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Computation of F-Reverse and Modified Reverse Indices of some Nanostructures

V.R.Kulli

Department of Mathematics
Gulbarga University, Gulbarga 585106, India
e-mail: vrkulli@gmail.com

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Abstract. In this paper, we introduce the modified first and second reverse indices of a graph. Also we present exact expressions for the modified first and second reverse indices, F-reverse index and F-reverse polynomial of certain nanostructures.

Keywords: modified reverse indices, F-reverse index, nanostructure.

AMS Mathematics Subject Classification (2010): 05C05, 05C07, 05C35

1. Introduction

A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. Chemical graph theory is a branch of Mathematical Chemistry which has an important effect on the development of Chemical Sciences. A topological index is a numeric value that is graph invariant. Numerous topological indices have found some applications in Theoretical Chemistry, especially in QSPR/QSAR study, see [1].

Let G be a finite, simple connected 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. Let $\Delta(G)$ denote the maximum degree among the vertices of G. The reverse vertex degree of a vertex v in G is defined as $c_v = \Delta(G) - d_G(v) + 1$. The reverse edge connecting the reverse vertices u and v will be denoted by uv. Any undefined term here may be found in Kulli [2].

In [3], Ediz introduced the first reverse Zagreb beta index and the second reverse Zagreb index of a graph. They are respectively defined as

$$CM_1(G) = \sum_{uv \in E(G)} (c_u + c_v), \qquad CM_2(G) = \sum_{uv \in E(G)} c_u c_v.$$

Recently, many reverse indices were studied, for example, in [4, 5, 6, 7, 8].

We introduce the modified first and second reverse indices of a graph G as

$$^{m}C_1(G) = \sum_{uv \in E(G)} \frac{1}{(c_u + c_v)} \tag{1}$$

$$^{m}C_2(G) = \sum_{uv \in E(G)} \frac{1}{c_u c_v}. \tag{2}$$

The forgotten topological index or F-index of a graph G is defined as

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

The F-index was studied by Furtula and Gutman in [9] and also it was studied, for example, in [10,11, 12, 13, 14, 15,16].

Motivated by the definition of the F-index and its applications, Kulli [17] introduced the F-reverse index and F-reverse polynomial of a graph as follows:

The F-reverse index of a graph G is defined as

$$FC(G)=\sum_{uv\in E(G)}\left(c_u^2+c_v^2\right). \quad (3)$$

The F-reverse polynomial of a graph G is defined as

$$FC(G,x)=\sum_{uv\in E(G)}x^{\left(c_u^2+c_v^2\right)}. \quad (4)$$

Some other F-indices were studied, for example, in [18,19,20].

In this paper, the modified first and second reverse indices, F-reverse index and F-reverse polynomial of certain nanostructures are computed. For more information about nanostructures see [21, 22].

2. Results for $KTUC_4C_8(S)$ nanotubes

In this section, we focus on the graph structure of a family of $TUC_4C_8(S)$ nanotubes. The 2-dimensional lattice of $TUC_4C_8(S)$ is denoted by $K=KTUC_4C_8[p,q]$ where p is the number of columns and q is the number of rows, see Figure 1.

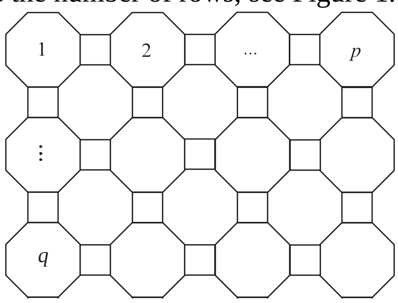

Figure 1: The graph of $KTUC_4C_8[p,q]$ nanotube

Let K be the graph of $KTUC_4C_8[p,q]$ nanotube. Clearly the vertices of K are either of degree 2 or 3. Thus $\Delta(K) = 3$. Therefore $c_u = \Delta(K) - d_K(u) + 1 = 4 - d_K(u)$. In K, by calculation, there are three types of edges as follows:

$E_{22} = \{uv \in E(K) \mid d_K(u) = d_K(v) = 2\}$, $|E_{22}| = 2p + 2q + 4$.

$E_{23} = \{uv \in E(K) \mid d_K(u) = 2, d_K(v) = 3\}$, $|E_{23}| = 4p + 4q - 8$.

$E_{33} = \{uv \in E(K) \mid d_K(u) = d_K(v) = 3\}$, $|E_{33}| = 12pq - 8p - 8q + 4$.

Thus there are three types of reverse edges as given in Table 1.

$c_u, c_v\backslash uv \in E(K)$	(2, 2)	(2, 1)	(1, 1)
Number of edges	$2p+2q+4$	$4p+4q-8$	$12pq - 8p - 8q+4$

Table 1: Reverse edge partition of K

Theorem 1. The modified first and second reverse indices of $KTUC_4C_8[p,q]$ nanotubes are given by

(i) ${}^mC_1(K) = 6pq - \frac{13}{6}(p+q) + \frac{1}{3}$. (ii) ${}^mC_2(K) = 12pq - \frac{11}{2}(p+q) + 1$.

Proof: (i) By using Table 1 and from equation (1), we deduce

$$ {}^mC_1(K) = \sum_{uv\in E(K)} \frac{1}{c_u + c_v} = \left(\frac{1}{2+2}\right)(2p+2q+4) + \left(\frac{1}{2+1}\right)(4p+4q-8) $$
$$ + \frac{1}{1+1}(12pq - 8p - 8q + 4) $$
$$ = 6pq - \frac{13}{6}(p+q) + \frac{1}{3}. $$

(ii) By using Table 1 and from equation (2), we deduce

$$ {}^mC_2(K) = \sum_{uv\in E(K)} \frac{1}{c_u c_v} = \left(\frac{1}{2\times2}\right)(2p+2q+4) + \left(\frac{1}{2\times1}\right)(4p+4q-8) $$
$$ + \frac{1}{1.1}(12pq - 8p - 8q + 4) $$
$$ = 12pq - \frac{11}{2}(p+q) + 1. $$

Theorem 2. The F-reverse index and F-reverse polynomial of $KTUC_4C_8[p,q]$ nanotubes are given by

(i) $FC(K) = 24pq + 20(p+q)$.

(ii) $FC(K, x) = (2p + 2q + 4)x^8 + (4p + 4q - 8)x^5 + (12pq - 8p - 8q + 4)x^2$.

Proof: (i) By using Table (1) and from equation (3), we derive

$$ FC(K) = \sum_{uv\in E(K)} \left(c_u^2 + c_v^2\right) $$
$$ = (2^2+2^2)(2p+2q+4)+(2^2+1^2)(4p+4q-8)+(1^2+1^2)(12pq-8p-8q+4) $$
$$ = 24pq + 20(p+q). $$

(ii) By using Table (1) and from equation (4), we derive

$$ FC(K,x) = \sum_{uv\in E(K)} x^{\left(c_u^2 + c_v^2\right)} $$
$$ = (2p+2q+4)x^{(2^2+2^2)} + (4p+4q-8)x^{(2^2+1^2)} + (12pq-8p-8q+4)x^{(1^2+1^2)} $$
$$ = (2p+2q+4)\,x^8 + (4p+4q-8)\,x^5 + (12pq-8p-8q+4)\,x^2. $$

3. Results for $GTUC_4C_8(S)$ nanotubes

In this section, we focus on the graph structure of family of $TUC_4C_8(S)$ nanotubes. The 2-dimensional lattice of $TUC_4C_8(S)$ is denoted by $G=GTUC_4C_8[p,q]$ where p is the number of columns and q is the number of rows, see Figure 2.

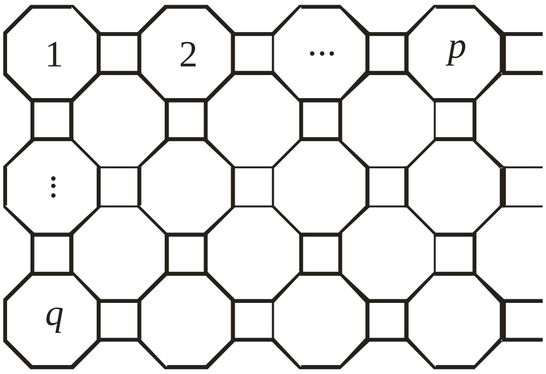

Figure 2: The graph of $GTUC_4C_8[4,3]$ nanotube

Let G be the molecular graph of $GTUC_4C_8[p,q]$ nanotube. From Figure 2, one can see that the vertices of G are either of degree 2 or 3. Thus $\Delta(G) = 3$. Therefore $c_u = \Delta(G) - d_G(u) + 1 = 4 - d_G(u)$. In G, by calculation, three types of edges as follows:

$E_{22} = \{uv \in E(K) \mid d_K(u) = d_K(v) = 2\}$, $|E_{22}| = 2p$.

$E_{23} = \{uv \in E(K) \mid d_K(u) = 2, d_K(v) = 3\}$, $|E_{23}| = 4p$.

$E_{33} = \{uv \in E(K) \mid d_K(u) = d_K(v) = 3\}$, $|E_{33}| = 12pq - 8p$.

Thus there are three types of reverse edges based on the degree of end reverse vertices of each reverse edge as given in Table 2.

$c_u, c_v \backslash uv \in E(G)$	(2, 2)	(2, 1)	(1, 1)
Number of edges	$2p$	$4p$	$12pq - 8p$

Table 2: Reverse edge partition of G

Theorem 3. The modified first and second reverse indices of $GTUC_4C_8[p,q]$ nanotubes are given by

(i) ${}^mC_1(G) = 6pq - \frac{13}{6}p.$ (ii) ${}^mC_2(G) = 12pq - \frac{11}{2}p.$

Proof: (i) By using Table 2 and from equation (1), we deduce

$${}^mC_1(G) = \sum_{uv\in E(G)} \frac{1}{c_u + c_v} = \left(\frac{1}{2+2}\right)2p + \left(\frac{1}{2+1}\right)4p + \left(\frac{1}{1+1}\right)(12pq - 8p)$$

$$= 6pq - \frac{13}{6}p.$$

(ii) By using Table 2 and from equation (2), we deduce

$${}^mC_2(G) = \sum_{uv\in E(G)} \frac{1}{c_u c_v} = \left(\frac{1}{2\times2}\right)2p + \left(\frac{1}{2\times1}\right)4p + \left(\frac{1}{1\times1}\right)(12pq - 8p)$$

$$= 12pq - \frac{11}{2}p.$$

Theorem 4. The F-reverse index and F-reverse polynomial of $GTUC_4C_8[p,q]$ nanotubes are given by

(i) $FC(G) = 24pq + 20p$.

(ii) $FC(G, x) = 2px^8 + 4px^5 + (12pq - 8p)x^2$.

Proof: (i) By using Table (2) and from equation (3), we derive

$$FC(G) = \sum_{uv \in E(G)} \left(c_u^2 + c_v^2\right)$$
$$= (2^2+2^2)2p + (2^2+1^2)4p + (1^2+1^2)(12pq - 8p)$$
$$= 24pq + 20p.$$

(ii) By using Table (2) and from equation (4), we derive

$$FC(G,x) = \sum_{uv \in E(G)} x^{\left(c_u^2 + c_v^2\right)}$$
$$= 2px^{(2^2+2^2)} + 4px^{(2^2+1^2)} + (12pq - 8p)x^{(1^2+1^2)}$$
$$= 2px^8 + 4px^5 + (12pq - 8p)\, x^2.$$

4. Results for $HTUC_4C_8(R)$ nanotorus

In this section, we focus on the graph structure of family of $HTC_4C_8(R)$ nanotorus. The 2-dimensional lattice of $HTUC_4C_8(R)$ is denoted by $H=HTUC_4C_8[p,q]$, where p is the number of columns and q is the number of rows, see Figure 3.

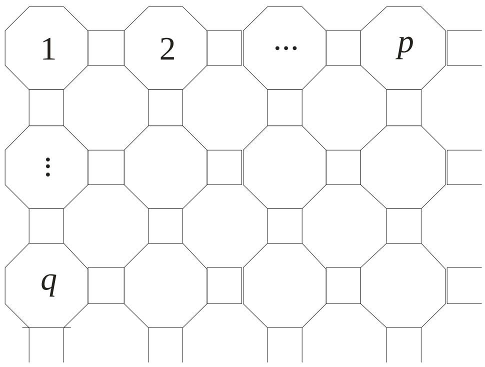

Figure 3: The graph of $HTUC_4C_8[p,q]$ nanotorus

Let H be the graph of $HTUC_4C_8[p,q]$ nanotorus. From Figure 3, we see that the degree of each vertex of H is 3. Thus $\Delta(H) = 3$. Therefore $c_u = \Delta(H) - d_H(u) + 1 = 4 - d_G(u)$. In G, there is only one type of edges as follows:

$E_{33} = \{uv \in E(H) \mid d_H(u) = d_H(v) = 3\}$, $|E_{33}| = 12pq$.

Thus there is only one type of reverse edges as follows:

$E_{33} = \{uv \in E(H) \mid c_u = c_v = 1\}$, $|RE_3| = 12pq$. (5)

Theorem 5. Let H be the graph of $HTUC_4C_8[p,q]$ nanotorus. Then

(i) ${}^{m}C_1(H) = 6pq$. (ii) ${}^{m}C_2(H) = 12pq$.

(iii) $FC(H) = 24pq$. (iv) $FC(H, x) = 12pqx^2$.

Proof: (i) By using (5) and from equation (1), we deduce

$$^{m}C_1(H) = \sum_{uv \in E(H)} \frac{1}{c_u + c_v} = \left(\frac{1}{1+1}\right) 12pq = 6pq.$$

(ii) By using (5) and from equation (2), we deduce

$$^{m}C_2(H) = \sum_{uv \in E(H)} \frac{1}{c_u c_v} = \left(\frac{1}{1 \times 1}\right) 12pq = 12pq.$$

(iii) By using (5) and from equation (3), we deduce

$$FC(H) = \sum_{uv \in E(H)} \left(c_u^2 + c_v^2\right) = \left(1^2 + 1^2\right) 12pq = 24pq.$$

(iv) By using (5) and from equation (4), we deduce

$$FC(H, x) = \sum_{uv \in E(H)} x^{\left(c_u^2 + c_v^2\right)} = 12pqx^{\left(1^2+1^2\right)} = 12pqx^2.$$

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