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Research article

Eccentric Connectivity Index of Nanostar Dendrimer $NS_3[N]$

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Abstract

Let G be a molecular graph. The eccentric connectivity index, $\zeta^c(G)$, is defined as, $\zeta^c(G) = \sum_{u \in V(G)} deg(u)ecc(u)$, where $deg(u)$ denotes the degree of vertex u and $ecc(u)$ is the largest distance between u and any other vertex v of G. In this paper, an exact formula for the eccentric connectivity index of nanostar dendrimer $NS_3[n]$ is given.

Keywords: Eccentric connectivity index, Nanostar dendrimer, Topological index

Mathematics Subject Classification (2020): 20D99

1 Introduction

Chemical graph theory is one of the branches of mathematical chemistry. In chemical graph theory, a variety of concepts from graph theory are used to model chemical phenomena graphically. In this modeling, each atom is represented by a vertex and each bond between two atoms is represented by an edge. A topological index for an undirected simple graph G is a numerical value that is invariant under all graph isomorphisms which correlates to its Physico-chemical properties. Topological indices are used for studying QSAR (quantitative structure-activity relationships) and QSPR (quantitative structure-property relationships) for foretelling many attributes of chemical compounds and their biological properties. Various studies have been performed on different topological indices [1–11].

Dendrimers are highly ordered, branched polymeric molecules. They have many applications in gene therapy, nanotechnology, medicine production, and other fields. Every dendrimer is a macromolecule which made of a core with tree-like arms or branches named dendrons. The zero generation of a dendrimer is the core molecule of dendrimer without dendrons. Each generation of a dendrimer is made by adding some new branches along the branches of the previous generation with a specific rule. Our aim in this study is to investigate a special topological property of dendrimers. The molecular graph of a molecule M is a graph with the finite set of all atoms as its vertex set and chemical bonds are the edges of this graph. We use the notations G (M), G for short, for this graph, V(G) for its vertex set, and E(G) for the set of all edges. For each vertex u, deg(u) denotes the degree of u. If $x, y \in V(G)$, then the length of a minimum path connecting x and y is named the distance between x and y and denoted by d(x,y).

Sharma, Goswami, and Madan proposed the eccentric connectivity index of the molecular graph G which is defined as

$$\zeta^c(G) = \sum_{u \in V(G)} deg(u)ecc(u),$$

where $ecc(u) = max\{d(u,v)|v \in V(G)\}$ [11].

Ashrafi and Saheli computed the eccentric connectivity index of nanostar dendrimers $NS_1[n]$ and $NS_2[n]$, see [3, 10] for details. In this study, we are going to comput the eccentric connectivity index of nanostar dendrimer $NS_3[n]$.

2 MAIN RESULTS AND DISCUSSION

$NS_1[n]$, $NS_2[n]$ and $NS_3[n]$ are three types of dendrimers with n generations. $NS_1[n]$ (for n=3) is depicted in Fig. 1 and its generator is shown in Fig. 2.

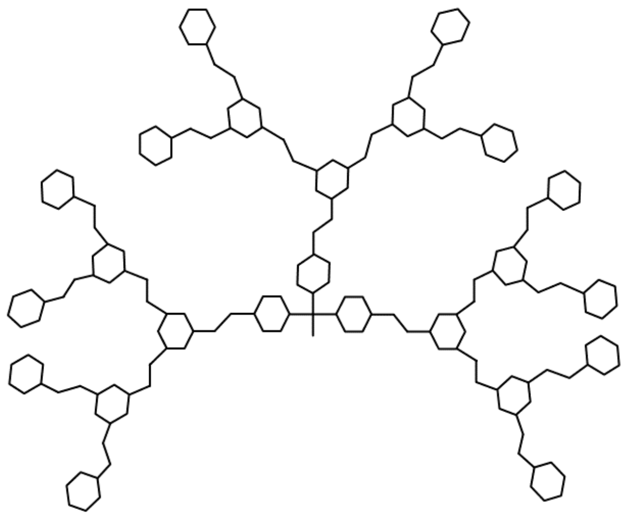

Figure 1. The molecular graph of $NS_1[3]$

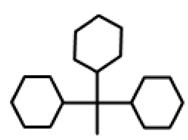

Figure 2. The core of $NS_1[n]$

In [10], Saheli and Ashrafi computed the eccentric connectivity index of nanostar dendrimer $NS_1[n]$ as

$$\zeta^c(NS_1[n]) = 135n \times 2^{n+2} + 135 \times 2^n - 50n + 179.$$

$NS_1[n]$ (for n=2), and its core, are shown in Figs. 3 and 4, respectively.
In [3], Ashrafi and Saheli computed the eccentric connectivity index of $NS_2[n]$ as

$$\zeta^c(NS_2[n]) = 420n \times 2^n + 60 \times 2^n - 110n + 40.$$

Now, we consider nanostar dendrimer where (Figs. 5 and 6). In the following we try to comput the eccentric connectivity index of $NS_3[n]$.

Theorem 1. *The eccentric connectivity index of nanostar dendrimer $NS_3[n]$, is computed as*

$$\zeta^c(NS_3[n]) = 29n \times 2^{n+5} + 741 \times 2^{n+1} - 104n - 98, n \geq 1.$$

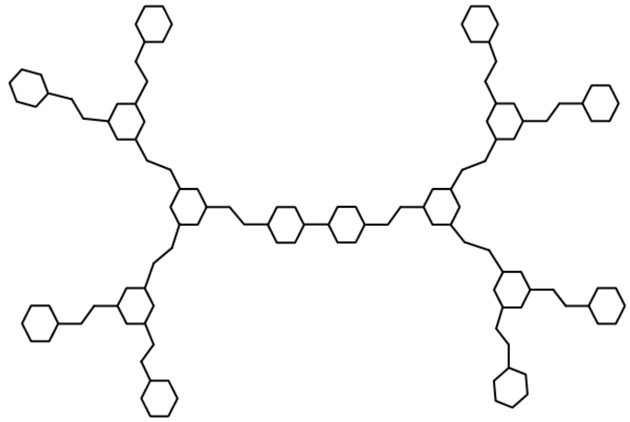

Figure 3. The molecular graph of $NS_2[2]$

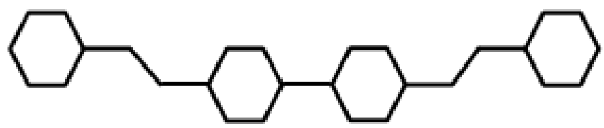

Figure 4. The core of $NS_2[n]$

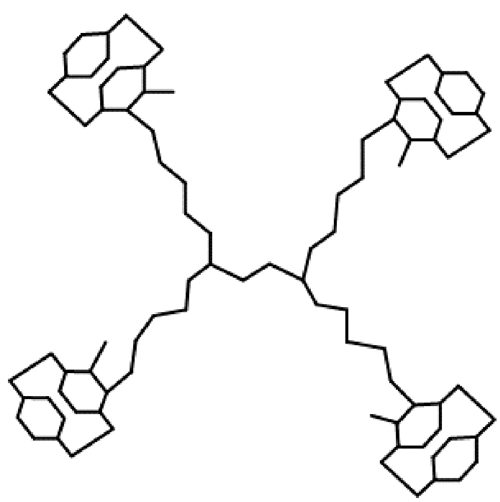

Figure 5. The molecular graph of $NS_3[1]$

Proof. Considering Figs. 7, 8 and Table 1. It can be seen that there exist 22 types of vertices in $NS_3[n]$, based on their positions in branches

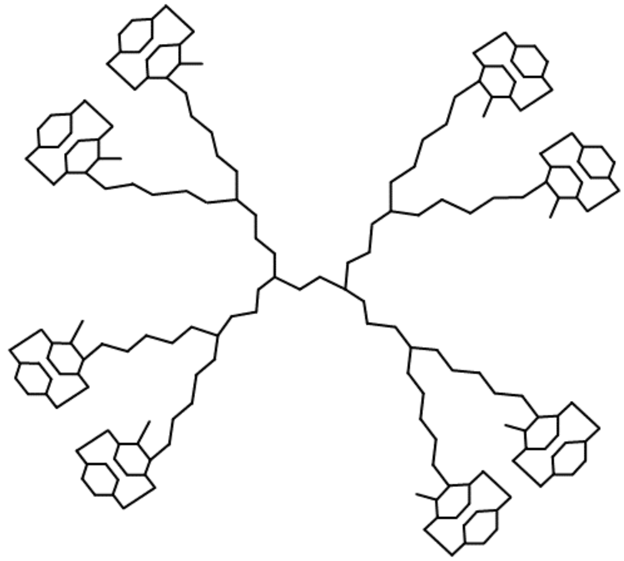

Figure 6. The molecular graph of $NS_3[2]$

of $NS_3[n]$ (Fig. 8). Therefore, we have:

$$
\begin{aligned}
\zeta^c(NS_3[n]) &= \sum_{u\in V(NS_3[n])} deg(u)ecc(u) \\
&= 2\times(8n+19)\times 2^{n+2} + 2\times(8n+18)\times 2^{2n+2} + 3\times(8n+17)\times 2^{n+1} \\
&+ 2\times(8n+16)\times 2^{n+1} + 2\times(8n+15)\times 2^{n+1} + 3\times(8n+14)\times 2^{2n+1} \\
&+ 2\times(8n+15)\times 2^{n+1} + 3\times(8n+13)\times 2^{n+1} + 3\times(8n+18)\times 2^{n+1} \\
&+ 2\times(8n+17)\times 2^{2n+1} + 2\times(8n+16)\times 2^{n+1} + 3\times(8n+15)\times 2^{n+1} \\
&+ 2\times(8n+16)\times 2^{n+1} + 3\times(8n+14)\times 2^{2n+1} + 1\times(8n+15)\times 2^{n+1} \\
&+ 2\times(8n+12)\times 2^{n+1} + 2\times(8n+11)\times 2^{n+1} \\
&+ 2\times\sum_{k=0}^{n-1}(8n-4k+10)\times(2^{n-k+1}) + 2\times\sum_{k=0}^{n-1}(8n-4k+9)\times(2^{n-k+1}) \\
&+ 2\times(8n+16)\times 2^{n+1} + 2\times\sum_{k=0}^{n-1}(8n-4k+8)\times(2^{n-k+1}) \\
&+ 3\times\sum_{k=0}^{n-2}(8n-4k+7)\times(2^{n-k}) + 3\times(4n+11)\times 2 + 2\times(4n+10)\times 2 \\
&= 29n\times 2^{n+5} + 741\times 2^{n+1} - 104n - 98
\end{aligned}
$$

□

Data Availability

The manuscript has no associated data or the data will not be deposited.

Conflicts of Interest

The author declares that there is no conflict of interest.

Table 1. Types of vertices in $NS_3[n]$.

Layer	Types of vertices	Frequences	ecc(u)	deg(u)
n	1	2^{n+2}	8n+19	2
n	2	2^{n+2}	8n+18	2
n	3	2^{n+1}	8n+17	3
n	4	2^{n+1}	8n+16	2
n	5	2^{n+1}	8n+15	2
n	6	2^{n+1}	8n+14	3
n	7	2^{n+1}	8n+13	3
n	8	2^{n+1}	8n+15	2
n	9	2^{n+1}	8n+18	3
n	10	2^{n+1}	8n+17	2
n	11	2^{n+1}	8n+16	2
n	12	2^{n+1}	8n+15	3
n	13	2^{n+1}	8n+16	2
n	14	2^{n+1}	8n+14	3
n	15	2^{n+1}	8n+15	1
n	16	2^{n+1}	8n+12	2
n	17	2^{n+1}	8n+11	2
n	18	2^{n+1}	8n+10	2
n	19	2^{n+1}	8n+9	2
n	20	2^{n+1}	8n+8	2
n	21	2^{n}	8n+8	3
For $1 \leq i \leq n-1$				
i	18	2^{i+1}	8i+14	2
i	19	2^{i+1}	8i+13	2
i	20	2^{i+1}	8i+12	2
i	21	2^{i}	8i+11	3
i	22	2	4i+10	2

Ethical Considerations

The author has diligently addressed ethical concerns, such as informed consent, plagiarism, data fabrication, misconduct, falsification, double publication, redundancy, submission, and other related matters.

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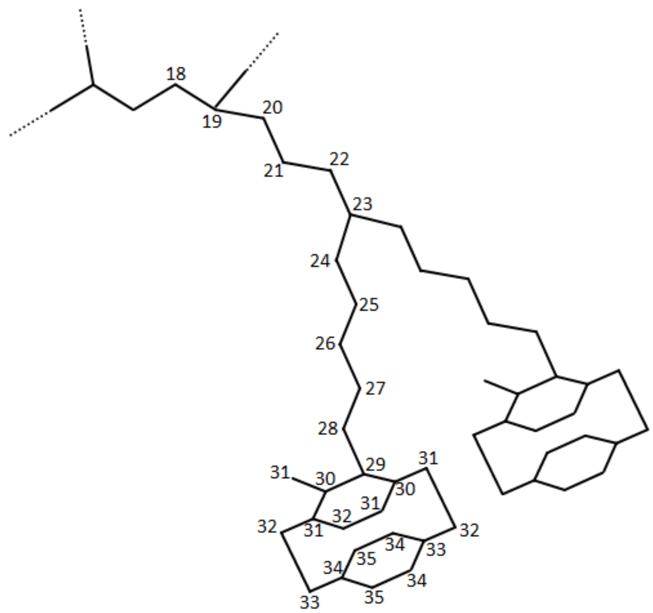

Figure 7. The eccentricity of vertices in a quarter of $NS_3[2]$

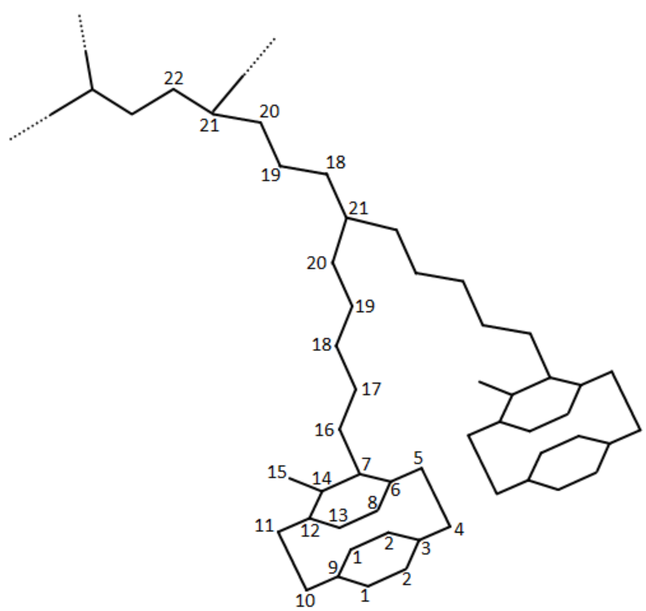

Figure 8. Types of vertices in a quarter of $NS_3[2]$

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