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The Wiener and Wiener Polarity Indices of a Class of Fullerenes with Exactly 12n Carbon Atoms

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Abstract

In this paper, the Wiener and Wiener polarity indices of a class of fullerenes with exactly 12n carbon atoms is computed. It is shown that the possibility of labeling of the fullerene molecule such that the resulting molecular graph is centrosymmetric plays a central role in our method. Some open questions are also presented.

1. Introduction

A ***molecular graph*** is a simple graph modeled a molecule M. In this graph atoms are vertices and chemical bonds are edges of the graph. In such a 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. It is well-known that an n–vertex fullerene graph has exactly *12* pentagonal and ($n/2 - 10$) hexagonal faces, where $20 \le n$ ($\neq 22$) is an

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even integer.

The most applicable fullerene is the ***Buckminsterfullerene*** C_{60}. It is the smallest fullerene in which no two pentagons share an edge. The buckminsterfullerene was discovered experimentally by Kroto et al. in 1985. It is no doubt that this was the most impressive events in carbon chemistry during the last 25 years [1,2]. When a new material is discovered, one of the fundamental works is the development of the necessary mathematics. The most important works on mathematics of fullerenes was done by Patrick Fowler [3−7]. We encourage the interested readers to consult [8−12] for more information on the mathematical properties of fullerene graphs as well as its computational techniques.

Suppose G is a connected graph and $x, y \in V(G)$, where $V(G)$ denotes the set of all vertices in G. The ***distance*** $d(x,y)$ between x and y is defined as the length of a minimal path connecting x and y. The maximum distance between two vertices of G is called the ***diameter*** of G, denoted by $diam(G)$. The ***Wiener index*** of G, $W(G)$, is defined as the summation of all distances between vertices of G [13].

The polynomial $H(G,x) = \Sigma_{x \neq y} x^{d(x,y)}$ is called the ***Hosoya polynomial*** of G. The name is used in honor of Haruo Hosoya, who discovered a new formula for the Wiener index in terms of graph distance [14]. We refer the interested readers to papers [15−21] for more information on this topic.

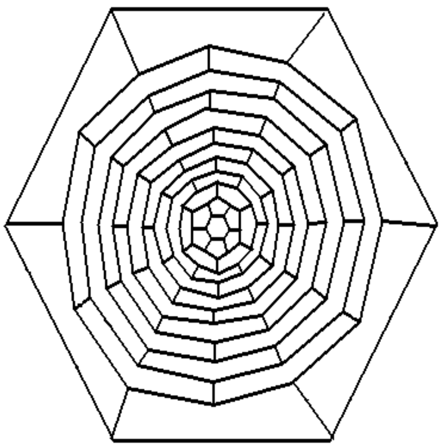

Figure 1. The Schelegel Diagram of a C_{12n} Fullerene Molecule.

2. Computational Details

Suppose F is the molecular graph of C_{12n} fullerene, as shown in 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 equal to the distance between vertices i and j for $i \neq j$, and zero otherwise.

To compute the Wiener index of F, we first draw F by HyperChem [22] and then apply TopoCluj software [23] of Diudea and his team to compute the adjacency and distance matrices of this graph. Finally, we provide a MATLAB program [24] 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 and Hosoya polynomial of the molecular graph under consideration. We begin with a labeling of F, which is important in our calculations. We label a C_{12n} fullerene by the method given in the Figure 2.

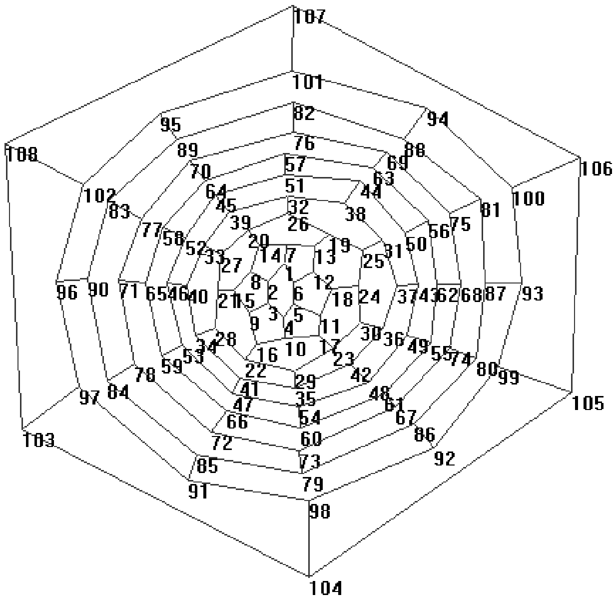

Figure 1. A Labeling of C_{108} Fullerene.

In an earlier paper, two of the present authors computed the Wiener index of a class of fullerenes with exactly 10n carbon atoms [25]. In this paper, we continue this program to compute the Wiener index of a class of fullerenes with exactly 12n carbon atoms, say C_{12n}. In [26, Theorem 2], it is proved that $diam(C_{12n}) = 2n - 1$, when $n \geq 5$. Moreover, $diam(C_{24}) = 5$, $diam(C_{36}) = 7$, $diam(C_{48}) = 8$ and $diam(C_{60}) = 10$.

To proceed further, we need some algebraic notions. Suppose that $A = [a_{i,j}]$ is an $n \times n$ matrix. A is called *symmetric* if $a_{ij} = a_{ji}$ and *centrosymmetric* if $a_{ij} = a_{(n-i+1)(n-j+1)}$, for $1 \leq i,j \leq n$. By considering above labeling, one can see that the distance matrix of our C_{12n} fullerene is centrosymmetric. In the next section, this fact helps us to partition the distance matrix of F in such a way that to compute its Hosoya polynomial.

3. Main Results and Discussion

Suppose F denotes the molecular graph of our C_{12n} fullerene and k is a positive integer such that $1 \leq k \leq diam(G)$, 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 $(d/dx)H(F,x)|_{x=1} = W(F) = \sum_k[k \times d(F,k)]$. Suppose $F[k] = [a_{ij}^k]$, $1 \leq k \leq diam(F)$, such that $a_{ij}^k = k$, when $k = d_F(i,j)$, and, 0; otherwise. In what follows twenty-one 6×6 matrices are presented by which it is possible to partition the distance matrix of F. In fact, those are the building blocks of $D[F]$.

$$E_1 = \begin{bmatrix} 0&1&0&0&0&0\\ 0&0&1&0&0&0\\ 0&0&0&1&0&0\\ 0&0&0&0&1&0\\ 0&0&0&0&0&1\\ 1&0&0&0&0&0 \end{bmatrix} \quad E_2 = \begin{bmatrix} 0&0&1&0&0&0\\ 0&0&0&1&0&0\\ 0&0&0&0&1&0\\ 0&0&0&0&0&1\\ 1&0&0&0&0&0\\ 0&1&0&0&0&0 \end{bmatrix} \quad E_3 = \begin{bmatrix} 0&0&0&1&0&0\\ 0&0&0&0&1&0\\ 0&0&0&0&0&1\\ 1&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&1&0&0&0 \end{bmatrix} \quad E_4 = \begin{bmatrix} 0&0&0&0&1&0\\ 0&0&0&0&0&1\\ 1&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&1&0&0&0\\ 0&0&0&1&0&0 \end{bmatrix}$$

$$E_5 = \begin{bmatrix} 0&0&0&0&0&1\\ 1&0&0&0&0&0\\ 0&1&0&0&0&0\\ 0&0&1&0&0&0\\ 0&0&0&1&0&0\\ 0&0&0&0&1&0 \end{bmatrix} \quad B_1 = \begin{bmatrix} 0&1&1&0&0&0\\ 0&0&1&1&0&0\\ 0&0&0&1&1&0\\ 0&0&0&0&1&1\\ 1&0&0&0&0&1\\ 1&1&0&0&0&0 \end{bmatrix} \quad B_2 = \begin{bmatrix} 0&0&1&1&0&0\\ 0&0&0&1&1&0\\ 0&0&0&0&1&1\\ 1&0&0&0&0&1\\ 1&1&0&0&0&0\\ 0&1&1&0&0&0 \end{bmatrix} \quad B_3 = \begin{bmatrix} 0&0&0&1&1&0\\ 0&0&0&0&1&1\\ 1&0&0&0&0&1\\ 1&1&0&0&0&0\\ 0&1&1&0&0&0\\ 0&0&1&1&0&0 \end{bmatrix}$$

$$B_4 = \begin{bmatrix} 0&0&0&0&1&1\\ 1&0&0&0&0&1\\ 1&1&0&0&0&0\\ 0&1&1&0&0&0\\ 0&0&1&1&0&0\\ 0&0&0&1&1&0 \end{bmatrix} \quad B_5 = \begin{bmatrix} 0&1&0&1&0&0\\ 0&0&1&0&1&0\\ 0&0&0&1&0&1\\ 1&0&0&0&1&0\\ 0&1&0&0&0&1\\ 1&0&1&0&0&0 \end{bmatrix} \quad B_6 = \begin{bmatrix} 0&0&1&0&1&0\\ 0&0&0&1&0&1\\ 1&0&0&0&1&0\\ 0&1&0&0&0&1\\ 1&0&1&0&0&0\\ 0&1&0&1&0&0 \end{bmatrix} \quad B_7 = \begin{bmatrix} 0&0&0&1&0&1\\ 1&0&0&0&1&0\\ 0&1&0&0&0&1\\ 1&0&1&0&0&0\\ 0&1&0&1&0&0\\ 0&0&1&0&1&0 \end{bmatrix}$$

$$B_8=\begin{bmatrix}0&1&0&0&1&0\\0&0&1&0&0&1\\1&0&0&1&0&0\\0&1&0&0&1&0\\0&0&1&0&0&1\\1&0&0&1&0&0\end{bmatrix}\quad B_9=\begin{bmatrix}0&0&1&0&0&1\\1&0&0&1&0&0\\0&1&0&0&1&0\\0&0&1&0&0&1\\1&0&0&1&0&0\\0&1&0&0&1&0\end{bmatrix}\quad G_1=\begin{bmatrix}1&0&0&0&1&1\\1&1&0&0&0&1\\1&1&1&0&0&0\\0&1&1&1&0&0\\0&0&1&1&1&0\\0&0&0&1&1&1\end{bmatrix}\quad G_2=\begin{bmatrix}1&1&1&0&0&0\\0&1&1&1&0&0\\0&0&1&1&1&0\\0&0&0&1&1&1\\1&0&0&0&1&1\\1&1&0&0&0&1\end{bmatrix}$$

$$C_1=\begin{bmatrix}1&0&0&1&1&1\\1&1&0&0&1&1\\1&1&1&0&0&1\\1&1&1&1&0&0\\0&1&1&1&1&0\\0&0&1&1&1&1\end{bmatrix}\quad C_2=\begin{bmatrix}1&1&1&1&0&0\\0&1&1&1&1&0\\0&0&1&1&1&1\\1&0&0&1&1&1\\1&1&0&0&1&1\\1&1&1&0&0&1\end{bmatrix}\quad J_1=\begin{bmatrix}1&0&1&1&1&1\\1&1&0&1&1&1\\1&1&1&0&1&1\\1&1&1&1&0&1\\1&1&1&1&1&0\\0&1&1&1&1&1\end{bmatrix}\quad J_2=\begin{bmatrix}1&1&1&1&1&0\\0&1&1&1&1&1\\1&0&1&1&1&1\\1&1&0&1&1&1\\1&1&1&0&1&1\\1&1&1&1&0&1\end{bmatrix}$$

$$J=\begin{bmatrix}1&1&1&1&1&1\\1&1&1&1&1&1\\1&1&1&1&1&1\\1&1&1&1&1&1\\1&1&1&1&1&1\\1&1&1&1&1&1\end{bmatrix}$$

Table 1: The Building Blocks of D[F], when $1 \le k \le diam(F)$.

Consider the $2n \times 2n$ block matrix $D[F] = [A_{ij}]$, where A_{ij} is a zero 6×6 matrix or one of the matrices presented in Table 1. If $12 \le k \le diam(F)$, 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,

$$F(k) = k \times \begin{bmatrix} 0_{6k\times 6k} & J_{6\times 6} & & & & \\ J_{6\times 6} & & J_{6\times 6} & & & \\ & J_{6\times 6} & & \cdot & & \\ & & \cdot & & \cdot & \\ & & & \cdot & & J_{6\times 6} \\ & & & J_{6\times 6} & & J_{6\times 6} \\ & & & & J_{6\times 6} & \end{bmatrix}_{2n\times 2n},$$

There are (2n – k) block J. Thus,

$$D(k,C_{12n}) = 36(2n-k) = 72n - 36k. \qquad (1)$$

$$F(11)=11\times\begin{bmatrix}
0 & . & 0 & 0 & J & & & & & & & & & \\
. & & & 0 & 0 & J & & & & & & & & \\
. & & & & E_5 & . & J & & & & & & & \\
0 & & & 0 & & 0 & . & J & & & & & & \\
J & 0 & E_1 & & & & E_5 & . & . & & & & & \\
 & J & . & 0 & & & & 0 & & . & & & & \\
 & & . & . & E_1 & & & & . & & . & & & \\
 & & & . & . & 0 & & & & . & & . & & \\
 & & & & . & . & . & & & & . & & J & \\
 & & & & & . & . & . & & & & E_5 & 0 & J \\
 & & & & & & . & . & 0 & & & & 0 & 0 \\
 & & & & & & & . & . & E_1 & & & & 0 \\
 & & & & & & & & J & 0 & 0 & & & \\
 & & & & & & & & & J & 0 & 0 & &
\end{bmatrix}$$

$$F(10)=10\times\begin{bmatrix}
0 & . & . & 0 & E_4 & J & & & & & & & & \\
. & & & & E_4 & 0 & J & & & & & & & \\
. & & & & & E_4 & 0 & J & & & & & & \\
0 & & & & & & . & . & . & & & & & \\
E_1 & E_1 & 0 & & & & & . & . & . & & & & \\
J & 0 & E_1 & & & & & & . & . & . & & & \\
 & J & 0 & . & & & & & & . & . & . & & \\
 & & J & . & . & & & & & & . & . & J & \\
 & & & . & . & . & & & & & & E_4 & 0 & J \\
 & & & & . & . & . & & & & & & E_4 & E_4 \\
 & & & & & . & . & & & & & & & 0 \\
 & & & & & & & . & & & & & & \\
 & & & & & & & J & 0 & E_1 & & & & \\
 & & & & & & & & J & E_1 & 0 & & &
\end{bmatrix}$$

Table 2: The Building Blocks of D[F], when k = 10 or 11.

Suppose k = 11. Then $A_{ij} = 0$, for $1 \leq i, j \leq 11$, and $A_{12,1} = A_{13,2} = \ldots = A_{2n,2n-11} = 11J$. Also, $A_{12,3} = A_{14,5} = \ldots = A_{2n-2,2n-11} = 11E_1$ and the other blocks are zero. So, the number of J,s are 2n–11 and number of E_1's are n–6. Hence,

$$D(11,C_{12n}) = 36\times(2n-11) + 6\times(n-6) = 78n - 432. \qquad (2)$$

Suppose k=10. Then $A_{ij} = 0$, for $1 \leq i,j \leq 9$, and $A_{10,1} = A_{10,2} = A_{11,3} = A_{12,4} = \ldots = A_{2n-1,2n-9} = A_{2n,2n-9} = 10E_1$. Also, $A_{11,1} = A_{12,2} = \ldots = A_{2n,2n-10} = 10J$ and the other blocks are zero. So, the number of J,s are 2n–10 and number of E_1,s are 2n–8. Hence,

$$D(10,C_{12n}) = 36\times(2n-10) + 6\times(2n-8) = 84n - 408. \qquad (3)$$

$$F(9)=9\times\begin{bmatrix}
0 & . & . & 0 & 0 & E_5 & J_2 & 0 & . & . & & & & 0\\
. & & & 0 & 0 & E_5 & 0 & J & 0 & . & . & & & \\
. & & & & E_4 & 0 & B_4 & & J_2 & . & . & . & & \\
0 & & & 0 & 0 & 0 & 0 & E_5 & & . & . & . & . & .\\
0 & 0 & E_2 & 0 & . & . & E_4 & . & B_4 & & . & . & . & .\\
E_1 & E_1 & . & 0 & . & . & 0 & 0 & & . & & . & 0 & .\\
J_1 & 0 & B_1 & 0 & E_2 & . & & 0 & . & & . & & J & 0\\
0 & J & . & E_1 & . & 0 & & & & . & & . & & J_2\\
. & 0 & J_1 & . & B_1 & 0 & . & & & & . & & E_5 & \\
. & . & 0 & J & . & . & . & . & & & & E_4 & & 0\\
. & . & . & 0 & . & . & . & . & 0 & & & & 0 & .\\
. & . & . & . & 0 & . & . & . & . & E_2 & 0 & . & . & 0\\
 & & . & . & & 0 & J & 0 & E_1 & 0 & 0 & & & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & J_1 & E_1 & 0 & . & . & & 0
\end{bmatrix}$$

$$F(8)=8\times\begin{bmatrix}
0 & . & . & 0 & 0 & 0 & B_4 & J_2 & & & & & & \\
. & & & & E_4 & . & B_4 & 0 & J_2 & & & & & \\
. & & & & 0 & E_4 & 0 & B_4 & . & . & & & & \\
0 & & & & & 0 & . & . & . & . & . & & & \\
0 & E_2 & & & & . & & . & . & . & . & . & & \\
0 & 0 & E_2 & & & & & & . & . & . & . & . & \\
B_1 & B_1 & 0 & . & & & & & & . & . & . & 0 & J_2\\
J_1 & 0 & . & . & . & & & & & & . & . & B_4 & B_4\\
0 & J_1 & . & . & . & . & & & & & & . & . & 0\\
. & & . & . & . & . & . & & & & & & E_4 & 0\\
 & & & . & . & . & . & . & & & & & & 0\\
 & & & & . & . & B_1 & . & . & & & & & \\
 & & & & & . & 0 & B_1 & 0 & E_2 & & & & \\
0 & & & & & 0 & j_1 & B_1 & 0 & 0 & 0 & & & 0
\end{bmatrix}$$

$$F(7)=7\times\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & E_4 & B_4 & C_2 & 0 & . & . & . & & 0\\
0 & 0 & 0 & 0 & E_4 & 0 & B_4 & 0 & J_2 & . & & & & \\
0 & 0 & . & E_3 & 0 & B_3 & . & B_7 & . & C_2 & & & & \\
0 & 0 & E_3 & . & 0 & 0 & E_4 & . & B_4 & . & J_2 & & & .\\
0 & E_2 & 0 & 0 & . & E_3 & . & . & . & . & . & . & & .\\
E_2 & 0 & B_2 & 0 & E_3 & . & 0 & . & . & . & . & . & . & 0\\
B_1 & B_1 & 0 & E_2 & . & 0 & . & . & . & . & . & . & . & C_2\\
C_1 & 0 & B_5 & 0 & . & . & . & . & . & . & . & . & B_4 & B_4\\
0 & J_1 & . & B_1 & 0 & . & . & . & . & . & . & B_3 & 0 & E_4\\
. & & C_1 & . & . & . & . & . & . & . & 0 & . & E_4 & 0\\
. & & & J_1 & . & . & . & . & . & 0 & . & E_3 & 0 & 0\\
. & & & & . & . & B_5 & . & B_2 & . & E_3 & . & 0 & 0\\
 & & & & & J_1 & . & B_1 & . & E_2 & 0 & 0 & 0 & 0\\
0 & & & & & 0 & C_1 & B_1 & E_2 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}$$

Table 3: Building Blocks of D[F], when k = 7, 8 or 9.

Suppose k=9. Then $A_{ij} = 0$, for $1 \le i,j \le 7$, and$A_{8,3}=A_{10,5}=\dots A_{2n-3,2n-7}=9E_2$ and $A_{9,1} = A_{9,2} = A_{11,4} = A_{13,6} = \dots = A_{2n,2n-8} = A_{2n-1,2n-8} = 9E_1$. Also, $A_{10,3} = A_{12,5} = \dots = A_{2n-2,2n-9} = 9B_1$ and $A_{10,1}=A_{12,3}=\dots=A_{2n,2n-9}=9J_1$ and $A_{11,2}=A_{13,4}=\dots=A_{2n-1,2n-10}=9J$ other blocks are zero. So, the number of J,s are (n–5) and number of J_1,s are (n–4)and the number of B_1,s are (n-5).and the number of E_1,s are (n-2) and the number of E_2,s are (n-4) Hence,

$$D(9,C_{12n}) = 36(n-5) + 30(n-4)+12(n-5)+6(n-2)+6(n-4) = 90n - 396. \quad (4)$$

Suppose k=8. Then $A_{ij} = 0$, for $1 \le i, j \le 5$, and$A_{6,2}=A_{7,3}=\ldots A_{2n-1,2n-5}=8E_2$ and $A_{8,1} = A_{8,2} = A_{9,3}=A_{10,4}= \ldots = A_{2n,2n-7}=A_{2n-1,2n-7} = 8B_1$. Also, $A_{9,1} = A_{10,2} = \ldots = A_{2n,2n-8} = 8J_1$ other blocks are zero. So, the number of J_1's are (2n−8), the number of B_1's are (2n−6) and the number of E_2's are (2n-6). Hence,

$$D(8,C_{12n}) = 30(2n-8) + 12(2n-6)+6(2n-6) = 96n - 348. \quad (5)$$

Suppose k=7. Then $A_{ij} = 0$, for $1 \le i, j \le 3$, and $A_{4,3}=A_{6,5}=\ldots A_{2n-2,2n-3}=7E_3$ and $A_{5,2} = A_{7,4} = A_{9,6}=A_{11,8}= \ldots = A_{2n-2,2n-4}=A_{6,1} = A_{2n,2n-5}= 7E_2$. Also, $A_{6,3} = A_{8,5} = \ldots = A_{2n-3,2n-5} = 7B_2$, $A_{7,1}=A_{7,2}=A_{9,4}=A_{11,6}=\ldots=A_{2n,2n-6}=A_{2n-1,2n-6}=7B_1$, $A_{8,3}=A_{10,5}=A_{12,7}=\ldots=A_{2n-2,2n-7}=7B_5$, $A_{8,1}=A_{10,3}=A_{12,5}=\ldots=A_{2n,2n-7}=7C_1$, $A_{9,2}=A_{11,4}=\ldots=A_{2n-1,2n-8}=7J_1$, other blocks are zero. So, the number of J_1's are (n−4), the number of B_1's are (n−1) and the number of C_1's are (n-3). Moreover, the number of E_2's are (n), the number of B_5's are (n-4), the number of B_2's are (n-3) and the number of E_3's are (n-2). Hence,

$$D(7,C_{12n}) = 30(n-4) + 12(n-1)+24(n-3)+6(n)+12(n-4)+12(n-3)+6(n-2) = 102n - 300 \quad (6).$$

If k = 6 then $A_{ij} = 0$, $1 \le i,j \le 2$, $A_{3,3} = A_{4,4} = A_{5,5} = A_{6,6} = \ldots = A_{2n-2,2n-2} = 6E_3$, $A_{4,2} = A_{5,3} = A_{6,4} = A_{7,5} = \ldots = A_{2n-1,2n-3} = 6B_2$,and $A_{5,1}=A_{2n,2n-4}=6E_2$ and $A_{6,1} = A_{6,2} = A_{7,3} = A_{8,4}= \ldots = A_{2n,2n-5}=A_{2n-1,2n-5} = 6B_5$ and $A_{7,1}=A_{8,2}=\ldots=A_{2n,2n-6}=6C_1$ the other blocks are zero. On the other hand, the number of E_3,s , B_2,s , E_2,s , B_5,s and C_1,s are (n-2),(2n−4),((2) , (2n-4) and (2n−6), respectively. Therefore,

$$D(6,C_{12n}) = 6(n-2)+12(2n-4)+2(6)+12(2n-4)+24(2n-6)=102n-240. \quad (7)$$

Suppose k = 5. Then $A_{2,2} = A_{n-1,n-1} = E_3$,$A_{3,2} = A_{5,4} = A_{7,6} = \ldots = A_{2n-1,2n-2} = B_2$, $A_{4,1} = A_{2n,2n-4} = B_2$, $A_{4,3} = A_{6,5} = A_{8,7} = \ldots = A_{2n-3,2n-4} = B_6$, $A_{5,2} = A_{7,4} = A_{9,6} = \ldots = A_{2n-1,2n-5} = B_5$, $A_{5,1} = A_{2n,2n-5} = B_5$, $A_{6,3} = A_{8,5} = A_{10,7} = \ldots = A_{2n-3,2n-6} = B_8$, $A_{6,1} = A_{8,3} = A_{10,5} = \ldots = A_{2n,2n-5} = G_1$ and $A_{7,2} = A_{9,4} = A_{11,6} = \ldots = A_{2n-1,2n-6} = C_1$, and the other blocks are zero. Also, the number of E_3, B_2, B_6, B_5, B_8,G_1 and C_1 are (1), (n+1), (n−2), (n), (n−3), (n-2) and (n-3), respectively. Therefore

$$D(5,C_{12n}) = 6(1)+12(n+1)+12(n-2)+12(n)+12(n-3)+18(n-2)+24(n-3)=90n-150 \quad (8)$$

$$F(6) = 6 \times \begin{bmatrix}
0 & 0 & 0 & 0 & E_4 & B_7 & C_2 & 0 & & & & & & \\
0 & 0 & 0 & B_3 & 0 & B_7 & 0 & C_2 & 0 & & & & & \\
0 & 0 & E_3 & . & B_3 & . & B_7 & . & C_2 & . & & & & \\
0 & B_2 & . & E_3 & . & . & . & . & . & . & . & & & \\
E_2 & 0 & B_2 & . & . & . & . & . & . & . & . & . & & \\
B_5 & B_5 & 0 & . & . & . & . & . & . & . & . & . & . & \\
C_1 & 0 & B_5 & . & . & . & . & . & . & . & . & . & . & 0 \\
0 & C_1 & 0 & . & . & . & . & . & . & . & . & . & 0 & C_2 \\
 & . & 0 & 0 & . & . & . & . & . & . & . & . & B_7 & B_7 \\
 & & . & . & . & . & . & . & . & . & . & B_3 & 0 & E_4 \\
 & & & . & . & . & . & . & . & . & E_3 & . & B_3 & 0 \\
 & & & & . & . & 0 & . & . & B_2 & . & E_3 & . & 0 \\
 & & & & & . & 0 & 0 & B_5 & 0 & B_2 & 0 & 0 & 0 \\
0 & & & & & & 0 & C_1 & B_5 & E_2 & 0 & 0 & 0 & 0
\end{bmatrix}$$

$$F(5) = 5 \times \begin{bmatrix}
0 & 0 & 0 & B_3 & B_7 & G_2 & 0 & 0 & . & . & & & & 0 \\
0 & E_3 & B_3 & 0 & B_7 & 0 & C_2 & 0 & . & & & & & \\
0 & B_2 & 0 & B_6 & 0 & B_9 & . & G_2 & 0 & . & & & & \\
B_2 & 0 & B_6 & 0 & B_3 & 0 & B_7 & . & C_2 & . & . & & & \\
B_5 & B_5 & 0 & B_2 & 0 & B_6 & & B_9 & . & . & . & . & & \\
G_1 & 0 & B_8 & 0 & B_6 & 0 & & & . & . & . & . & . & \\
0 & C_1 & 0 & B_5 & 0 & B_2 & . & & & . & . & . & C_2 & 0 \\
. & 0 & G_1 & 0 & B_8 & 0 & . & . & & & . & . & 0 & G_2 \\
. & . & 0 & C_1 & 0 & B_5 & . & . & . & & & D & B_7 & B_7 \\
. & . & . & 0 & G_1 & 0 & . & . & . & & & & I_2 & B_3 \\
. & . & . & . & . & C_1 & . & . & . & . & & & & 0 \\
 & . & . & . & . & . & . & . & B_8 & . & B_6 & & & \\
 & . & . & . & . & . & . & C_1 & 0 & B_5 & 0 & B_2 & E_3 & \\
0 & . & . & . & . & . & . & 0 & G_1 & B_5 & B_2 & 0 & 0 & 0
\end{bmatrix}$$

$$F(4) = 4 \times \begin{bmatrix}
0 & E_3 & B_3 & B_9 & G_2 & 0 & . & . & . & 0 \\
E_3 & B_6 & 0 & B_9 & 0 & . & 0 & . & . & 0 \\
B_2 & 0 & B_6 & 0. & B_9 & 0 & . & 0 & . & 0 \\
B_8 & B_8 & 0 & . & . & . & 0 & . & . & 0 \\
G_1 & 0 & B_8 & 0 & . & . & . & . & . & 0 \\
0 & . & . & . & . & . & . & . & 0 & G_2 \\
. & . & . & . & . & . & . & . & B_9 & B_9 \\
. & . & . & . & . & . & . & B_6 & 0 & B_3 \\
. & . & . & . & . & 0 & B_8 & 0 & B_6 & E_3 \\
0 & . & . & . & 0 & G_1 & B_8 & B_2 & E_3 & 0
\end{bmatrix}$$

Table 4: Building Blocks of D[F], when k = 4, 5 or 6.

Finally, we assume that k = 4. Then $A_{11} = 0$, $A_{2,2} = A_{3,3} = A_{4,4} = A_{5,5} = \ldots = A_{2n-1,2n-1} = 4B_6$, $A_{2,1}=A_{n,n-1}=E_3$, $A_{3,1}=A_{n,n-2}=B_2$, $A_{4,1}=A_{4,2} = A_{5,3} = A_{6,4} = \ldots = A_{2n-1,2n-4} = A_{2n,2n-4} = 4B_8$, $A_{5,1} = A_{6,2} = A_{7,3} = \ldots = A_{2n,2n-5} = 4G_1$ and the other blocks are zero. On the other hand, the number of B_6, E_3, B_2 , B_8 and G_1 are (n-1), (2), (2) and (2n-4), respectively. Therefore,

$$D(4,C_{12n}) = 12(n-1) + 6(2) + 12(2) + 18(2n-4) = 72n-72. \quad (9)$$

The Wiener polarity index of the molecular graph G, $W_P(G)$, is defined as $W_p(G) = d(G,3)$ [13,28]. In the best of our knowledge, the Wiener had some information about the applicability of this topological index. We now apply our calculations to compute the Wiener and Wiener polarity index of the fullerene graph C_{12n}.

Theorem. The Wiener and Wiener polarity indices of C_{12n}, $n > 5$, are computed as follows:

$$W(C_{12n}) = 48n^3 + 828n - 1632 \ \& \ \ W_P(C_{12n}) = 54n - 30.$$

Proof. By Eq. (1), the well-known relation $W(F) = \sum_k[k \times d(F,k)]$ and the fact that $diam(C_{12n}) = 2n - 1$, we deduce that

$$\sum_{i=12}^{i=2n-1} i \times D(i, C_{12n}) = \sum_{i=10}^{2n-1} i \times (72n - 36i) = 48n^3 - 4764n + 18216.$$

On the other hand, $D(1,C_{12n}) = 18n$, $D(2,C_{12n}) = 36n$ and $D(3,C_{12n}) = 54n-30$, where $n \geq 2$. Also, by Eqs. (2)– (9), we obtain $\sum_{i=1}^{11} i \times D(i, C_{12n}) = 5592n - 19848$. 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 Hosoya polynomial and then the Wiener index of this class 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_{12n} 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 cubic polynomial.

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