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Multiplicative Atom Bond Sum Connectivity Index of Certain Nanotubes

V.R.Kulli

Department of Mathematics
Gulbarga University, Gulbarga 585 106, India
E-mail: vrkulli@gmail.com

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Abstract. We put forward the multiplicative atom bond sum connectivity index of a graph. We determine the atom bond sum connectivity index and the multiplicative atom bond sum connectivity index for some chemical nanostructures such as armchair polyhex nanotubes, zigzag polyhex nanotubes and carbon nanocone networks.

Keywords: multiplicative atom bond sum connectivity index, nanotube.

AMS Mathematics Subject Classification (2010): 05*C*07, 05*C*09, 05*C*92

1. Introduction

Let $G = (V, E)$ be a finite, simple connected graph. Let $d(u)$ denote the degree of a vertex u [1].

In the modelling of Mathematics, a molecular or a chemical graph is a simple graph related to the structure of a chemical compound. Each vertex of this graph represents an atom of the molecule and its edges to the bonds between atoms. Topological indices are useful for finding correlations between the structure of a chemical compound and its physicochemical properties [2].

In [3], Ali et al. introduced the atom bond sum connectivity index of graph G, defined as

$$ABS(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}}.$$

We define the multiplicative atom bond sum connectivity index as

$$ABSII(G) = \prod_{uv \in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}}.$$

The atom bond connectivity index has been found to be a useful predictive indicator in the research on heat generation in octanes and heptanes [4]. The atom bond connectivity indices have been researched in the past [5, 6, 7, 8, 9, 10, 11, 12, 13, 14].In this paper, we compute the atom bond sum connectivity index and multiplicative atom bond sum connectivity index of armchair polyhex nanotubes, zigzag polyhex nanotubes and carbon nanocone networks.

2. Armchair Polyhex nanotubes

Carbon polyhex nanotubes exist in nature with remarkable stability and possess very interesting electrical, thermal and mechanical properties. The molecular graph of armchair polyhex nanotube $TUAC_6\,[p, q]$ is shown in Figure 1.

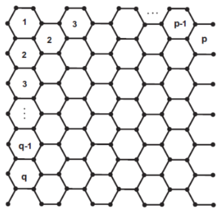

Figure 1

The graphs of armchair polyhex nanotubes have $2p(q+1)$ vertices and $3pq + 2p$ edges are shown in the above graph. Let $A= TUAC_6[p, q]$.

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

$d(u), d(v) \setminus uv \in E(A)$	(2, 2)	(2, 3)	(3, 3)
Number of edges	P	$2p$	$3pq- p$

Theorem 1. The atom bond sum connectivity index of $TUAC_6\,[p, q]$ is

$$ABS(A) = \sqrt{6}pq + \left(\frac{1}{\sqrt{2}} + 2\sqrt{\frac{3}{5}} - \sqrt{\frac{2}{3}}\right)p.$$

Proof: Applying definition and edge partition of $TUAC_6\,[p, q]$, we conclude

$$ABS(G) = \sum_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}}$$

$$= p\left(\sqrt{\frac{2+2-2}{2+2}}\right) + 2p\left(\sqrt{\frac{2+3-2}{2+3}}\right) + (3pq-p)\left(\sqrt{\frac{3+3-2}{3+3}}\right).$$

By solving the above equation, we get the desired result.

Theorem 2. The multiplicative atom bond sum connectivity index of $TUAC_6\,[p, q]$ is

$$ABSII(A) = \left(\frac{1}{2}\right)^{\frac{1}{2}p} \times \left(\frac{3}{5}\right)^{p} \times \left(\frac{2}{3}\right)^{\frac{1}{2}(3pq-p)}.$$

Proof: Applying definition and edge partition of $TUAC_6\,[p, q]$, we conclude

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

$$= \left(\sqrt{\frac{2+2-2}{2+2}}\right)^{p} \times \left(\sqrt{\frac{2+3-2}{2+3}}\right)^{2p} \times \left(\sqrt{\frac{3+3-2}{3+3}}\right)^{(3pq-p)}.$$

By solving the above equation, we obtain the desired result.

3. ZigZag Polyhex nanotubes

The molecular graph of zigzag polyhex nanotube $TUZC_6$ $[p, q]$ is depicted in below graph.

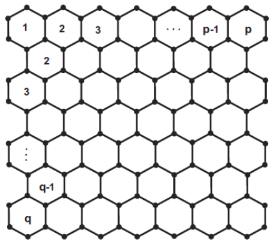

Figure 2

The graphs of zigzag polyhex nanotubes have $2p(q+1)$ vertices and $3pq + 2p$ edges are shown in the above graph. Let $B = TUZC_6[p, q]$.

We obtain that $\{d(u), d(v): uv \in E(B)\}$ has three edge set partitions.

$d(u), d(v) \setminus uv \in E(B)$	(2, 3)	(3, 3)
Number of edges	$4p$	$3pq - 2p$

Theorem 3. The atom bond sum connectivity index of $TUZC_6$ $[p, q]$ is given by

$$ABS(B) = \sqrt{6}pq + \left(4\sqrt{\frac{3}{5}} - 2\sqrt{\frac{2}{3}}\right)p.$$

Proof: Applying definition and edge partition of $TUZC_6$ $[p, q]$, we conclude

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

$$= 4p\left(\sqrt{\frac{2+3-2}{2+3}}\right) + (3pq - 2p)\left(\sqrt{\frac{3+3-2}{3+3}}\right).$$

By solving the above equation, we get the desired result.

Theorem 4. The multiplicative atom bond sum connectivity index of $TUZC_6$ $[p, q]$ is given by

$$ABSII(B) = \left(\frac{3}{5}\right)^{2p} \times \left(\frac{2}{3}\right)^{\frac{1}{2}(3pq-2p)}.$$

Proof: Applying definition and edge partition of $TUZC_6$ $[p, q]$, we conclude

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

$$= \left(\sqrt{\frac{2+3-2}{2+3}}\right)^{4p} \times \left(\sqrt{\frac{3+3-2}{3+3}}\right)^{(3pq-2p)}.$$

By solving the above equation, we get the necessary result.

4. Carbon Nanocone networks

The molecular graph of pentagonal nanocone network $CNC_5[n]$ is depicted in below graph.

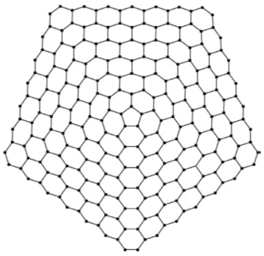

Figure 3

The graphs of pentagonal nanocone networks have $5(n+1)^2$ vertices and $\frac{15}{2}n^2+\frac{25}{2}n+5$ edges are shown in the above graph. Let $C = CNC_5[n]$.

We obtain that $\{d(u), d(v): uv\in E(C)\}$ has three edge set partitions.

$d(u), d(v) \backslash uv\in E(C)$	(2, 2)	(2, 3)	(3, 3)
Number of edges	5	$10n$	$\frac{15}{2}n^2+\frac{5}{2}n$

Theorem 5. The multiplicative atom bond sum connectivity index of $CNC_5[n]$ is

$$ABS(C)=\frac{15}{\sqrt{6}}n^2+\left(10\sqrt{\frac{3}{5}}+\frac{5}{\sqrt{6}}\right)n+\frac{5}{\sqrt{2}}.$$

Proof: Applying definition and edge partition of $CNC_5[n]$, we conclude

$$ABS(C)=\sum_{uv\in E(C)}\sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}}$$

$$=5\left(\sqrt{\frac{2+2-2}{2+2}}\right)+10n\left(\sqrt{\frac{2+3-2}{2+3}}\right)+\left(\frac{15}{2}n^2+\frac{5}{2}n\right)\left(\sqrt{\frac{3+3-2}{3+3}}\right).$$

By solving the above equation, we obtain the desired result.

Theorem 6. The multiplicative atom bond sum connectivity index of $CNC_5[n]$ is

$$ABSII(C)=\left(\frac{1}{\sqrt{2}}\right)^5\times\left(\frac{3}{5}\right)^{5n}\times\left(\frac{2}{3}\right)^{\frac{15}{4}n^2+\frac{5}{4}n}.$$

Proof: Applying definition and edge partition of $CNC_5[n]$, we conclude

$$ABSII(C)=\prod_{uv\in E(C)}\sqrt{\frac{d(u)+d(v)-2}{d(u)+d(v)}}$$

$$=\left(\sqrt{\frac{2+2-2}{2+2}}\right)^{5}\times\left(\sqrt{\frac{2+3-2}{2+3}}\right)^{10n}\times\left(\sqrt{\frac{3+3-2}{3+3}}\right)^{\frac{15}{2}n^{2}+\frac{5}{2}n}.$$

By solving the above equation, we get the desired result.

5. Conclusion

We have introduced the multiplicative atom bond sum connectivity index of a graph. Also, we have determined the atom bond sum connectivity index and the multiplicative atom bond sum connectivity index for some important chemical structures.

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Conflict of interest. The paper is written by single author so there is no conflict of interest.

Authors' Contributions. It is a single author paper. So, full credit goes to the author.

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