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Distance Property of Fullerenes

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ABSTRACT

Fullerenes are closed–cage carbon molecules formed by 12 pentagonal and *n/2 – 10* hexagonal faces, where *n* is the number of carbon atoms. Patrick Fowler in his lecture in MCC 2009 asked about the Wiener index of fullerenes in general. In this paper we respond partially to this question for an infinite class of fullerenes with exactly *10n* carbon atoms. Our method is general and can be applied to fullerene graphs with centrosymmetric adjacency matrix.

Keywords: Fullerene, Wiener index, centrosymmetric matrix.

1. INTRODUCTION

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. A ***fullerene graph*** is the molecular graph of a fullerene molecule. It is a cubic planar graph having pentagonal or hexagonal faces. From Euler's theorem, one can deduce that an *n*–vertex fullerene graph has exactly *12* pentagonal and (*n/2 – 10*) hexagonal faces, where $20 \leq n$ ($\neq 22$) is an even integer. It was elected as the "***Molecule of the Year***" by *Science, 1991*. The C_{60} fullerene was discovered experimentally by Kroto et al. in 1985. It presents a new form of existence of carbon other than graphite, diamond and amorphous carbon [1,2]. We encourage the reader to consult [3–7] for more information on the mathematical properties of fullerene graphs and papers [8–11] for computational techniques.

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Suppose G is a graph and $x, y \in V(G)$, the set of vertices of G. The distance $d(x,y)$ between x and y is defined as the length of a minimal path connecting them. The Wiener index [12] of G, $W(G)$, is summation of all distances between vertices of G. It is the first graph invariant defined by distance function $d: V(G) \times V(G) \longrightarrow \mathbb{R}$ applicable in chemistry. 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.

Diudea and his co–workers [13,14] computed the Wiener index of armchair and zig–zag polyhex nanotubes. After publication of these papers, some researchers published hundreds of papers in the problem of computing distance–based topological indices of nanostructures, but by the best of our knowledge, there is not a published paper which presents exact formula for computing the Wiener index of fullerenes in general.

On the other hand, P. W. Fowler, one of the pioneers of fullerene graphs, in a lecture in MCC 2009 asked about Wiener index of fullerenes in general. This paper is partially response to this question. To do this, we compute exact formula for the Wiener index of an infinite class of fullerenes with exactly $10n$ carbon atoms, Figures 1.

2. COMPUTATIONAL DETAILS

Suppose F is the molecular graph of C_{10n} fullerene, Figure 1. The adjacency matrix of F is an $n \times n$ matrix $A = [a_{ij}]$ defined by $a_{ij} = 1$, if vertices i and j are connected by an edge and, $a_{ij} = 0$, otherwise. The distance matrix $D = [d_{ij}]$ of F is another $n \times n$ matrix in which d_{ij} is the length of a minimal path connecting vertices i and j, $i \neq j$, and zero otherwise.

To compute the Wiener index of F, we first draw F by HyperChem [15] and then apply TopoCluj software [16] of Diudea and his team to compute the adjacency and distance matrices of this graph. Finally, we provide a MATLAB program [17] to calculate the number of pair of vertices in a given distance. This program is accessible from authors upon request. By these numbers and in a simple way, one can compute the Wiener index of molecular graphs under consideration.

We begin by a labeling of F which is important in our calculations. We label a C_{10n} fullerene by method given in the Figure 1.

An $n \times n$ matrix $A = [a_{i,j}]$ is called s*ymmetric* if $a_{ij} = a_{ji}$ and *centrosymmetric* when its entries satisfy $a_{ij} = a_{n-i+1,n-j+1}$ for $1 \leq i,j \leq n$. By above labeling one can see that the distance matrix of our C_{10n} fullerene is centrosymmetric. In next section this help us to partition the distance matrix of F to compute its Wiener index. The main result of this paper is as follows:

Theorem. The Wiener index of C_{10n} is $W(C_{10n}) = 100/3n^3 + 1175/3n - 670$.

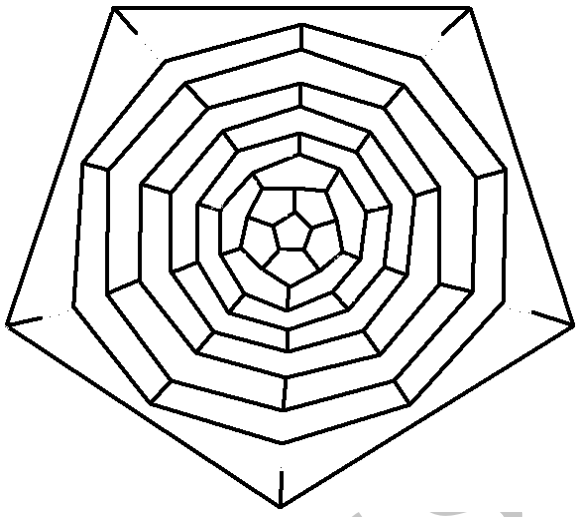

Figure 1. The Schelegel Diagram of a C_{10n} Fullerene Molecule.

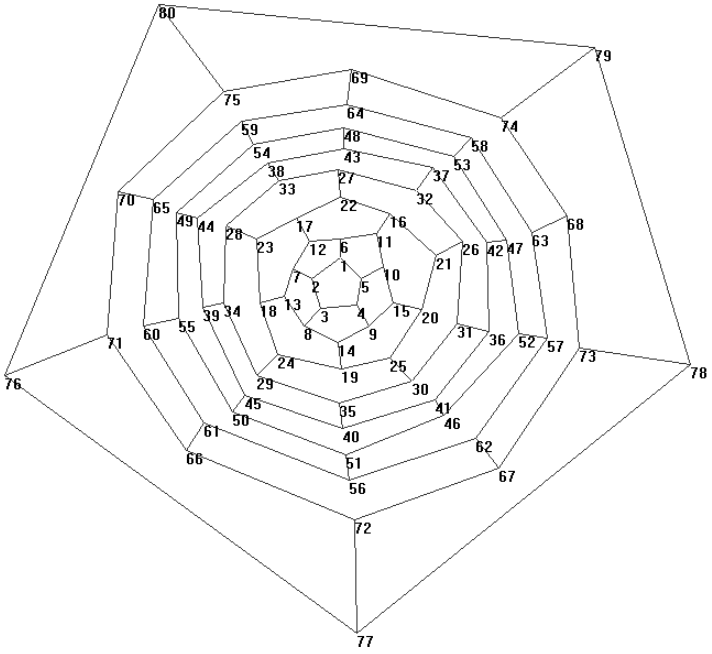

Figure 2. A Labeling of C_{80} Fullerene.

3. MAIN RESULTS AND DISCUSSION

Suppose F denotes the molecular graph of our C_{10n} fullerene and k is a positive integer such that $1 \le k \le diam(G)$, where $diam(G)$ is defined as the maximum distance between vertices of F. The aim of this section is to compute the Wiener index of F. To do this, we first introduce some notions which are crucial in this paper. The number of unordered pairs of vertices u and v of F such that $d_F(u, v) = k$ is denoted by $d(F,k)$. It is clear that $W(F) = \sum_k [k \times d(F,k)]$. Suppose $F[k] = \left[a_{ij}^k\right]$, $1 \le k \le diam(F)$, such that $a_{ij}^k = k$, when $k = d_F(i,j)$, and, 0; otherwise. In what follows fifteen 5×5 matrices are presented by which it is possible to partition the distance matrix of F. These are as follows:

$$M = \begin{bmatrix} 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \end{bmatrix} \quad B = \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 \end{bmatrix} \quad J^* = \begin{bmatrix} 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 1 \end{bmatrix} \quad D = \begin{bmatrix} 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \end{bmatrix}$$

$$E = \begin{bmatrix} 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \end{bmatrix} \quad Y = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 \end{bmatrix} \quad F = \begin{bmatrix} 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \end{bmatrix} \quad J' = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \end{bmatrix}$$

$$C = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 \end{bmatrix} \quad I = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \quad I_1 = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix} \quad I_2 = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{bmatrix}$$

$$I_3 = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix} \quad I_4 = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix} \quad J = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

We have to prove these matrices are the building blocks of $D[F]$. To do this, we consider the $2n \times 2n$ block matrix $D[F] = [A_{ij}]$, where A_{ij} is a zero 5×5 matrix or one of the matrices presented in Table 1. If $10 \le k \le diam(F)$, then $A_{ij} = 0$, $1 \le i, j \le k$, and $A_{k+1,1} =$

$A_{k+2,2} = \ldots = A_{2n,2n-k} = k \times J$ and the other blocks are zero. Since the matrix is symmetric, $A_{1,k+1} = A_{2,k+2} = \ldots = A_{2n-k,2n} = k \times J$. We have,

$$F(k) = k \times \begin{bmatrix} 0_{5k\times 5k} & J_{5\times 5} & & & & & & & \\ J_{5\times 5} & & J_{5\times 5} & & & & & & \\ & J_{5\times 5} & & \ddots & & & & & \\ & & \ddots & & \ddots & & & & \\ & & & \ddots & & J_{5\times 5} & & & \\ & & & & J_{5\times 5} & & J_{5\times 5} & & \\ & & & & & J_{5\times 5} & & & \end{bmatrix}_{2n\times 2n}$$

There are (2n – k) blocks equal to J. Thus,

$$D(k,C_{10n}) = 25(2n - k) = 50n - 25k. \qquad (1)$$

On the other hand, we have:

$$F(9) = 9 \times \begin{bmatrix} 0 & \ldots & 0 & J & & & & & & & \\ \vdots & & & 0 & J & & & & & & \\ \vdots & & & I_1 & \ddots & J & & & & & \\ 0 & & 0 & & 0 & \ddots & J & & & & \\ J & 0 & I_4 & & & I_1 & \ddots & \ddots & & & \\ & J & \ddots & 0 & & & 0 & \ddots & & & \\ & & \ddots & \ddots & I_4 & & & \ddots & \ddots & & \\ & & & \ddots & \ddots & 0 & & & \ddots & \ddots & \\ & & & & \ddots & \ddots & \ddots & & & J & \\ & & & & & \ddots & \ddots & \ddots & I_1 & & J \\ & & & & & & \ddots & 0 & & 0 & \\ & & & & & & & I_4 & & & 0 \\ & & & & & & J & 0 & 0 & & \\ & & & & & & & J & 0 & 0 & \end{bmatrix}$$

$$F(8) = 8 \times \begin{bmatrix} 0 & \ldots & 0 & I_1 & J & & & & & & \\ \vdots & & & I_1 & 0 & J & & & & & \\ \vdots & & & & I_1 & 0 & J & & & & \\ 0 & & & & & \ddots & \ddots & \ddots & & & \\ I_4 & I_4 & & & & & \ddots & \ddots & \ddots & & \\ J & 0 & I_4 & & & & & \ddots & \ddots & \ddots & \\ & J & 0 & \ddots & & & & & \ddots & \ddots & \ddots \\ & & J & \ddots & \ddots & & & & & \ddots & J \\ & & & \ddots & \ddots & \ddots & & & & I_1 & 0 & J \\ & & & & \ddots & \ddots & \ddots & & & & I_1 & I_1 \\ & & & & & \ddots & \ddots & & & & & 0 \\ & & & & & & & \ddots & & & & \\ & & & & & & J & 0 & I_4 & & & \\ & & & & & & & J & I_4 & 0 & & \end{bmatrix}$$

$$F(7)=7\times\begin{bmatrix}
0 & . & . & 0 & 0 & I_1 & J' & & & & & & \\
. & & & 0 & 0 & I_1 & 0 & J & & & & & \\
. & & & & I_2 & 0 & C & 0 & J' & & & & \\
0 & & & & & 0 & . & I_1 & . & J & & & \\
0 & 0 & I_3 & & & & I_2 & . & C & . & . & & \\
I_4 & I_4 & 0 & 0 & & & & 0 & . & . & . & . & \\
J^* & 0 & B & 0 & I_3 & & & & . & . & . & 0 & J \\
 & J & 0 & I_4 & . & 0 & & & & . & . & C & 0 & J' \\
 & & J^* & . & B & . & . & & & & 0 & 0 & I_1 & I_1 \\
 & & & . & . & . & . & . & & & & I_2 & 0 & 0 \\
 & & & & . & . & . & . & . & & & & 0 & 0 \\
 & & & & & . & & B & . & I_3 & & & & 0 \\
 & & & & & & J & 0 & I_4 & 0 & 0 & & & \\
 & & & & & & & J^* & I_4 & 0 & 0 & 0 & &
\end{bmatrix}$$

Suppose k=9. Then $A_{ij} = 0$, for $1 \le i,j \le 9$, and $A_{10,1} = A_{11,2} = \ldots = A_{2n,2n-9} = 9J$. Also, $A_{10,3} = A_{12,4} = \ldots = A_{2n-2,2n-9} = 9I_4$ and the other blocks are zero. So, the number of J,s are 2n–9 and number of I_4,s are n–5. Hence,

$$D(9,C_{10n}) = 25\times(2n-9) + 5\times(n-5) = 55n - 250. \qquad (2)$$

We now compute F(4), F(5) and F(6) as follows:

$$F(6)=6\times\begin{bmatrix}
0 & . & . & 0 & 0 & 0 & C & J' & & & & & \\
. & & & & I_2 & 0 & C & 0 & J' & & & & \\
. & & & & & I_2 & 0 & C & 0 & J' & & & \\
0 & & & & & & 0 & . & . & . & & & \\
0 & I_3 & & & & & & . & . & . & . & & \\
0 & 0 & I_3 & & & & & & . & . & . & . & \\
B & B & . & . & & & & & & . & . & . & J' \\
J^* & 0 & B & . & . & & & & & & . & C & C \\
 & J^* & 0 & B & . & . & & & & & I_2 & 0 & 0 \\
 & & . & . & . & . & . & & & & & I_2 & 0 \\
 & & & . & . & . & . & . & & & & & 0 \\
 & & & & . & . & B & . & . & & & & \\
 & & & & & . & 0 & B & 0 & I_3 & & & \\
 & & & & & & J^* & B & 0 & o & 0 & &
\end{bmatrix}$$

$$F(5)=5\times\begin{bmatrix}
0 & . & . & 0 & 0 & I_2 & C & Y & & & & & \\
. & & & & I_2 & 0 & C & 0 & J' & & & & \\
. & & & & & D & . & F & 0 & Y & & & \\
0 & & & & & & I_2 & . & C & . & . & & \\
0 & I_3 & & & & & & D & . & F & . & . & \\
I_3 & 0 & D & & & & & & . & . & . & J' & \\
B & B & 0 & I_3 & & & & & & . & . & 0 & Y \\
X & 0 & E & . & D & & & & & & . & C & C \\
 & J^* & 0 & B & . & . & & & & & D & 0 & I_2 \\
 & & X & . & E & . & . & & & & & I_2 & 0 \\
 & & & . & . & . & . & . & & & & & 0 \\
 & & & & . & . & . & . & D & & & & \\
 & & & & & J^* & 0 & B & 0 & I_3 & & & \\
 & & & & & & X & B & I_3 & 0 & 0 & &
\end{bmatrix}$$

$$F(4) = 4\times\begin{bmatrix} 0 & 0 & I_2 & M & Y & & & & & \\ 0 & D & 0 & M & 0 & . & & & & \\ I_3 & 0 & D & . & . & . & . & & & \\ E & E & o & . & . & . & . & . & & \\ X & 0 & E & & . & . & . & . & . & \\ & . & . & . & & . & . & . & 0 & Y \\ & & . & . & . & & . & . & M & M \\ & & & . & . & . & & D & 0 & I_2 \\ & & & & . & 0 & E & & D & 0 \\ & & & & & X & E & I_3 & & 0 \end{bmatrix}.$$

If k=8, then $A_{ij} = 0,\ 1 \le i,j \le 7,\ A_{8,1} = A_{8,2} = A_{9,3} = A_{10,4} = \ldots = A_{2n-2,2n-8} = A_{2n-1,2n-7} = 8I_4,\ A_{9,1} = A_{10,2} = \ldots = A_{2n,2n-8} = 8J$ and the other blocks are zero. Hence, there are 2n–6 sub–matrix I_4 and 2n–8 sub–matrix J. So,

$$D(8,C_{10n}) = 5\times(2n-6) + 25\times(2n-8) = 60n-230. \quad (3)$$

We now assume that k = 7. Then $A_{ij} = 0,\ 1 \le i,j \le 5,\ A_{6,3} = A_{8,5} = A_{10,7} = A_{12,9} = \ldots = A_{2n-2,2n-5} = 7I_3,\ A_{7,1} = A_{7,2} = A_{9,4} = A_{11,6} = A_{13,8} = \ldots = A_{2n-1,2n-6} = A_{2n,2n-6} = 7I_4,\ A_{8,3} = A_{10,5} = A_{12,7} = \ldots = A_{2n-2,2n-7} = 7B,\ A_{8,1} = A_{10,3} = A_{12,5} = \ldots = A_{2n,2n-7} = 7J^*,\ A_{9,2} = A_{11,4} = A_{13,6} = \ldots = A_{2n-1,2n-8} = 7J$ and the other blocks are zero. One can see that the number of J, J^*, B, I_4 and I_3 are (n–4) , (n–3), (n–4) , (n–1) and (n–3), respectively. Therefore,

$$D(7,C_{10n}) = 25\times(n-4) + 20\times(n-3) + 10\times(n-4) + 5\times(n\times1) + 5\times(n-3) = 65n-220. \quad (4)$$

If k = 6 then $A_{ij} = 0,\ 1 \le i,j \le 3,\ A_{4,2} = A_{5,3} = A_{6,4} = A_{7,5} = \ldots = A_{2n-1,2n-3} = 6I_3,\ A_{6,1} = A_{6,2} = A_{7,3} = A_{8,4} = \ldots = A_{2n-1,2n-5} = A_{2n,2n-5} = 6B,\ A_{7,1} = A_{8,2} = A_{9,3} = \ldots = A_{2n,2n-6} = 6J^*$ and the other blocks are zero. On the other hand, the number of J^*, B and I_3 are (2n–6), (2n–4) and (2n–4), respectively. Therefore,

$$D(6,C_{10n}) = 20\times(2n-6) + 10\times(2n-4) + 5(2n-4) = 70n-180. \quad (5)$$

Suppose k = 5. Then $A_{ij} = 0,\ 1 \le i,j \le 2,\ A_{4,1} = A_{3,2} = A_{5,4} = A_{7,6} = A_{9,8} = \ldots = A_{2n-1,2n-2} = 5I_3,\ A_{5,1} = A_{5,2} = A_{7,4} = A_{9,6} = \ldots = A_{2n-1,2n-4} = A_{2n,2n-4} = 5B$, and $A_{7,2} = A_{9,4} = A_{11,6} = \ldots = A_{2n-1,2n-6} = 5J^*,\ A_{4,3} = A_{6,5} = A_{8,7} = \ldots = A_{2n-2,2n-3} = 5D,\ A_{6,3} = A_{8,5} = \ldots = A_{2n-2,2n-5} = 5E,\ A_{6,1} = A_{8,3} = \ldots = A_{2n,2n-5} = 5X$ and the other blocks are zero. Also, the number of J^*, B, D, E, X and I_3 are (n–3), n, (n–2), (n–3), (n–2) and (n+1), respectively. Therefore

$$D(5,C_{10n}) = 20\times(n-3) + 10n + 10\times(n-2) + 10\times(n-3) + 15\times(n-2) + 5\times(n+1) = 70n-135. \quad (6)$$

Finally, we assume that k = 4. Then $A_{11} = 0$, $A_{2,2} = A_{3,3} = A_{4,4} = A_{5,5} = \ldots = A_{2n-1,2n-1} = 4D$, $A_{3,1} = A_{2n,2n-2} = 4I_3$, $A_{4,1} = A_{4,2} = A_{5,3} = A_{6,4} = \ldots = A_{2n-1,2n-3} = A_{2n,2n-3} = 4E$, $A_{5,1} = A_{6,2} = A_{7,3} = \ldots = A_{2n,2n-4} = 4X$ and the other blocks are zero. On the other hand, the number of D, E, X and I_3 are (2n–2), (2n–2), (2n–4) and 2, respectively. Therefore,

$$D(4,C_{10n}) = 10\times(n-1) + 10\times(2n-2) + 15\times(2n-4) + 5\times 2 = 60n-80. \quad (7)$$

We are now ready to state our main result:

Theorem. The Wiener index of C_{10n} is computed as follows:

$$W(C_{10n}) = \frac{100}{3}n^3 + \frac{1175}{3}n - 670.$$

Proof. By above calculations, $diam(C_{10n}) = 2n - 1$.

Apply Eq. (1) and $W(F) = \sum_k [k \times d(F,k)]$, we have $\sum_{i=10}^{i=2n-1} i \times D(i, C_{10n}) = \sum_{i=10}^{2n-1} i \times (50n - 25i) = \frac{100}{3}n^3 - \frac{6775}{3}n + 7125$. On the other hand, $D(1,C_{10n}) = 15n$, $D(2,C_{10n}) = 30n$ and $D(3,C_{10n}) = 45n-30$, where $n \geq 2$. Also, by Eqs. (2–7), $\sum_{i=1}^{9} i \times D(i, C_{10n}) = 2650n - 7795$. This completes our proof. ■

4. CONCLUDING REMARKS

In the MCC 2009, P. W. Fowler asked about formula for computing Wiener index of fullerenes. In this paper a class of fullerene graphs with exactly 10n vertices is considered. A matrix method is presented by which it is possible to compute the Wiener index of Fullerenes. We believe that our matrix method is general and can be applied to other class of fullerenes. By our calculation one can easily compute the Hosoya polynomial of C_{10n} fullerenes. Moreover, our calculations suggest the following conjectures:

Conjecture 1: The adjacency matrix of fullerene graphs is centrosymmetric.

Conjecture 2: If X_n is an infinite sequence of fullerenes then $W(X_n)$ is a polynomial of degree 3.

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