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SOME MULTIPLICATIVE REDUCED INDICES OF CERTAIN NANOSTRUCTURES

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ABSTRACT

A topological index is a numeric quantity from structural graph of a molecule. In this paper, we define the multiplicative reduced second Zagreb-index, multiplicative reduced second hyper-Zagreb index and general multiplicative reduced second Zagreb index and compute exact formulas for certain nanostructures.

Keywords: multiplicative reduced second Zagreb index, multiplicative reduced second hyper-Zagreb index, general multiplicative reduced second Zagreb index, nanostructure.

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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 the Chemical Sciences. Numerous topological indices have been considered in Theoretical Chemistry and have found some applications.

We consider only finite, simple and connected graph G 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. We refer to [1] for undefined term and notation.

Furtula et al., in [2] proposed the reduced second Zagreb index, defined as

$$RM_{2}(G) = \sum_{uv \in E(G)} (d_{G}(u) - 1) (d_{G}(v) - 1).$$

In [3] Kulli introduced the reduced second hyper-Zagreb index, defined as

$$RHM_{2}(G) = \sum_{uv \in E(G)} \left[\left(d_{G}(u) - 1 \right) \left(d_{G}(v) - 1 \right) \right]^{2}.$$

Recently, some reduced indices were studied, for example, in [4, 5, 6, 7].

Inspired by work on reduced indices, we introduce the multiplicative reduced second Zagreb index, multiplicative reduced second hyper-Zagreb index, general multiplicative reduced second Zagreb index as follows:

The multiplicative reduced second Zagreb index of a graph G is defined as

$$RM_{2}H(G) = \prod_{uv \in E(G)} (d_{G}(u) - 1)(d_{G}(v) - 1).$$

The multiplicative reduced second hyper-Zagreb index of a graph G is defined as

$$RHM_{2}II(G) = \prod_{uv \in E(G)} \left[(d_{G}(u) - 1) (d_{G}(v) - 1) \right]^{2}.$$

Corresponding Author: V. R. Kulli. Department of Mathematics, Gulbarga University, Gulbarga, 585106, India. The general multiplicative reduced second Zagreb index of a graph G is defined as

$$RM_{2}^{a}II(G) = \prod_{uv \in E(G)} \left[\left(d_{G}(u) - 1 \right) \left(d_{G}(v) - 1 \right) \right]^{a}.$$

$$\tag{1}$$

where *a* is a real number.

Recently many other multiplicative indices were studied, for example, in [8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24].

In this paper, the multiplicative reduced second Zagreb index, multiplicative reduced second hyper-Zagreb index and general multiplicative reduced second Zagreb index for certain nanostructures are determined. For more information about nanostructures see [25, 26].

2. *KTUC*₄*C*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 with 12pq - 2p - 2q. In *K*, by calculation, there are three types of edges based on the degree of end vertices of each edge as given in Table 1.

$d_k(u), d_k(v) \setminus uv \in E(K)$	(2, 2)	(2, 3)	(3, 3)
Number of edges	2p+2q+4	4p + 4q - 8	12pq - 8p - 8q + 4
	Table-1: Edge p	partition of K	

In the following theorem, we compute the general multiplicative reduced second Zagreb index of K.

Theorem 1: The general multiplicative reduced second Zagreb index $KTUC_4C_8[p,q]$ nanotube is given by $RM_2^a II(K) = 2^{a(4p+4q-8)} \times 4^{a(12pq-8p-8q+4)}$.

Proof: Let *K* be the graph of $KTUC_4C_8[p,q]$ nanotube. From equation (1) and Table 1, we deduce.

$$RM_{2}^{a}II(K) = \prod_{uv \in E(K)} \left[\left(d_{K}(u) - 1 \right) \left(d_{K}(v) - 1 \right) \right]^{a}.$$

= $\left[(2-1)(2-1) \right]^{a(2p+2q-4)} \times \left[(2-1)(3-1) \right]^{a(4p+4q-8)} \times \left[(3-1)(3-1) \right]^{a(12pq-8p-8q+4)}$
= $2^{a(4p+4q-8)} \times 4^{a(12pq-8p-8q+4)}.$

We obtain the following results by using Theorem 1.

Corollary 1.1: The multiplicative reduced second Zagreb index of $KTUC_4C_8[p,q]$ nanotube is $RM_2II(K) = 2^{4p+4q-8} \times 4^{12pq-8p-8q+4}$.

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

Corollary 1.2: The multiplicative reduced second hyper-Zagreb index of $KTUC_4C_8[p,q]$ nanotube is $RHM_2II(K) = 2^{8p+8q-16} \times 4^{24pq-16p-16q+8}$.

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

(2)

3. $GTUC_4C_8(S)$ 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 $GTUC_4C_8[p, q]$ nanotube

Let G be the molecular graph of $GTUC_4C_8[p,q]$ nanotube with 12pq - 2p edges. In G, by calculation, there are three types of edges based on the degree of end vertices of each edge as given in Table 2.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(2, 2)	(2, 3)	(3, 3)		
Number of edges	2p	4p	12pq - 8p		
Table-2: Edge partition of G					

Theorem 2: The general multiplicative reduced second Zagreb index of $GTUC_4C_8[p,q]$ nanotube is

$$RM_2^a II(G) = 2^{4pa} \times 4^{a(12pq-8p)}.$$

Proof: Let G be the graph of $GTUC_4C_8[p,q]$ nanotube. From equation (1) and Table 2, we deduce

$$\begin{split} RM_2^a II(G) &= \prod_{uv \in E(G)} \left[\left(d_G(u) - 1 \right) \left(d_G(v) - 1 \right) \right]^a. \\ &= \left[(2 - 1)(2 - 1) \right]^{a2p} \times \left[(2 - 1)(3 - 1) \right]^{a4p} \times \left[(3 - 1)(3 - 1) \right]^{a(12pq - 8p)} \\ &= 2^{4pa} \times 4^{a(12pq - 8p)}. \end{split}$$

We obtain the following results by using Theorem 2.

Corollary 2.1: The multiplicative reduced second Zagreb index of $GTUC_4C_8[p,q]$ is $RM_2II(G) = 2^{4p} \times 4^{12pq-8p}$.

Proof: Put a = 1 in equation (3), we get the desired result.

Corollary 2.2: The multiplicative reduced second hyper-Zagreb index of $GTUC_4C_8[p,q]$ is $RHM_2II(G) = 2^{8p} \times 4^{24pq-16p}$.

Proof: Put a = 2 in equation (3), we get the desired result.

4. HTUC₄C₈(R) Nanotorus

In this section, we focus on the graph structure of a family of $HTUC_4C_8(R)$ 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

(3)

Let *H* be the graph of $HTUC_4C_8[p,q]$ nanotorus with 12pq edges. In *H*, there is only one type of edges as given in Table 3.

$d_G(u), d_G(v) \setminus uv \in E(G)$	(3, 3)
Number of edges	12 <i>pq</i>
Table-2: Edge part	ition of <i>H</i>

Theorem 3: The general multiplicative reduced second Zagreb index of $HTUC_4C_8[p, q]$ nanotorus is $RM_2^a II(H) = 4^{12apq}$.

Proof: Let *H* be the graph of $HTUC_4C_8[p,q]$ nanotorus. From equation (1) and Table 3, we derive

$$RM_2^a II(H) = \prod_{uv \in E(H)} \left[\left(d_H(u) - 1 \right) \left(d_H(v) - 1 \right) \right]^a.$$

= $\left[(3-1)(3-1) \right]^{a12pq} = 4^{12apq}.$

We obtain the following results by using Theorem 3.

Corollary 3.1: The multiplicative reduced second Zagreb index of $HTUC_4C_8[p,q]$ nanotorus is $RM_2II(H) = 4^{12pq}$.

Proof: Put a = 1 in equation (4), we get the desired result.

Corollary 3.2: The multiplicative reduced second hyper-Zagreb index of $HTUC_4C_8[p,q]$ nanotorus is $RHM_2II(H) = 4^{24pq}$.

Proof: Put a = 2 in equation (4), we get the desired result.

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