International Journal of Mathematics and Computer Research

ISSN: 2320-7167

Volume 11 Issue 02 February 2023, Page no. – 3230-3235

Index Copernicus ICV: 57.55, Impact Factor: 8.187

DOI: 10.47191/ijmcr/v11i2.01

Neighborhood Sum Atom Bond Connectivity Indices of Some Nanostar Dendrimers

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ARTICLE INFO

Published Online:
08 February 2023
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ABSTRACT

In this paper, we introduce the neighborhood sum atom bond connectivity index and the multiplicative neighborhood sum atom bond connectivity index of a graph. Also we compute these indices for certain dendrimers.

KEYWORDS: neighborhood sum atom bond connectivity index, multiplicative neighborhood sum atom bond connectivity index, dendrimer.

I. INTRODUCTION

Let $K = (V(K), E(K))$ be a finite, simple connected graph. A molecular graph is a simple graph related to the structure of a chemical compound. Each vertex of a molecular graph represents an atom of the molecule and its edges to the bonds between atoms. Let $s(u)$ denote the sum of the degrees of all vertices adjacent to a vertex u. For other undefined notations, readers may refer to [1].

Chemical Graph Theory has an important effect on the development of Chemical Sciences. Topological index is a numerical parameter mathematically derived from the graph structure. Numerous topological indices have been considered in Theoretical Chemistry, especially in quantitative structure activity (*QSAR*) and quantitative structure property (*QSPR*) study, see [2, 3].

The fourth atom bond connectivity index [4] is

$$ABC_4(K) = \sum_{uv \in E(K)} \sqrt{\frac{s(u)+s(v)-2}{s(u)s(v)}}.$$

Recently some atom bond connectivity indices were studied in [5, 6, 7, 8, 9. 10, 11, 12, 13, 14].

We define the neighborhood sum atom bond connectivity index as

$$NSA(K) = \sum_{uv \in E(K)} \sqrt{\frac{s(u)+s(v)-2}{s(u)+s(v)}}.$$

The fourth multiplicative atom bond connectivity index [15] is

$$ABC_4II(K) = \prod_{uv \in E(K)} \sqrt{\frac{s(u)+s(v)-2}{s(u)s(v)}}.$$

Recently some multiplicative atom bond connectivity indices were studied, for example, in [16, 17, 18, 9, 20, 21, 22, 23, 24, 25, 26, 27].

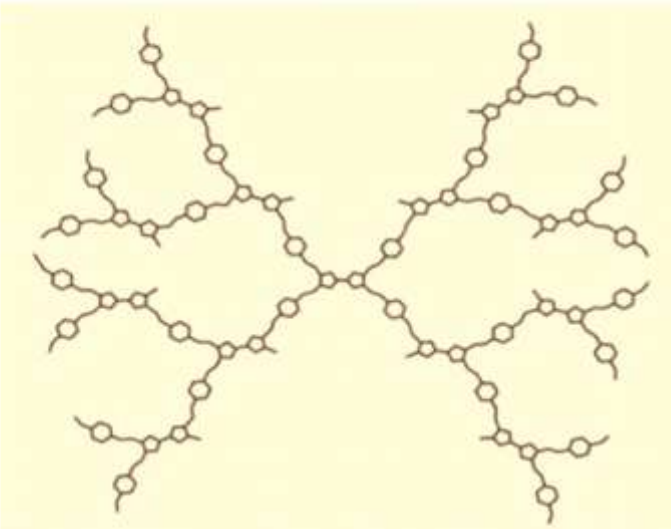
Now we define the multiplicative neighborhood sum atom bond connectivity index as

$$NSAII(K) = \prod_{uv \in E(K)} \sqrt{\frac{s(u)+s(v)-2}{s(u)+s(v)}}.$$

In this paper, we compute the neighborhood sum atom bond connectivity index and the multiplicative neighborhood sum atom bond connectivity index of tetrathiafulvalene, POPAM, $NS_2[n]$ and $NS_3[n]$ dendrimers.

II. TETRATHIAFULVALENE DENDRIMERS $TD_2[n]$

The molecular graph of tetrathiafulvalene dendrimers $TD_2[n]$ is shown in the below graph.



The graphs of $TD_2[n]$ have $31\times 2^{n+2} - 74$ vertices and $35\times 2^{n+2} - 85$ edges are shown in the above graph. Let $A = TD_2[n]$.

We obtain that $\{s(u), s(v): uv \in E(A)\}$ has nine edge set partitions.

$s(u), s(v)\backslash uv\in E(A)$	Number of edges
(2, 4)	2^{n+2}
(3, 6)	$2^{n+2} - 4$
(4, 6)	2^{n+2}
(5, 5)	$7\times 2^{n+2} - 16$
(5, 6)	$11\times 2^{n+2} - 24$
(5, 7)	$3\times 2^{n+2} - 8$
(6, 6)	$2^{n+2} - 4$
(6, 7)	$8\times 2^{n+2} - 24$
(7, 7)	$2\times 2^{n+2} - 5$

Theorem 1. The neighborhood sum atom bond connectivity index of $TD_2[n]$ is

$$NSA(A) = 2^{n+2}\left(\sqrt{\frac{2}{3}}\right) + \left(2^{n+2}-4\right)\left(\frac{\sqrt{7}}{3}\right) + \left(8\times 2^{n+2}-16\right)\left(\frac{2}{\sqrt{5}}\right) + \left(11\times 2^{n+2}-24\right)\left(\frac{3}{\sqrt{11}}\right) + \left(4\times 2^{n+2}-12\right)\left(\sqrt{\frac{5}{6}}\right) + \left(8\times 2^{n+2}-24\right)\left(\sqrt{\frac{11}{13}}\right) + \left(2\times 2^{n+2}-5\right)\left(\sqrt{\frac{6}{7}}\right).$$

Proof: Applying definition and edge partition of $TD_2[n]$, we conclude

$$NSA(A) = \sum_{uv\in E(A)} \sqrt{\frac{s(u)+s(v)-2}{s(u)+s(v)}}$$

$$= 2^{n+2}\left(\sqrt{\frac{2+4-2}{2+4}}\right) + \left(2^{n+2}-4\right)\left(\sqrt{\frac{3+6-2}{3+6}}\right) + 2^{n+2}\left(\sqrt{\frac{4+6-2}{4+6}}\right) + \left(7\times 2^{n+2}-16\right)\left(\sqrt{\frac{5+5-2}{5+5}}\right)$$
$$+\left(11\times 2^{n+2}-24\right)\left(\sqrt{\frac{5+6-2}{5+6}}\right) + \left(3\times 2^{n+2}-8\right)\left(\sqrt{\frac{5+7-2}{5+7}}\right) + \left(2^{n+2}-4\right)\left(\sqrt{\frac{6+6-2}{6+6}}\right) + \left(8\times 2^{n+2}-24\right)\left(\sqrt{\frac{6+7-2}{6\times 7}}\right)$$
$$+\left(2\times 2^{n+2}-5\right)\left(\sqrt{\frac{7+7-2}{7\times 7}}\right)$$

gives the desired result by solving the above equation.

Theorem 2. The multiplicative neighborhood sum atom bond connectivity index of $TD_2[n]$ is

$$NSAII(A) = \left(\sqrt{\frac{2}{3}}\right)^{2^{n+2}} \times \left(\frac{\sqrt{7}}{3}\right)^{2^{n+2}-4} \times \left(\frac{2}{\sqrt{5}}\right)^{8\times 2^{n+2}-16} \times \left(\frac{3}{\sqrt{11}}\right)^{11\times 2^{n+2}-24} \times \left(\sqrt{\frac{5}{6}}\right)^{4\times 2^{n+2}-12} \times \left(\sqrt{\frac{11}{13}}\right)^{8\times 2^{n+2}-24} \times \left(\sqrt{\frac{6}{7}}\right)^{2\times 2^{n+2}-5}.$$

Proof: Applying definition and edge partition of $TD_2[n]$, we conclude

$$NSAII(A) = \prod_{uv\in E(A)} \sqrt{\frac{s(u)+s(v)-2}{s(u)+s(v)}}$$

$$= \left(\sqrt{\frac{2+4-2}{2+4}}\right)^{2^{n+2}} \times \left(\sqrt{\frac{3+6-2}{3+6}}\right)^{2^{n+2}-4} \times \left(\sqrt{\frac{4+6-2}{4+6}}\right)^{2^{n+2}} \times \left(\sqrt{\frac{5+5-2}{5+5}}\right)^{7\times 2^{n+2}-16}$$

$$\times\left(\sqrt{\frac{5+5-2}{5+5}}\right)^{7\times 2^{n+2}-16}\times\left(\sqrt{\frac{5+6-2}{5+6}}\right)^{11\times 2^{n+2}-24}$$

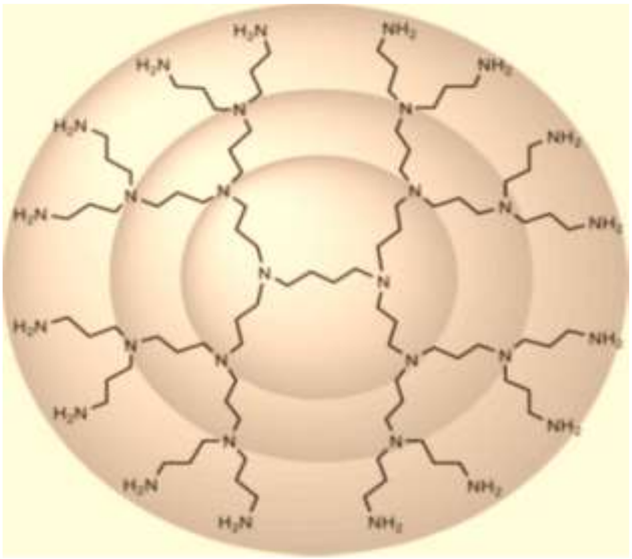
$$\times\left(\sqrt{\frac{5+7-2}{5+7}}\right)^{3\times 2^{n+2}-8}\times\left(\sqrt{\frac{6+6-2}{6+6}}\right)^{2^{n+2}-4}$$

$$\times\left(\sqrt{\frac{6+7-2}{6+7}}\right)^{8\times 2^{n+2}-24}\times\left(\sqrt{\frac{7+7-2}{7+7}}\right)^{2\times 2^{n+2}-5}$$

gives the desired result by solving the above equation.

III. POPAM DENDRIMERS $TD_2[n]$

The molecular graph of POPAM dendrimers $POD_2[n]$ is shown in the below graph.



The graphs of $POD_2[n]$ have $2^{n+5} - 10$ vertices and $2^{n+5} - 11$ edges are shown in the above graph. Let $B = POD_2[n]$.

We obtain that $\{s(u), s(v): uv$ □ $E(B)\}$ has five edge set partitions.

$s(u), s(v) \setminus uv \in E(B)$	Number of edges
(2, 3)	2^{n+2}
(3, 4)	2^{n+2}
(4, 4)	1
(4, 5)	$3\times 2^{n+2} - 6$
(5, 6)	$3\times 2^{n+2} - 6$

Theorem 3. The neighborhood sum atom bond connectivity index of $POD_2[n]$ is

$$NSA(B)=2^{n+2}\left(\sqrt{\frac{3}{5}}\right)+2^{n+2}\left(\sqrt{\frac{5}{7}}\right)+\left(\sqrt{\frac{3}{4}}\right)$$
$$+\left(3\times 2^{n+2}-6\right)\left(\frac{\sqrt{7}}{3}\right)+\left(3\times 2^{n+2}-6\right)\left(\frac{3}{\sqrt{11}}\right).$$

Proof: Applying definition and edge partition of $POD_2[n]$, we conclude

$$NSA(B)=\sum_{uv\in E(B)}\sqrt{\frac{s(u)+s(v)-2}{s(u)+s(v)}}$$

$$=2^{n+2}\left(\sqrt{\frac{2+3-2}{2+3}}\right)+2^{n+2}\left(\sqrt{\frac{3+4-2}{3+4}}\right)$$
$$+\left(\sqrt{\frac{4+4-2}{4+4}}\right)+\left(\sqrt{\frac{4+4-2}{4+4}}\right)$$
$$+\left(3\times 2^{n+2}-6\right)\left(\sqrt{\frac{4+5-2}{4+5}}\right)$$
$$+\left(3\times 2^{n+2}-6\right)\left(\sqrt{\frac{5+6-2}{5+6}}\right)$$

gives the desired result by solving the above equation.

Theorem 4. The multiplicative neighborhood sum atom bond connectivity index of $POD_2[n]$ is

$$NSAII(B)=\left(\sqrt{\frac{3}{5}}\right)^{2^{n+2}}\times\left(\sqrt{\frac{5}{7}}\right)^{2^{n+2}}$$
$$\times\left(\sqrt{\frac{3}{4}}\right)\times\left(\frac{\sqrt{7}}{3}\right)^{3\times 2^{n}-6}\times\left(\frac{3}{\sqrt{11}}\right)^{3\times 2^{n}-6}.$$

Proof: Applying definition and edge partition of $POD_2[n]$, we conclude

$$NSAII(B)=\prod_{uv\in E(B)}\sqrt{\frac{s(u)+s(v)-2}{s(u)+s(v)}}$$

$$=\left(\sqrt{\frac{2+3-2}{2+3}}\right)^{2^{n+2}}\times\left(\sqrt{\frac{3+4-2}{3+4}}\right)^{2^{n+2}}$$
$$\times\left(\sqrt{\frac{4+4-2}{4+4}}\right)^{1}\times\left(\sqrt{\frac{4+5-2}{4+5}}\right)^{3\times 2^{n+2}-6}$$
$$\times\left(\sqrt{\frac{5+6-2}{5+6}}\right)^{3\times 2^{n+2}-6}$$

gives the desired result by solving the above equation.

IV. $NS_2[n]$ DENDRIMERS

The molecular graph of $NS_2[n]$ dendrimers is shown in the below graph.

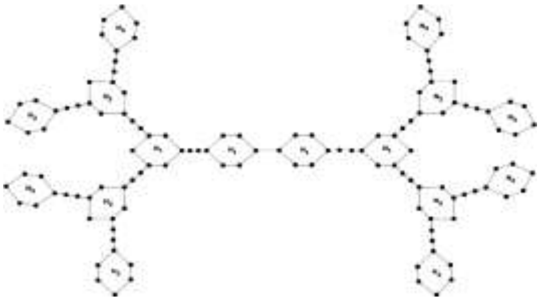


Figure 3. The molecular structure of $NS_2[3]$

The graphs of $NS_2[n]$ have $16\times 2^n - 4$ vertices and $18\times 2^n - 5$ edges are shown in the above graph. Let $C = NS_2[n]$.

We obtain that {*s(u), s(v): uv* □ *E*(*C*)} has five edge set partitions.

$s(u), s(v) \setminus uv \in E(C)$	Number of edges
(4, 4)	2×2^n
(5, 4)	2×2^n
(5, 5)	$2\times 2^n +2$
(5, 6)	6×2^n
(7, 7)	1
(5, 7)	4
(6, 6)	$6\times 2^n - 12$

Theorem 5. The neighborhood sum atom bond connectivity index of a $NS_2[n]$ dendrimer is

$$NSA(C)=\left(\frac{\sqrt{3}}{2}+\frac{\sqrt{7}}{3}+\frac{2}{\sqrt{5}}+\frac{9}{\sqrt{11}}+3\sqrt{\frac{5}{6}}\right)2\times 2^n$$
$$-\frac{4}{\sqrt{5}}+\left(\sqrt{\frac{6}{7}}\right)-8\sqrt{\frac{5}{6}}.$$

Proof: Applying definition and edge partition of $NS_2[n]$, we conclude

$$NSA(C)=\sum_{uv\in E(C)}\sqrt{\frac{s(u)+s(v)-2}{s(u)+s(v)}}$$
$$=2\times 2^n\left(\sqrt{\frac{4+4-2}{4+4}}\right)+2\times 2^n\left(\sqrt{\frac{5+4-2}{5+4}}\right)$$
$$+\left(2\times 2^n+2\right)\left(\sqrt{\frac{5+5-2}{5+5}}\right)+6\times 2^n\left(\sqrt{\frac{5+6-2}{5+6}}\right)$$
$$+\left(\sqrt{\frac{7+7-2}{7+7}}\right)+4\left(\sqrt{\frac{5+7-2}{5+7}}\right)$$
$$+\left(6\times 2^n-12\right)\left(\sqrt{\frac{6+6-2}{6+6}}\right)$$

gives the desired result by solving the above equation.

Theorem 6. The multiplicative neighborhood sum atom bond connectivity index of $NS_2[n]$ is

$$NSAII(C)=\left(\frac{\sqrt{3}}{2}\right)^{2\times 2^n}\times\left(\frac{\sqrt{7}}{3}\right)^{2\times 2^n}\times\left(\frac{2}{\sqrt{5}}\right)^{2\times 2^n-2}$$
$$\times\left(\frac{3}{\sqrt{11}}\right)^{6\times 2^n}\times\left(\sqrt{\frac{6}{7}}\right)\times\left(\sqrt{\frac{5}{6}}\right)^{6\times 2^n-12}.$$

Proof: Applying definition and edge partition of $NS_2[n]$ based on $S_G(u)$, $S_G(v)$, we conclude

$$NSAII(C)=\prod_{uv\in E(C)}\sqrt{\frac{s(u)+s(v)-2}{s(u)+s(v)}}$$
$$=\left(\sqrt{\frac{4+4-2}{4+4}}\right)^{2\times 2^n}\times\left(\sqrt{\frac{5+4-2}{5+4}}\right)^{2\times 2^n}$$
$$\times\left(2\times 2^n+2\right)\left(\sqrt{\frac{5+5-2}{5+5}}\right)^{2\times 2^n+2}\times\left(\sqrt{\frac{5+6-2}{5+6}}\right)^{6\times 2^n}$$
$$\times\left(\sqrt{\frac{7+7-2}{7+7}}\right)^{1}\times\left(\sqrt{\frac{5+7-2}{5+7}}\right)^{4}$$
$$\times\left(\sqrt{\frac{6+6-2}{6+6}}\right)^{6\times 2^n-12}$$

gives the desired result by solving the above equation.

IV. $NS_3[n]$ DENDRIMERS

The molecular graph of $NS_3[n]$ dendrimers is shown in the below graph.

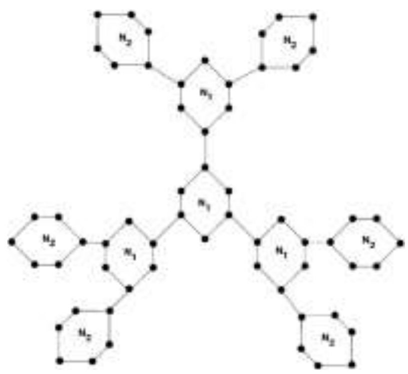


Figure 4. The molecular structure of $NS_3[2]$

The graphs of $NS_3[n]$ have $18\times 2^n - 12$ vertices and $21\times 2^n - 15$ edges are shown in the above graph. Let $D = NS_3[n]$.

We obtain that $\{s(u), s(v): uv \in E(D)\}$ has five edge set partitions.

$S_G(u), S_G(v) \setminus uv \in E(D)$	Number of edges
(4, 4)	3×2^n
(4, 5)	3×2^n
(5, 7)	3×2^n
(6, 7)	$9\times 2^n - 12$
(7, 7)	$3\times 2^n - 3$

Theorem 7. The neighborhood sum atom bond connectivity index of $NS_3[n]$ is

$$NSA(D)=\left(\frac{\sqrt{3}}{2}+\frac{\sqrt{7}}{3}+\sqrt{\frac{5}{6}}+3\sqrt{\frac{11}{13}}+\sqrt{\frac{6}{7}}\right)3\times 2^n$$
$$-12\sqrt{\frac{11}{13}}-3\left(\sqrt{\frac{6}{7}}\right).$$

Proof: Applying definition and edge partition of $NS_3[n]$, we conclude

$$NSA(D)=\sum_{uv\in E(D)}\sqrt{\frac{s(u)+s(v)-2}{s(u)+s(v)}}$$
$$=3\times 2^n\left(\sqrt{\frac{4+4-2}{4+4}}\right)+3\times 2^n\left(\sqrt{\frac{4+5-2}{4+5}}\right)$$
$$+3\times 2^n\left(\sqrt{\frac{5+7-2}{5+7}}\right)+\left(9\times 2^n-12\right)\left(\sqrt{\frac{6+7-2}{6+7}}\right)$$
$$+\left(3\times 2^n-3\right)\left(\sqrt{\frac{7+7-2}{7+7}}\right)$$

gives the desired result by solving the above equation.

Theorem 8. The multiplicative neighborhood sum atom bond connectivity index of $NS_3[n]$ is

$$NSAII(D)=\left(\frac{\sqrt{3}}{2}\right)^{3\times 2^n}\times\left(\frac{\sqrt{7}}{3}\right)^{3\times 2^n}\times\left(\sqrt{\frac{5}{6}}\right)^{3\times 2^n}$$
$$\times\left(\sqrt{\frac{11}{13}}\right)^{9\times 2^n-12}\times\left(\sqrt{\frac{6}{7}}\right)^{3\times 2^n-3}.$$

Proof: Applying definition and edge partition of $NS_3[n]$ based on $S_G(u)$, $S_G(v)$, we conclude

$$NSAII(D)=\prod_{uv\in E(D)}\sqrt{\frac{s(u)+s(v)-2}{s(u)+s(v)}}$$
$$=\left(\sqrt{\frac{4+4-2}{4+4}}\right)^{3\times 2^n}\times\left(\sqrt{\frac{4+5-2}{4+5}}\right)^{3\times 2^n}$$
$$\times\left(\sqrt{\frac{5+7-2}{5+7}}\right)^{3\times 2^n}\times\left(\sqrt{\frac{6+7-2}{6+7}}\right)^{9\times 2^n-12}$$
$$\times\left(\sqrt{\frac{7+7-2}{7+7}}\right)^{3\times 2^n-3}$$

gives the desired result by solving the above equation.

V. CONCLUSION

In this paper, we have determined the neighborhood sum atom bond connectivity index and the multiplicative neighborhood sum atom bond connectivity index of certain dendrimers.

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