

Edge Version of F -index, General Sum Connectivity Index of Certain Nanotubes

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Abstract. Chemical graph theory is a branch of graph theory whose focus of interest is to finding topological indices of chemical graphs which correlate well with chemical properties of the chemical molecules. In this paper, we define the edge version of F -index, the edge version of the general sum connectivity index of a graph and compute exact formulas for some families of nanotubes.

Keywords: F -index, hyper-Zagreb index, sum connectivity index, nanotubes.

AMS Mathematics Subject Classification (2010): 05C05, 05C12

1. Introduction

A molecular 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. A topological index is a numerical parameter mathematically derived from the graph structure. Numerous topological indices have been considered in Theoretical Chemistry and have some applications, especially in *QSPR/QSAR* research [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 a graph 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 F -index of a graph G is defined as

$$F(G) = \sum_{u \in V(G)} d_G(u)^3 \quad \text{or} \quad F(G) = \sum_{uv \in E(G)} [d_G(u)^2 + d_G(v)^2].$$

This index was introduced in [4]. In [5], Furtula and Gutman studied this index and called it forgotten topological index

In [6], Shirdel et al. introduced the hyper-Zagreb index of a graph G . It is defined as

$$HM(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^2.$$

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In [7], Zhou and Trinajstić introduced the sum connectivity index of a graph G and it is defined as

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

The general sum connectivity index was introduced by Zhou and Trinajstić in [8]. This index is defined as

$$M_1^a(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^a.$$

where a is a real number.

The above mentioned indices were also studied in [9,10]. Recently many other topological indices were studied, for example, in [11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25].

We define the edge version of F -index, edge version of sum connectivity index, edge version of hyper-Zagreb index, edge version of general sum connectivity index of a molecular graph G as follows:

The edge version of the F -index of a graph G is defined as

$$F_e(G) = \sum_{uv \in E(L(G))} d_{L(G)}(e)^3.$$

or
$$F_e(G) = \sum_{ef \in E(L(G))} [d_{L(G)}(e)^2 + d_{L(G)}(f)^2].$$

The edge version of sum connectivity index of a graph G is defined as

$$X_e(G) = \sum_{ef \in E(L(G))} \frac{1}{\sqrt{d_{L(G)}(e) + d_{L(G)}(f)}}.$$

The edge version of hyper-Zagreb index of a graph G is defined as

$$HM_e(G) = \sum_{ef \in E(L(G))} [d_{L(G)}(e) + d_{L(G)}(f)]^2.$$

The edge version of these indices were studied, for example, in [26, 27].

In this paper, we compute the edge version of F -index, edge version of sum connectivity index, hyper Zagreb index and edge version of general sum connectivity index of $TUC_4C_6C_8[p, q]$ nanotubes, $TUSC_4C_8(S)[p, q]$ nanotubes. For more information about these nanotubes see [28].

2. Results for $TUC_4C_6C_8[p, q]$ nanotube

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

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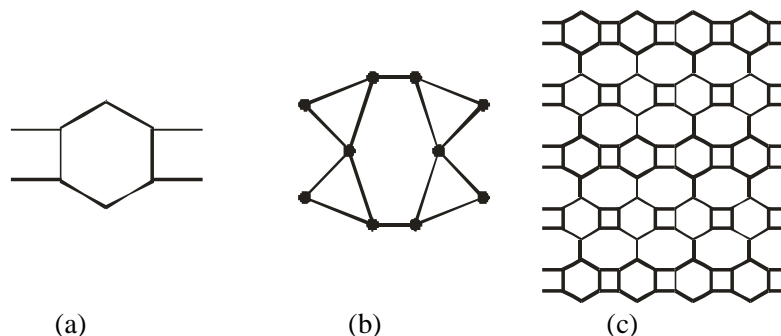


Figure 1:

Let G be the graph of 2-dimensional lattice of $TUC_4C_6C_8[p, q]$ nanotube. By calculation, we obtain that the line graph of $TUC_4C_6C_8[p, q]$ has $18pq - 4p$ edges. In $L(TUC_4C_6C_8[p, q])$, there are three types of edges based on the degree of the vertices of each edge. Thus by calculation, we obtain edge partitions of $L(TUC_4C_6C_8[p, q])$ based on the sum of degrees of the end vertices of each edge 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: Edge partition of $L(G)$

In the following theorem, we compute the exact value of $F_e(TUC_4C_6C_8[p, q])$.

Theorem 1. Let G be the graph of $TUC_4C_6C_8[p, q]$ nanotube. Then

$$F_e(TUC_4C_6C_8[p, q]) = 576pq - 212p.$$

Proof: We have $F_e(G) = \sum_{ef \in E(L(G))} [d_{L(G)}(e)^2 + d_{L(G)}(f)^2]$.

By using Table 1, we have

$$\begin{aligned} F_e(G) &= (3^2 + 3^2)2p + (3^2 + 4^2)8p + (4^2 + 4^2)(18pq - 14p) \\ &= 576pq - 212p. \end{aligned}$$

In the next theorem, we compute the exact value of the edge version of the general sum connectivity index of $TUC_4C_6C_8[p, q]$ nanotube.

Theorem 2. Let G be the graph of $TUC_4C_6C_8[p, q]$ nanotube. Then

$$M_{1e}^a(TUC_4C_6C_8[p, q]) = 18 \times 8^a pq + (2 \times 6^a + 8 \times 7^a - 14 \times 8^a)p. \quad (1)$$

Proof: We have $M_{1e}^a(G) = \sum_{ef \in E(L(G))} [d_{L(G)}(e) + d_{L(G)}(f)]^a$.

By using Table 1, we have

$$M_{1e}^a(G) = (3+3)^a 2p + (3+4)^a 8p + (4+4)^a (18pq - 14p)$$

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$$= 18 \times 8^a pq + (2 \times 6^a + 8 \times 7^a - 14 \times 8^a) p.$$

We obtain the following results by using Theorem 2.

Corollary 2.1. The edge version of the sum connectivity index of $TUC_4C_6C_8[p, q]$ nanotube is given by

$$M_{1e}^a(TUC_4C_6C_8[p, q]) = \frac{9}{\sqrt{2}} pq + \left(\frac{2}{\sqrt{6}} + \frac{8}{\sqrt{7}} - \frac{7}{\sqrt{2}} \right) p.$$

Proof: Put $a = -\frac{1}{2}$ in equation (1), we get the desired result.

Corollary 2.2. The edge version of the hyper-Zagreb index of $TUC_4C_6C_8[p, q]$ nanotube is given by

$$HM_e(TUC_4C_6C_8[p, q]) = 1152 pq - 432 p.$$

Proof: Put $a = 2$ in equation (1), we get the desired result.

3. Results for $TUSC_4C_8(S)[p, q]$ nanotube

We consider the graph of 2-dimensional lattice of $TUSC_4C_8(S)[p, q]$ nanotube with p columns and q rows. The graph of 2-dimensional lattice of $TUSC_4C_8(S)[1,1]$ nanotube is shown in Figure 2(a). The line graph of $TUSC_4C_8(S)[1,1]$ nanotube is shown in Figure 2(b). Also the graph of $TUSC_4C_8(S)[p, q]$ is shown in Figure 2(c).

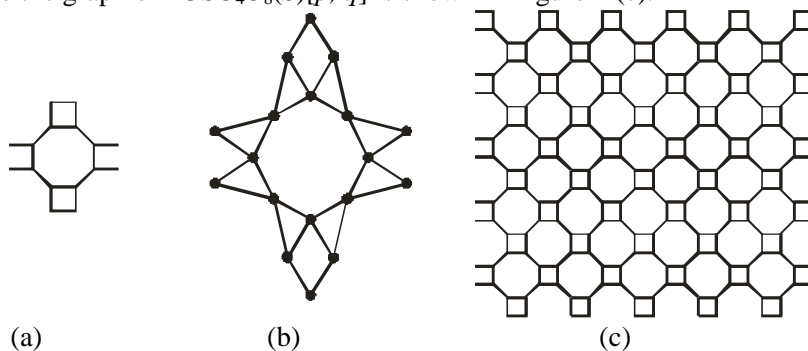


Figure 2:

Let G be the graph of 2-dimensional lattice of $TUSC_4C_8(S)[p, q]$ nanotube. By calculation, we obtain that the line graph of $TUSC_4C_8(S)[p, q]$ has $24pq + 4p$ edges. In $L(TUSC_4C_8(S)[p, q])$, there are three types of edges based on the degree of the vertices of each edge. Thus by calculation, we obtain that edge partitions of $L(TUSC_4C_8(S)[p, q])$ based on the sum of degrees of the end vertices of each edge 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	$4p$	$8p$	$24pq - 8p$

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

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In the following theorem, we compute the exact value of the edge version of F -index of $TUSC_4C_8(S)[p, q]$ nanotube.

Theorem 3. Let G be the graph of $TUSC_4C_8(S)[p, q]$ nanotube. Then

$$F_e(TUSC_4C_8(S)[p, q]) = 768pq - 4p.$$

Proof: We have $F_e(G) = \sum_{ef \in E(L(G))} [d_{L(G)}(e)^2 + d_{L(G)}(f)^2]$.

By using Table 2, we have

$$\begin{aligned} F_e(TUSC_4C_8(S)[p, q]) &= (2^2 + 3^2)4p + (3^2 + 4^2)8p + (4^2 + 4^2)(24pq - 8p) \\ &= 768pq - 4p. \end{aligned}$$

In the next theorem, we compute the exact value of the edge version of the general sum connectivity index of $TUSC_4C_8(S)[p, q]$ nanotube.

Theorem 4. Let G be the graph of $TUSC_4C_8(S)[p, q]$ nanotube. Then

$$M_{1e}^a(TUSC_4C_8(S)[p, q]) = 24 \times 8^a pq + (4 \times 5^a + 8 \times 7^a - 8 \times 8^a) p. \quad (2)$$

Proof: We have $M_{1e}^a(G) = \sum_{ef \in E(L(G))} [d_{L(G)}(e) + d_{L(G)}(f)]^a$.

By using Table 2, we have

$$\begin{aligned} M_{1e}^a(TUSC_4C_8(S)[p, q]) &= (2+3)^a 4p + (3+4)^a 8p + (4+4)^a (24pq - 8p) \\ &= 24 \times 8^a pq + (4 \times 5^a + 8 \times 7^a - 8 \times 8^a) p. \end{aligned}$$

We obtain the following results by using Theorem 4.

Corollary 4.1. The edge version of the sum connectivity index of $TUSC_4C_8(S)[p, q]$ nanotube is given by

$$X_e(TUSC_4C_8(S)[p, q]) = 3\sqrt{8}pq + \left(\frac{4}{\sqrt{5}} + \frac{8}{\sqrt{7}} - \sqrt{8} \right) p.$$

Proof: Put $a = -\frac{1}{2}$ in equation (2), we get the desired result.

Corollary 4.2. The edge version of the hyper-Zagreb index of $TUSC_4C_8(S)[p, q]$ nanotube is given by

$$HM_e(TUSC_4C_8(S)[p, q]) = 1536pq - 20p.$$

Proof: Put $a = 2$ in equation (2), we get the desired result.

5. Conclusion

Chemical Graph Theory is an important tool for studying molecular structures. At present, the study of topological indices is one of the active research fields in chemical graph theory. In this paper, we have obtained some theoretical results on "Edge version

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of F-index, general sum connectivity index of certain nanotubes". These formulas make it possible to correlate chemical structure of nanotubes with an information about their physical features.

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