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On multiplicative universal Zagreb and its subsequent indices of C_4C_8 carbon nanostructures

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Mathematical chemistry studies the chemical structure of molecules. Topological indices are numerical values which associates the chemical structure with the physical and chemical properties. Multiplicative Universal Zagreb indices are generalized degree-based topological indices which gave rise to several indices like first and second multiplicative, Zagreb and hyper-Zagreb indices, multiplicative sum and product conductivity indices. This research is designed to study the first and second multiplicative Universal Zagreb indices of carbon nanostructures (carbon nanosheet, nanotube and nanotorus) of the same chemical formula C_4C_8. We also depict the values of first and second multiplicative, Zagreb and hyper-Zagreb indices as well as multiplicative sum and product connectivity indices for the mentioned structures. The graphical comparison for each of the multiplicative Zagreb indices is presented for all the carbon nanostructures with the same chemical formula C_4C_8.

Keywords: First and second multiplicative Universal Zagreb indices; C_4C_8 carbon nanosheet; C_4C_8 carbon nanotube; C_4C_8 carbon nanotorus.

Mathematics Subject Classification 2020: 05C07, 05C90, 92E10

1. Introduction

Mathematical chemistry interprets the chemical structure of molecules using graphs called molecular graph. A molecular graph presents atoms as vertices and chemical bonds as edges. Topological indices are the graph invariants depending usually

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either on degrees of vertices or distance between the vertices. It is well known that the distance-based topological indices are difficult to investigate as compared to the degree-based topological indices [1, 2]. Degree-based topological indices determine the physical and chemical properties of chemicals [3,4]. Literature reveals the investigations regarding topological indices of drugs for curing COVID-19 patients [5–11].

Carbon nanosheet (CNS) is a two-dimensional ornament with utmost chemical, mechanical, magnetic, thermal stability and flexibility. They are consumed in industry in many processes [12–16]. A carbon nanotube (CNTu) is a special carbon allotrope of cylindrical form. The elastic modulus and tensile strength make CNTu the hardest and strongest nanomaterial. A carbon nanotorus (CNTo) is formed from bending carbon CNTu into a ring-shaped structure [17]. The major and minor radii influence mechanical properties like deformation, vibration, buckling of structures. CNTo has structural properties as light weight, stability, flexibility, low cost, high efficiency, energy harvesting and energy storage.

The famous degree-based topological indices are a class of Zagreb indices describing the molecular complexity, chirality, ZE-isomorphism and heterosystems [18, 19]. The generalized multiplicative Zagreb indices for Eulerian graphs, cycle graphs, (n, m)-graphs, David derived structures, double graphs of subdivision graphs, graphs with bridges and F-Sum graphs were calculated [20–26]. The general Zagreb index was found for cactus chain [27]. The general Zagreb and (a, b)-Zagreb indices for probabilistic neural network are depicted [28]. The general Zagreb indices and other degree-based indices have been computed and correlated with the physical properties of boron B12 [29]. The multiplicative generalized Zagreb and geometric arithmetic indices are found for alcohol [30]. Multiplicative degree-based indices of hyaluronic acid paclitaxel conjugates, tungsten trioxide nano-multilayer structure are computed [31,32]. Moreover, the generalized Zagreb indices of different formulae of silicon carbide have been calculated [33, 34].

The multiplicative sum and product connectivity indices with other multiplicative degree-based indices of magnesium iodide, H-Naphtalenic and $TUC4[m, n]$ nanotubes were found [35, 36]. Generalized and fifth multiplicative Zagreb indices of dendrimer structures are calculated [37, 38]. The multiplicative Zagreb, hyper-Zagreb, sum and product connectivity indices of Phenylenic, Naphatalenic, Anthracene and Tetracenic Nanotubes were computed [39]. The multiplicative redefined first, second, third and augmented Zagreb index of carbon nanocones $CNC_k[n]$, nanotori $C_4C_6C_8(p, q)$, nanostructures of bridge graphs, dendrimer nanostars were determined [40–42]. The subsequent indices of multiplicative generalized Zagreb indices are estimated for $TUC_4C_6C_8[m, n]$, phenylenic, naphatalenic, anthracene and tetracenic nanotubes and $C_4C_6C_8[m, n]$ nanotori [39, 43].

The objective of this study is to derive the first and second Universal Zagreb indices for the three C_4C_8 nanostructures, CNS, CNTu and CNTo. These Universal Zagreb indices lead to the first and second multiplicative Zagreb and hyper-Zagreb indices as well as the sum and product conductivity indices. Section 2 contains the methodology to derive the Universal Zagreb indices. Section 3 contains the computational results in the form of theorems and corollaries. Section 4 consists of discussion and calculations of subsequent indices from multiplicative Universal Zagreb indices. The last section concludes the research work.

2. Methodology

A mathematical description of a molecular graph is a simple graph $\mathbb{G}$: $(V(\mathbb{G}),\ E(\mathbb{G}))$ where $V(\mathbb{G})$ is the vertex set and $E(\mathbb{G})$ is the edge set of $\mathbb{G}$. Consider any two adjacent vertices f and g of $\mathbb{G}$ with the incident edge (f, g). Let d_f and M_f correspond to the degree of vertex f and sum of degrees at the end vertex f of edge (f, g), respectively. These two notations d_f and M_f are considered as the basis of many degree-based topological indices.

The molecular structures of the C_4C_8 carbon nanostructures (CNS, CNTu, CNT) can be mathematically modeled as molecular graphs. We shall introduce a special subdivision scheme for drawing these graphs. Moreover, the multiplicative Universal Zagreb indices and their subsequent indices can be calculated following the steps mentioned below:

- Consider the graph of the C_4C_8 carbon nanostructure with p number of squares in each row and q number of squares in each column, respectively.
- Split each edge into two by embedding a single vertex. The resultant graph is homeomorphic to the base graph.
- Calculate the degree of each vertex.

Table 1. Subsequent indices derived from multiplicative Universal Zagreb indices.

Sr. No.	Specific value of α	Index name	Mathematical formula
1	$\alpha = 1$	First multiplicative Zagreb index	$MZ_1^1(\mathbb{G})$: $II_1 = \prod_{(f,g)\in E(\mathbb{G})}(d_f + d_g)$
		Second multiplicative Zagreb index	$MZ_2^1(\mathbb{G})$: $II_2 = \prod_{(f,g)\in E(\mathbb{G})}(d_f \times d_g)$
2	$\alpha = 2$	First multiplicative hyper-Zagreb index	$MZ_1^2(\mathbb{G})$: $HII_1 = \prod_{(f,g)\in E(\mathbb{G})}(d_f + d_g)^2$
		Second multiplicative hyper-Zagreb index	$MZ_2^2(\mathbb{G})$: $HII_2 = \prod_{(f,g)\in E(\mathbb{G})}(d_f \times d_g)^2$
3	$\alpha = -\frac{1}{2}$	Multiplicative sum connectivity index	$MZ_1^{-\frac{1}{2}}(\mathbb{G})$: $SCII = \prod_{(f,g)\in E(\mathbb{G})}(d_f + d_g)^{-\frac{1}{2}}$
		Multiplicative product connectivity index	$MZ_2^{-\frac{1}{2}}(\mathbb{G})$: $PCII = \prod_{(f,g)\in E(\mathbb{G})}(d_f \times d_g)^{-\frac{1}{2}}$

- The first and second multiplicative Universal Zagreb indices can be calculated using the formulae [30]:

$$MZ_1^{\alpha}(\mathbb{G}) = \prod_{(f,g)\in E(\mathbb{G})} (d_f + d_g)^{\alpha}, \tag{1}$$

$$MZ_2^{\alpha}(\mathbb{G}) = \prod_{(f,g)\in E(\mathbb{G})} (d_f \times d_g)^{\alpha}. \tag{2}$$

- The first and second multiplicative Zagreb, hyper-Zagreb, multiplicative sum and product conductivity indices can be calculated as in Table 1.

3. Computational Results

We shall calculate the multiplicative Universal Zagreb indices of C_4C_8 carbon nanostructures (CNS, CNTu, CNT). Further, the subsequent degree-based topological indices including the first and second multiplicative Zagreb and hyper-Zagreb indices, the sum and productivity indices would be derived. The results are presented in the form of theorems and corollaries.

4. Results for Carbon Nanosheet C_4C_8

The homeomorphic graph of CNS $HAC_4C_8[p, q]$ obtained by adding a single vertex to each edge is shown in Fig. 1.

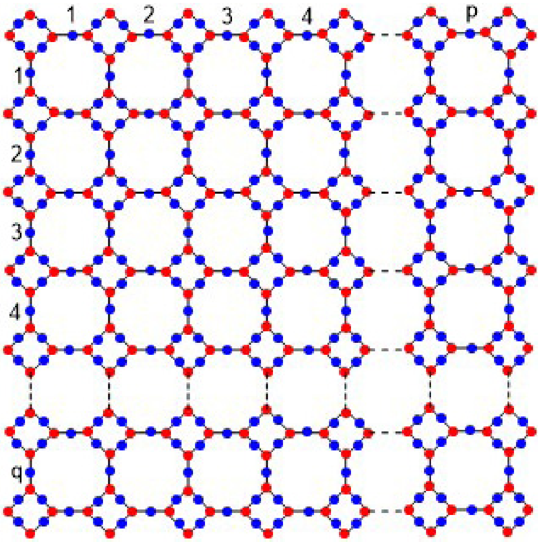

Fig. 1. Graph of CNS subdivision $HAC_4C_8[p, q]$.

For the graph in Fig. 1, the number of vertices and the number edges of CNS $HAC_4C_8[p,q]$ are calculated as

$$\begin{aligned} |V(HAC_4C_8[p,q])| &= 10pq - p - q, \\ |E(HAC_4C_8[p,q])| &= 12pq - 2p - 2q. \end{aligned} \tag{3}$$

Theorem 1. *Let $\mathbb{G}_1 \cong HAC_4C_8[p,q]$ be the graph of C_4C_8 CNS, then the first and the second multiplicative Universal Zagreb indices are, respectively, equal to*

$$MZ_1^{\alpha}(HAC_4C_8[p,q]) = (20)^{\alpha}(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2), \tag{4}$$

$$MZ_2^{\alpha}(HAC_4C_8[p,q]) = (24)^{\alpha}(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2). \tag{5}$$

Proof. Consider the CNS with subdivision $HAC_4C_8[p,q]$, $(p,q \geq 1)$ given in Fig. 1. The edge partitioning table of the graph is given as Table 2.

Substituting values in mathematical formula of the first multiplicative Universal Zagreb index (Eq. (1)) gives

$$\begin{aligned} MZ_1^{\alpha}(HAC_4C_8[p,q]) &= \prod_{(f,g)\in E(\mathbb{G})} (d_f + d_g)^{\alpha} \\ MZ_1^{\alpha}(HAC_4C_8[p,q]) &= (2+2)^{\alpha}(4p+4q)(2+3)^{\alpha}(12pq - 6p - 6q) \\ &= (4)^{\alpha}(4p+4q)(5)^{\alpha}(12pq - 6p - 6q) \\ &= (20)^{\alpha}(4p+4q)(12pq - 6p - 6q) \\ &= (20)^{\alpha}(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2). \end{aligned} \tag{6}$$

The mathematical formula of the second multiplicative Universal Zagreb index (Eq. (2)) leads to

$$\begin{aligned} MZ_2^{\alpha}(HAC_4C_8[p,q]) &= \prod_{(f,g)\in E(\mathbb{G})} (d_f \times d_g)^{\alpha}, \\ MZ_2^{\alpha}(HAC_4C_8[p,q]) &= (2\times 2)^{\alpha}(4p+4q)(2\times 3)^{\alpha}(12pq - 6p - 6q) \\ &= (4)^{\alpha}(4p+4q)(6)^{\alpha}(12pq - 6p - 6q) \\ &= (24)^{\alpha}(4p+4q)(12pq - 6p - 6q) \\ &= (24)^{\alpha}(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2). \end{aligned} \tag{7}$$

□

Table 2. Edge partition of CNS subdivision $HAC_4C_8[p,q]$.

Case	(d_f, d_g) where $f\ g \in E(\mathbb{G})$	Number of edges
1	$(2,2)$	$4p + 4q$
2	$(2,3)$	$12pq - 6p - 6q$

Corollary 1. *Let $\mathbb{G}_1 \cong HAC_4C_8[p,q]$ be the graph of C_4C_8 CNS, then the first and the second multiplicative Zagreb and hyper-Zagreb, multiplicative sum and product conductivity indices are, respectively, equal to*

$$II_1(HAC_4C_8[p,q]) = 960p^2q - 480p^2 - 960pq + 960pq^2 - 480q^2, \tag{8}$$

$$II_2(HAC_4C_8[p,q]) = 1152p^2q + 1152pq^2 - 576p^2 - 1152pq - 576q^2, \tag{9}$$

$$\begin{aligned} HII_1(HAC_4C_8[p,q]) &= 19200p^2q + 19200pq^2 - 9600p^2 \\ &\quad - 19200pq - 9600q^2, \end{aligned} \tag{10}$$

$$\begin{aligned} HII_2(HAC_4C_8[p,q]) &= 27648p^2q + 27648pq^2 - 13824p^2 \\ &\quad - 27648pq - 13824q^2, \end{aligned} \tag{11}$$

$$SCII(HAC_4C_8[p,q]) = \frac{12}{\sqrt{5}}(2p^2q + 2pq^2 - p^2 - 2pq - q^2), \tag{12}$$

$$PCII(HAC_4C_8[p,q]) = 2\sqrt{6}(2p^2q + 2pq^2 - p^2 - 2pq - q^2). \tag{13}$$

Proof. Substituting $\alpha = 1$ in Eqs. (4) and (5), respectively, leads to the first and second multiplicative Zagreb indices for C_4C_8 CNS $HAC_4C_8[p,q]$ as

$$\begin{aligned} II_1(HAC_4C_8[p,q]) &= (20)^1(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2) \\ &= 20(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2) \\ &= 960p^2q + 960pq^2 - 480p^2 - 960pq - 480q^2, \\ II_2(HAC_4C_8[p,q]) &= (24)^1(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2) \\ &= 24(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2) \\ &= 1152p^2q + 1152pq^2 - 576p^2 - 1152pq - 576q^2. \end{aligned} \tag{14}$$

Substituting $\alpha = 2$ in Eqs. (4) and (5), respectively, provides the first and second multiplicative hyper-Zagreb indices for C_4C_8 CNS $HAC_4C_8[p,q]$ as

$$\begin{aligned} HII_1(HAC_4C_8[p,q]) &= (20)^2(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2) \\ &= 400(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2) \\ &= 19200p^2q + 19200pq^2 - 9600p^2 - 19200pq - 9600q^2, \end{aligned} \tag{15}$$

$$\begin{aligned} HII_2(HAC_4C_8[p,q]) &= (24)^2(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2) \\ &= 576(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2) \\ &= 27648p^2q + 27648pq^2 - 13824p^2 - 27648pq - 13824q^2. \end{aligned} \tag{16}$$

Substituting $\alpha = -\frac{1}{2}$ in Eqs. (4) and (5), respectively, gives the sum and product connectivity indices for C_4C_8 CNS $HAC_4C_8[p,q]$ as

$$\begin{aligned} SCII(HAC_4C_8[p,q]) &= (20)^{-\frac{1}{2}}(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2) \\ &= \frac{1}{(20)^{\frac{1}{2}}}(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2) \\ &= \frac{1}{2\sqrt{5}}(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2) \\ &= \frac{12}{\sqrt{5}}(2p^2q + 2pq^2 - p^2 - 2pq - q^2), \end{aligned} \tag{17}$$

$$\begin{aligned} PCII(HAC_4C_8[p,q]) &= (24)^{-\frac{1}{2}}(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2) \\ &= \frac{1}{(24)^{\frac{1}{2}}}(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2) \\ &= \frac{1}{2\sqrt{6}}(48p^2q + 48pq^2 - 24p^2 - 48pq - 24q^2) \\ &= 2\sqrt{6}(2p^2q + 2pq^2 - p^2 - 2pq - q^2). \end{aligned} \tag{18}$$

□

5. Results for Carbon Nanotube C_4C_8

The homeomorphic graph of CNTu $TUC_4C_8[p,q]$ obtained by adding a single vertex to each edge as shown in Fig. 2.

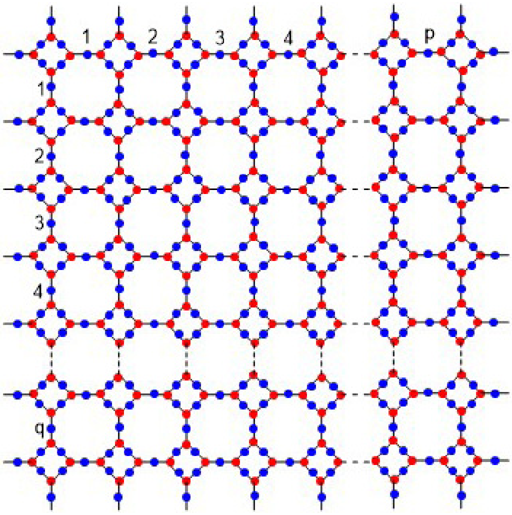

Fig. 2. Graph of CNTu subdivision $TUC_4C_8[p,q]$.

For the graph in Fig. 2, the number of vertices and the number edges of CNTu $TUC_4C_8[p,q]$ are calculated as

$$\begin{aligned}|V(TUC_4C_8[p,q])| &= 10pq - p,\\ |E(TUC_4C_8[p,q])| &= 12pq - 2p.\end{aligned} \tag{19}$$

Theorem 2. *Let $\mathbb{G}_2 \cong TUC_4C_8[p,q]$ be the graph of C_4C_8 CNTu, then the first and the second multiplicative Universal Zagreb indices are, respectively, equal to*

$$MZ_1^{\alpha}(TUC_4C_8[p,q]) = (20)^{\alpha}(48p^2q - 24p^2), \tag{20}$$

$$MZ_2^{\alpha}(TUC_4C_8[p,q]) = (24)^{\alpha}(48p^2q - 24p^2). \tag{21}$$

Proof. Consider the CNTu with subdivision $TUC_4C_8[p,q]$, $(p,q \geq 1)$ given in Fig. 2. The edge partitioning table of the graph is given as Table 3.

Substituting values in mathematical formula of the first multiplicative Universal Zagreb index (Eq. (1)) gives

$$\begin{aligned}MZ_1^{\alpha}(TUC_4C_8[p,q]) &= \prod_{(f,g)\in E(\mathbb{G})} (d_f + d_g)^{\alpha},\\ MZ_1^{\alpha}(TUC_4C_8[p,q]) &= (2+2)^{\alpha}(4p)(2+3)^{\alpha}(12pq - 6p)\\ &= (4)^{\alpha}(4p)(5)^{\alpha}(12pq - 6p)\\ &= (20)^{\alpha}(4p)(12pq - 6p)\\ &= (20)^{\alpha}(48p^2q - 24p^2).\end{aligned} \tag{22}$$

The mathematical formula of the second multiplicative Universal Zagreb index (Eq. (2)) leads to

$$\begin{aligned}MZ_2^{\alpha}(TUC_4C_8[p,q]) &= \prod_{(f,g)\in E(\mathbb{G})} (d_f \times d_g)^{\alpha},\\ MZ_2^{\alpha}(TUC_4C_8[p,q]) &= (2\times 2)^{\alpha}(4p)(2\times 3)^{\alpha}(12pq - 6p)\\ &= (4)^{\alpha}(4p)(6)^{\alpha}(12pq - 6p)\\ &= (24)^{\alpha}(4p)(12pq - 6p)\\ &= (24)^{\alpha}[(4p)(12pq) + (4p)(-6p)]\\ &= (24)^{\alpha}(48p^2q - 24p^2).\end{aligned} \tag{23}$$

□

Table 3. Edge partition of CNTu subdivision $TUC_4C_8[p,q]$.

Case	(d_f, d_g) where $f\ g \in E(\mathbb{G})$	Number of edges
1	$(2,2)$	$4p$
2	$(2,3)$	$12pq - 6p$

Corollary 2. *Let $\mathbb{G}_2 \cong TUC_4C_8[p,q]$ be the graph of C_4C_8 CNTu, then the first and the second multiplicative Zagreb and hyper-Zagreb, multiplicative sum and product conductivity indices are, respectively, equal to*

$$II_1(TUC_4C_8[p,q]) = 960p^2q - 480p^2, \tag{24}$$

$$II_2(TUC_4C_8[p,q]) = 1152p^2q - 576p^2, \tag{25}$$

$$HII_1(TUC_4C_8[p,q]) = 19200p^2q - 9600p^2, \tag{26}$$

$$HII_2(TUC_4C_8[p,q]) = 27648p^2q - 13824p^2, \tag{27}$$

$$SCII(TUC_4C_8[p,q]) = \frac{1}{2\sqrt{5}}(48p^2q - 24p^2), \tag{28}$$

$$PCII(TUC_4C_8[p,q]) = \frac{1}{2\sqrt{6}}(48p^2q - 24p^2). \tag{29}$$

Proof. Substituting $\alpha = 1$ in Eqs. (20) and (35), respectively, leads to the first and second multiplicative Zagreb indices for C_4C_8 CNTu $TUC_4C_8[p,q]$ as

$$\begin{aligned} MZ_1^1(TUC_4C_8[p,q]) &= II_1(TUC_4C_8[p,q]) = (20)^1(48p^2q - 24p^2) \\ &= 20(48p^2q - 24p^2) = 960p^2q - 480p^2, \end{aligned} \tag{30}$$

$$\begin{aligned} MZ_2^1(TUC_4C_8[p,q]) &= II_2(TUC_4C_8[p,q]) = (24)^1(48p^2q - 24p^2) \\ &= 24(48p^2q - 24p^2) = 1152p^2q - 576p^2. \end{aligned} \tag{31}$$

Substituting $\alpha = 2$ in Eqs. (20) and (35), respectively, provides the first and second multiplicative hyper-Zagreb indices for C_4C_8 CNTu $TUC_4C_8[p,q]$ as

$$\begin{aligned} MZ_1^2(TUC_4C_8[p,q]) &= HII_1(TUC_4C_8[p,q]) = (20)^2(48p^2q - 24p^2) \\ &= 400(48p^2q - 24p^2) = 19200p^2q - 9600p^2, \end{aligned} \tag{32}$$

$$\begin{aligned} MZ_2^2(TUC_4C_8[p,q]) &= HII_2(TUC_4C_8[p,q]) = (24)^2(48p^2q - 24p^2) \\ &= 576(48p^2q - 24p^2) = 27648p^2q - 13824p^2. \end{aligned} \tag{33}$$

Substituting $\alpha = -\frac{1}{2}$ in Eqs. (20) and (35), respectively, gives the sum and product connectivity indices for C_4C_8 CNTu $TUC_4C_8[p,q]$ as

$$\begin{aligned} MZ_1^{-\frac{1}{2}}(TUC_4C_8[p,q]) &= SCII(TUC_4C_8[p,q]) = (20)^{-\frac{1}{2}}(48p^2q - 24p^2) \\ &= \frac{1}{(20)^{\frac{1}{2}}}(48p^2q - 24p^2) \\ &= \frac{1}{2\sqrt{5}}(48p^2q - 24p^2), \end{aligned} \tag{34}$$

$$MZ_2^{-\frac{1}{2}}(TUC_4C_8[p,q]) = PCII(TUC_4C_8[p,q]) = (24)^{-\frac{1}{2}}(48p^2q - 24p^2)$$
$$= \frac{1}{(24)^{\frac{1}{2}}}(48p^2q - 24p^2) = \frac{1}{2\sqrt{6}}(48p^2q - 24p^2). \qquad (35)$$
□

6. Results for Carbon Nanotorus C_4C_8

The homeomorphic graph of CNTo $TC_4C_8[p,q]$ obtained by adding a single vertex to each edge is shown in Fig. 3.

For the graph in Fig. 3, the number of vertices and the number of edges of CNTo $TC_4C_8[p,q]$ are calculated as

$$|V(TC_4C_8[p,q])| = 10pq,$$
$$|E(TC_4C_8[p,q])| = 12pq.$$

Theorem 3. *Let* $\mathbb{G}_3 \cong TC_4C_8[p,q]$ *be the graph of* C_4C_8 *CNTo, then the first and the second multiplicative Universal Zagreb indices are, respectively, equal to*

$$MZ_1^{\alpha}(TC_4C_8[p,q]) = (5)^{\alpha}(12pq), \qquad (36)$$
$$MZ_2^{\alpha}(TC_4C_8[p,q]) = (6)^{\alpha}(12pq). \qquad (37)$$

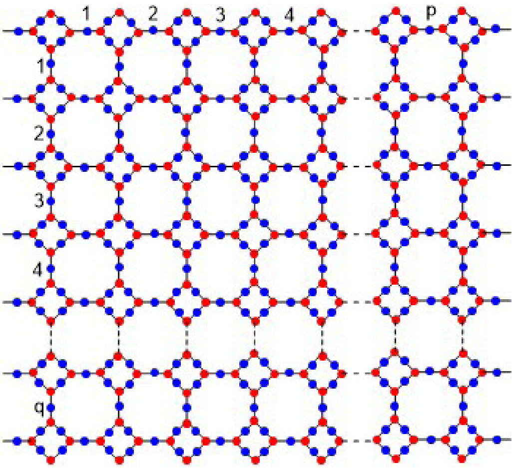

Fig. 3. Graph of CNTo subdivision $TC_4C_8[p,q]$.

Table 4. Edge partition of CNTo subdivision $TC_4C_8[p,q]$.

Case	(d_f, d_g) where $fg \in E(\mathbb{G})$	Number of edges
1	$(2,3)$	$12pq$

Proof. Consider the CNTo with subdivision $TC_4C_8[p,q]$, $(p,q \geq 1)$ given in Fig. 3. The edge partitioning table of the graph is given as Table 4.

Substituting values in mathematical formula of the first multiplicative Universal Zagreb index (Eq. (1)) gives

$$\begin{aligned} MZ_1^{\alpha}(TC_4C_8[p,q]) &= \prod_{(f,g)\in E(\mathbb{G})} (d_f + d_g)^{\alpha}, \\ MZ_1^{\alpha}(\mathbb{G}_3) &= (2+3)^{\alpha}(12pq) \\ &= (5)^{\alpha}(12pq). \end{aligned} \tag{38}$$

The mathematical formula of the second multiplicative Universal Zagreb index (Eq. (2)) leads to

$$\begin{aligned} MZ_2^{\alpha}(TC_4C_8[p,q]) &= \prod_{(f,g)\in E(\mathbb{G})} (d_f \times d_g)^{\alpha}, \\ MZ_2^{\alpha}(\mathbb{G}_3) &= (2\times 3)^{\alpha}(12pq) \\ &= (6)^{\alpha}(12pq). \end{aligned} \tag{39}$$

□

Corollary 3. *Let $\mathbb{G}_3 \cong TC_4C_8[p,q]$ be the graph of C_4C_8 CNTo, then the first and the second multiplicative Zagreb and hyper-Zagreb, multiplicative sum and product conductivity indices are, respectively, equal to*

$$II_1(TC_4C_8[p,q]) = 60pq, \tag{40}$$

$$II_2(TC_4C_8[p,q]) = 72pq, \tag{41}$$

$$HII_1(TC_4C_8[p,q]) = 300pq, \tag{42}$$

$$HII_2(TC_4C_8[p,q]) = 432pq. \tag{43}$$

$$SCII(TC_4C_8[p,q]) = \frac{12}{\sqrt{5}}pq, \tag{44}$$

$$PCII(TC_4C_8[p,q]) = 2\sqrt{6}pq. \tag{45}$$

Proof. Substituting $\alpha = 1$ in Eqs. (36) and (37), respectively, leads to the first and second multiplicative Zagreb indices for C_4C_8 CNTo $TC_4C_8[p,q]$ as

$$\begin{aligned} MZ_1^{1}(TC_4C_8[p,q]) &= II_1(TC_4C_8[p,q]) = (5)^1(12pq) \\ &= 5(12pq) \\ &= 60pq, \end{aligned} \tag{46}$$

$$\begin{aligned} MZ_2^{1}(TC_4C_8[p,q]) &= II_2(TC_4C_8[p,q]) = (6)^1(12pq) \\ &= 6(12pq) \\ &= 72pq. \end{aligned} \tag{47}$$

Substituting $\alpha = 2$ in Eqs. (36) and (37), respectively, provides the first and second multiplicative hyper-Zagreb indices for C_4C_8 CNTo $TC_4C_8[p,q]$ as

$$\begin{aligned} MZ_1^2(TC_4C_8[p,q]) &= HII_1(TC_4C_8[p,q]) = (5)^2(12pq) \\ &= 25(12pq) \\ &= 300pq, \end{aligned} \tag{48}$$

$$\begin{aligned} MZ_2^2(TC_4C_8[p,q]) &= HII_2(TC_4C_8[p,q]) = (6)^2(12pq) \\ &= 36(12pq) \\ &= 432pq. \end{aligned} \tag{49}$$

Substituting $\alpha = -\frac{1}{2}$ in Eqs. (36) and (37), respectively, gives the sum and product connectivity indices for C_4C_8 CNTo $TC_4C_8[p,q]$ as

$$\begin{aligned} MZ_1^{-\frac{1}{2}}(TC_4C_8[p,q]) &= SCII(TC_4C_8[p,q]) = (5)^{-\frac{1}{2}}(12pq) \\ &= \frac{1}{(5)^{\frac{1}{2}}}(12pq) \\ &= \frac{12}{2\sqrt{5}}pq \\ &= \frac{6}{\sqrt{5}}pq, \end{aligned} \tag{50}$$

$$\begin{aligned} MZ_2^{-\frac{1}{2}}(TC_4C_8[p,q]) &= PCII(TC_4C_8[p,q]) = (6)^{-\frac{1}{2}}(12pq) \\ &= \frac{1}{(6)^{\frac{1}{2}}}(12pq) \\ &= \frac{12}{2\sqrt{6}}pq \\ &= 2\sqrt{6}pq. \end{aligned} \tag{51}$$

□

7. Discussion

We have computed the first and second multiplicative Universal indices for the C_4C_8 carbon nanostructures CNS ($HAC_4C_8[p,q]$), CNTu ($TUC_4C_8[p,q]$), CNTo ($TC_4C_8[p,q]$) with p and q the number of squares in each row and column, respectively. These indices play the role as parents for computing many degree-based topological indices including multiplicative Zagreb and hyper-Zagreb indices, multiplicative sum and product connectively indices.

The first multiplicative Zagreb, second multiplicative Zagreb, first multiplicative hyper-Zagreb, second multiplicative hyper-Zagreb, multiplicative sum and multiplicative product connectivity indices for the three carbon nanostructures (CNS, CNTu and CNTo) are presented in Figs. 4–8. In all these figures, the plots for CNS $HAC_4C_8[p,q]$, CNTu $TUC_4C_8[p,q]$ and CNTo $TC_4C_8[p,q]$ are presented in green, blue and yellow colors, respectively.

Figure 4 demonstrates that when p and q rise, the first multiplicative Zagreb index would rise for C_4C_8 CNS, CNTu and CNTo. This indicates that when carbon nanostructure size increases, so do the values of topological indices. The first multiplicative Zagreb index has the largest values for the CNTo, relatively lower for the CNT, and the lowest for the CNS.

Figure 5 exhibits that the second multiplicative Zagreb index increases as p and q rise. It implies that as the size of the carbon nanostructures increases, so do the

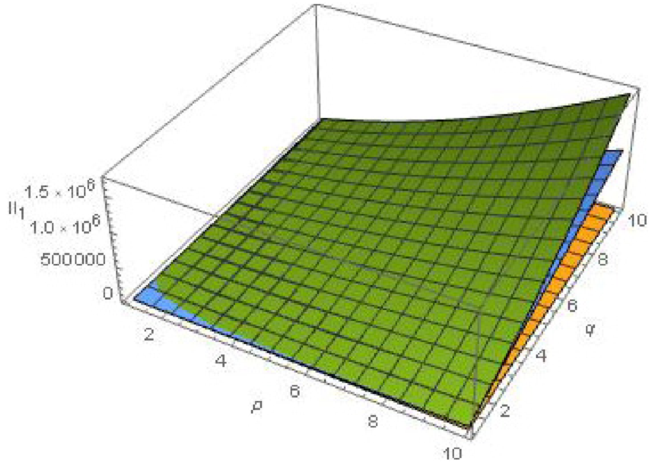

Fig. 4. Graphs of first multiplicative Zagreb index of C_4C_8 carbon nanostructures.

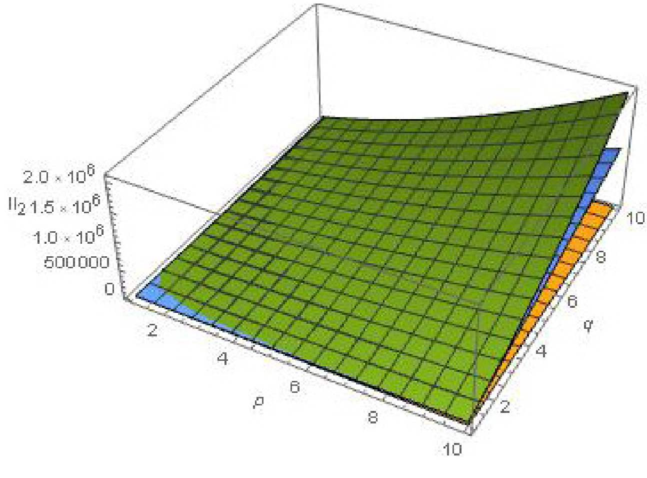

Fig. 5. Graphs of second multiplicative Zagreb index of C_4C_8 carbon nanostructures.

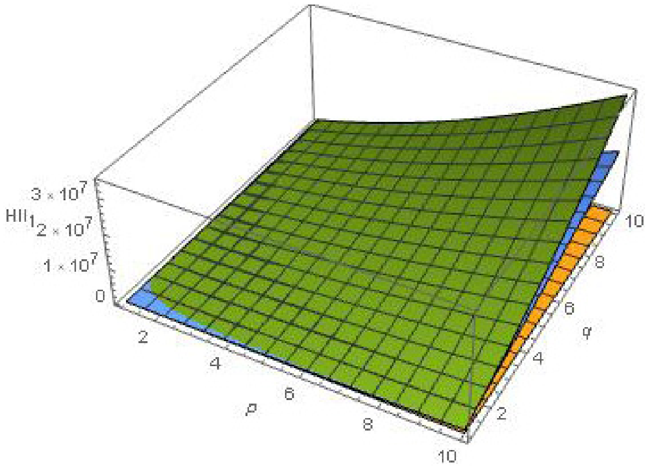

Fig. 6. Graphs of first multiplicative hyper-Zagreb index of C_4C_8 carbon nanostructures.

values of second multiplicative Zagreb index. The CNTo has the greatest values of second multiplicative Zagreb index, whereas those of the CNT and CNS are lower.

Figure 6 shows that when p and q grow, the first multiplicative hyper-Zagreb index rise. It implies that when carbon nanostructures grow in size, the values of first multiplicative hyper-Zagreb index rise as well. The values of the first multiplicative hyper-Zagreb index are the highest for the CNTo, relatively lower for the CNT, and the lowest for the CNS.

Figure 7 depicts that the second multiplicative hyper-Zagreb index rises with the increase in p and q. This indicates that when the size of carbon nanostructure

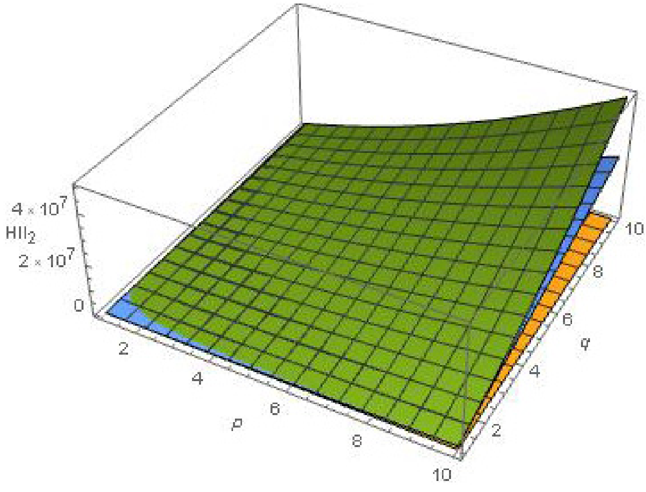

Fig. 7. Graphs of second multiplicative hyper-Zagreb index of C_4C_8 carbon nanostructures.

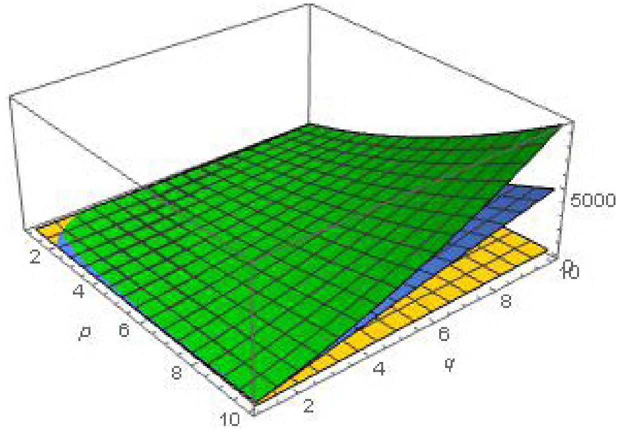

Fig. 8. Graphs of multiplicative sum connectivity index of C_4C_8 carbon nanostructures.

increases, so do the values of the second multiplicative hyper-Zagreb index. Additionally, the second multiplicative hyper-Zagreb index admits largest values for the CNTo, lower for the CNT and the lowest for the CNS.

Figure 8 indicates that the multiplicative sum connectivity index is growing as p and q rise. It implies that as the size of the carbon nanostructures increases, so do the values of the multiplicative sum connectivity index. Moreover, the CNTo has the greatest values of the multiplicative sum connectivity index, whereas the CNT and CNS have lower values.

Figure 9 indicates that the values of multiplicative product connectivity index are increasing with an increase in p and q. It means that the values of multiplicative product connectivity index increase with the increase in size of the carbon nanostructures. Moreover, the values of multiplicative product connectivity index are the highest for the CNTo, less for CNT and the least for the CNS.

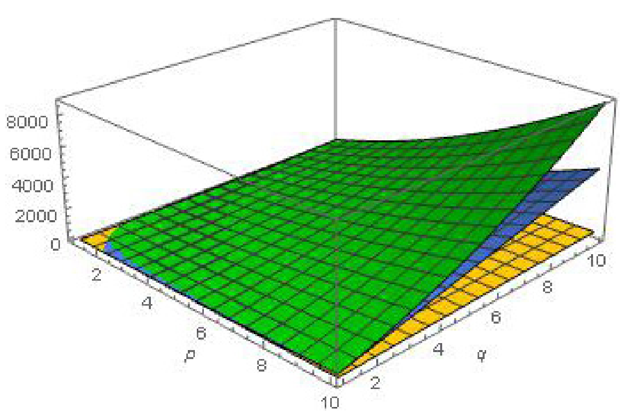

Fig. 9. Graphs of multiplicative product connectivity index of C_4C_8 carbon nanostructures.

Since the value of the power α plays an important role in determining the value of multiplicative degree-based indices from the multiplicative Universal Zagreb index, the values of multiplicative sum and product connectivity indices are lowest, the values of first and second multiplicative Zagreb indices are the higher and the first and second multiplicative hyper-Zagreb indices are the highest for all the C_4C_8 carbon nanostructures.

8. Conclusion

Topological indices represent several physiochemical properties of molecular structures using a single numeric. The vertex degree indicating the number of bonds concerning a single atom significantly plays its role in determining these properties. Thus, the degree-based topological indices are important. The Zagreb indices and their variants are well known to represent the chemical properties of molecular structures. The Universal Zagreb indices are a general representation of Zagreb, hyper-Zagreb, the sum and product conductivity indices. Carbon nanostructures C_4C_8 CNS, CNTu, CNTo are potentially used in industry due to their stability, flexibility, light weight, low cost, high efficiency, electromagnetic and energy storage properties. Therefore, the Universal Zagreb indices of these nanostructures become the center of interest. The first and second, multiplicative Zagreb and multiplicative hyper-Zagreb, multiplicative sum and product conductivity indices of these structures are also derived from the formulae of Universal Zagreb indices. These indices can be compared graphically.

Figures 4–8 show that the multiplicative topological indices are increasing as p and q increase. It means that the values of topological indices increase with the increase in size of the carbon nanostructures. Moreover, the values of all the multiplicative topological indices are highest for the CNTo, less for CNT and least for the CNS. Since the value of α plays an important role in determining the value of multiplicative degree-based indices from the multiplicative Universal Zagreb index, the values of multiplicative sum and product connectivity indices are lowest, the values of first and second multiplicative Zagreb indices are the higher and the first and second multiplicative hyper-Zagreb indices are the highest for all the C_4C_8 carbon nanostructures.

The results obtained in this work are novel and are a significant contribution in QSAR and QSPR studies of carbon nanostructures.

This work can be extended to calculate other degree-based multiplicative topological indices of the same nanostructures. Moreover, the multiplicative Universal Zagreb indices of other carbon nanostructures can be investigated.

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