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NEW EDGE VERSION OF ARITHMETIC GEOMETRIC INDEX

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ABSTRACT

We introduce the edge version of arithmetic geometric index of a molecular graph. In this paper, we determine the edge version of arithmetic-geometric index for some families of nanotubes and nanotori.

Keywords: *molecular graph, arithmetic-geometric index, nanotubes, nanotori.*

Mathematics Subject Classification: *05C05, 05C12, 05C35.*

1. INTRODUCTION

A molecular graph is a graph such that its vertices correspond to the atoms and edges to the bonds. A single number that can be computed from the molecular graph and used to characterize some property of the underlying molecule is said to be a topological index or molecular structure descriptor. Numorous such descriptors have been considered in theoretical chemistry and have found some applications, especially in *QSPR/QSAR* research see [1].

The arithmetic geometric index [2] of a graph G is defined as

$$AG(G) = \sum_{uv \in E(G)} \frac{d_G(u) + d_G(v)}{2\sqrt{d_G(u) d_G(v)}}$$

where $d_G(u)$ denotes the degree of a vertex u in G.

The line graph $L(G)$ of a graph G is the graph whose vertex set corresponds to the edges G such that two vertices of $L(G)$ are adjacent if the corresponding edges of G are adjacent. We refer to [3] for undefined term and notation.

Motivated by previous research on topological indices, we now propose the edge version of arithmetic geometric index of a graph as follows:

The edge version of arithmetic geometric index of a graph G is defined as

$$AG_e(G) = \sum_{ef \in E(L(G))} \frac{d_{L(G)}(e) + d_{L(G)}(f)}{2\sqrt{d_{L(G)}(e) d_{L(G)}(f)}}$$

where $d_{L(G)}(e)$ denotes the degree of an edge e in G.

Many other arithmetic geometric indices were studied, for example, in [4, 5, 6, 7]. The edge version of multiplicative atom bond connectivity index and the edge version of the product and sum connectivity indices were studied respectively in [8] and [9].

In this paper, we compute the edge version of arithmetic-geometric index of some families of nanotubes and nanotorus. For more information about nanotubes and nanotorus; see [10].

2. $TUC_4C_6C_8[p, q]$ NANOTUBES

Consider the graph of $TUC_4C_6C_8[p, q]$ nanotube with p columns and q rows. The graph of $TUC_4C_6C_8[4, 5]$ is shown in Figure 1 (a). Now consider the graph of 2-D lattice of $TUC_4C_6C_8[1, 1]$ nanotube as shown in Figure 1(b). The line graph of $TUC_4C_6C_8[1, 1]$ is shown in Figure 1 (c).

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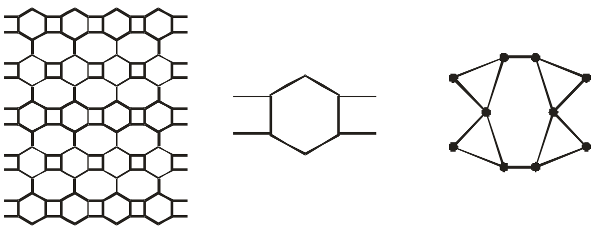


(a) (b) (c)

Figure-1

In the following theorem, we determine the edge version of arithmetic-geometric index for $TUC_4C_6C_8[p,q]$ nanotube.

Theorem 1: The edge version of arithmetic geometric index of $TUC_4C_6C_8[p, q]$ nanotube is given by

$$AG_e\left(TUC_4C_6C_8\left[p,q\right]\right)=18pq+\left(\frac{14}{\sqrt{3}}-12\right)p.$$

Proof: Let G be the graph of $TUC_4C_6C_8[p, q]$ nanotube. By algebraic method, we obtain that the line graph of $TUC_4C_6C_8[p, q]$ nanotube has $18pq - 4p$ edges. In $L(G)$, there are three types of edges based on the degree of the vertices of each edge. The graphic properties on the degree sum of vertices for each edge imply the edge partition of $L(G)$. Table 1 explains such partition.

$d_{L(G)}(e), d_{L(G)}(f)\backslash ef \in E(L(G))$	(3, 3)	(3, 4)	(4, 4)
Number of edges	$2p$	$8p$	$18pq - 14p$

Table-1: Edge partition of $L(G)$

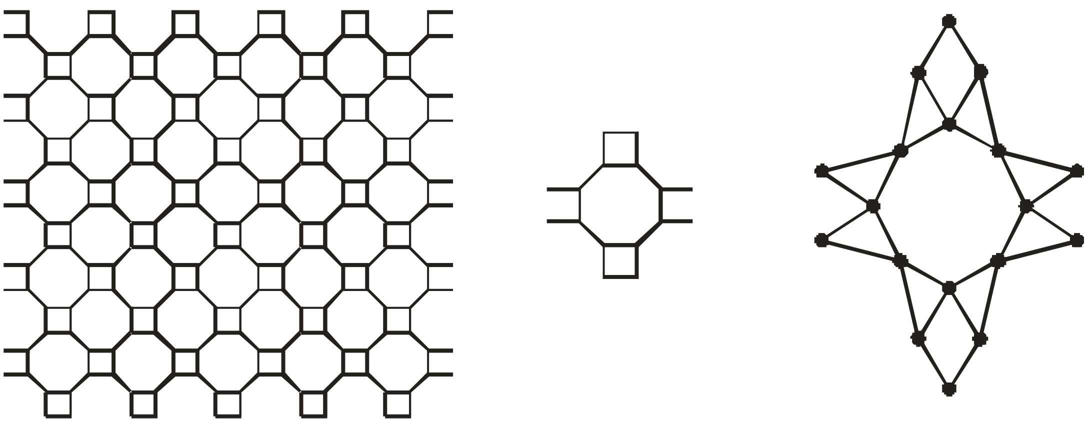
Table 1 and $AG_e\left(G\right)=\sum_{ef\in E(L(G))}\frac{d_{L(G)}(e)+d_{L(G)}(f)}{2\sqrt{d_{L(G)}(e)d_{L(G)}(f)}}$, we have

$$AG_e\left(TUC_4C_6C_8\left[p,q\right]\right)=2p\left(\frac{3+3}{2\sqrt{3\times 3}}\right)+8p\left(\frac{3+4}{2\sqrt{3\times 4}}\right)+\left(18pq-14p\right)\left(\frac{4+4}{2\sqrt{4\times 4}}\right)$$

$$=18pq+\left(\frac{14}{\sqrt{3}}-12\right)p.$$

3. $TUSC_4C_8(S)[m, n]$ NANOTUBES

Consider the graph of $TUSC_4C_8(S)[m, n]$ nanotube with m columns and n rows. The graph of $TUSC_4C_8(S)[5, 4]$ nanotube is shown in Figure 2 (a). Now consider the graph of 2-D lattice of $TUSC_4C_8(S)$ [1, 1] nanotube as shown in Figure 2(b). The line graph of $TUSC_4C_8(S)[1, 1]$ is shown in Figure 2(c).



(a) (b) (c)

Figure-2

In the following theorem, we determine the edge version of arithmetic-geometric index for $TUSC_4C_8(S)[m, n]$ nanotube.

Theorem 2: The edge version of arithmetic-geometric index of $TUSC_4C_8(S)[m, n]$ nanotube is given by

$$AG_e\left(TUSC_4C_8\left(S\right)\left[m,n\right]\right) = 24mn + \left(\frac{10}{\sqrt{6}} + \frac{14}{\sqrt{3}} - 8\right)m.$$

Proof: Let G be the graph of $TUSC_4C_8(S)[m, n]$ nanotube. By algebraic method, the line graph of $TUSC_4C_8(S)[m, n]$ has $24mn + 4m$ edges. In $L(G)$, there are three types of edges based on the degree of the vertices for each edge imply the edge partition of $L(G)$. Table 2 explains such partition.

$d_{L(G)}(e), d_{L(G)}(f) \backslash ef \in E(L(G))$	(2, 3)	(3, 4)	(4, 4)
Number of edges	$4m$	$8m$	$24mn - 8m$

Table-2: Edge partition of $L(G)$

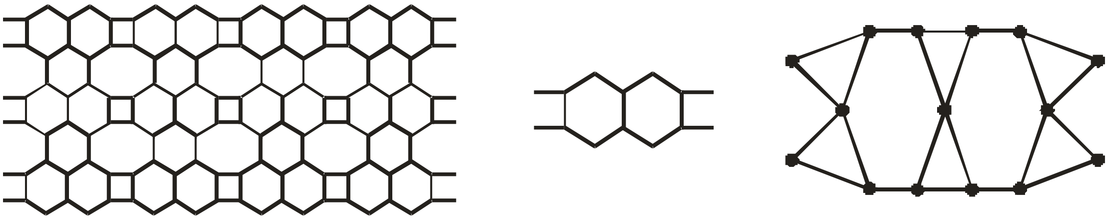
Table 2 and $AG_e(G) = \sum_{ef \in E(L(G))} \frac{d_{L(G)}(e) + d_{L(G)}(f)}{2\sqrt{d_{L(G)}(e)d_{L(G)}(f)}}$, we have

$$AG_e\left(TUSC_4C_8\left(S\right)\left[m,n\right]\right) = 4m\left(\frac{2+3}{2\sqrt{2\times 3}}\right) + 8m\left(\frac{3+4}{2\sqrt{3\times 4}}\right) + \left(24mn - 8m\right)\left(\frac{4+4}{2\sqrt{4\times 4}}\right)$$

$$= 24mn + \left(\frac{10}{\sqrt{6}} + \frac{14}{\sqrt{3}} - 8\right)m.$$

4. *H*-NAPHTALENIC *NPHX* [*m, n*] NANOTUBE

Consider the graph of H-Naphtalenic $NPHX[m, n]$ nanotube with m columns and n rows. The graph of H-Naphtalenic $NPHX[4, 3]$ nanotube is shown in Figure 3(a). Now consider the graph of 2-D lattice of H- Naphtalenic $NPHX[1, 1]$ nanotube as shown in Figure 3(b). The line graph of H-Naphtalenic $NPHX[1, 1]$ is shown in Figure 3(c).



(a) (b) (c)

Figure-3

In the following theorem, we determine the edge version of arithmetic geometric index for H-Naphtalenic $NPHX[m, n]$ nanotube.

Theorem 3: The edge version of arithmetic-geometric index of H-Naphtalenic $NPHX[m, n]$ nanotube is given by

$$AG_e\left(NPHX\left[m,n\right]\right) = 30mn + \left(\frac{21}{\sqrt{3}} - 20\right)m.$$

Proof: Let G be the graph of H-Naphtalenic $NPHX$ $[m, n]$ nanotube. By algebraic method, the line graph of H-Naphtalenic $NPHX[m, n]$ nanotube has $30mn - 8m$ edges. In $L(G)$, there are three types of edges based on the degree of the vertices for each edge imply the edge partition of $L(G)$. Table 3 explains such partition.

$d_{L(G)}(e), d_{L(G)}(f) \backslash ef \in E(L(G))$	(3, 3)	(3, 4)	(4, 4)
Number of edges	$6m$	$12m$	$30mn - 26m$

Table-3: Edge partition of $L(G)$

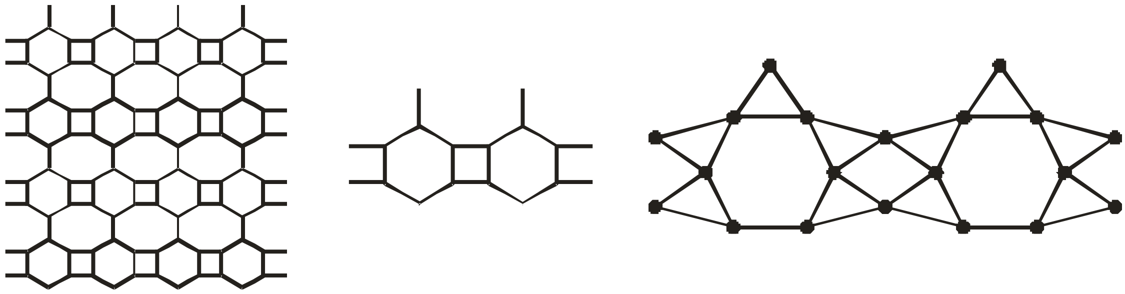
Table 3 and $AG_e\left(G\right) = \sum_{ef \in E\left(L(G)\right)} \frac{d_{L(G)}\left(e\right) + d_{L(G)}\left(f\right)}{2\sqrt{d_{L(G)}\left(e\right)d_{L(G)}\left(f\right)}}$, we have

$$AG_e\left(NPHX\left[m,n\right]\right) = 6m\left(\frac{3+3}{2\sqrt{3\times 3}}\right) + 12m\left(\frac{3+4}{2\sqrt{3\times 4}}\right) + \left(30mn - 26m\right)\left(\frac{4+4}{2\sqrt{4\times 4}}\right)$$

$$= 30mn + \left(\frac{21}{\sqrt{3}} - 20\right)m.$$

5. $C_4C_6C_8[p, q]$ NANOTORI

Consider the graph of $C_4C_6C_8[p, q]$ nanotori with p columns and q rows. The graph of $C_4C_6C_8[4, 4]$ nanotori is shown in Figure 4 (a). Now consider the graph of 2-*D* lattice of $C_4C_6C_8[2, 1]$ nanotori as shown in Figure 4(b). The line graph of $C_4C_6C_8[2, 1]$ is shown in Figure 4 (c).



(a) (b) (c)

Figure-4

In the following theorem, we determine the edge version of arithmetic geometric index for $C_4C_6C_8[p,q]$ nanotori.

Theorem 4: The edge version of arithmetic-geometric index of $C_4C_6C_8[p, q]$ nanotori is given by

$$AG_e\left(C_4C_6C_8[p,q]\right) = 18pq + \left(\frac{3}{\sqrt{2}} + \frac{7}{\sqrt{3}} - 8\right)p.$$

Proof: Let G be the graph of $C_4C_6C_8[p, q]$ nanotori. By algebraic method, the line graph of $C_4C_6C_8[p,q]$ nanotori has $18pq - 2p$ edges. In $L(G)$, there are four types of edges based on the degree of the vertices for each edge imply the edge partition of $L(G)$. Table 4 explains such partition.

$d_{L(G)}(e), d_{L(G)}(f) \backslash ef \in E(L(G))$	(2, 4)	(3, 3)	(3, 4)	(4, 4)
Number of edges	$2p$	p	$4p$	$18pq - 9p$

Table-4: Edge partition of $L(G)$

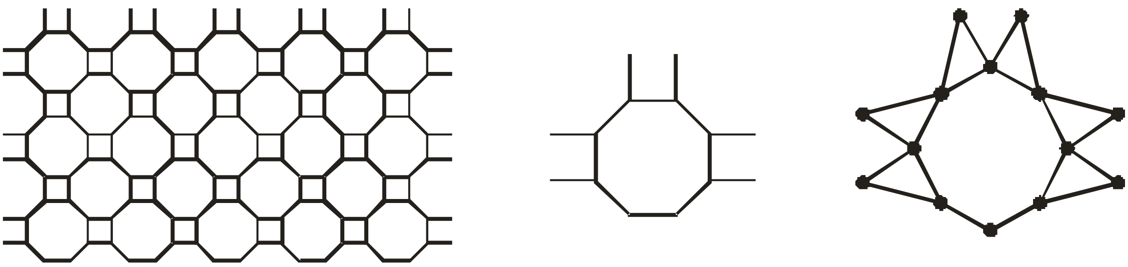
Table 4 and $AG_e(G) = \sum_{ef \in E(L(G))} \frac{d_{L(G)}(e) + d_{L(G)}(f)}{2\sqrt{d_{L(G)}(e)\, d_{L(G)}(f)}}$, we have

$$AG_e\left(C_4C_6C_8[p,q]\right) = 2p\left(\frac{2+4}{2\sqrt{2\times 4}}\right) + p\left(\frac{3+3}{2\sqrt{3\times 3}}\right) + 4p\left(\frac{3+4}{2\sqrt{3\times 4}}\right) + (18pq - 9p)\left(\frac{4+4}{2\sqrt{4\times 4}}\right)$$

$$= 18pq + \left(\frac{3}{\sqrt{2}} + \frac{7}{\sqrt{3}} - 8\right)p.$$

6. $TC_4C_8(S)\,[p, q]$ NANOTORI

Consider the graph of $TC_4C_8(S)[p, q]$ nanotori with p columns and q rows. The graph of $TC_4C_8(S)[5, 3]$ nanotori is shown in Figure 5(a). Now consider the graph of 2-*D* lattice of $TC_4C_8(S)$ [1, 1] nanotori as shown in Figure 5(b). The line graph of $TC_6C_8(S)[1, 1]$ nanotori is shown in Figure 5 (c).



(a) (b) (c)

Figure-5

In the next theorem, we determine the edge version of arithmetic geometric index for $TC_4C_8(S)[p, q]$ nanotori.

Theorem 5: The edge version of arithmetic geometric index of $TC_4C_8(S)[p, q]$ nanotori is given by

$$AG_e\left(TC_4C_8\left(S\right)\left[p,q\right]\right)=24pq+\left(\frac{5}{\sqrt{6}}+\frac{6}{\sqrt{2}}+\frac{7}{\sqrt{3}}-14\right)p.$$

Proof: Let G be the graph of $TC_4C_8(S)[p, q]$ nanotori has $24pq - 4p$ edges. In $L(G)$, there are four types of edges based on the degree of the vertices for each edge imply the edge partition of $L(G)$. Table 5 explains such partition.

$d_{L(G)}(e), d_{L(G)}(f) \setminus ef \in E(L(G))$	(2, 3)	(2, 4)	(3, 4)	(4, 4)
Number of edges	$2p$	$4p$	$4p$	$24pq - 14p$

Table-5: Edge partition of $L(G)$.

Table 5 and $AG_e = \sum_{ef\in E(L(G))} \frac{d_{L(G)}(e)+d_{L(G)}(f)}{\sqrt{d_{L(G)}(e)d_{L(G)}(f)}}$, we have

$$AG_e\left(TC_4C_8\left(S\right)\left[p,q\right]\right)=2p\left(\frac{2+3}{2\sqrt{2\times3}}\right)+4p\left(\frac{2+4}{2\sqrt{2\times4}}\right)+4p\left(\frac{3+4}{2\sqrt{3\times4}}\right)+\left(24pq-14p\right)\left(\frac{4+4}{2\sqrt{4\times4}}\right)$$

$$=24pq+\left(\frac{5}{\sqrt{6}}+\frac{6}{\sqrt{2}}+\frac{7}{\sqrt{3}}-14\right)p.$$

7. CONCLUSION

Numerous topological indices have been considered in theoretical chemistry and have found some applications especially in *QSPR/QSAR* research. In this paper, we computed the edge version of arithmetic- geometric index of $TUC_4C_6C_8[p, q]$, $TUSC_4C_8(S)[m, n]$, $NPHX[m, n]$ nanotubes and $C_4C_6C_8[p, q]$, $TC_4C_8(S)[p, q]$ nanotori.

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