Computing Wiener Index of C_{12n} Fullerenes

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Abstract. Since the Wiener index has a successful in study of benzenoid systems and boiling point of alkanes it is natural to examine this number for study of fullerenes, which most of its cycles are hexagons. This topological index is equal to the sum of distances between all pairs of vertices of the respective graph. It was introduced in 1947 by one of the pioneer of this area e. g, Harold Wiener who realized that there are correlations between the boiling points of paraffin and the structure of the molecules. The present paper is the first attempt to compute the Wiener index of an infinite class of fullerene. Further, we obtain a correlation between the values of Wiener index and the boiling point of such a fullerene for the first time.

MSC: 05C40, 05C90

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

1. Introduction

The Wiener index is a distance-based topological invariant much used in the study of the structure-property and the structure-activity relationships of various classes of biochemically interesting compounds. It has been also much researched from the purely mathematical viewpoint, giving rise to a vast corpus of literature over the last decades. A number of derivative invariants have been investigated and many formulas for particular classes of graphs were obtained. We refer the reader to a comprehensive survey of results for trees by Dobrynin, Entringer and Gutman as an illustration of that effort [1]. Most of the results on Wiener index are obtained by working on other features of the graph; for more details about Wiener index see [2-5].

The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. In a molecular graph, it is convenient to omit hydrogen atoms. 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. Although the Wiener index was first defined by Wiener to obtain the sum of distances between carbon atoms in saturated hydrocarbons, [6] it was Hosoya who introduced the formula for Wiener index

$$W(G) = \sum d(u,v).$$

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It is the first graph, invariant defined by distance function $d: V(G) \times V(G) \rightarrow \mathbb{R}$ applicable in chemistry. Diudea and his co–workers [7, 8] computed the Wiener index of armchair and zig–zag polyhex nanotubes. After publication of these papers, many researchers work on it, but the Wiener index of fullerene graphs is also an unsolved problem. This is an attempt to solve this problem. Graovac et al, [9] computed the Wiener index of an infinite class of fullerenes, but the methods described here are completely different. Throughout this paper all graphs considered are simple and connected. Our notation is standard and mainly taken from [10 – 12].

2. Main Results and Discussion

A fullerene is any molecule composed entirely of carbon, in the form of a hollow sphere, ellipsoid, or tube. Spherical fullerenes are also called buckyballs and cylindrical ones are called carbon nanotubes or buckytubes. Fullerenes are similar in structure to graphite, which is composed of stacked graphene sheets of linked hexagonal rings; but they may also contain pentagonal rings. 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 to be discovered, and the family's namesake, was buckminsterfullerene C_{60}, made in 1985 by Robert Curl, Harold Kroto and Richard Smalley, [13, 14].

The Wiener Index, or the Wiener number, is one of the quantities associated with a molecular graph that correlates nicely to physical and chemical properties, and has been studied in depth. In other words, some physical properties, such as the boiling point, are related to the geometric structure of the compound. The first investigations into 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. Since then it has become one of the most frequently used topological indices in chemistry, as molecules are usually modeled as undirected graphs, especially trees.

The goal of this paper is to compute the Wiener index of an infinite class of fullerene graphs with exactly $12n$ ($n = 2, 3, \ldots$) vertices. For this we denote this family of fullerenes by C_{12n}. The first member of this family can be obtained by putting $n = 2$, see Figure 1.

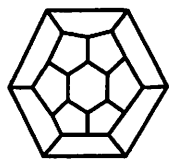

Figure 1: 2 – D graph of fullerene C_{12n}, $n = 2$.

In this paper we prove that the Wiener index of this class of fullerenes for $n \geq 6$ is as follows:

$$W(C_{12}) = 48n^3 + 828n - 1632.$$

The Wiener index of this class of fullerene is computed for the first time in this paper. We can also apply our method to compute the other classes of fullerene graphs. In [15] a method is described to obtain a fullerene graph from a zig – zag or armchair nanotubes. Here by continuing his method we construct an infinite class of

fullerenes and then we obtain its Wiener number. Denoted by $T_Z[m, n]$ means a zig – zag nanotube with m rows and n columns of hexagons, see Figure 2.

An IPR fullerene is a fullerene satisfies in the isolated pentagon rule. In other words, in this structure none of the pentagons make contact with each other, otherwise we say the fullerene is non IPR, see Figure 4.

Combine a nanotube $T_Z[6, n]$ with two copies of caps B (Figure 3) as shown in Figure 4, the resulted graph is a non IPR fullerene, which has $12n$ vertices and exactly $6n$ - 10 hexagonal faces.

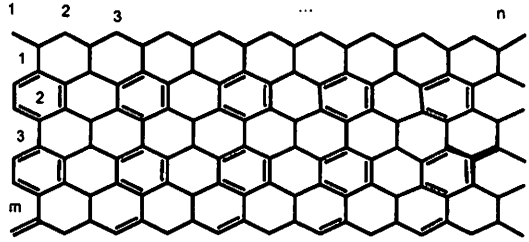

Figure 2. 2 – D graph of zig – zag nanotube $T_z[m, n]$, for $m = 5$, $n = 10$.

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. In the following Theorem the Wiener index of the $G = T_Z[6, n]$ nanotube for $n \geq 7$ is computed, see Figure 5.

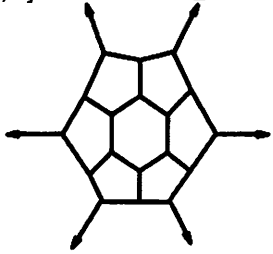

Figure 3. Caps B.

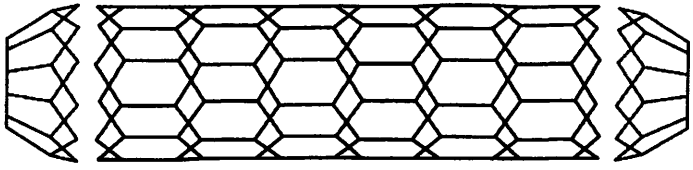

Figure 4. Fullerene C_{12n} constructed by combining two copies of caps B and the zigzag nanotube $T_Z[6, n]$.

Theorem 1.

$$W(G) = 48n^3 - 144n^2 + 972n - 2136.$$

Proof. According to the Figure 5, it is to see that there are $n + 1$ rows of vertices. We suppose the vertices of the last row are $U = \{u_1, u_2, \ldots, u_{12}\}$. To compute the Wiener index of this nanotube we use from a recursive sequence method. Let t_n be

the two times of Wiener index of $G = T_Z[6, n]$. By using definition of the Wiener index and the concept of recursive sequence one can see that:

$$2W(G) = t_n = \sum_{x,y\in U} d(x,y) + \sum_{x,y\in V\setminus U} d(x,y) + 2 \sum_{x\in U, y\in V\setminus U} d(x,y)$$

$$= 432 + t_{n-1} + 2 \sum_{x\in U, y\in V\setminus U} d(x,y).$$

To compute the summation $\sum_{x\in V, y\in V\setminus U} d(x,y)$ by using the symmetry of graph we have

$$\sum_{x\in U, y\in V\setminus U} d(x,y) = 6(d(u_1) + d(u_2)),$$

where, $d(u_1) = \sum_{v\in V\setminus U} d(u_1, v)$ and $d(u_2)$ defines similarly, see Figure 5. By computing these values one can see that:

$$d(u_1) = 12n^2 - 42n + 106,$$

$$d(u_2) = 12n^2 - 30n + 52.$$

This implies that $t_{n+1} = t_n + 432 + 12[d(u_1) + d(u_2)]$. By solving this recursive sequence we have:

$$W(G) = 48n^3 - 144n^2 + 972n - 2136.$$

Finally, by computing the Wiener index of special cases of G, namely $T_Z[6, n]$ for $n = 3,4,5$ as reported in Table 1, the proof is completed.

n	Wiener Index
3	1020
4	2592
5	5136

Table 1. The values of Wiener index for special cases.

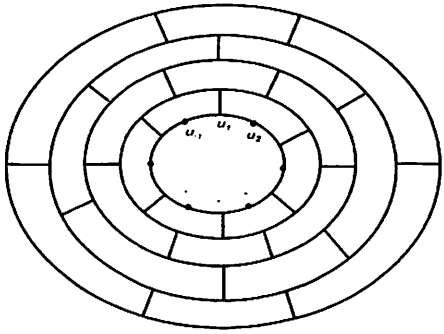

Figure 5. 2 - D graph of nanotube $T_Z[6, n]$.

Theorem 2.

$$W(C_{12}) = 48n^3 + 828n - 1632.$$

Proof. From Figure 4, one can see that the distance matrix of fullerene C_{12n} can be written as a block matrix form as follows:

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 first caps, vertices of $T_Z[6, n]$ and vertices of the second caps, respectively. The distance matrix D can be broken to 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 caps with the vertices of the first caps, vertices of $T_Z[6, n]$ and vertices of the second caps. The matrix U is the distance matrix of vertices $\{u_1, \ldots, u_s\}$. In other words, U is the distance matrix of $T_Z[6, n]$.This matrix computed in Theorem 1. It is easy to see that the Wiener index is equal to the half-sum of distances of the distance matrix D between all pairs of vertices. For any fullerene graph C_{12n}, the matrix V is constant and it is as follows:

$$V = \begin{bmatrix} 0 & 2 & 4 & 6 & 4 & 2 & 1 & 3 & 5 & 5 & 3 & 1 \\ 2 & 0 & 2 & 4 & 6 & 4 & 1 & 1 & 3 & 5 & 5 & 3 \\ 4 & 2 & 0 & 2 & 4 & 6 & 3 & 1 & 1 & 3 & 5 & 5 \\ 6 & 4 & 2 & 0 & 2 & 4 & 5 & 3 & 1 & 1 & 3 & 5 \\ 4 & 6 & 4 & 2 & 0 & 2 & 5 & 5 & 3 & 1 & 1 & 3 \\ 2 & 4 & 6 & 4 & 2 & 0 & 3 & 5 & 5 & 3 & 1 & 1 \\ 1 & 1 & 3 & 5 & 5 & 3 & 0 & 2 & 4 & 6 & 4 & 2 \\ 3 & 1 & 1 & 3 & 5 & 5 & 2 & 0 & 2 & 4 & 6 & 4 \\ 5 & 3 & 1 & 1 & 3 & 5 & 4 & 2 & 0 & 2 & 4 & 6 \\ 5 & 5 & 3 & 1 & 1 & 3 & 6 & 4 & 2 & 0 & 2 & 4 \\ 3 & 5 & 5 & 3 & 1 & 1 & 4 & 6 & 4 & 2 & 0 & 2 \\ 1 & 3 & 5 & 5 & 3 & 1 & 2 & 4 & 6 & 4 & 2 & 0 \end{bmatrix}.$$

The summation of entries of matrix V is 432. Obviously, the distance matrices B, U and W are dependant to the number of rows in the nanotube $T_Z[6, n]$. In other words, if w_n and w_{n-1} be the Wiener indices of the fullerenes C_{12n} and $C_{12(n-1)}$, respectively, then similar to the proof of the Theorem 1, for $n \geq 6$ we have

$$w_7 - w_8 = 6924,$$
$$w_8 - w_9 = 8940,$$
$$w_9 - w_{10} = 11244,$$
$$w_{10} - w_{11} = 13836.$$

By using a recursive sequence one can deduce the following formula for the Wiener index of fullerene C_{12n}:

$$w_n - w_{n-1} = 144n^2 - 144n + 876.$$

By solving this recursive sequence, it is easy to see that

$$W(C_{12}) = 48n^3 + 828n - 1632.$$

The Wiener indices of C_{12n} for $n = 2, \ldots, 8$ are reported in Table 2 and this completes the proof.

As a result of Theorem 2, one can see that there is a correlation between the values of Wiener indices and the boiling points of fullerene C_{12n}. In other words, by

using the values reported in Table 2 the correlation between these numbers is R = 0.868. It should be noted that, this is the first attempt to guess the boiling point of fullerene graphs, respect to the Wiener index. We can also apply our method to compute the Wiener index of other nanostructures.

n	Wiener Number	Boiling Point
2	804	443.5
3	2292	601.7
4	4788	733.6
5	8514	849
6	13704	953
7	20628	1048
8	41184	1136

Table 2. The Wiener indices and boiling points of C_{12n}, for n = 2, ..., 8.

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