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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.

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

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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.

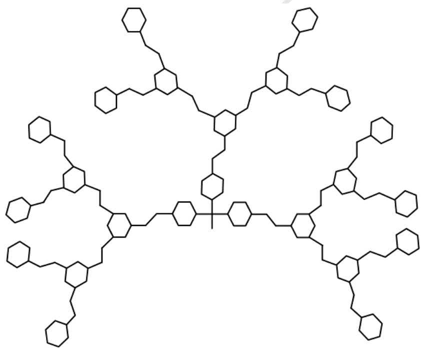

Fig. 1 The molecular graph of $NS_1[3]$

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

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

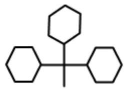

Fig. 2 The core of $NS_1[n]$

$NS_1[n]$ (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

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

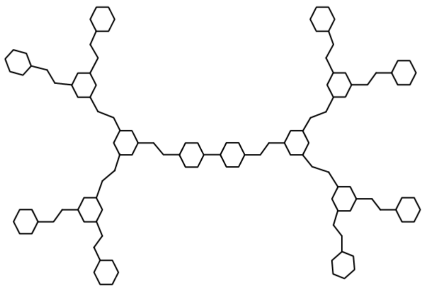

Fig. 3 The molecular graph of $NS_2[2]$

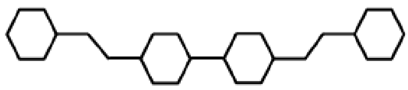

Fig. 4 The core of $NS_2[n]$

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*

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

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 of $NS_3[n]$

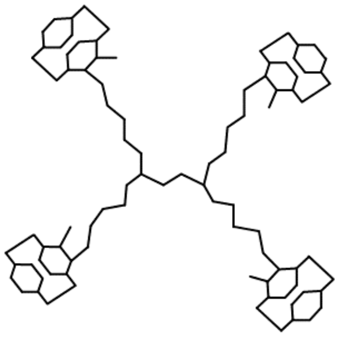

Fig. 5 The molecular graph of $NS_3[1]$

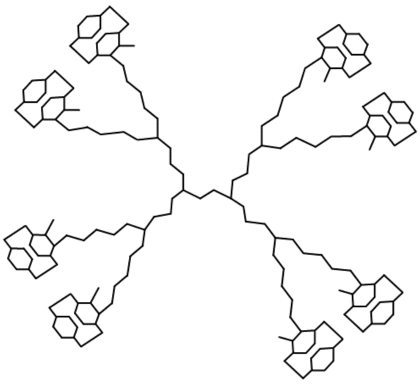

Fig. 6 The molecular graph of $NS_3[2]$

(Fig. 8). Therefore, we have:

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

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

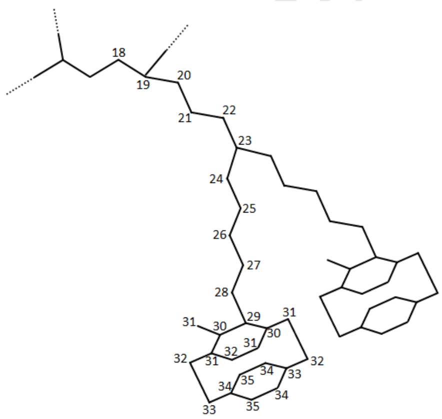

Fig. 7 The eccentricity of vertices in a quarter of $NS_3[2]$

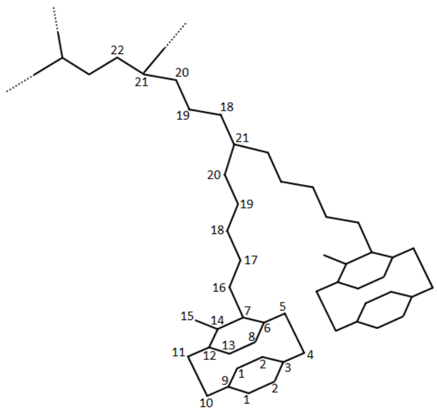

Fig. 8 Types of vertices in a quarter of $NS_3[2]$

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