of this class can be obtained by putting $n = 0$, see Figure 1.

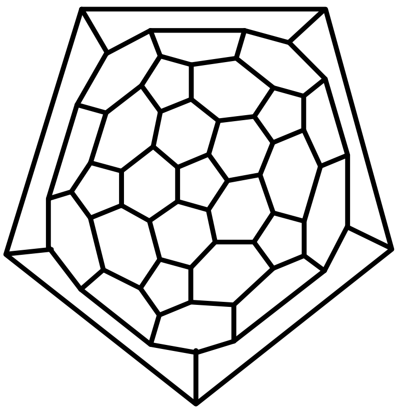

Figure 1. 2 – D graph of fullerene $C_{20n + 60}$, $n = 0$.

In this paper we prove that the Wiener index of this class of fullerenes for $n \geq 8$ is as follows:

$$W\left(C_{20n+60}\right) = 10(40n^3 + 360n^2 + 310n + 663)/3.$$

We can also apply our method to compute the Wiener index in other classes of fullerene graphs. Zhang et al. [15] is described a method to obtain a fullerene graph from a zig–zag or armchair nanotubes.

Denote by $T_Z[n, m]$ a zig–zag nanotube with n rows and m columns of hexagons, see Figure 2. Combine a nanotube $T_Z[n, 10]$ with two copies of the cap B (Figure 3) as shown in Figure 4, the resulted graph being an IPR fullerene, which has $20n + 60$ vertices and exactly $10n + 20$ hexagonal faces.

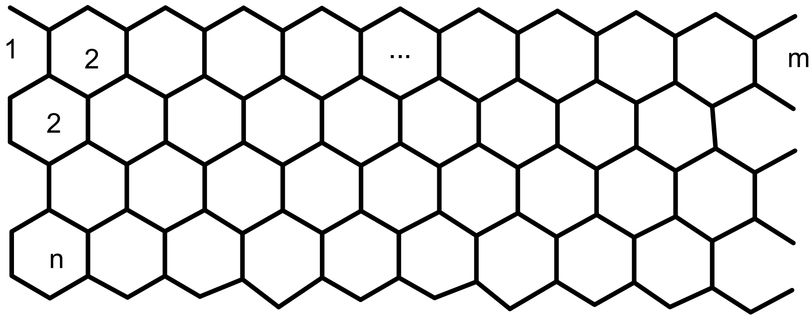

Figure 2. 2 – *D* graph of zig – zag nanotube $T_z[n, m]$, for $m = 10$ and $n = 6$.

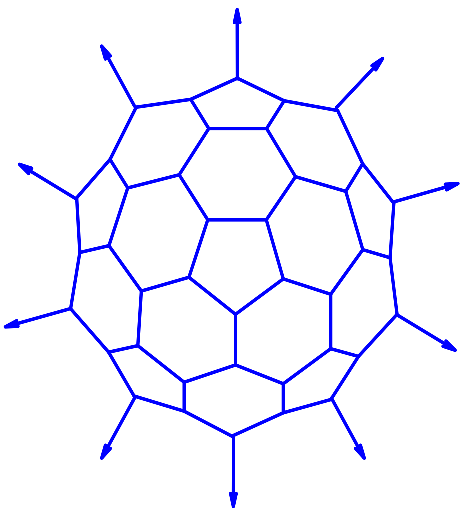

Figure 3. Cap *B.*

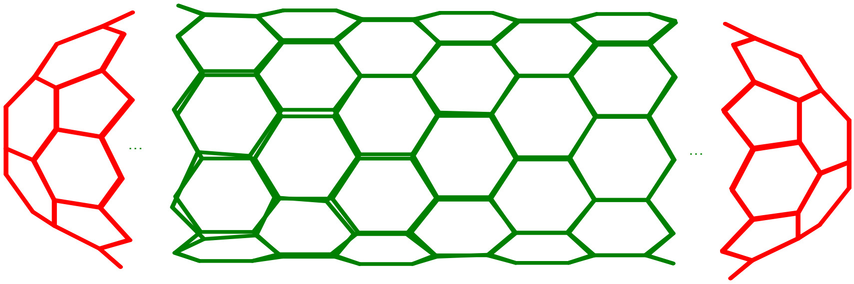

Figure 4. Fullerene C_{20n+60} constructed by combining two copies of caps B and the zigzag nanotube $T_Z[n, 10]$.

A block matrix is a matrix whose entries are again a matrix. In other words, the block matrix can be written in terms of smaller matrices. By using the concept of the block matrices, we stated

Theorem 1. The Wiener index of the $G = T_Z[n, 10]$ nanotube for $n \geq 9$ is calculated as:

$$W(G) = \frac{484}{3}n^3 + 484n^2 + \frac{30371}{3}n - 16819.$$

Proof. According to Figure 5, it is easy to see that $T_Z[n, 10]$ nanotube has $n + 1$ layers of vertices. Let $U = \{u_1, u_2, \ldots, u_{10}\}$ be the vertices of the last row. To compute the Wiener index of this nanotube we make use of a recursive sequence method. Let also U_n be the Wiener index of $G = T_Z[n, 10]$. By using definition of the Wiener index one can see that:

$$\begin{aligned} 2W(G) = U_n &= \sum\nolimits_{x,y\in U} d(x,y) + \sum\nolimits_{x,y\in V\setminus U} d(x,y) \\ &\quad + \sum\nolimits_{x\in V, y\in V\setminus U} d(x,y) \\ &= 90 + U_{n-1} + \sum\nolimits_{x\in V, y\in V\setminus U} d(x,y). \end{aligned}$$

Thus, it is enough to compute the summation $\sum_{x\in V, y\in V\setminus U} d(x,y)$, but by using the symmetry of this graph we have:

$$\sum\nolimits_{x\in V, y\in V\setminus U} d(x,y) = 5[d(u_1) + d(u_2)],$$

where, $d(u_1) = \sum_{v\in V\setminus U} d(u_1, v)$ and $d(u_2)$ can be defined by a similar way. By computing these values one can see that:

$$\begin{aligned} d(u_1) &= 437 + 199(n-2) + 30(n-2)(n-3) + (n-2)(n-3)(n-4), \\ d(u_2) &= 431 + 193(n-2) + 28(n-2)(n-3) + (n-2)(n-3)(n-4). \end{aligned}$$

This implies that $U_{n+1} = U_n + 90 + 5[d(u_1) + d(u_2)] = 10n^3 + 200n^2 + 770n + 1920$. By solving this recursive sequence we have:

$$W(G) = \frac{484}{3}n^3 + 484n^2 + \frac{30371}{3}n - 16819.$$

Finally, by computing the Wiener index of $T_Z[n, 10]$ for $n = 1, \ldots, 8$, as reported in Table 1, the proof is completed.

As a corollary of Theorem 1, we can compute the Wiener index of C_{20n+60} fullerenes as follows:

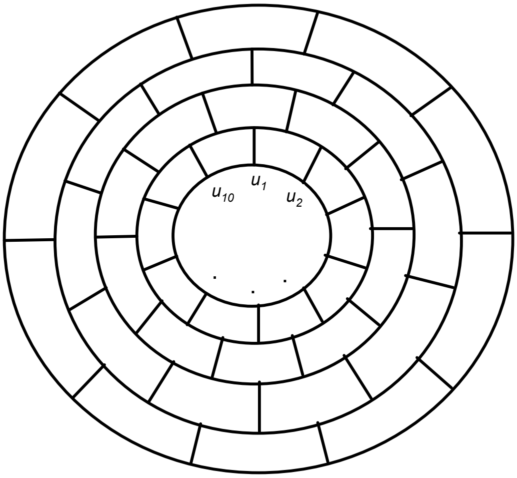

Figure 5. The 2D graph of the nanotube $T_Z[n,10]$.

Table 1. The values of Wiener index for special cases

n	Wiener Index
1	4420
2	14047
3	20400
4	3400
5	52100
6	75320
7	133232
8	177771

Theorem 2.

$$W(C_{20n+60}) = 10(40n^3 + 360n^2 + 310n + 663)/3.$$

Proof. The distance matrix of fullerene C_{20n+60} can be written as a block matrix by the following way, see Figure 4:

Suppose $\{v_1, v_2, \ldots, v_r\}$, $\{u_1, \ldots, u_s\}$ and $\{w_1, \ldots, w_r\}$ be the set of vertices of the left caps, vertices of $T_Z[n, 10]$ and vertices of the second cap, respectively. The distance matrix D can be written in the following form:

$$D = \begin{pmatrix} V & B & W \\ B & U & B \\ W & B & V \end{pmatrix},$$

where V, B and W are distances between vertices of the first cap with the vertices of the first cap, vertices of $T_Z[n, 10]$ and vertices of the right cap. The matrix U is the distance matrix of vertices $\{u_1, \ldots, u_s\}$. In other words, U is the distance matrix of $T_Z[n, 10]$ and this matrix was computed in Theorem 1. It is easy to see that the Wiener index is equal to the half-sum of distances between all pairs of vertices of D. Notice that for any fullerene graph C_{20n+60}, the matrix V is constant. Obviously, the distance matrices B, U and W are dependant to the number of rows in the nanotube $T_Z[n, 10]$. In other words, if W_n and W_{n-1} are the Wiener indices of the fullerenes C_{20n+60} and $C_{20(n-1)+60}$, respectively, then similar to the proof of the Theorem 1, for $n \geq 8$ we have:

$$W_9 - W_8 = 59700,$$
$$W_{10} - W_9 = 69300,$$
$$W_{11} - W_{10} = 79700,$$
$$W_{12} - W_{11} = 90900,$$
$$W_{13} - W_{12} = 102900.$$

By using a recursive sequence, we have the following formula for the Wiener index of fullerene C_{20n+60}:

$$W_n - W_{n-1} = 400n^2 + 1200n + 7700.$$

If we solve this recursive sequence then, the resulted values represent the Wiener index:

$$W\left(C_{20n+60}\right) = 10(40n^3 + 360n^2 + 310n + 663)/3.$$

The Wiener index of C_{20n+60} for $n = 0, \ldots, 7$ is also reported in Table 2 and this completes the proof of the Theorem.

In the third column of table 2, the boiling pont of a series of fullerenes C_{20n+60}, for $n = 0, \ldots, 8$ is listed. These values are obtained by ACD/LABS software [16]. One can see that there is a correlation of R = 0.913 between the values of Wiener index and the boiling point of fullerene C_{20n+60}. This result is mainly because the distances in the molecules are related to the molecular size.

Table 2. The Wiener index of C_{20n+60}, for n = 0, …, 8.

n	W	*BP*
0	11089	849
1	17600	1017
2	30770	1296
3	48625	1417
4	71800	1530
5	100870	1635
6	136455	1735
7	179320	1829
8	230210	1933

CONCLUSIONS

The Wiener index, representing the sum of distances of a connected graph, provided good correlation with some size-dependent physic-chemical or biological properties. In the present paper, we computed, by a recursive method, the Wiener index of an infinite class of fullerenes and tested its correlating ability with the (computed) boiling point of these fullerenes.

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