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Wiener Index of a New Type of Nanostar Dendrimer

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ABSTRACT

Let G be a molecular graph. The Wiener index of G is defined as the summation of all distances between vertices of G. In this paper, an exact formula for the Wiener index of a new type of nanostar dendrimer is given.

Keywords: Nanostar dendrimer, molecular graph, Wiener index.

1. INTRODUCTION

The nanostar dendrimer is part of a new group of macromolecules that appear to be photon funnels just like artificial antennas. The topological study of these macromolecules is the aim of this article.

Throughout this paper graph means finite simple graph without multiple edges and loops. The set of vertices and edges of a graph G are denoted by V(G) and E(G), respectively. The distance $d_G(u,v)$ (d(u,v) for short) between two vertices u, v ∈ V(G) of a connected graph G is the length of a shortest path connecting them. Suppose $\mathfrak{I}$ denotes the set of all finite graphs and $\mathfrak{R}$ is the set of real numbers. A map Top from $\mathfrak{I}$ into $\mathfrak{R}$ is called a topological index, if Top(H) = Top(G), for all pairs (H,G) of isomorphic graphs.

The concept of "topological index" was first proposed by Hosoya [1] for characterizing the topological nature of a graph. Such graph invariants are usually related to the distance function d(−,−). Recently, this part of Mathematical Chemistry named "Metric Graph Theory". The first topological index of this type was proposed in 1947 by the chemist Harold Wiener [2]. It is defined as the sum of all distances between vertices of the

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graph under consideration. In the last meeting of International Academy of Mathematical Chemistry, professor Roberto Todeschini announced that he and his team improved MOLE db – Molecular Descriptors Data Base [3,4] for working with more than thousand molecular descriptors. The MOLE db is a free on-line database constituted of 1124 molecular descriptors calculated on 234773 molecules allows the user to search for a specific group of molecules and analyze the corresponding values of molecular descriptors and also to save in an output file the values of a block of molecular descriptors calculated on a group of molecules.

Suppose G is a graph with the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. In Metric Graph Theory, the distance matrix of G is defined as $D(G) = [d_{ij}]$, where $d_{ij} = d(v_i, v_j)$. We refer to the book of Harary [5] for describing the connectivity in directed graphs.

The problem of computing the topological indices of nanostructures was raised by Diudea and his co-authors. In some research papers [6–12] they computed the Wiener index of nanotubes and tori. In [13,14], the authors presented some methods for calculation of the Wiener index and resonance energy of benzenoid systems which are extendable to nano–materials. In recent years, some authors worked on computing the Wiener, PI, Schultz and Szeged indices of the chemical graphs of some nano–materials [15–25].

This paper addresses the problem of computing the Wiener index of an infinite class of nanostar dendrimers. Our notation is standard and taken mainly from the standard books of graph theory.

2. RESULT AND DISCUSSION

Throughout this paper NS[n] denotes the molecular graph of a nanostar dendrimer with exactly n generation, Figures 1–2, [27]. At first, we introduce two concepts which are important in our calculations. Suppose G and H are graphs such that $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. Then we call H to be a subgraph of G. H is called isometric, if for each $x, y \in V(H)$, $d_H(x,y) = d_G(x,y)$.

To calculate the Wiener index of NS[n], we first notice that $|V(NS[n])| = 8.2^{n+1} + 52$. In Figure 3, four isometric subgraphs of NS[n] are depicted. From this figure, it is clear that NS[n] is constructed from the subgraphs isomorphic to B and the core, Figure 2. To compute the Wiener index of NS[n], we calculate matrices WA_1, WA_2, WA_3 and WB which are the Wiener matrices of the subgraphs A_1, A_2, A_3 and B, respectively. Suppose D_i and D_i' are 8×8 and 8×68 matrices in which each entry is equal to i and M is the Wiener matrix of the core.

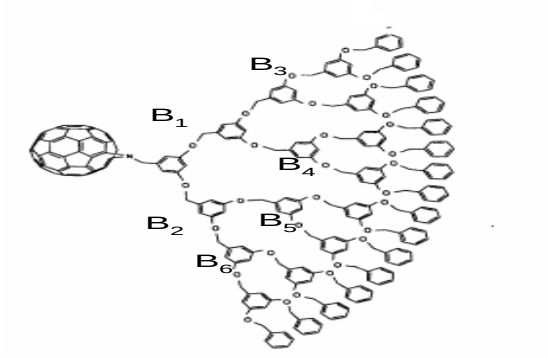

Figure 1. The Molecular Graph of NS[1].

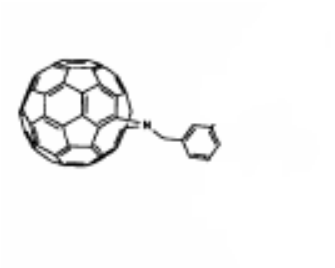

Figure 2. The Core of NS[n].

To construct the Wiener matrix of NS[n], it is enough to calculate the distance matrix between a subgraph isomorphic to B and core, distance matrix between two subgraphs isomorphic to B (see A_2 and A_3 in Figure 3) and the Wiener matrix of the core. The distance matrix between a subgraph isomorphic to B and core is equal to the sum of the Wiener matrix of the subgraph A_1, WA_1, and the matrix D_i', where $i = l(P) - 1$ such that P is a minimum path connecting a vertex of core to a vertex of B and l(P) denotes the length of P. We now calculate the distance matrix between two subgraphs isomorphic to B. To do this, we assume that B_1 and B_2 are two subgraphs isomorphic to B and P is a minimum path connecting a vertex of B_1 to a vertex of B_2. Obviously, there are two separate cases that one of the end vertices of P is a vertex of a hexagon of NS[n] or two end vertices of P are not belong to a hexagon. In the first case, we calculate the distance matrix $D(B_1,B_2)$ between B_1 and B_2. It is enough to compute the following three matrices which are important for calculation of the Wiener matrix of NS[n].

$$B_{Win}=\begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 & 4 & 5 \\ 1 & 0 & 1 & 2 & 3 & 2 & 3 & 4 \\ 2 & 1 & 0 & 1 & 2 & 3 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 \\ 1 & 2 & 3 & 2 & 1 & 0 & 3 & 4 \\ 4 & 3 & 2 & 1 & 2 & 3 & 0 & 1 \\ 5 & 4 & 3 & 2 & 3 & 4 & 1 & 0 \end{bmatrix} \quad A_{2Win}=\begin{bmatrix} 5 & 4 & 3 & 4 & 5 & 6 & 2 & 1 \\ 6 & 5 & 4 & 5 & 6 & 7 & 3 & 2 \\ 7 & 6 & 5 & 6 & 7 & 8 & 4 & 3 \\ 8 & 7 & 6 & 7 & 8 & 9 & 5 & 4 \\ 9 & 8 & 7 & 8 & 9 & 10 & 6 & 5 \\ 10 & 9 & 8 & 9 & 10 & 11 & 7 & 6 \\ 9 & 8 & 7 & 8 & 9 & 10 & 6 & 5 \\ 8 & 7 & 6 & 7 & 8 & 9 & 5 & 4 \end{bmatrix} \quad A_{3Win}=\begin{bmatrix} 6 & 5 & 4 & 3 & 4 & 5 & 2 & 1 \\ 7 & 6 & 5 & 4 & 5 & 6 & 3 & 2 \\ 8 & 7 & 6 & 5 & 6 & 7 & 4 & 3 \\ 9 & 8 & 7 & 6 & 7 & 8 & 5 & 4 \\ 8 & 7 & 6 & 5 & 6 & 7 & 4 & 3 \\ 7 & 6 & 5 & 4 & 5 & 6 & 3 & 2 \\ 10 & 9 & 8 & 7 & 8 & 9 & 6 & 5 \\ 11 & 10 & 9 & 8 & 9 & 10 & 7 & 6 \end{bmatrix}$$

For example, the distance matrix of the nanostar dendrimer NS[2], is as follows:

	C	B_1	B_2	B_3	B_4	B_5	B_6
C	C	A_1	A_1	A_1+D_5'	A_1+D_5'	A_1+D_5'	A_1+D_5'
B_1	A_1	B	A_2+D_3	A_3	A_3	A_2+D_8	A_2+D_8
B_2	A_1	A_2+D_3	B	A_2+D_8	A_2+D_8	A_3	A_3
B_3	A_1+D_5'	A_3	A_2+D_8	B	A_2+D_3	A_2+D_{13}	A_2+D_{13}
B_4	A_1+D_5'	A_3	A_2+D_8	A_2+D_3	B	A_2+D_{13}	A_2+D_{13}
B_5	A_1+D_5'	A_2+D_8	A_3	A_2+D_{13}	A_2+D_{13}	B	A_2+D_3
B_6	A_1+D_5'	A_2+D_8	A_3	A_2+D_{13}	A_2+D_{13}	A_2+D_3	B

Table 1. The Wiener Matrix of NS[2].

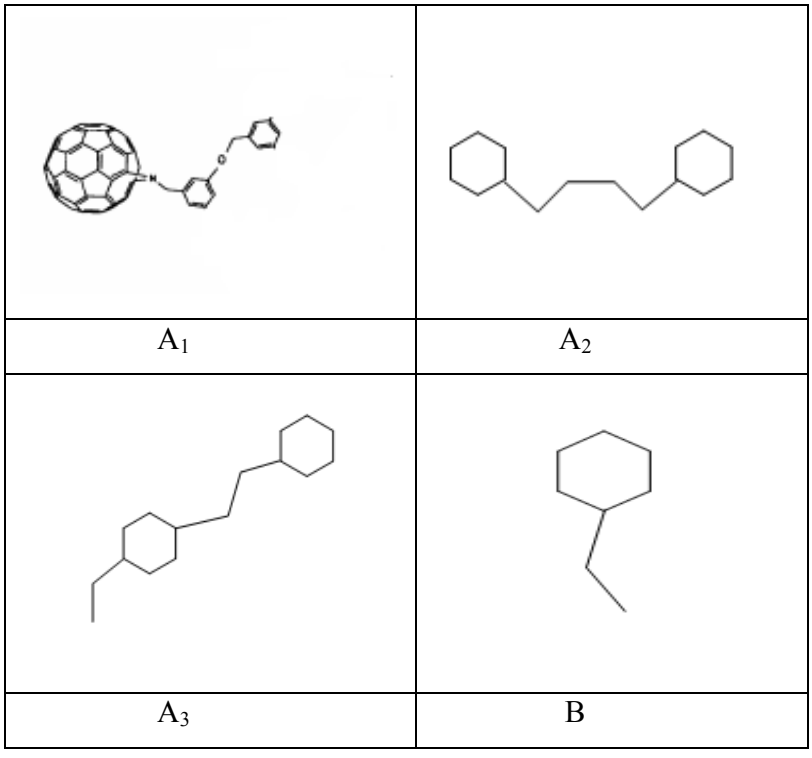

Figure 3. Some Subgraphs of NS[n].

We are now ready to state our main result.

Theorem. The Wiener index of NS[n] is computed as follows:

$$Win(NS[n]) = 9435 + 5488.2^n + 5600.n.2^n - 2624.4^n + 1280.4^n.n.$$

Proof. By definition of A_1, A_2, A_3, B, M, D_i and D_i' and above calculations, we have in the following table the number of appearance of submatrices in the distance matrix of NS[n] are computed.

$s_1 = 64.\sum_{j=3}^{n} 2^{2(j-1)}.(13+(j-2)10)\sum_{i=j}^{n} 2^{i-j}$ $= \frac{-7808}{9}.4^n + \frac{1280}{3}.4^n.n - 768.2^n + \frac{29696}{9}$
$s_2 = 368.\sum_{j=3}^{n} 2^{2(j-1)}\sum_{i=j}^{n} 2^{i-j} = \frac{832}{3}.4^n - 1664.2^n + \frac{6656}{3}$
$s_3 = 64.\sum_{j=3}^{n} 2^i = 2^{n+1} - 8$
$s_4 = 416.\sum_{j=3}^{n}\sum_{i=1}^{j-1}(2^j - 2^{j-i}).2^i = 416.(-n.2^{(n+1)} - \frac{16}{3} + \frac{1}{3}.2^{2n+2})$
$s_5 = 368.\sum_{j=3}^{n}\sum_{i=1}^{j-1}(2^{j-i}).2^i = 368.(n-2).2^{n+1}$
$s_6 = 64.\sum_{k=3}^{n}\sum_{j=1}^{k-2}\sum_{i=1}^{j} 2^{k+1+i-1}.(5k+3)+10(i-1)-5(j-1)$ $= \frac{-23296}{9}.4^n + \frac{2560}{3}.4^n.n + 768.2^n + 2432.n.2^n - 640.2^n n^2 + \frac{16384}{9}.$
$s_7 = 64.\sum_{j=3}^{n}\sum_{i=1}^{j-1}(2^j).(5(i-1)) + 64\sum_{j=3}^{n}\sum_{i=1}^{j-1} 2^j.(5i+3)$ $= 3072.2^n - 2176.2^n.n + 640.2^n.n^2 - 5120$ $68.8.\sum_{i=3}^{n} 2^i.(5(i-1)) = -8160.2^{n+1} + 2720.2^{n+1}.(n+1)$
$s_8 = 68.8\sum_{i=3}^{n} 2^i.(5(i-1)) = -8160.2^{n+1} + 2720.2^{n+1}.(n+1)$
$s_9 = 6600.\sum_{i=3}^{n} 2^i = 6600(2^{n+1} - 8)$
$s_{10} = (2.3.64 + 4.13.64).\sum_{i=3}^{n} 2^{i-2} = 3712.(\frac{1}{4}.2^{n+1} - 2) = 928.2^{n+1} - 7424$
$s_{11} = (6.416).\sum_{i=3}^{n} 2^{i-2} = 624.2^{n+1} - 4992$

By a simple calculation with Maple, one can see that

$$s_1 + s_2 + ...s_{11} = 9435 + 5488 .2^n + 5600 .n.2^n - 2624 .4^n + 1280 .4^n.n.$$

Therefore,

$$Win(NS[n]) = 75163 + 64.(2^{n+1} - 8) + (\frac{-7808}{9}.4^n + \frac{1280}{3}.4^n.n - 768.2^n + \frac{29696}{9}) + (\frac{832}{3}.4^n - 1664.2^n$$
$$+ \frac{6656}{3}) + (\frac{-23296}{9}.4^n + \frac{2560}{3}.4^n.n + 768.2^n + 2432n.2^n - 640.2^n.n^2 + \frac{16384}{9}) + (624.2^{n+1} - 4992)$$
$$+ (928.2^{n+1} - 7424) + (3072.2^n - 2176.2^n.n + 640.2^n.n^2 - 5120) + (-416.n.2^{n+1} - \frac{6656}{3}) + \frac{416}{3}.2^{2n+2}$$
$$+ (368.(n-2).2^{n+1}) + (-8160.2^{n+1} + 2720.2^{n+1}.(n+1)) + 6600.2^{n+1} - 8$$
$$= 9435 + 5488.2^n + 5600.n.2^n - 2624.4^n + 1280.4^n.n$$

3. CONCLUSIONS

In this paper a novel method for computing the Wiener matrix of chemical graphs are presented. If a molecular graph G can be decomposed into cycles and paths then a similar method as given in the paper can be applied to compute the Wiener matrix of G. So, the method given in this paper is general for such molecular graphs.

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