International Research Journal of Pure Algebra-7(11), 2017, 855-858
Available online through www.rjpa.info ISSN 2248–9037

EDGE VERSION OF INVERSE SUM INDEG INDEX OF CERTAIN NANOTUBES AND NANOTORI

V. R. KULLI*

Department of Mathematics,
Gulbarga University, Gulbarga 585106, India.

(Received On: 10-11-17; Revised & Accepted On: 28-11-17)

ABSTRACT

Chemical graph theory is a branch of graph theory whose focus of interest is to finding topological indices of chemical molecular graphs, which correlate well with chemical properties of the chemical molecules. A topological index is a numerical parameter mathematically derived from the graph structure. In this paper, we compute the edge version of inverse sum indeg index of certain nanotubes and nanotori.

Key words: *molecular graph, inverse sum indeg index, nanotubes, nanotori.*

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

1. INTRODUCTION

Let G be a finite, simple graph with vertex set $V(G)$ and edge set $E(G)$. 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 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 [1] for undefined term and notation.

Chemical graph theory is a branch of Mathematical chemistry which has an important effect on the development of the chemical sciences. A topological index is a numerical parameter mathematically derived from the graph structure. Numerous such topological indices or descriptors have been considered in Theoretical Chemistry and have found some applications, especially in *QSPR/QSAR* studies, see [2, 3].

The inverse sum indeg index [4] of a graph G is defined as

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

The edge version of the inverse sum indeg index [5] of a graph G is defined as

$$ISI_e(G) = \sum_{ef \in E(L(G))} \frac{d_{L(G)}(e)d_{L(G)}(f)}{d_{L(G)}(e)+d_{L(G)}(f)}. \qquad (2)$$

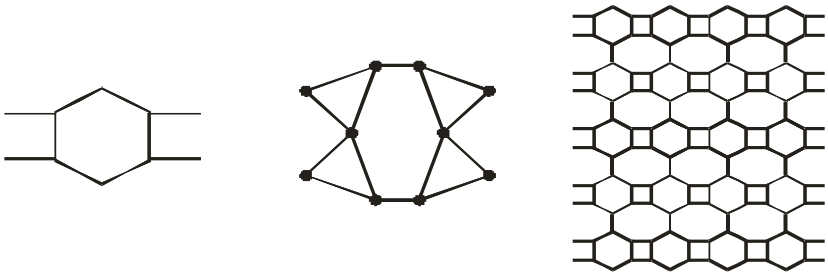
Very recently the inverse sum indeg index was also studied, for example, in [6]. Many other edge version of indices were studied, for example, in [7, 8, 9, 10].

In this paper, the edge version of the inverse sum indeg index for certain nanotubes and nanotori are determined, For more information about nanotubes and nanotori see [11].

2. RESULTS FOR $TUC_4C_6C_8$ [p, q] NANOTUBE

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

Corresponding Author: V. R. Kulli*
Department of Mathematics, Gulbarga University, Gulbarga 585106, India.



(a) (b) (c)

Figure-1

Let G be the graph of 2-D lattice of $TUC_4C_6C_8$ [p, q] nanotube. By calculation, we obtain $|E(L(TUC_4C_6C_8\ [p, q]))| = 18pq - 4p$. 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 that the edge partitions of the line graph of $TUC_4C_6C_8$ [p, q] based on the sum of degrees of the end vertices of each edge as given in Table 1.

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

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

Theorem 1: The edge version of inverse sum indeg index of $TUC_4C_6C_8$ [p, q] nanotube is given by

$$ISI_e\left(TUC_4C_6C_8\left[p,q\right]\right) = 36pq - \frac{79}{7}p.$$

Proof: Let G be the graph of $TUC_4C_6C_8$ [p, q] nanotube. From equation (2) and by cardinalities of the edge partitions of $L(G)$, we have

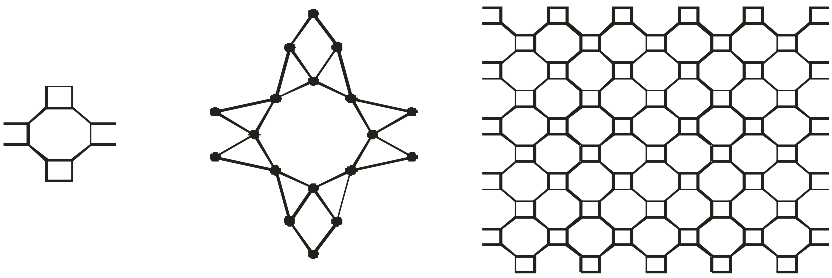
$$ISI_e\left(TUC_4C_6C_8\left[p,q\right]\right) = \sum_{ef\in E(L(G))} \frac{d_{L(G)}(e)d_{L(G)}(f)}{d_{L(G)}(e)+d_{L(G)}(f)}.$$

$$= 2p\left(\frac{3\times3}{3+3}\right) + 8p\left(\frac{3\times4}{3+4}\right) + \left(18pq - 14p\right)\left(\frac{4\times4}{4+4}\right)$$

$$= 36pq - \frac{79}{7}p.$$

3. RESULTS OF $TUSC_4C_8(S)$ [p, q] NANOTUBE

We consider the graph of 2-D lattice of $TUSC_4C_8(S)$ [p, q] nanotube with p columns and q rows. The graph of 2-D 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 $TUSC_4C_8(S)$ [4, 5] is shown in Figure 2(c).



(a) (b) (c)

Figure-2

Let G be the graph of 2-D lattice of $TUSC_4C_8(S)[p\ q]$) nanotube. By calculation, we obtain $|E(L(TUSC_4C_8(S)[p, q])| = 24pq + 4p$. 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 the 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.

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

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

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

Theorem 2: The edge version of inverse sum indeg index of $TUSC_4C_8(S)[p, q]$ nanotube is given by

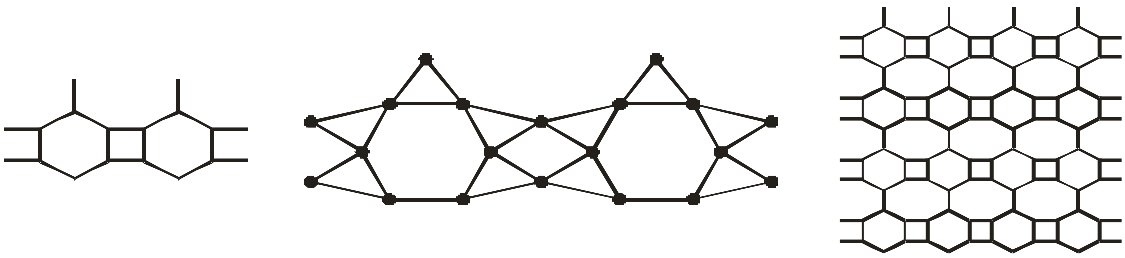
$$ISI_e\left(TUSC_4C_8\left(S\right)\left[p,q\right]\right)=48pq+\frac{88}{35}p.$$

Proof: Let G be the graph of $TUSC_4C_8(S)[p, q]$ nanotube. From equation (2) and by cardinalities of the edge partitions of $L(G)$, we have

$$\begin{aligned}ISI_e\left(TUSC_4C_8\left(S\right)\left[p,q\right]\right)&=\sum_{ef\in E(L(G))}\frac{d_{L(G)}(e)d_{L(G)}(f)}{d_{L(G)}(e)+d_{L(G)}(f)}\\&=4p\left(\frac{2\times3}{2+3}\right)+8p\left(\frac{3\times4}{3+4}\right)+\left(24pq-8p\right)\left(\frac{4\times4}{4+4}\right)\\&=48pq+\frac{88}{35}p.\end{aligned}$$

4. RESULTS FOR $C_4C_6C_8$ [p, q] NANOTORI

We consider the graph of 2-D lattice of $C_4C_6C_8$ [p, q] nanotori with p columns and q rows. The graph of 2-D lattice of $C_4C_6C_8$ [2, 1] nanotori is shown Figure 3(a). The line graph of 2-D lattice of $C_4C_6C_8$[2,1] nanotori is shown in Figure 3(b). Also the graph of 2-D lattice of $C_4C_6C_8$[4,4] nanotori is shown in Figure 3(c).



(a) (b) (c)

Figure-3

Let G be the graph of 2-D lattice of $C_4C_6C_8$ [p, q] nanotori. By calculation, we obtain $|E(L(C_4C_6C_8[p,q]))|= 18pq - 2p$. In $L(C_4C_6C_8 [p, q])$, there are four types of edges based on the degree of the vertices of each edge. Thus by calculation, we obtain that the edge partitions of the line graph of $C_4C_6C_8[p,q]$ based on the sum of degrees of the end vertices of each edge as given in Table 3.

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

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

In the next theorem, we compute the exact value of ISI_e index of $C_4C_6C_8$ [p, q] nanotori.

Theorem 3: The edge version of the inverse sum indeg index of $C_4C_6C_8$ [p, q] is given by

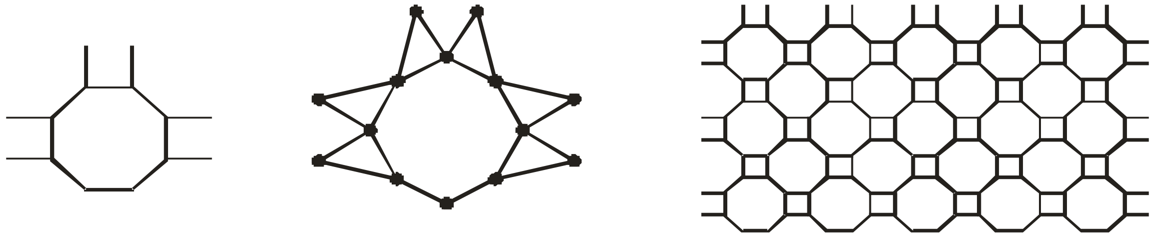
$$ISI_e\left(C_4C_6C_8\left[p,q\right]\right)=36pq-\frac{293}{42}p.$$

Proof: Let G be the graph of $C_4C_6C_8$ [p, q] nanotori. From equation (2) and by cardinalities of the edge partitions of $L(G)$, we have

$$\begin{aligned}ISI_e\left(C_4C_6C_8\left[p,q\right]\right)&=\sum_{ef\in E(L(G))}\frac{d_{L(G)}(e)d_{L(G)}(f)}{d_{L(G)}(e)+d_{L(G)}(f)}\\&=2p\left(\frac{2\times4}{2+4}\right)+p\left(\frac{3\times3}{3+3}\right)+4p\left(\frac{3\times4}{3+4}\right)+\left(18pq-9p\right)\left(\frac{4\times4}{4+4}\right)\\&=36pq-\frac{293}{42}p.\end{aligned}$$

5. RESULTS FOR TC_4C_8 (S) [p, q] NANOTORI

We consider the graph of 2-*D* lattice of TC_4C_8 (S) [p, q] nanotori with p columns and q rows. The graph of 2-*D* lattice of TC_4C_8 (S) [1, 1] nanotori is shown in Figure 4(a). The line graph of 2-*D* lattice of TC_4C_8 (S) [1, 1] nanotori is shown in Figure 4(b). Also the graph of 2-*D* lattice of TC_4C_8 (S) [5, 3] nanotori is shown in Figure 4(c).



(a) (b) (c)

Figure-4

Let G be the graph of 2-*D* lattice of TC_4C_8 (S) [p, q] nanotori. By calculation, we obtain $|E(L(TC_4C_8(S)[p, q]))| = 24pq – 4p$. In $L(TC_4C_8$ (S) [p, q]), there are four types of edges based on the degree of the vertices of each edge. Thus by calculation, we obtain that the edge partitions of the line graph of TC_4C_8 (S) [p, q] based on the sum of degrees of the end vertices of each edge as given in Table 4.

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

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

In the following theorem, we compute the exact value of ISI_e index of TC_4C_8 (S) [p, q] nanotori.

Theorem 4: The edge version of inverse sum indeg index of TC_4C_8 (S) [p, q] nanotori is given by

$$ISI_e\left(TC_4C_8\left(S\right)\left[p,q\right]\right) = 48pq - \frac{1408}{105}p.$$

Proof: Let G be the graph of $TC_4C_8(S)[p, q]$ nanotori. From equation (2) and by cardinalities of the edge partitions of $L(G)$, we have

$$ISI_e\left(TC_4C_8\left(S\right)\left[p,q\right]\right) = \sum_{ef \in E(L(G))} \frac{d_{L(G)}(e)\, d_{L(G)}(f)}{d_{L(G)}(e) + d_{L(G)}(f)}$$

$$= 2p\left(\frac{2\times3}{2+3}\right) + 4p\left(\frac{2\times4}{2+4}\right) + 4p\left(\frac{3\times4}{3+4}\right) + \left(24pq - 14p\right)\left(\frac{4\times4}{4+4}\right)$$

$$= 48pq - \frac{1408}{105}p.$$

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Source of Support: Nil, Conflict of interest: None Declared

