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Multiplicative Product Connectivity and Sum Connectivity Indices of Chemical Structures in Drugs

[*1]V. R. Kulli, [2]B. Chaluvaraju and [3]T. V. Asha

[1]*Professor of Mathematics(Rtd.), Gulbarga University, Gulbarga (India)*
[2]*Professor of Mathematics, Bangalore University, Bangalore (India)*
[3]*Research Scholar, Department of Mathematics, Bangalore University, Bangalore (India)*

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***Corresponding Author**
Email: bchaluvaraju@gmail.com

ABSTRACT

In Chemical sciences, the multiplicative connectivity indices are used in the analysis of drug molecular structures which are helpful for chemical and medical scientists to find out the chemical and biological characteristics of drugs. In this paper, we compute the multiplicative product and sum connectivity indices of some important nanostar dendrimers which appeared in nanoscience.

1. Introduction

Let $G = (V,E)$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree (or, valency) $d_G(v)$ of a vertex v is the number of vertices adjacent to v. For all further notation and terminology, we refer the reader to [4].

A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. Then chemical molecular structure of drug can be expressed by a molecular graph. In the field of nanoscience, concerning the definition of the topological index on the molecular graph and corresponding medical, chemical, pharmaceutical properties of drugs can be studied by the topological index calculation. To understand the nature of the drug, this procedure does not depend on the laboratory equipments and reagents.

One of the best known and widely used topological index is the product connectivity index (or Randi´c index, connectivity index) by Randi´c [23], who has shown this index to reflect molecular branching. The product connectivity index of a graph G is defined as

$$P(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}$$

Motivated by Randi´c definition of the product connectivity index, the sum connectivity index was initiated by Zhou and Trinajstic [24] and [25], which is defined by

$$S(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)+d_G(v)}}$$

There are many contributions on different types of degree based indices of certain molecular structures and they can be referred to [1, 2, 3, 5, 6, 7, 8, 9, 10, 11] and [21].

Analogously, Kulli [12] introduced the multiplicative product connectivity and multiplicative sum connectivity indices of a graph G, defined as

$$P\prod(G) = \prod_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}$$

and

$$S\prod(G) = \prod_{uv \in E(G)} \frac{1}{\sqrt{d_G(u)+d_G(v)}}$$

Several papers contributed to different kinds of multiplicative structures and they can be referred from [13, 14, 15, 16, 17, 18, 19, 20].

In this paper, the multiplicative product connectivity and multiplicative sum connectivity indices for certain infinite families of nanostar dendrimers are determined. For more information about naostar dendrimers, see [22].

2. Results For $NS_1[n]$ Nanostar Dendrimers

In this section, we focus on the first class of nanostar dendrimers, denoted by $NS_1[n]$, where n is the steps of growth in this type of dendrimer. The graph of $NS_1[n]$ nanostar dendrimer is depicted in Figure-1.

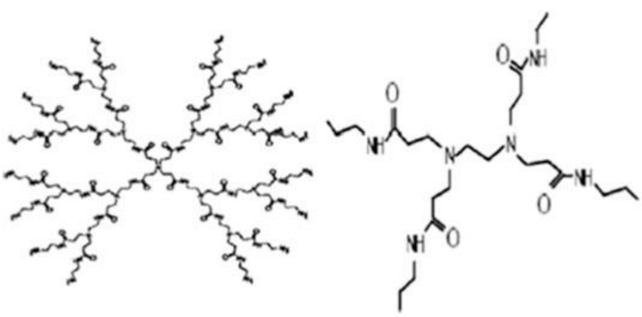

FIGURE-1. The structure of $NS_1[n]$.

Let G be the graph of $NS_1[n]$ nanostar dendrimer. By calculation, we obtain that G has $32 \times 2^n - 29$ edges. Also by calculation, we obtain that G has four types of edges based on the degree of end vertices of each edge as given in Table-1.

$d_G(u), d_G(v)$: $uv \in E(G)$	(1,2)	(1,3)	(2,2)	(2,3)
Number of edges	$2x2^n$	$4x2^n$-4	$12x2^n$-11	$14x2^n$-14

Table-1. Edge partition of $NS_1[n]$.

In the following theorems, we compute the multiplicative product connectivity and multiplicative sum connectivity indices of $NS_1[n]$.

Theorem 2.1. The multiplicative product connectivity index of a polypropylenimine octaamine dendrimer $NS_1[n]$ is

$$P\prod(NS_1[n]) = \left(\frac{1}{2}\right)^{13\times 2^n - 11} \times \left(\frac{1}{3}\right)^{2\times 2^n - 2} \times \left(\frac{1}{6}\right)^{7\times 2^n - 7}$$

Proof: Let G be the molecular graph of $NS_1[n]$. By using the multiplicative product connectivity index and Table-1, we deduce

$$P\prod(NS_1[n]) = \prod_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}$$
$$= \left(\frac{1}{\sqrt{1\times 2}}\right)^{2\times 2^n} \times \left(\frac{1}{\sqrt{1\times 3}}\right)^{4\times 2^n - 4}$$
$$\times \left(\frac{1}{\sqrt{2\times 2}}\right)^{12\times 2^n - 11} \times \left(\frac{1}{\sqrt{2\times 3}}\right)^{14\times 2^n - 14}$$
$$= \left(\frac{1}{2}\right)^{13\times 2^n - 11} \times \left(\frac{1}{3}\right)^{2\times 2^n - 2} \times \left(\frac{1}{6}\right)^{7\times 2^n - 7}$$

Theorem 2.2. The multiplicative sum connectivity index of a polypropylenimine octaamine dendrimer $NS_1[n]$ is

$$S\prod(NS_1[n]) = \left(\frac{1}{\sqrt{3}}\right)^{2\times 2^n} \times \left(\frac{1}{2}\right)^{16\times 2^n - 15} \times \left(\frac{1}{\sqrt{5}}\right)^{14\times 2^n - 14}$$

Proof: Let G be the molecular graph of $NS_1[n]$. By using the multiplicative sum connectivity index and Table-1, we deduce

$$S\prod(NS_1[n]) = \prod_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)+d_G(v)}}$$
$$= \left(\frac{1}{\sqrt{1+2}}\right)^{2\times 2^n} \times \left(\frac{1}{\sqrt{1+3}}\right)^{4\times 2^n - 4}$$
$$\times \left(\frac{1}{\sqrt{2+2}}\right)^{12\times 2^n - 11} \times \left(\frac{1}{\sqrt{2+3}}\right)^{14\times 2^n - 14}$$
$$= \left(\frac{1}{\sqrt{3}}\right)^{2\times 2^n} \times \left(\frac{1}{2}\right)^{16\times 2^n - 15} \times \left(\frac{1}{\sqrt{5}}\right)^{14\times 2^n - 14}$$

3. Results For $NS_2[n]$ Nanostar Dendrimers

In this section, we focus on the second type of nanostar dendrimers, denoted by $NS_2[n]$, where n is the steps of growth in this type of dendrimer. The graph of $NS_2[n]$ nanostar dendrimer is shown in Figure-2.

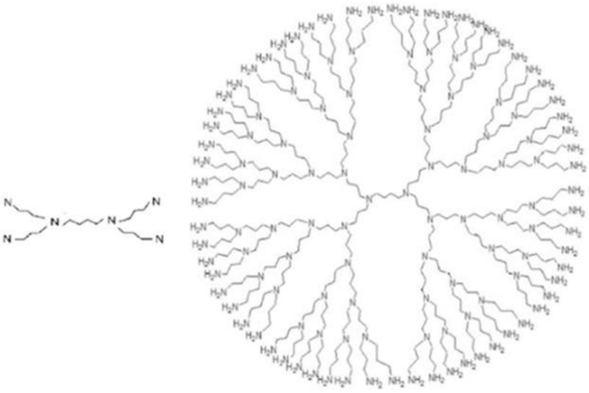

FIGURE 2. The structure of $NS_2[n]$.

Let G be the graph of $NS_2[n]$ polypropylenimine octaamine dendrimer. By calculation, we obtain that G has $16x2^n$ -11 edges. Also by calculation, we obtain that G has three types of edges based on the degree of end vertices of each edge as given in Table-2.

$d_G(u), d_G(v)$: $uv \in E(G)$	(1,2)	(2,2)	(2,3)
Number of edges	$2x2^n$	$8x2^n$-5	$6x2^n$-6

Table-2. Edge partition of $NS_2[n]$.

In the following theorems, we compute the multiplicative product connectivity and multiplicative sum connectivity indices of $NS_2[n]$.

Theorem 3.1. The multiplicative product connectivity index of a polypropylenimine octaamine dendrimer $NS_2[n]$ is

$$P\prod(NS_2[n]) = \left(\frac{1}{2}\right)^{9\times 2^n - 5} \times \left(\frac{1}{6}\right)^{3\times 2^n - 3}$$

Proof: Let G be the molecular graph of $NS_2[n]$. By using the multiplicative product connectivity index and Table-1, we obtain

$$P\prod(NS_2[n]) = \prod_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}$$
$$= \left(\frac{1}{\sqrt{1\times 2}}\right)^{2\times 2^n} \times \left(\frac{1}{\sqrt{2\times 2}}\right)^{8\times 2^n - 5}$$
$$\times \left(\frac{1}{\sqrt{2\times 3}}\right)^{6\times 2^n - 6}$$

$$P\prod(NS_2[n]) = \left(\frac{1}{2}\right)^{9\times 2^n - 5} \times \left(\frac{1}{6}\right)^{3\times 2^n - 3}$$

Theorem 3.2. The multiplicative sum connectivity index of a polypropylenimine octaamine dendrimer $NS_2[n]$ is

$$S\prod(NS_2[n]) = \left(\frac{1}{3}\right)^{2^n} \times \left(\frac{1}{2}\right)^{8\times 2^n - 5} \times \left(\frac{1}{5}\right)^{3\times 2^n - 3}$$

Proof: Let G be the molecular graph of $NS_2[n]$. By using the multiplicative sum connectivity index and Table-1, we deduce

$$S\prod(NS_2[n]) = \prod_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)+d_G(v)}}$$
$$= \left(\frac{1}{\sqrt{1+2}}\right)^{2\times 2^n} \times \left(\frac{1}{\sqrt{2+2}}\right)^{8\times 2^n - 5} \times \left(\frac{1}{\sqrt{2+3}}\right)^{6\times 2^n - 6}$$
$$= \left(\frac{1}{3}\right)^{2^n} \times \left(\frac{1}{2}\right)^{8\times 2^n - 5} \times \left(\frac{1}{5}\right)^{3\times 2^n - 3}$$

4. Results For $NS_3[n]$ Polymer Dendrimers

In this section, we focus on the class of polymer dendrimers, denoted by $NS_3[n]$, where n is the steps of growth in this type of dendrimer. The graph of $NS_3[n]$ polymer dendrimer is presented in Figure-3.

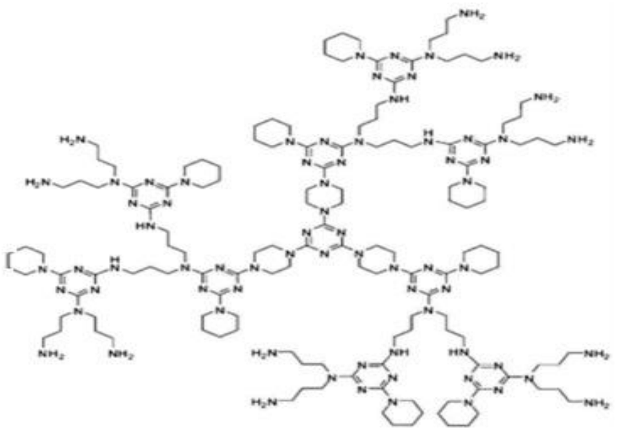

FIGURE 3. The structure of $NS_3[n]$

Let G be the graph of $NS_3[n]$ polymer dendrimer. By calculation, we obtain that G has $69 \times 2^n - 90$ edges. Also by calculation, we obtain that G has four types of edges based on the degree of end vertices of each edge as give in Table-3.

$d_G(u), d_G(v)$: $uv \in E(G)$	(1,2)	(2,2)	(2,3)	(3,3)
Number of edges	$3x2^n$	$27x2^n$-24	$33x2^n$+114	$6x2^n$

Table-3. Edge partition of $NS_3[n]$

In the following theorems, we compute the multiplicative product connectivity and multiplicative sum connectivity indices of $NS_3[n]$.

Theorem 4.1. The multiplicative product connectivity index of a polymer dendrimer $NS_3[n]$ is

$$P\prod(NS_3[n]) = \left(\frac{1}{\sqrt{2}}\right)^{57\times 2^n-48} \times \left(\frac{1}{\sqrt{6}}\right)^{33\times 2^n+114} \times \left(\frac{1}{3}\right)^{6\times 2^n}$$

Proof: Let G be the molecular graph of $NS_3[n]$. By using the multiplicative product connectivity index and Table-3, we derive

$$P\prod(NS_3[n]) = \prod_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}$$
$$= \left(\frac{1}{\sqrt{1\times 2}}\right)^{3\times 2^n} \times \left(\frac{1}{\sqrt{2\times 2}}\right)^{27\times 2^n-24}$$
$$\times \left(\frac{1}{\sqrt{2\times 3}}\right)^{33\times 2^n+114} \times \left(\frac{1}{\sqrt{3\times 3}}\right)^{6\times 2^n}$$
$$= \left(\frac{1}{\sqrt{2}}\right)^{57\times 2^n-48} \times \left(\frac{1}{\sqrt{6}}\right)^{33\times 2^n+114} \times \left(\frac{1}{3}\right)^{6\times 2^n}$$

Theorem 4.2. The multiplicative sum connectivity index of a polymer dendrimer $NS_3[n]$ is

$$S\prod(NS_3[n]) = \left(\frac{1}{\sqrt{3}}\right)^{3\times 2^n} \times \left(\frac{1}{2}\right)^{27\times 2^n-24} \times \left(\frac{1}{\sqrt{5}}\right)^{33\times 2^n+114} \times \left(\frac{1}{\sqrt{6}}\right)^{6\times 2^n}$$

Proof: Let G be the molecular graph of $NS_3[n]$. By using the multiplicative sum connectivity index and Table-3, we derive

$$S\prod(NS_3[n]) = \prod_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)+d_G(v)}}$$
$$= \left(\frac{1}{\sqrt{1+2}}\right)^{3\times 2^n} \times \left(\frac{1}{\sqrt{2+2}}\right)^{27\times 2^n-24}$$
$$\times \left(\frac{1}{\sqrt{2+3}}\right)^{33\times 2^n+114} \times \left(\frac{1}{\sqrt{3+3}}\right)^{6\times 2^n}$$
$$= \left(\frac{1}{\sqrt{3}}\right)^{3\times 2^n} \times \left(\frac{1}{2}\right)^{27\times 2^n-24} \times \left(\frac{1}{\sqrt{5}}\right)^{33\times 2^n+114}$$
$$\times \left(\frac{1}{\sqrt{6}}\right)^{6\times 2^n}$$

5. Results For $NS_4[n]$ Fullerene Dendrimers

In this section, we focus on the class of fullerene dendrimers, denoted by $NS_4[n]$, where n is the steps of growth in this type of dendrimer. The graph of $NS_4[n]$ fullerene dendrimer is presented in Figure-4.

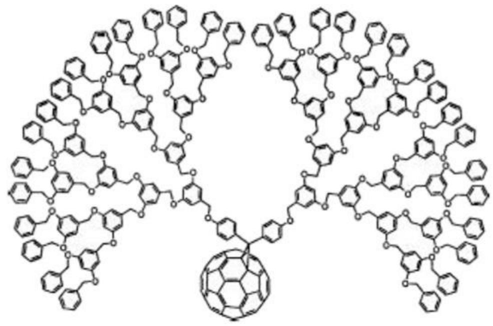

FIGURE 4. The structure of $NS_4[n]$

Let G be the graph of $NS_4[n]$ fullerene dendrimer. By calculation, we obtain that G has $20 \times 2^n + 89$ edges. Also by calculation, we obtain that G has six types of edges based on the degree of end vertices of each edge as given in Table-4.

$d_G(u), d_G(v)$:$uv \in E(G)$	(1,2)	(2,2)	(2,3)	(3,3)	(3,4)	(4,4)
Number of edges	$2x2^n$	$2x2^n$+2	$16x2^n$-8	86	6	3

Table-4. Edge partition of $NS_4[n]$

We determine the multiplicative product connectivity and multiplicative sum connectivity indices of $NS_4[n]$.

Theorem 5.1. The multiplicative product connectivity index of a fullerene dendrimer $NS_4[n]$ is

$$P\prod(NS_4[n]) = \left(\frac{1}{2}\right)^{3\times 2^n+2} \times \left(\frac{1}{\sqrt{6}}\right)^{16\times 2^n-8} \times \left(\frac{1}{3}\right)^{86} \times \left(\frac{1}{\sqrt{12}}\right)^{6} \times \left(\frac{1}{4}\right)^{3}$$

Proof: Let G be the molecular graph of $NS_4[n]$. By using the multiplicative product connectivity index and Table-4, we deduce

$$P\prod(NS_4[n]) = \prod_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}$$
$$= \left(\frac{1}{\sqrt{1\times 2}}\right)^{2\times 2^n} \times \left(\frac{1}{\sqrt{2\times 2}}\right)^{2\times 2^n+2} \times \left(\frac{1}{\sqrt{2\times 3}}\right)^{16\times 2^n-8}$$
$$\times \left(\frac{1}{\sqrt{3\times 3}}\right)^{86} \times \left(\frac{1}{\sqrt{3\times 4}}\right)^{6} \times \left(\frac{1}{\sqrt{4\times 4}}\right)^{3}$$
$$= \left(\frac{1}{2}\right)^{3\times 2^n+2} \times \left(\frac{1}{\sqrt{6}}\right)^{16\times 2^n-8} \times \left(\frac{1}{3}\right)^{86} \times \left(\frac{1}{\sqrt{12}}\right)^{6}$$
$$\times \left(\frac{1}{4}\right)^{3}$$

Theorem 5.2. The multiplicative sum connectivity index of a fullerene dendrimer $NS_4[n]$ is

$$S\prod(NS_4[n]) = \left(\frac{1}{\sqrt{3}}\right)^{2\times2^n} \times \left(\frac{1}{2}\right)^{2\times2^n+2} \times \left(\frac{1}{\sqrt{5}}\right)^{16\times2^n-8} \times \left(\frac{1}{\sqrt{6}}\right)^{86} \times \left(\frac{1}{\sqrt{7}}\right)^{6} \times \left(\frac{1}{\sqrt{8}}\right)^{3}$$

Proof: Let *G* be the molecular graph of $NS_4[n]$. By using the multiplicative sum connectivity index and Table-4, we deduce

$$S\prod(NS_4[n]) = \prod_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)+d_G(v)}}$$

$$= \left(\frac{1}{\sqrt{1+2}}\right)^{2\times2^n} \times \left(\frac{1}{\sqrt{2+2}}\right)^{2\times2^n+2} \times \left(\frac{1}{\sqrt{2+3}}\right)^{16\times2^n-8} \times \left(\frac{1}{\sqrt{3+3}}\right)^{86} \times \left(\frac{1}{\sqrt{3+4}}\right)^{6} \times \left(\frac{1}{\sqrt{4+4}}\right)^{3}$$

$$= \left(\frac{1}{\sqrt{3}}\right)^{2\times2^n} \times \left(\frac{1}{2}\right)^{2\times2^n+2} \times \left(\frac{1}{\sqrt{5}}\right)^{16\times2^n-8} \times \left(\frac{1}{\sqrt{6}}\right)^{86} \times \left(\frac{1}{\sqrt{7}}\right)^{6} \times \left(\frac{1}{\sqrt{8}}\right)^{3}$$

6. Results For $NS_5[n]$ Polymer Dendrimers

In this section, we consider the class of polymer dendrimers, denoted by $NS_5[n]$, where *n* is the steps of growth in this type of dendrimers. The graph of $NS_5[n]$ polymer dendrimer is presented in Figure-5.

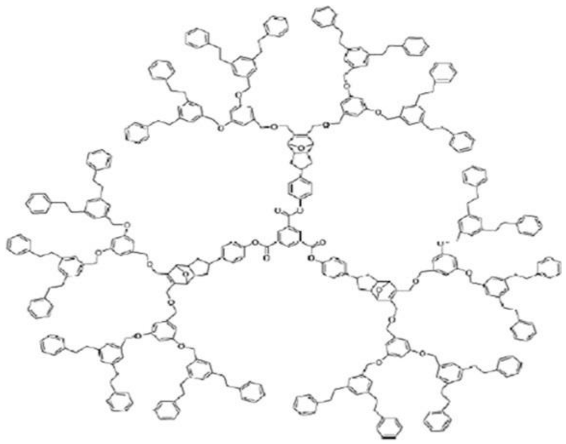

FIGURE 5. The structure of $NS_5[n]$

Let *G* be the graph of $NS_5[n]$ polymer dendrimer. By calculation, we obtain that *G* has $60 \times 2^n + 27$ edges. Also by calculation, we obtain the edge set *E*(*G*) can be divided into four partitions as given in Table-5.

$d_G(u), d_G(v)$: $uv \in E(G)$	(1,3)	(2,2)	(2,3)	(3,3)
Number of edges	$6x2^n+3$	$6x2^n+6$	$48x2^n-6$	24

Table-5. Edge partition of $NS_5[n]$

We compute the multiplicative product connectivity and multiplicative sum connectivity indices of $NS_5[n]$.

Theorem 6.1. The multiplicative product connectivity index of a polymer dendrimer $NS_5[n]$ is

$$P\prod(NS_5[n]) = \left(\frac{1}{\sqrt{3}}\right)^{6\times2^n+3} \times \left(\frac{1}{2}\right)^{6\times2^n+6} \times \left(\frac{1}{\sqrt{6}}\right)^{48\times2^n-6} \times \left(\frac{1}{3}\right)^{24}$$

Proof: Let *G* be the molecular graph of $NS_5[n]$. By using the multiplicative product connectivity index and Table-5, we derive

$$P\prod(NS_5[n]) = \prod_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}$$

$$= \left(\frac{1}{\sqrt{1\times3}}\right)^{6\times2^n+3} \times \left(\frac{1}{\sqrt{2\times2}}\right)^{6\times2^n+6} \times \left(\frac{1}{\sqrt{2\times3}}\right)^{48\times2^n-6} \times \left(\frac{1}{\sqrt{3\times3}}\right)^{24}$$

$$= \left(\frac{1}{\sqrt{3}}\right)^{6\times2^n+3} \times \left(\frac{1}{2}\right)^{6\times2^n+6} \times \left(\frac{1}{\sqrt{6}}\right)^{48\times2^n-6} \times \left(\frac{1}{3}\right)^{24}$$

Theorem 6.2. The multiplicative sum connectivity index of a polymer dendrimer $NS_5[n]$ is

$$S\prod(NS_5[n]) = \left(\frac{1}{2}\right)^{12\times2^n+9} \times \left(\frac{1}{\sqrt{5}}\right)^{48\times2^n-6} \times \left(\frac{1}{\sqrt{6}}\right)^{24}$$

Proof: Let G be the molecular graph of $NS_5[n]$. By using the multiplicative sum connectivity index and Table-5, we derive

$$S\prod(NS_5[n]) = \prod_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)+d_G(v)}}$$

$$= \left(\frac{1}{\sqrt{1+3}}\right)^{6\times2^n+3} \times \left(\frac{1}{\sqrt{2+2}}\right)^{6\times2^n+6} \times \left(\frac{1}{\sqrt{2+3}}\right)^{48\times2^n-6} \times \left(\frac{1}{\sqrt{3+3}}\right)^{24}$$

$$= \left(\frac{1}{2}\right)^{12\times2^n+9} \times \left(\frac{1}{\sqrt{5}}\right)^{48\times2^n-6} \times \left(\frac{1}{\sqrt{6}}\right)^{24}$$

7. Results For $NS_6[n]$ Nanostar Dendrimers

In this section, we focus on the class of nanostar dendrimers, denoted by $NS_6[n]$, where n is the steps of growth. The graph of $NS_6[n]$ nanostar dendrimer is depicted in Figure-6.

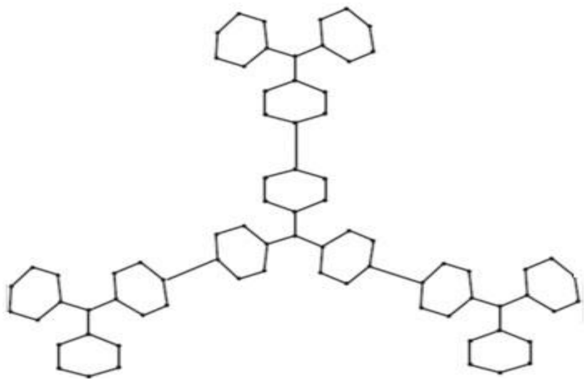

FIGURE 6. The structure of $NS_6[n]$

Let *G* be the graph of $NS_6[n]$ nanostar dendrimer. By calculation, we obtain that *G* has $33 \times 2^n - 45$ edges. Also by calculation, we obtain that the edge set *E*(*G*) can be divided into three partitions as given in Table-6.

$d_G(u), d_G(v)$: $uv \in E(G)$	(2,2)	(2,3)	(3,3)
Number of edges	$12x2^n-12$	$15x2^n-24$	$6x2^n-9$

Table-6. Edge partition of $NS_6[n]$

In the following theorems, we compute the multiplicative product connectivity and multiplicative sum connectivity indices of $NS_6[n]$.

Theorem 7.1. The multiplicative product connectivity index of a nanostar dendrimer $NS_6[n]$ is

$$P\prod(NS_6[n]) = \left(\frac{1}{2}\right)^{12\times2^n-12} \times \left(\frac{1}{\sqrt{6}}\right)^{15\times2^n-24} \times \left(\frac{1}{3}\right)^{6\times2^n-9}$$

Proof: Let *G* be the molecular graph of $NS_6[n]$. By using the multiplicative product connectivity index and Table-6, we obtain

$$P\prod(NS_6[n]) = \prod_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)d_G(v)}}$$

$$= \left(\frac{1}{\sqrt{2\times2}}\right)^{12\times2^n-12} \times \left(\frac{1}{\sqrt{2\times3}}\right)^{15\times2^n-24} \times \left(\frac{1}{\sqrt{3\times3}}\right)^{6\times2^n-9}$$

$$= \left(\frac{1}{2}\right)^{12\times2^n-12} \times \left(\frac{1}{\sqrt{6}}\right)^{15\times2^n-24} \times \left(\frac{1}{3}\right)^{6\times2^n-9}$$

Theorem 7.2. The multiplicative sum connectivity index of a nanostar dendrimer $NS_6[n]$ is

$$S\prod(NS_6[n]) = \left(\frac{1}{2}\right)^{12\times2^n-12} \times \left(\frac{1}{\sqrt{5}}\right)^{15\times2^n-24} \times \left(\frac{1}{\sqrt{6}}\right)^{6\times2^n-9}$$

Proof: Let *G* be the molecular graph of $NS_6[n]$. By using the multiplicative sum connectivity index and Table-6, we deduce

$$S\prod(NS_6[n]) = \prod_{uv\in E(G)} \frac{1}{\sqrt{d_G(u)+d_G(v)}}$$

$$= \left(\frac{1}{\sqrt{2+2}}\right)^{12\times2^n-12} \times \left(\frac{1}{\sqrt{2+3}}\right)^{15\times2^n-14} \times \left(\frac{1}{\sqrt{3+3}}\right)^{6\times2^n-9}$$

$$= \left(\frac{1}{2}\right)^{12\times2^n-12} \times \left(\frac{1}{\sqrt{5}}\right)^{15\times2^n-24} \times \left(\frac{1}{\sqrt{6}}\right)^{6\times2^n-9}$$

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