Eccentric Connectivity and Augmented Eccentric Connectivity indices of N-branched Phenylacetylenes Nanostar Dendrimers

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ABSTRACT

A topological index of a molecular graph G is a numeric quantity related to G which is invariant under symmetry properties of G. Let G be a molecular graph. The eccentric connectivity index $\xi(G)$ is defined as $\xi(G) = \sum_{u\in V(G)} \deg(u)\,\varepsilon(u)$, where $deg(u)$ denotes the degree of vertex u in G and $\varepsilon(u)$ is the largest distance between u and any other vertex v of G. The augmented eccentric connectivity index, ${}^{A}\xi(G)$ is defined as ${}^{A}\xi(G) = \sum_{u\in V(G)} \frac{M(u)}{\varepsilon(u)}$, where $M(u)$ denotes the product of degrees of all neighbors of vertex u. In this paper, exact formulas for the eccentric connectivity and augmented eccentric connectivity indices of an infinite family of nanostar dendrimer are computed.

Keywords: Eccentric connectivity index, augmented eccentric connectivity index, nanostar.

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1 INTRODUCTION

A graph G consists of a set of vertices $V(G)$ and a set of edges $E(G)$. A chemical graph is a graph such that, each vertex represents an atom of the molecule, and covalent bonds between atoms are represented by edge between the corresponding vertices. If the vertices $u, v \in V(G)$ are connected by an edge e then we write $e = uv$. A topological index is a numeric quantity from the structure of a graph which is invariant under automorphisms of the graph under consideration. One of the most famous topological indices is the Wiener index was introduced by Harold Wiener [1]. The Wiener index of G is the sum of distances between all unordered pairs of vertices of G, $W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v)$.

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Nanostar dendrimer is a kind of nanostructure. One type of nanostar dendrimers is N-branched phenylacetylenes and it is shown by NSB[n], some topological indices were obtained in [2]. In Figure 1, the molecular graph of NSB[1] and in Figure 2, the molecular graph of NSB[2] are shown.

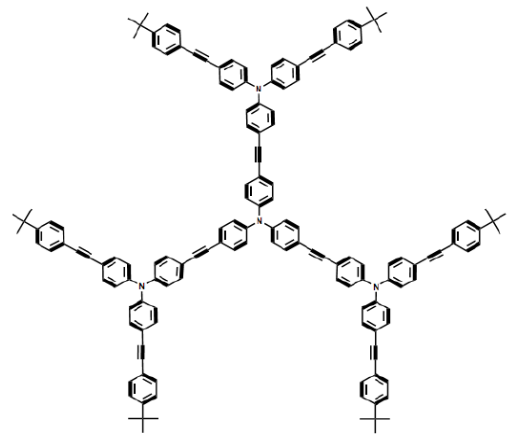

Figure 1. The Molecular Graph of NSB[1].

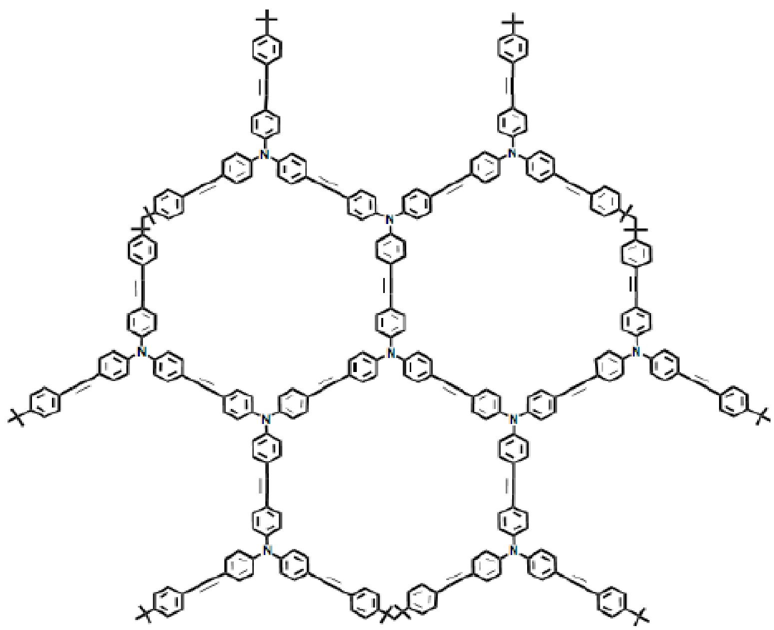

Figure 2. The molecular graph of NSB[2].

Suppose u and v are vertices of a graph G. We define their distance d(u,v) as the length of a shortest path connecting u and v. For a given vertex u of V(G), its eccentricity

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$\varepsilon(u)$ is the largest distance between u and any other vertex v of G. The maximum eccentricity over all vertices of G is called the diameter of G and denoted by d(G) and the minimum eccentricity among the vertices of G is called radius of G and denoted by r(G). The vertex u is called a central vertex if $\varepsilon(u)=r(G)$. The center of G, $C(G)$ is defined as $C(G)=\{u\in V(G)\,|\,\varepsilon(u)=r(G)\}$. The eccentric connectivity index is a topological index that has been much used in study of various properties of many classes of chemical compounds. This index is defined as $\xi(G)=\sum_{u\in V(G)}\deg(u)\,\varepsilon(u)$, where $\deg(u)$ denotes the degree of vertex u in G and $\varepsilon(u)$ is its eccentricity. It was introduced by Madan et al. and used in a series of papers concerned with QSAR/QSPR studies. Its mathematical properties started to be studied only recently, see [3] for details. The investigation of its mathematical properties started only recently, and so far results in determining the extremal values of the invariant and the extremal graphs where those values are achieved, also in a number of explicit formulas for the eccentric connectivity index of several classes of graphs, see [4−8].

Another topological index that we attend it in this paper is augmented eccentric connectivity index. This is defined as the summation of the quotients of the product of adjacent vertex degrees and eccentricity of the concerned vertex, for all vertices in the hydrogen-suppressed molecular graph, see [9]. It is expressed as

$$\xi(G)=\sum_{u\in V(G)}\frac{M(u)}{\varepsilon(u)},$$

where M(u) denotes the product of degrees of all neighbors of vertex u, see [10].

In this paper we present explicit formula for eccentric connectivity and augmented eccentric connectivity indices of N-branched phenylacetylenes nanostar dendrimer. For terms and concepts not defined here we refer the reader to any of several standard monographs, such as [11, 12].

2 Main Results

In this section at first we compute the eccentricity of each vertex then by using them, we can obtain the eccentric connectivity index.

Lemma 1. [2] The number of vertices and edges of dendrimer NSB[n] are given as:

$$|V(NSB[n])| = 87\times 2^n - 38,\ |E(NSB[n])| = 99\times 2^n - 45.$$

In the following lemma the eccentricity of each vertex of NSB[n] is obtained, by using the eccentricity of the central vertex.

Lemma 2. Let v_0 be the central vertex and u is a vertex of NSB[n], such that $d(u,v_0)=k$.

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Then

$$\varepsilon(v_0) = 9n + 10 \text{ and } \varepsilon(u) = 9n + k + 10.$$

Proof. Let v_0 be the central vertex of NSB[n], it is clear that the eccentricity of this vertex is attained at a leaf. Assume that u_0 is a leaf, then $\varepsilon(v_0) = d(v_0, u_0) = 9n + 10$. Now let u be a vertex of NSB[n], such that $d(u,v_0) = k$. The eccentricity of this vertex is also attained at a leaf, and if u_0 is a leaf, then $\varepsilon(u) = d(u,u_0) = d(u,v_0) + d(v_0,u_0) = 9n + k + 10$. □

By Lemma 1 and 2, we can compute the eccentric connectivity index of N-branched phenylacetylenes.

Theorem 3. The eccentric connectivity index of NSB[n] is computed as follows:

$$\xi(NSB[n]) = \left(945n + \frac{3015}{2}\right)2^{n+1} - 810n - 1359 + 837\sum_{i=1}^{n} i2^i.$$

Proof. By definition of eccentric connectivity index, $\xi(NSB[n]) = \sum_{u \in V(NSB[n])} \deg(u)\varepsilon(u)$. Let v_0 be the central vertex of NSB[n] and u_i be vertex that $d(u_i, v_0) = i$. Then

$$\begin{aligned}
\xi(NSB[n]) &= \deg(v_0)\varepsilon(v_0) + \sum_{\substack{u \in V(NSB[n]) \\ u \neq v_0}} \deg(u)\varepsilon(u) \\
&= 3(9n+10) + \sum_{i=1}^{9n+10} \sum_{u_i \in V(NSB[n])} \deg(u_i)\varepsilon(u_i) \\
&= 3(9n+10) + \sum_{i=1}^{9n+10} \sum_{u_i \in V(NSB[n])} \deg(u_i)(9n+i+10) \\
&= 3(9n+10) + 3\sum_{i=1}^{n} 2^i(279n + 279i + 463) \\
&= \left(945n + \frac{3015}{2}\right)2^{n+1} - 810n - 1359 + 837\sum_{i=1}^{n} i2^i.
\end{aligned}$$

This completes the proof of theorem. □

In the following theorem, the augmented eccentric connectivity index of NSB[n] is computed.

Theorem 4. The augmented eccentric connectivity index of NSB[n] is given by the following formula:

$$^{A}\xi(NSB[n]) = 3^2.2^2\sum_{i=0}^{n}\sum_{j=2}^{9}\frac{2^i}{9(n-i)+10+j} + 3^4\sum_{i=0}^{n-1}\frac{1}{9(n+i)+19} + \frac{3^2.2^n}{18n+19} + \frac{3^2.2^{n+1}+3^3}{9n+10}.$$

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Proof. By definition of augmented eccentric connectivity index, ${}^{A}\xi(NSB[n]) = \sum_{u \in V(NSB[n])} \frac{M(u)}{\varepsilon(u)}$. We may partition the vertex set of NSB[n] into central vertex with three isomorphic subgraphs $N_1[n]$, $N_2[n]$ and $N_3[n]$. Let v_0 be the central vertex and u_i be vertex that $d(u_i, v_0)=i$. Then, we can compute the above summation as follows,

$$
\begin{aligned}
{}^{A}\xi(NSB[n]) &= \frac{M(v_0)}{\varepsilon(v_0)} + 3\sum_{u \in V(N_1[n])} \frac{M(u)}{\varepsilon(u)} \\
&= \frac{27}{9n+10} + 3\sum_{i=1}^{9n+10} \sum_{u_i \in V(N_1[n])} \frac{M(u_i)}{9n+i+10} \\
&= 3^2.2^2 \sum_{i=0}^{n} \sum_{j=2}^{9} \frac{2^i}{9(n-i)+10+j} \\
&+ 3^4 \sum_{i=0}^{n-1} \frac{1}{9(n+i)+19} + \frac{3^2.2^n}{18n+19} + \frac{3^2.2^{n+1}+3^3}{9n+10}.
\end{aligned}
$$

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