

Edge Version of Multiplicative Atom Bond Connectivity Index of Certain Nanotubes and Nanotorus

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Abstract: We define the edge version of multiplicative atom bond connectivity index of a molecular graph. In this paper, we compute this index for different chemically interesting nanotubes and nanotorus.

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1. Introduction

Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. A molecular graph is a finite simple graph such that its vertices correspond to the atoms and the edges to the bonds. A topological index is a numerical parameter mathematically derived from the graph structure. There are several topological indices that have some applications in theoretical chemistry, especially in *QSPR/QSAR* study [1, 2]. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v . The degree of an edge $e = uv$ in G is defined by $d_G(e) = d_G(u) + d_G(v) - 2$. The line graph $L(G)$ of G is the graph whose vertex set corresponds to the edges of 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. The multiplicative atom bond connectivity index [4] of a graph G is defined as

$$ABCII(G) = \prod_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u) d_G(v)}}$$

This index was also studied, for example, in [5, 6]. We now define the edge version of multiplicative atom bond connectivity index of a graph G as follows:

The edge version of multiplicative atom bond connectivity index of a molecular graph G is defined as

$$ABCII_e(G) = \prod_{ef \in E(L(G))} \sqrt{\frac{d_{L(G)}(e) + d_{L(G)}(f) - 2}{d_{L(G)}(e) d_{L(G)}(f)}}$$

Many other multiplicative topological indices were studied, for example, in [7–19]. Edge version of indices were also studied, for example, in [20, 21]. In this paper, we compute the edge version of multiplicative atom bond connectivity index of $TUC_4C_6C_8[p, q]$, $TUSC_4C_8(S)[m, n]$, $NPHX[m, n]$ nanotubes and $C_4C_6C_8[p, q]$, $TC_4C_8(S)[p, q]$ nanotorus. For more information about nanotubes and nanotori see [22].

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2. Results for Nanotubes

2.1. $TUC_4C_6C_8[p, q]$ Nanotube

We consider the graph 2- D lattice of $TUC_4C_6C_8[1, 1]$ nanotube as depicted in Figure 1(a). The line graph of $TUC_4C_6C_8[1, 1]$ is shown in Figure 1(b). Also we 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(c).

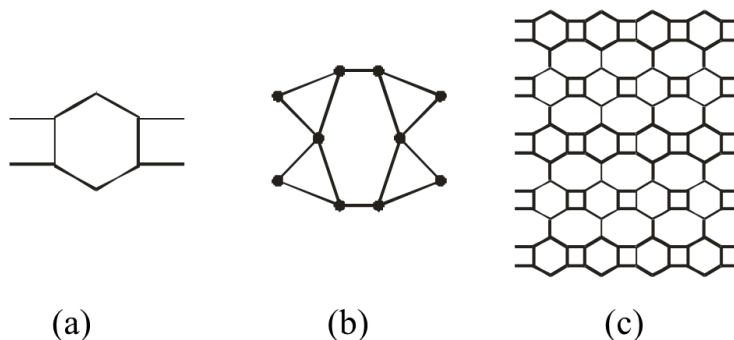


Figure 1.

We determine the edge version of multiplicative atom bond connectivity index for $TUC_4C_6C_8[p, q]$ nanotube.

Theorem 2.1. *The edge version of multiplicative atom bond connectivity index of $TUC_4C_6C_8[p, q]$ nanotube is*

$$ABCII_e(TUC_4C_6C_8[p, q]) = \left(\frac{2}{3}\right)^{2p} \left(\frac{5}{12}\right)^{4p} \left(\frac{3}{8}\right)^{9pq-7p}.$$

Proof. Let G be the graph of $TUC_4C_6C_8[p, q]$ nanotube. By algebraic method, the line graph of $TUC_4C_6C_8[p, q]$ has $18pq - 4p$ edges. Also we obtain that the edge set $E(L(G))$ can be divided into three partitions as given in Table 1.

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

Table 1. Partitions of the edge set $E(L(G))$

Thus, using the definition of edge version of multiplicative atom bond connectivity index, we obtain

$$\begin{aligned} ABCII_e(TUC_4C_6C_8[p, q]) &= \left(\sqrt{\frac{3+3-2}{3 \times 3}}\right)^{2p} \left(\sqrt{\frac{3+4-2}{3 \times 4}}\right)^{8p} \left(\sqrt{\frac{4+4-2}{4 \times 4}}\right)^{18pq-14p} \\ &= \left(\frac{2}{3}\right)^{2p} \left(\frac{5}{12}\right)^{4p} \left(\frac{3}{8}\right)^{9pq-7p}. \end{aligned}$$

□

2.2. $TUSC_4C_8(S)[m, n]$ Nanotube

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

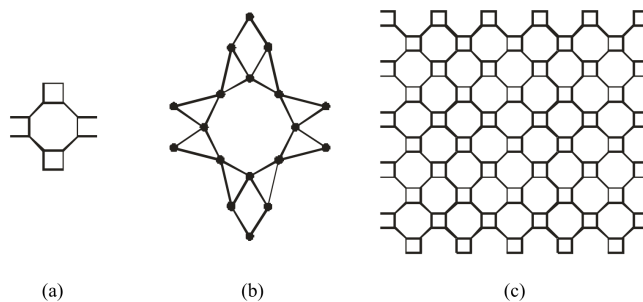


Figure 2.

In the following theorem, we determine the edge version of multiplicative atom bond connectivity index for $TUSC_4C_8(S)[m, n]$ nanotube.

Theorem 2.2. *The edge version of multiplicative atom bond connectivity index of $TUSC_4C_8(S)[m, n]$ nanotube is*

$$ABCII_e(TUSC_4C_8(S)[m, n]) = \left(\frac{1}{2}\right)^{2m} \left(\frac{5}{12}\right)^{4m} \left(\frac{3}{8}\right)^{12mn-4m}.$$

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. Also we obtain that the edge set $E(L(G))$ can be divided into three partitions as given in Table 2.

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

Table 2. Partitions of the edge set $E(L(G))$

Thus using the definition of edge version of multiplicative atom bond connectivity index, we obtain

$$\begin{aligned} ABCII_e(TUSC_4C_8(S)[m, n]) &= \left(\sqrt{\frac{2+3-2}{2 \times 3}}\right)^{4m} \left(\sqrt{\frac{3+4-2}{3 \times 4}}\right)^{8m} \left(\sqrt{\frac{4+4-2}{4 \times 4}}\right)^{24mn-8m} \\ &= \left(\frac{1}{2}\right)^{2m} \left(\frac{5}{12}\right)^{4m} \left(\frac{3}{8}\right)^{12mn-4m}. \end{aligned}$$

□

2.3. H-Naphtalenic $NPHX[m, n]$ Nanotube

We consider the graph 2-D lattice of H-Naphtalenic $NPHX[1, 1]$ nanotube as shown in Figure 3(a). The line graph of H-Naphtalenic $NPHX[1, 1]$ is shown in Figure 3(b). Also we consider the graph of H-Naphtalenic $NPHX[4, 3]$ nanotube as shown in Figure 3(c).

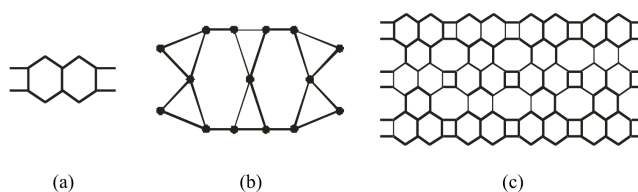


Figure 3.

In the following theorem, we determine the edge version of multiplicative atom bond connectivity index for $NPHX[m, n]$ nanotube.

Theorem 2.3. The edge version of multiplicative atom bond connectivity index of $NPHX[m, n]$ nanotube is

$$ABCII_e(NPHX[m, n]) = \left(\frac{2}{3}\right)^{6m} \left(\frac{5}{12}\right)^{6m} \left(\frac{3}{8}\right)^{15mn-13m}.$$

Proof. Let G be the graph of $NPHX[m, n]$ nanotube. By algebraic method, the line graph of $NPHX[m, n]$ nanotube has $30mn - 8m$ edges. Also we obtain that the edge set $E(L(G))$ can be divided into three partitions as given in Table 3.

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

Table 3. Partitions of edge set $E(L(G))$

Thus, using the definition of edge version of multiplicative atom bond connectivity index, we obtain

$$\begin{aligned} ABCII_e(NPHX[m, n]) &= \left(\sqrt{\frac{3+3-2}{3 \times 3}}\right)^{6m} \left(\sqrt{\frac{3+4-2}{3 \times 4}}\right)^{12m} \left(\sqrt{\frac{4+4-2}{4 \times 4}}\right)^{30mn-26m} \\ &= \left(\frac{2}{3}\right)^{6m} \left(\frac{5}{12}\right)^{6m} \left(\frac{3}{8}\right)^{15mn-13m}. \end{aligned}$$

□

3. Results for Nanotorus

3.1. $C_4C_6C_8[p, q]$ Nanotori

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

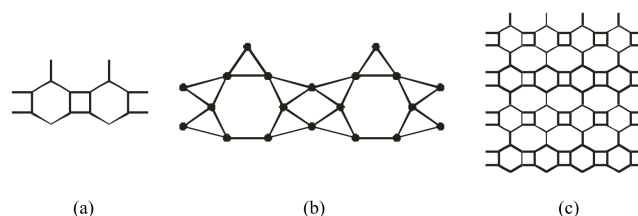


Figure 4.

Theorem 3.1. The edge version of multiplicative atom bond connectivity index of $C_4C_6C_8[p, q]$ is

$$ABCII_e(C_4C_6C_8[p, q]) = \left(\frac{1}{2}\right)^p \left(\frac{2}{3}\right)^p \left(\frac{5}{12}\right)^{2p} \left(\frac{\sqrt{6}}{4}\right)^{18pq-9p}.$$

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. Also we obtain that the edge set $E(L(G))$ can be divided into four partitions as given in Table 4.

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

Table 4. Partitions of the edge set $E(L(G))$

Thus using the definition of edge version of multiplicative atom bond connectivity index, we obtain

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

$$= \left(\frac{1}{2}\right)^p \left(\frac{2}{3}\right)^p \left(\frac{5}{12}\right)^{2p} \left(\frac{\sqrt{6}}{4}\right)^{18pq-9p}.$$

□

3.2. $TC_4C_8(S)[p, q]$ Nanotori

Consider the graph of 2-D lattice of $TC_4C_8(S)[1, 1]$ nanotori as shown in Figure 5(a). The line graph of $TC_4C_8(S)[1, 1]$ nanotori is shown in Figure 5(b). Also we consider the graph of 2-D lattice of $TC_4C_8(S)[5, 3]$ nanotori as shown in Figure 5(c).

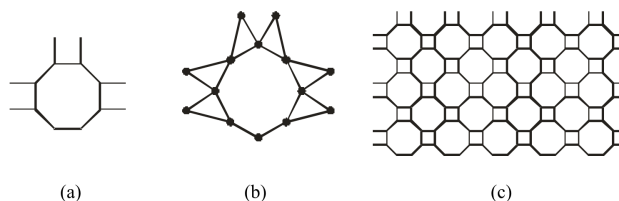


Figure 5.

In the following theorem, we determine the edge version of multiplicative atom bond connectivity index for $TC_4C_8(S)[p, q]$ nanotori.

Theorem 3.2. *The edge version of multiplicative atom bond connectivity index of $TC_4C_8(S)[p, q]$ nanotori is*

$$ABCI_e(TC_4C_8(S)[p, q]) = \left(\frac{1}{2}\right)^{3p} \left(\frac{5}{12}\right)^{4p} \left(\frac{3}{8}\right)^{12pq-7p}.$$

Proof. Let G be the graph of $TC_4C_8(S)[p, q]$ nanotori. By algebraic method, the line graph of $TC_4C_8(S)[p, q]$ nanotori has $24pq - 4p$ edges. Also we obtain that the edge set $E(L(G))$ can be divided into four partitions as given in Table 5.

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

Table 5. Partitions of the edge set $E(L(G))$

Thus, using the definition of edge version of multiplicative atom bond connectivity index, we obtain

$$\begin{aligned} ABCI_e(TC_4C_8(S)[p, q]) &= \left(\sqrt{\frac{2+3-2}{2 \times 3}}\right)^{2p} \left(\sqrt{\frac{2+4-2}{2 \times 4}}\right)^{4p} \left(\sqrt{\frac{3+4-2}{3 \times 4}}\right)^{4p} \left(\sqrt{\frac{4+4-2}{4 \times 4}}\right)^{24pq-14p} \\ &= \left(\frac{1}{2}\right)^{3p} \left(\frac{5}{12}\right)^{4p} \left(\frac{3}{8}\right)^{12pq-7p}. \end{aligned}$$

□

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