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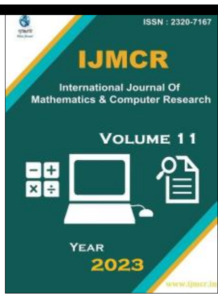

Edge Version of Sombor and Nirmala Indices of Some Nanotubes and Nanotori

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ABSTRACT

Chemical Graph Theory is a branch of Mathematical Chemistry whose focus of interest is to finding topological indices of chemical graphs which correlate well with chemical properties of the chemical molecules. In this study, we define the edge version of Sombor index, the edge version of modified Sombor index and, the edge version of Nirmala index of a graph and compute exact formulas for certain families of nanotubes and nanotori.

KEYWORDS: edge version of Sombor index, edge version of modified Sombor index, edge version of Nirmala index, nanotube, nanotori.

I. INTRODUCTION

We consider only simple, finite, connected graphs. Let G be such a graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u. The edge e connecting the vertices u and v is denoted by uv. If $e=uv$ is an edge of G, then the vertex u and edge e are incident as are v and e. Let $d_G(e)$ denote the degree of an edge e in G, which is defined by $d_G(e) = d_G(u) + d_G(v) – 2$ with $e=uv$. 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. For term and concept not given here, we refer [1].

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 [2] have been considered in Theoretical Chemistry and have some applications, especially in *QSPR/QSAR* research [3].

The edge version of the F-index [4] of a graph G is defined as

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

The edge versions of indices were studied, for example, in [5, 6, 7].

We define the edge version of Sombor index, edge version of modified Sombor index, edge version of Nirmala index of a molecular graph G as follows:

We define the edge version of Sombor index of a graph G as

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

Recently, some Sombor indices were studied, for example, in [8, 9, 10, 11, 12, 13, 14].

We define the edge version of modified Sombor index of a graph G as

$$^{m}SO_e(G) = \sum_{ef \in E(L(G))} \frac{1}{\sqrt{d_{L(G)}(e)^2 + d_{L(G)}(f)^2}}.$$

We define the edge version of Nirmala index of a graph G as

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

Recently, some Nirmala indices were studied, for example, in [15, 16, 17, 18, 19, 20, 21, 22, 23, 24].

The edge version of sum connectivity index [4] of a graph G is defined as

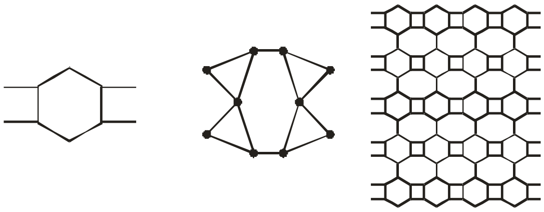
$$X_e(G)=\sum_{ef\in E(L(G))}\frac{1}{\sqrt{d_{L(G)}(e)+d_{L(G)}(f)}}.$$

We call this index as edge version of modified Nirmala index.

In this paper, we compute the edge version of Sombor index, edge version of modified Sombor index and edge version of Nirmala index of $TUC_4C_6C_8[p, q]$ nanotubes, $TUSC_4C_8(S)[p, q]$ nanotubes, H-Naphtalenic $NPHX[m, n]$ nanotubes, $C_4C_6C_8[p, q]$ nanotori and $TC_4C_8(S)[p, q]$ nanotori.

II. 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).



(a) (b) (c)

Figure 1

Let G be the graph of 2-dimensional lattice of $TUC_4C_6C_8[p,q]$ nanotube. The graphs of $L(TUC_4C_6C_8[p,q])$ have $18pq - 4p$ edges. Let $G = TUC_4C_6C_8[p,q]$. We obtain that { $d_{L(G)}(e)$, $d_{L(G)}(f)$ \ ef □□$E(L(G))$ } has three edge set partitions.

Table 1. Edge partition of $L(G)$

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

We compute the exact value of $SO_e(TUC_4C_6C_8[p,q])$.

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

$$SO_e(G)=72\sqrt{2}pq+\left(40-50\sqrt{2}\right)p.$$

Proof: By using the definition and the edge partition of $L(G)$, we deduce

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

$$=\sqrt{3^2+3^2}\,2p+\sqrt{3^2+4^2}\,8p+\sqrt{4^2+4^2}\,(18pq-14p)$$

$$=72\sqrt{2}pq+\left(40-50\sqrt{2}\right)p.$$

We compute the exact value of the edge version of the modified Sombor 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

$${}^mSO_e(G)=\frac{9}{2\sqrt{2}}pq+\left(\frac{2}{3\sqrt{2}}+\frac{8}{5}-\frac{7}{2\sqrt{2}}\right)p.$$

Proof: By using the definition and the edge partition of $L(G)$, we deduce

$${}^mSO_e(G)=\sum_{ef\in E(L(G))}\frac{1}{\sqrt{d_{L(G)}(e)^2+d_{L(G)}(f)^2}}$$

$$=\frac{1}{\sqrt{3^2+3^2}}2p+\frac{1}{\sqrt{3^2+4^2}}8p+\frac{1}{\sqrt{4^2+4^2}}(18pq-14p)$$

$$=\frac{9}{2\sqrt{2}}pq+\left(\frac{2}{3\sqrt{2}}+\frac{8}{5}-\frac{7}{2\sqrt{2}}\right)p.$$

We compute the exact value of $N_e(TUC_4C_6C_8[p,q])$.

Theorem 3. Let G be the graph of $TUC_4C_6C_8[p, q]$ nanotube. Then

$$N_e(G)=36\sqrt{2}pq+\left(2\sqrt{6}+8\sqrt{7}-28\sqrt{2}\right)p.$$

Proof: By using the definition and the edge partition of $L(G)$, we deduce

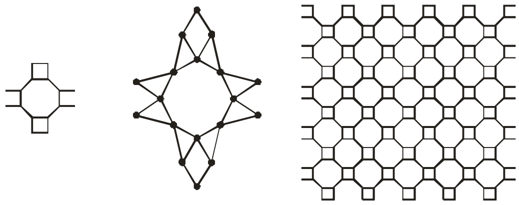
$$N_e(G)=\sum_{ef\in E(L(G))}\sqrt{d_{L(G)}(e)+d_{L(G)}(f)}$$

$$=\sqrt{3+3}2p+\sqrt{3+4}8p+\sqrt{4+4}(18pq-14p)$$

$$=36\sqrt{2}pq+\left(2\sqrt{6}+8\sqrt{7}-28\sqrt{2}\right)p.$$

III. 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).



(a) **(b)** **(c)**

Figure 2

Let G be the graph of 2-dimensional lattice of $TUSC_4C_8(S)[p,q]$ nanotube.

The graphs of $L(TUSC_4C_8(S)[p,q])$ have $24pq - 8p$ edges. Let $G = TUC_4C_6C_8[p,q]$.

We obtain that $\{ d_{L(G)}(e), d_{L(G)}(f) \setminus ef \in E(L(G)) \}$ has three edge set partitions.

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

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

We compute the exact value of $SO_e(TUSC_4C_8(S)[p,q])$

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

$$SO_e(G) = 96\sqrt{2}pq + \left(4\sqrt{13} + 40 - 32\sqrt{2}\right)p.$$

Proof: By using the definition and the edge partition of $L(G)$, we deduce

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

$$= \sqrt{2^2+3^2}\,4p + \sqrt{3^2+4^2}\,8p + \sqrt{4^2+4^2}\,(24pq - 8p)$$

$$= 96\sqrt{2}pq + \left(4\sqrt{13} + 40 - 32\sqrt{2}\right)p.$$

We compute the exact value of the edge version of the modified Sombor index of $TUSC_4C_8(S)[p,q]$ nanotube.

Theorem 5. Let G be the graph of $TUSC_4C_8(S)[p,q]$ nanotube. Then

$${}^{m}SO_e(G) = \frac{6}{\sqrt{2}}pq + \left(\frac{4}{\sqrt{13}} + \frac{8}{5} - \frac{2}{\sqrt{2}}\right)p.$$

Proof: By using the definition and the edge partition of $L(G)$, we deduce

$${}^{m}SO_e(G) = \sum_{ef \in E(L(G))} \frac{1}{\sqrt{d_{L(G)}(e)^2 + d_{L(G)}(f)^2}}$$

$$= \frac{1}{\sqrt{2^2+3^2}}4p + \frac{1}{\sqrt{3^2+4^2}}8p + \frac{1}{\sqrt{4^2+4^2}}(24pq - 8p)$$

$$= \frac{6}{\sqrt{2}}pq + \left(\frac{4}{\sqrt{13}} + \frac{8}{5} - \frac{2}{\sqrt{2}}\right)p.$$

We compute the exact value of $N_e(TUC_4C_6C_8[p,q])$.

Theorem 6. Let G be the graph of $TUSC_4C_8(S)[p,q]$ nanotube. Then

$$N_e(G) = 48\sqrt{2}pq + \left(4\sqrt{5} + 8\sqrt{7} - 16\sqrt{2}\right)p.$$

Proof: By using the definition and the edge partition of $L(G)$, we deduce

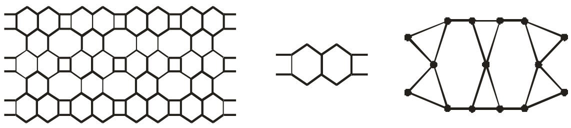
$$N_e(G) = \sum_{ef \in E(L(G))} \sqrt{d_{L(G)}(e) + d_{L(G)}(f)}$$

$$= \sqrt{2+3}\,4p + \sqrt{3+4}\,8p + \sqrt{4+4}\,(24pq - 8p)$$

$$= 48\sqrt{2}pq + \left(4\sqrt{5} + 8\sqrt{7} - 16\sqrt{2}\right)p.$$

IV. RESULTS FOR *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

Let G be the graph of 2-dimensional lattice of H-Naphtalenic $NPHX\ [m, n]$ nanotube.

The graphs of $L(NPHX\ [m, n])$ have $30mn - 8m$ edges. Let $G = NPHX\ [m, n]$.

We obtain that $\{ d_{L(G)}(e), d_{L(G)}(f) \setminus ef \in E(L(G)) \}$ has three edge set partitions.

Table 3. Edge partition of $L(G)$

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

We determine the edge version of Sombor index for H-Naphtalenic $NPHX[m, n]$ nanotube.

Theorem 7. Let G be the graph of $NPHX[m, n]$ nanotube. Then

$$SO_e(G) = 120\sqrt{2}mn + \left(60 - 86\sqrt{2}\right)m.$$

Proof: By using the definition and the edge partition of $L(G)$, we deduce

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

$$=\sqrt{3^2+3^2}\,6m+\sqrt{3^2+4^2}\,12m+\sqrt{4^2+4^2}\,(30mn-26m)$$

$$=120\sqrt{2}mn+\left(60-86\sqrt{2}\right)m.$$

We compute the exact value of the edge version of the modified Sombor index of *NPHX*[*m*, *n*] nanotube.

Theorem 8. Let *G* be the graph of $TUSC_4C_8(S)[p,q]$ nanotube. Then

$$^{m}SO_e(G)=\frac{15}{2\sqrt{2}}mn+\left(\frac{2}{\sqrt{2}}+\frac{12}{5}-\frac{13}{2\sqrt{2}}\right)m.$$

Proof: By using the definition and the edge partition of *L*(*G*), we deduce

$$^{m}SO_e(G)=\sum_{ef\in E(L(G))}\frac{1}{\sqrt{d_{L(G)}(e)^2+d_{L(G)}(f)^2}}$$

$$=\frac{1}{\sqrt{3^2+3^2}}6m+\frac{1}{\sqrt{3^2+4^2}}12m$$

$$+\frac{1}{\sqrt{4^2+4^2}}(30mn-26m)$$

$$=\frac{15}{2\sqrt{2}}mn+\left(\frac{2}{\sqrt{2}}+\frac{12}{5}-\frac{13}{2\sqrt{2}}\right)m.$$

We compute the exact value of $N_e(TUC_4C_6C_8[p,q])$.

Theorem 9. Let *G* be the graph of $TUSC_4C_8(S)[p,q]$ nanotube. Then

$$N_e(G)=48\sqrt{2}pq+\left(4\sqrt{5}+8\sqrt{7}-16\sqrt{2}\right)p.$$

Proof: By using the definition and the edge partition of *L*(*G*), we deduce

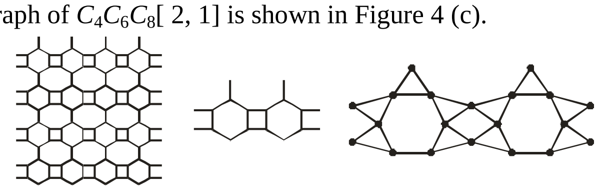
$$N_e(G)=\sum_{ef\in E(L(G))}\sqrt{d_{L(G)}(e)+d_{L(G)}(f)}$$

$$=\sqrt{3+3}\,6m+\sqrt{3+4}\,12m+\sqrt{4+4}\,(30mn-26m)$$

$$=60\sqrt{2}mn+\left(6\sqrt{6}+12\sqrt{7}-52\sqrt{2}\right)m.$$

V. RESULTS FOR $C_4C_6C_8[p, q]$ 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

Let *G* be the graph of 2-dimensional lattice of $C_4C_6C_8[p, q]$ nanotori.

The graphs of $L(C_4C_6C_8[p, q])$ have $18pq - 2p$ edges. Let $G = C_4C_6C_8[p, q]$.

We obtain that { $d_{L(G)}(e)$, $d_{L(G)}(f)$ \ *ef* □□$E(L(G))$ } has four edge set partitions.

Table 4. Edge partition of *L*(*G*)

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

We determine the edge version of Sombor index of $C_4C_6C_8[p,q]$ nanotori.

Theorem 10. Let *G* be the graph of $C_4C_6C_8[p,q]$ nanotori. Then

$$SO_e(G)=72\sqrt{2}pq+\left(4\sqrt{5}+20-33\sqrt{2}\right)p.$$

Proof: By using the definition and the edge partition of *L*(*G*), we deduce

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

$$=\sqrt{2^2+4^2}\,2p+\sqrt{3^2+3^2}\,p+\sqrt{3^2+4^2}\,4p$$

$$+\sqrt{4^2+4^2}\,(18pq-9p)$$

$$=72\sqrt{2}pq+\left(4\sqrt{5}+20-33\sqrt{2}\right)p.$$

We compute the exact value of the edge version of the modified Sombor index of $C_4C_6C_8[p,q]$ nanotori.

Theorem 11. Let *G* be the graph of $C_4C_6C_8[p,q]$ nanotori. Then

$$^{m}SO_e(G)=\frac{9}{2\sqrt{2}}pq+\left(\frac{1}{\sqrt{5}}+\frac{1}{3\sqrt{2}}+\frac{4}{5}-\frac{9}{4\sqrt{2}}\right)p.$$

Proof: By using the definition and the edge partition of *L*(*G*), we deduce

$$^{m}SO_e(G)=\sum_{ef\in E(L(G))}\frac{1}{\sqrt{d_{L(G)}(e)^2+d_{L(G)}(f)^2}}$$

$$=\frac{1}{\sqrt{2^2+4^2}}2p+\frac{1}{\sqrt{3^2+3^2}}p+\frac{1}{\sqrt{3^2+4^2}}4p$$

$$+\frac{1}{\sqrt{4^2+4^2}}(18pq-9p)$$

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

We compute the exact value of $N_e(TUC_4C_6C_8[p,q])$.

Theorem 12. Let G be the graph of $C_4C_6C_8[p,q]$ nanotori. Then

$$N_e(G) = 36\sqrt{2}pq + \left(3\sqrt{6} + 4\sqrt{7} - 18\sqrt{2}\right)p.$$

Proof: By using the definition and the edge partition of $L(G)$, we deduce

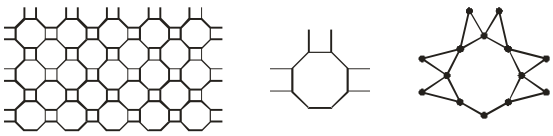
$$N_e(G) = \sum_{ef \in E(L(G))} \sqrt{d_{L(G)}(e) + d_{L(G)}(f)}$$

$$= \sqrt{2+4}2p + \sqrt{3+3}p + \sqrt{3+4}4p + \sqrt{4+4}(18pq - 9p)$$

$$= 36\sqrt{2}pq + \left(3\sqrt{6} + 4\sqrt{7} - 18\sqrt{2}\right)p.$$

VI. RESULTS FOR $TC_4C_8(S)$ [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

Let G be the graph of 2-dimensional lattice of $TC_4C_8(S)[p, q]$ nanotori.

The graphs of $L(TC_4C_8(S)[p, q])$ have $24pq - 4p$ edges. Let $G = TC_4C_8(S)[p, q]$.

We obtain that { $d_{L(G)}(e)$, $d_{L(G)}(f)$ \ ef □□$E(L(G))$ } has four edge set partitions.

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

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

We determine the edge version of Sombor index of $C_4C_6C_8[p,q]$ nanotori.

Theorem 13. Let G be the graph of $TC_4C_8(S)[p, q$ nanotori. Then

$$SO_e(G) = 96\sqrt{2}pq + \left(2\sqrt{13} + 8\sqrt{5} + 20 - 56\sqrt{2}\right)p.$$

Proof: By using the definition and the edge partition of $L(G)$, we deduce

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

$$= \sqrt{2^2+3^2}\,2p + \sqrt{2^2+4^2}\,4p + \sqrt{3^2+4^2}\,4p$$

$$+ \sqrt{4^2+4^2}\,(24pq - 14p)$$

$$= 96\sqrt{2}pq + \left(2\sqrt{13} + 8\sqrt{5} + 20 - 56\sqrt{2}\right)p.$$

We compute the exact value of the edge version of the modified Sombor index of $TC_4C_8(S)[p, q]$ nanotori.

Theorem 14. Let G be the graph of $TC_4C_8(S)[p, q$ nanotori. Then

$${}^mSO_e(G) = \frac{6}{\sqrt{2}}pq + \left(\frac{2}{\sqrt{13}} + \frac{2}{\sqrt{5}} + \frac{4}{5} - \frac{7}{2\sqrt{2}}\right)p.$$

Proof: By using the definition and the edge partition of $L(G)$, we deduce

$${}^mSO_e(G) = \sum_{ef \in E(L(G))} \frac{1}{\sqrt{d_{L(G)}(e)^2 + d_{L(G)}(f)^2}}$$

$$= \frac{1}{\sqrt{2^2+4^2}}2p + \frac{1}{\sqrt{3^2+3^2}}p + \frac{1}{\sqrt{3^2+4^2}}4p$$

$$+ \frac{1}{\sqrt{4^2+4^2}}(18pq - 9p)$$

$$= \frac{6}{\sqrt{2}}pq + \left(\frac{2}{\sqrt{13}} + \frac{2}{\sqrt{5}} + \frac{4}{5} - \frac{7}{2\sqrt{2}}\right)p.$$

We compute the exact value of $N_e(TUC_4C_6C_8[p,q])$.

Theorem 15. Let G be the graph of $TC_4C_8(S)[p, q$ nanotori. Then

$$N_e(G) = 48\sqrt{2}pq + \left(2\sqrt{5} + 4\sqrt{6} + 4\sqrt{7} - 56\sqrt{2}\right)p.$$

Proof: By using the definition and the edge partition of $L(G)$, we deduce

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

$$= \sqrt{2+3}2p + \sqrt{2+4}4p + \sqrt{3+4}4p$$

$$+ \sqrt{4+4}(24pq - 14p)$$

$$= 48\sqrt{2}pq + \left(2\sqrt{5} + 4\sqrt{6} + 4\sqrt{7} - 56\sqrt{2}\right)p.$$

VII. CONCLUSION

In this paper, we have determined the edge version of Sombor index, the edge version of modified Sombor index and the edge version of Nirmala index of certain nanotubes and nanotori.

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