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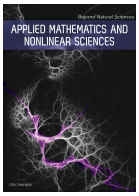

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Computation of certain topological coindices of graphene sheet and $C_4C_8(S)$ nanotubes and nanotorus

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Abstract

Topological indices are widely used for quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR). Topological coindices are topological indices that considers the non adjacent pairs of vertices. Here, we consider the following five well-known topological coindices: the first and second Zagreb coindices, the first and second multiplicative Zagreb coindices and the F-coindex. By using graph structural analysis and derivation, we study the above-mentioned topological coindices of some chemical molecular graphs that frequently appear in medical, chemical, and material engineering such as graphene sheet and $C_4C_8(S)$ nanotubes and nanotorus and obtain the computation formulae of the coindices of these graphs. Furthermore, we analyze the results by MATLAB and obtain the relationship of the coindices which they describe the physcio-chemical properties and biological activities.

Keywords: Molecular graph, topological coindex, graphene sheet, nanotubes, nanotorus
AMS 2010 codes: 05C90, 90C35.

1 Introduction

In the fields of chemical graph theory, molecular topology, and mathematical chemistry, a topological index also known as a connectivity index is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound. Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant. Topological indices are used for example in the development

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of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure [1].

Graphene is an allotrope (form) of carbon consisting of a single layer of carbon atoms arranged in a hexagonal lattice. Graphene can be considered as an indefinitely large aromatic molecule, the ultimate case of the family of flat polycyclic aromatic hydrocarbons. Graphite, the most common allotrope of carbon, is basically a stack of graphene layers held together with weak bonds. Fullerenes and carbon nanotubes, two other forms of carbon, have structures similar to that of graphene; which can also be viewed as a fullerene or nanotube of infinitely large size.

In present report, authors computed several degree-based topological indices of graphene sheet, nanotube and nanotori.

Let G be the molecular graph which is simple connected graph with vertex (atom) set $V(G)$ and edge (bond) set $E(G)$ respectively. The degree $d_G(v)$ of a vertex $v \in V(G)$ is the number of neighbour vertices to v. A graph G is called regular of degree r, if each and every vertices of G has precisely r-neighbours. The complement of a graph G which is denoted by $\overline{G}$ is the simple graph with the same vertex set $V(G)$ and any two vertices $uv \in E(\overline{G})$ if and only if $uv \notin E(G)$.

Wiener index, first and second Zagreb indices and Randic index are among the oldest and most thoroughly studied graph-based molecular structure descriptors with a number of applications. The first (M_1) and second (M_2) Zagreb indices were introduced in 1972 by Gutman and Trinajstić [2] with in a study of the structure-dependency of the total π-electron energy (ε) where approximate formulas for the total π -electron energy (ε) were obtained. These indices provide a measure of the branching of the carbon-atom skeleton. These quantities are defined as

$$M_1(G) = \sum_{u \in V(G)} d_G(u)^2 = \sum_{uv \in E(G)} (d_G(u) + d_G(v))$$

and

$$M_2(G) = \sum_{uv \in E(G)} (d_G(u) d_G(v))$$

For details of the theory and applications of these indices we refer the reader to [3–7] and the references cited therein. In [2] another degree based topological index which is also a measure of branching was encountered but for unknown reason it was not further studied. After more than 40 years, Furtula and Gutman [8] re-initiated and establish some basic properties of it. This index is denoted by $F(G)$ and named as forgotten topological index or F-index. It is defined as

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

According to Furtula and Gutman [8], the predictive ability of the F-index is quite similar to that of M_1 and in the case of entropy and acentric factor, both M_1 and F yield correlation coefficients greater than 0.95. Some studies on F-index can be referred to [9, 10].

Most degree based topological indices are viewed as the contributions of pairs of adjacent vertices. But through time scientists introduced some degree based topological indices that considers the non-adjacent pairs of vertices for computing some topological properties of graphs and named as coindices.

The first $(\overline{M}_1)$ and second $(\overline{M}_2)$ Zagreb coindices were introduced by Došlic [11] while computing weighted Wiener polynomial of certain composite graphs. They are defined as

$$\overline{M}_1(G) = \sum_{uv \in E(\overline{G})} (d_G(u) + d_G(v))$$

and

$$\overline{M}_2(G) = \sum_{uv \in E(\overline{G})} (d_G(u) d_G(v))$$

Xu et al. [12] defined the first and second multiplicative Zagreb coindices which are considered as the multiplicative versions of Zagreb coindices and discussed some properties and upper and lower bounds of molecular graphs. They are defined respectively as

$$\overline{\prod}_1(G) = \prod_{uv \in E(\overline{G})} (d_G(u) + d_G(v))$$

and

$$\overline{\prod}_2(G) = \prod_{uv \in E(\overline{G})} (d_G(u) d_G(v))$$

Recently, De et al. [13] introduced the F-coindex of a graph G, denoted by $\overline{F}$, after testifying that the correlation coefficients between the logarithm of octanol-water partition coefficient ($log(P)$) and the corresponding F-coindex values of octane isomers is found to be 0.996 which shows F-coindex can predict the $log(P)$ values with high accuracy. It is defined as

$$\overline{F}(G) = \sum_{uv \in E(\overline{G})} (d_G(u)^2 + d_G(v)^2)$$

Some studies on the mentioned coindices can be refered to [14–19]. Even though there are several research reports contributing on the computation of degree and distance based topological indices of molecular graphs, the studies on the computation of topological coindices of molecular graphs are largely limited. Thus, in this paper we develop an exact formula of certain coindices such as the first and second Zagreb coindices, the first and second multiplicative Zagreb coindices, and the forgotten topological coindex, of certain nanomaterials such as graphene sheet, $TUC_4C_8(S)$ nanotubes and $TUC_4C_8(S)$ nanotorus. MATLAB script that calculates all the mentioned coindices values of these nanomaterals as well as graphical and tabular comparisons are included.

2 Preliminaries

Let $\delta(G)$ (resp. $\Delta(G)$) be the minimum (resp. maximum) degrees of the molecular graph G. The vertex set $V(G)$ and edge sets $E(G)$, and $E(\overline{G})$ can be divided into several partitions: for any degrees i and j in G with $\delta(G) \leq i, j \leq \Delta(G)$, in this paper we use the following notations.
Let $n_i = |V_i|$ for $V_i = \{v \in V(G) | d_G(v) = i\}$,
$m_{ij} = |E_{ij}|$ for $E_{ij} = \{uv \in E(G) | d_G(v) = i, \text{ and } d_G(u) = j\}$, and
$\overline{m}_{ij} = |\overline{E}_{ij}|$ for $\overline{E}_{ij} = \{uv \in E(\overline{G}) | d_G(v) = i, \text{ and } d_G(u) = j\}$

Lemma 1. *Let G be a connected graph of order n and let n_i be the number of vertices of degree i and m_{ij} be the number of edges connecting the vertices of degrees i and j. Then, for $\overline{E}_{ij} = \{uv \in E(\overline{G}) | d_G(v) = i, \text{ and } d_G(u) = j\}$*

$$\overline{m}_{ij} = |\overline{E}_{ij}| = \begin{cases} n_i(n_i - 1)/2 - m_{ii} & \text{for } i = j. \\ n_i \cdot n_j - m_{ij} & \text{for } i < j. \end{cases}$$

Proof. Let G be a graph of order n.
Define $\overline{E}_{ij} = \{uv \in E(\overline{G}) : d_G(u) = i, d_G(v) = j\}$
With out loss of generality, we assume that $i \leq j$
If $i = j$, then it is clear that $\overline{m}_{ii} = n_i(n_i - 1)/2 - m_{ii}$
If $i < j$, since degree i comes from a set of vertex of size n_i and for each choice of degree i there are n_j choices for degree j, by incorporating the multiplication principle we obtained $\overline{m}_{ij} = n_i \cdot n_j - m_{ij}$. □

Theorem 1. *Let G be a graph of order n with $V_i = \{v \in V(G) : d_G(v) = i\}$ and $E_{ij} = \{uv \in E(G) : d_G(u) = i, d_G(v) = j\}$. Then*

(i). $\overline{F}(G) = \sum_{\delta \le i \le j \le \Delta} \overline{m}_{ij}(i^2 + j^2)$

(ii). $\overline{M}_1(G) = \sum_{\delta \le i \le j \le \Delta} \overline{m}_{ij}(i + j)$

(iii). $\overline{M}_2(G) = \sum_{\delta \le i \le j \le \Delta} \overline{m}_{ij}(i \cdot j)$

(iv). $\overline{\prod}_1(G) = \prod_{\delta \le i \le j \le \Delta} (i + j)^{\overline{m}_{ij}}$

(v). $\overline{\prod}_2(G) = \prod_{\delta \le i \le j \le \Delta} (i \cdot j)^{\overline{m}_{ij}}$

Where $\overline{m}_{ij}$ is as defined in lemma 1.

Proof. Let G be a graph of order n. With out loss of generality, assume that $i \le j$. Then, By the definition of F-coindex

$$\begin{aligned}
\overline{F}(G) &= \sum_{uv \in E(\overline{G})} (d_G(u)^2 + d_G(v)^2) \\
&= \sum_{uv \in E(\overline{G}), i=j} (d_G(u)^2 + d_G(v))^2 + \sum_{uv \in E(\overline{G}), i<j} (d_G(u)^2 + d_G(v)^2) \\
&= \sum_{i=\delta}^{\Delta} (i^2 + i^2) \cdot \overline{m}_{ii} + \sum_{\delta \le i < j \le \Delta} (i^2 + j^2) \cdot \overline{m}_{ij} \\
&= \sum_{\delta \le i \le j \le \Delta} \overline{m}_{ij} \cdot (i^2 + j^2)
\end{aligned}$$

Similarly, by using the definitions of each topological coindices and lemma 1, we can proof the remaining parts of the theorem. □

Corollary 1. *Let G be an r- regular graph of order n. Then*

(i). $\overline{F}(G) = r^2 n(n - r - 1)$

(ii). $\overline{M}_1(G) = rn(n - r - 1)$

(iii). $\overline{M}_2(G) = r^2 n(n - r - 1)/2$

(iv). $\overline{\prod}_1(G) = (2r)^{n(n-r-1)/2}$

(v). $\overline{\prod}_2(G) = r^{n(n-r-1)}$

Proof. In r-regular graph of order n, $\overline{m}_{rr} = |E(\overline{G})| = n(n - r - 1)/2$. Thus, the results follow immediately. □

Corollary 2. *Let G be an r- regular graph of order n. Then we have the following relations.*

(i). $\overline{F}(G) = r\overline{M}_1(G) = 2\overline{M}_2(G)$

3 Main Results and discussions

3.1 The Graphene sheet

Graphene sheet is an atomic-scale honeycomb lattice composed of carbon atoms linked in hexagonal shapes, as shown in Fig. 1, with each carbon atom covalently bonded to three other carbon atoms.

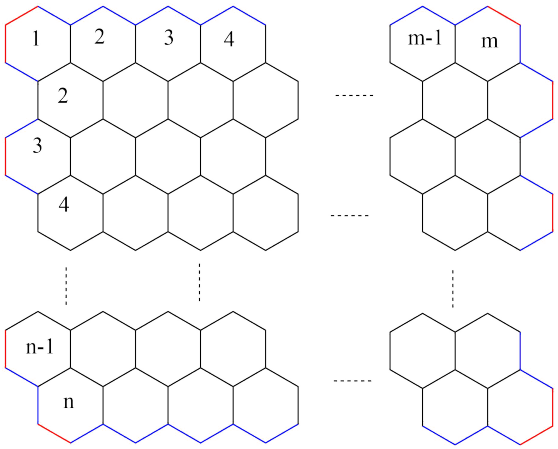


Fig. 1 Graphene sheet $G(n,m)$ where, n and m denotes the number of hexagons in rows and columns.

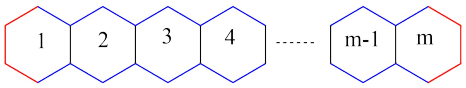


Fig. 2 Graphene sheet $G(1,m)$.

Graphene has excellent optical transmittance ($\sim 97.7\%$), high young's modulus ($\sim 1\,TPa$), large theoretical specific surface area ($2630\,m^2\,g^{-1}$), good thermal conductivity ($\sim 5000\,W\,m^{-1}\,K^{-1}$), high intrinsic carrier mobility ($200,000\,cm^2\,v^{-1}\,s^{-1}$) [21], intrinsic electrical conductivity of ($10^6\,S\,cm^{-1}$) [20, 23], good mechanical flexibility, high theoretical gravimetric capacitance ($550\,F\,g^{-1}$) [21], and splendid theoretical lithium storage capacity ($744\,mA\,h\,g^{-1}$) [21, 23]. This shows, graphene is much stronger than diamond and conducts electricity and heat better than any material ever discovered. Thus, due to such impressive optical, mechanical, thermal and morphological properties, graphene has attracted the attention of scientists, researchers, and industries worldwide and it will play an important role in different aspects such as aerospace, automobile, communications, solar, electronics, energy storage, and sensor. Sridhara et al. [24] determined some topological indices of graphene such as the atom-bond connectivity index, fourth atom-bond connectivity index, sum connectivity index, Randic connectivity index, geometric-arithmetic connectivity and fifth geometric-arithmetic connectivity index. Jagadeesh et al. [25] studied first and second Zagreb indices, first and second multiplicative Zagreb indices, augmented Zagreb index, harmonic index and hyper-Zagreb index of graphene. Similarly, Gao et al. [26] studied the F-index of graphene. Consider the graphene sheet $G(n,m)$ in Fig.1 and Fig.2. It is bi-degreed graph with vertices of degree two and degree three and based on the end vertices of each edge, there are exactly three partitions of edges: m_{22} (the edges in red colours), m_{23} (the edges in blue colours), and m_{33} (the edges in black colours). Since the graphene sheet for $n \neq 1$ (Fig 1) and $n = 1$ (Fig. 2) behaves different on the number of partitions of edges, there are two cases to consider. The number of vertices and edges of the graphene sheet for $n \neq 1$ is presented in Table 1 and that of $n = 1$ is presented in Table 2. By using lemma 1 and results in Table 1 and Table 2, we further obtained the edge partitions: $\overline{m}_{22}$, $\overline{m}_{23}$, and $\overline{m}_{33}$ of the complement graph $\overline{G}(n,m)$ with respect to the vertex degrees of $G(n,m)$ and the results are also presented in Table 3 for $n \neq 1$ and in Table 4 for $n = 1$.

Table 1 Vertex and edge partitions of graphene sheet for $n \neq 1$

Row	n_2	n_3	m_{22}	m_{23}	m_{33}
1	$m+3$	$3m-1$	3	$2m$	$3m-2$
2	2	$2m$	1	2	$3m-1$
3	2	$2m$	1	2	$3m-1$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$n-1$	2	$2m$	1	2	$3m-1$
n	$m+3$	$m-1$	3	$2m$	$m-1$
Total	$2m+2n+2$	$2mn-2$	$n+4$	$4m+2n-4$	$3nm-2m-n-1$

Table 2 Vertex and edge partitions of graphene sheet for $n = 1$

n_2	n_3	m_{22}	m_{23}	m_{33}
$2m+4$	$2m-2$	6	$4m-4$	$m-1$

Table 3 The edge partitions $\overline{m}_{ij}$ of $\overline{G}$ based on the vertex degrees of G, for $n \neq 1$

$(d_G(u), d_G(v))$ where $uv \in E(G)$	Number of edges in $\overline{G}$
$(2,2)$	$2m^2+2n^2+4mn+3m+2n-3$
$(3,3)$	$2(mn)^2-8mn+2m+n+4$
$(2,3)$	$4m^2n+4mn^2+4mn-8m-6n$

Table 4 The edge partitions $\overline{m}_{ij}$ of $\overline{G}$ based on the vertex degrees of G, for $n = 1$

$(d_G(u), d_G(v))$ where $uv \in E(G)$	Number of edges in $\overline{G}$
$(2,2)$	$2m^2+7m$
$(3,3)$	$2m^2-6m+4$
$(2,3)$	$4m^2-4$

Theorem 2. *Let $G(n,m)$ be a graphene sheet with n rows and m columns. Then*

$$\overline{F}(G) = \begin{cases} 36(mn)^2 + 52mn^2 + 52nm^2 + 16m^2 + \\ 16n^2 - 60mn - 44m - 44n + 48. & \text{for } n \neq 1. \\ 104m^2 - 52m + 20 & \text{for } n = 1. \end{cases}$$

Proof. Let G be the graphene sheet $G(n,m)$. We find the edge partition of $\overline{G}$ based on the vertex degrees of G. Table 3 and Table 4 explains such partitions of $\overline{G}$. Consider the following cases.
Case.1 For $n \neq 1$
By using Theorem 1 **(i)** and Table 3 we obtain.

$$\begin{aligned} \overline{F}(G) &= \sum_{2\leq i\leq j\leq 3} \overline{m}_{ij} \cdot (i^2 + j^2) \\ &= 8\overline{m}_{22} + 13\overline{m}_{23} + 18\overline{m}_{33} \\ &= 8(2m^2 + 2n^2 + 4mn + 3m + 2n - 3) + 13(4m^2n + 4mn^2 + 4mn - 8m - 6n) \\ &+ 18(2(mn)^2 - 8mn + 2m + n + 4) \\ &= 36(mn)^2 + 52mn^2 + 52nm^2 + 16m^2 + 16n^2 - 60mn - 44m - 44n + 48. \end{aligned}$$

Case.2 For $n = 1$
By using Theorem 1 **(i)** and Table 4 we obtain the required one.

$$\begin{aligned} \overline{F}(G) &= \sum_{2\leq i\leq j\leq 3} \overline{m}_{ij} \cdot (i^2 + j^2) \\ &= 8\overline{m}_{22} + 13\overline{m}_{23} + 18\overline{m}_{33} \\ &= 8(2m^2 + 7m) + 13(4m^2 - 4) + 18(2m^2 - 6m + 4) \\ &= 104m^2 - 52m + 20. \end{aligned}$$

□

Theorem 3. *Let $G(n,m)$ be a graphene sheet with n rows and m columns. Then*

$$\overline{M}_1(G) = \begin{cases} 12(mn)^2 + 20mn^2 + 20nm^2 + 8m^2 + \\ 8n^2 - 12mn - 16m - 16n + 12. & \text{for } n \neq 1. \\ 40m^2 - 8m + 4 & \text{for } n = 1. \end{cases}$$

Proof. Let G be the graphene sheet $G(n,m)$. By using Theorem 1 **(ii)** and Table 3 we can obtain the result for the case $n \neq 1$ and by using Theorem 1 **(ii)** and Table 4 we can also get the result for the case $n = 1$. □

Theorem 4. *Let $G(n,m)$ be a graphene sheet with n rows and m columns. Then*

$$\overline{M}_2(G) = \begin{cases} 18(mn)^2 + 24mn^2 + 24nm^2 + 8m^2 + 8n^2 \\ -32mn - 18m - 19n + 24. & \text{for } n \neq 1. \\ 50m^2 - 26m + 12 & \text{for } n = 1. \end{cases}$$

Proof. Let G be the graphene sheet $G(n,m)$. By using Theorem 1 **(iii)** and Table 3 we can obtain the required result for the case $n \neq 1$ and by using Theorem 1 **(iii)** and Table 4 we can obtain the result for the remaining case. □

Theorem 5. *Let $G(n,m)$ be a graphene sheet with n rows and m columns. Then*

$$\overline{\prod}_1(G) = \begin{cases} 4^{(2m^2+2n^2+4mn+3m+2n-3)} \cdot 5^{(4m^2n+4mn^2+4mn-8m-6n)} \\ \cdot 6^{(2(mn)^2-8mn+2m+n+4)} & for\ n \neq 1. \\ 4^{(2m^2+7m)} \cdot 5^{(4m^2-4)} \cdot 6^{(2m^2-6m+4)} & for\ n = 1. \end{cases}$$

Proof. Let G be the graphene sheet $G(n,m)$. We find the edge partition of the complement graph of G based on vertex degrees of G. Consider the following cases.
Case.1 For $n \neq 1$
By using Theorem 1**(iv)** and Table 3 we obtain

$$\begin{aligned} \overline{\prod}_1(G) &= \prod_{\delta \leq i \leq j \leq \Delta} (i+j)^{\overline{m}_{ij}} \\ &= 4^{\overline{m}_{22}} \cdot 5^{\overline{m}_{23}} \cdot 6\overline{m}_{33} \\ &= 4^{(2m^2+2n^2+4mn+3m+2n-3)} \cdot 5^{(4m^2n+4mn^2+4mn-8m-6n)} \cdot 6^{(2(mn)^2-8mn+2m+n+4)} \end{aligned}$$

Case.2 For $n = 1$
By using Theorem 1**(iv)** and Table 4 we obtain

$$\begin{aligned} \overline{\prod}_1(G) &= \prod_{\delta \leq i \leq j \leq \Delta} (i+j)^{\overline{m}_{ij}} \\ &= 4^{\overline{m}_{22}} \cdot 5^{\overline{m}_{23}} \cdot 6^{\overline{m}_{33}} \\ &= 4^{(2m^2+7m)} \cdot 5^{(4m^2-4)} \cdot 6^{(2m^2-6m+4)} \end{aligned}$$

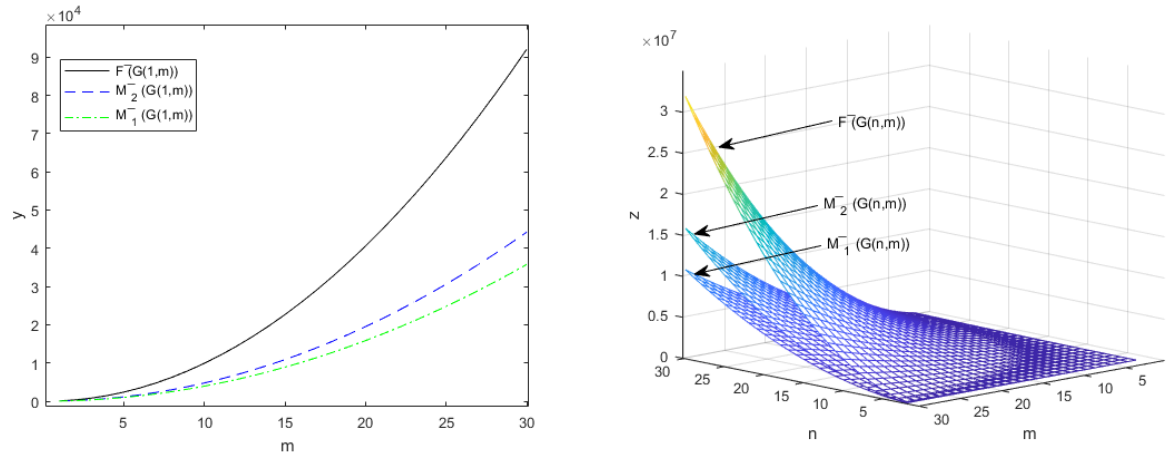
□

Theorem 6. *Let $G(n,m)$ be a graphene sheet with n rows and m columns. Then*

$$\overline{\prod}_2(G) = \begin{cases} 4^{(2m^2+2n^2+4mn+3m+2n-3)} \cdot 6^{(4m^2n+4mn^2+4mn-8m-6n)} \\ \cdot 9^{(2(mn)^2-8mn+2m+n+4)} & for\ n \neq 1. \\ 4^{(2m^2+7m)} \cdot 6^{(4m^2-4)} \cdot 9^{(2m^2-6m+4)} & for\ n = 1. \end{cases}$$

Proof. Let G be the graphene sheet $G(n,m)$. Result on case $n \neq 1$ can be obtained by using Theorem 1 **(v)** and Table 3 and that of the remaining case by using Theorem 1 **(v)** and Table 4. □

% MATLAB script to calculate $\overline{F}, \overline{M}_2, \overline{M}_1, \overline{\prod}_1$ and $\overline{\prod}_2$ of an n by m dimensional graphene sheet $G(n,m)$.
function [ ]=Topological_coindices_of_graphene_sheet(n,m)
disp('——-')
disp(' m n $\overline{F}$ $\overline{M}_2$ $\overline{M}_1$ $\overline{\prod}_1$ $\overline{\prod}_2$ ')
disp('——-')
for $i = 1 : n$
for $j = 1 : m$
if $i == 1$
$\overline{F} = 104 * j^2 - 52 * j + 20;$
$\overline{M}_2 = 50 * j^2 - 26 * j + 12;$
$\overline{M}_1 = 40 * j^2 - 8 * j + 4;$
$\overline{\prod}_1 = 4^{(2*j^2+7*j)} * 5^{(4*j^2-4)} * 6^{(2*j^2-6*j+4)};$
$\overline{\prod}_2 = 4^{(2*j^2+7*j)} * 6^{(4*j^2-4)} * 9^{(2*j^2-6*j+4)};$
else
$\overline{F} = 36 * (i^2) * (j^2) + 52 * j * (i^2) + 52 * i * (j^2) + 16 * i^2 + 16 * j^2 - 60 * j * i - 44 * j - 44 * i + 48;$



(a) (b)

Fig. 3 Comparative model for different coindices of the graphene sheet $G(n,m)$ (a) for $n = 1$ and (b) for $n \neq 1$

$\overline{M}_2 = 18*(i^2)*(j^2)+24*j*(i^2)+24*i*(j^2)+8*j^2+8*i^2-32*j*i-18*j-19*i+24;$
$\overline{M}_1 = 12*(i^2)*(j^2)+20*j*(i^2)+20*i*(j^2)+8*j^2+8*i^2-12*j*i-16*j-16*i+12;$
$\overline{\prod}_1 = 4^{(2*j^2+2*i^2+4*j*i+3*j+2*i-3)} * 5^{(4*j^2*i+4*i*j^2+4*j*i-8*j-6*i)} * 6^{(2*(j*i)^2-8*j*i+2*j+i+4)};$
$\overline{\prod}_2 = 4^{(2*j^2+2*i^2+4*j*i+3*j+2*i-3)} * 6^{(4*j^2*i+4*i*j^2+4*j*i-8*j-6*i)} * 9^{(2*(j*i)^2-8*j*i+2*j+i+4)};$

```
            end
fprintf(%2d\t %2d %12d %12d %12d %22d %22d \n', i, j, F, M2, M1, ∏1, ∏2)
        end
    end
disp('----------')
```

Table 5 MATLAB illustration: » Topological_coindices_of_graphene_sheet(3,3)

n	m	$\overline{F}$	$\overline{M}_2$	$\overline{M}_1$	$\overline{\prod}_1$	$\overline{\prod}_2$
1	1	72	36	36	262144	262144
1	2	332	160	148	$4.294967e+21$	$3.829436e+22$
1	3	800	384	340	$9.119789e+48$	$1.578155e+52$
2	1	332	160	148	$1.099512e+16$	$2.279947e+16$
2	2	1168	558	476	$4.057816e+67$	$3.066407e+73$
2	3	2532	1212	996	$2.518170e+156$	$1.557022e+173$
3	1	800	383	340	$1.593799e+32$	$3.330579e+33$
3	2	2532	1211	996	$7.383353e+122$	$6.934815e+135$
3	3	5256	2523	2004	$3.208625e+277$	Inf

In Table 5 the illustration of the out put of the above MATLAB script that calculates all the studied coindices for n by m dimensional graphene sheet (in this case for 3 by 3) is presented. It shows that values of first and second multiplicative Zagreb coindices are found to be much higher (Inf) than the requirement needed for valid molecular descriptors, where as the corresponding values of F-coindex and first and second Zagreb coindices are in the suitable numerical range. This may suggest that the F-coindex and Zagreb coindices are suitable for studying the quantitative structure-property(activity) relationships.

Fig. 3 models the three degree based coindices from Theorems 2,3 and 4 of the graphene sheet (for both cases

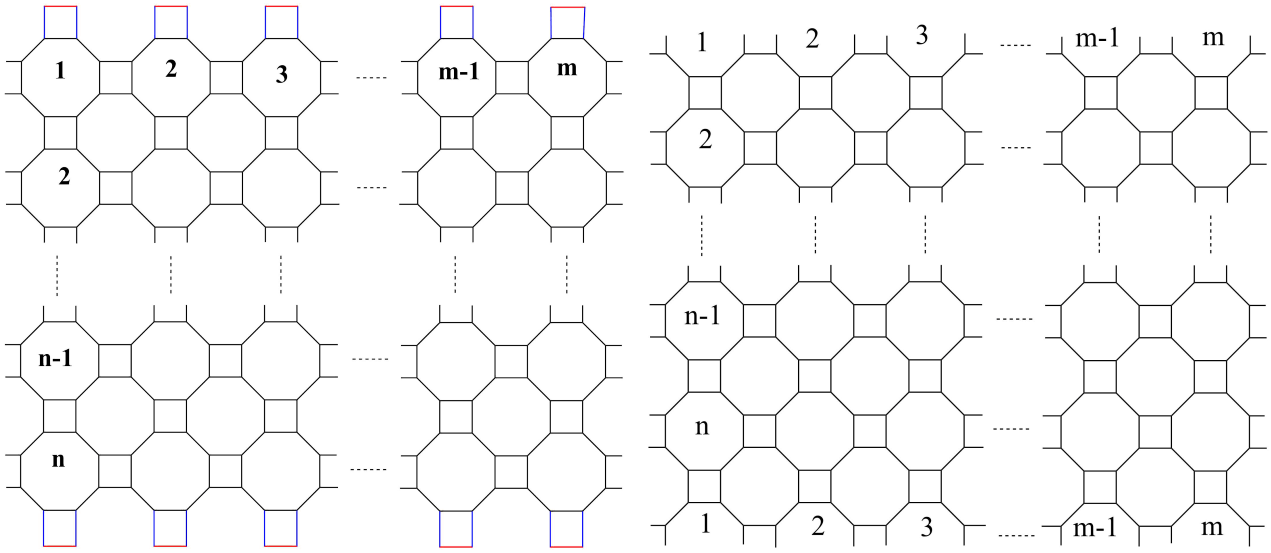


Fig. 4 Two-dimensions of $TUC_4C_8(S)[m,n]$ (a) nanotube and (b) nanotorus

considered). All the coindex values are increasing with an increasing extent of the dimensions of the graphene sheet. We can see that for both cases i.e ($n = 1$ and $n \neq 1$) of the $G(n,m)$ graphene sheet, the F-coindex is dominating over the first and second Zagreb coindices.

3.2 The $C_4C_8(S)$ nanotubes and nanotorus

Nanotube is a nanometer-scale tube like structure. The best and widely used nanotubes are carbon nanotubes (CNTs). Carbon nanotubes are the strongest and stiffest materials yet discovered in terms of tensile strength and elastic modulus, respectively. Nanotubes have interesting electrical, mechanical and thermal properties. Nanotorus is bended nanotube found to have extraordinary properties, such as very high magnetic moments and its properties vary widely as radius of the tours and radius of the tube varies [27]. A C_4C_8 net is a trivalent decoration made by alternating squares C_4 and octagons C_8. This net covers either a tube (denoted by $TUC_4C_8(S/R)$ nanotube) or a torus (denoted by $TUC_4C_8(S/R)$ nanotorus). These families of carbon structures can be derived from a square net by the leapfrog operation. [28] In recent years there has been considerable interest in the general problem of determining topological indices of nanotubes and nanotorus and many researchers are studied different degree and distance based topological indices of these and related nanostructures, for details see [29–40] and references cited there in. In Fig. 5(a) the $TUC_4C_8(S)[m,n]$ nanotube and in Fig. 5(b) the $TUC_4C_8(S)[m,n]$ nanotorus are depicted.
Let $G = TUC_4C_8(S)[m,n]$ and $H = TUC_4C_8(S)[m,n]$ be the molecular graphs of $C_4C_8(S)$ nanotube and nanotorus, in which n and m represents the number of octagons in a row and in a fixed column respectively. The order and size of G is found to be $8nm+4m$ and $12nm+4m$ respectively. We also noted that H is 3-regular graph with exactly $8mn$ vertices. The vertex and edge partitions of G are summarised in Table 6. By using

Table 6 Vertex and edge partitions of G

n_2	n_3	m_{22}	m_{23}	m_{33}
$4m$	$8nm$	$2m$	$4m$	$12nm-2m$

lemma 1 and results in Table 6, we further obtained the edge partitions $\overline{m}_{22}$, $\overline{m}_{23}$, and $\overline{m}_{33}$ of the complement

graph $\overline{G}$ with respect to the vertex degrees of G and results are presented in Table 7.

Table 7 The edge partitions $\overline{m}_{ij}$ of $\overline{G}$ based on the vertex degrees of G.

(d_u, d_v) where $uv \in E(G)$	Number of edges in $\overline{G}$
$(2,2)$	$8m^2 - 4m$
$(3,3)$	$32(mn)^2 - 16mn + 2m$
$(2,3)$	$32nm^2 - 4m$

Theorem 7. *Let G be the $TUC_4C_8(S)[m,n]\,(\forall\, m,n \geq 2)$ nanotube. Then*

(i). $\overline{F}(G) = 576(mn)^2 + 416nm^2 + 64m^2 - 288nm - 48m.$

(ii). $\overline{M}_1(G) = 192(mn)^2 + 160nm^2 + 32m^2 - 96nm - 24m.$

(iii). $\overline{M}_2(G) = 288(mn)^2 + 192nm^2 + 32m^2 - 144nm - 22m.$

(iv). $\overline{\prod}_1(G) = 4^{(8m^2-4m)} \cdot 5^{(32nm^2-4m)} \cdot 6^{(32(mn)^2-16mn+2m)}.$

(v). $\overline{\prod}_2(G) = 4^{(8m^2-4m)} \cdot 6^{(32nm^2-4m)} \cdot 9^{(32(mn)^2-16mn+2m)}.$

Proof. Let G be the $TUC_4C_8(S)[m,n]\,(\forall\, m,n \geq 2)$ nanotube. By using Theorem 1 **(i)** and Table 7 we have

$$\begin{aligned}\overline{F}(G) &= \sum_{2\leq i\leq j\leq 3} \overline{m}_{ij} \cdot (i^2 + j^2) \\ &= 8\overline{m}_{22} + 13\overline{m}_{23} + 18\overline{m}_{33} \\ &= 8(8m^2 - 4m) + 13(32nm^2 - 4m) + 18(32(mn)^2 - 16mn + 2m) \\ &= 576(mn)^2 + 416nm^2 + 64m^2 - 288nm - 48m.\end{aligned}$$

Similarly, by using Theorem 1 **(ii-v)** and results in Table 7 we can proof the remaining parts. □

Theorem 8. *Let H be the $TUC_4C_8(S)[m,n]\,(\forall\, m,n \geq 2)$ nanotorus. Then*

(i). $\overline{F}(H) = 576(nm)^2 - 288nm.$

(ii). $\overline{M}_1(H) = 192(nm)^2 - 96nm.$

(iii). $\overline{M}_2(H) = 288(nm)^2 - 144nm.$

(iv). $\overline{\prod}_1(H) = 6^{32(mn)^2-16mn}.$

(v). $\overline{\prod}_2(H) = 3^{64(mn)^2-32mn}.$

Proof. Since H is 3-regular graph of order $8mn$, we can obtained the required results by applying corrollary 1 **(i-v)**. □

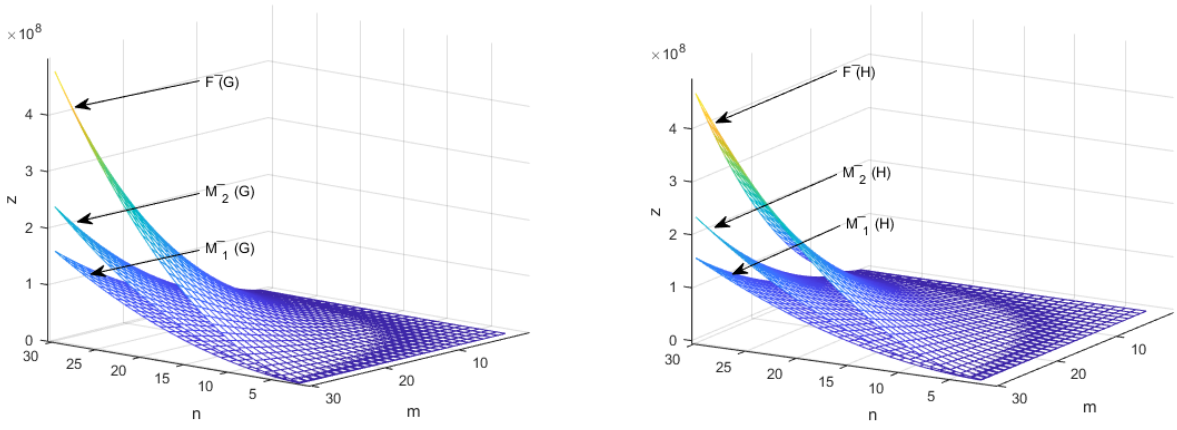
In Table 8 and Table 9, some coindex values for the formulas reported in Theorem 7 for the nanotube and Theorem 8 for the nanotorus are presented respectively. In both tables it shows that values of first and second multiplicative Zagreb coindices are found to be much higher (Inf) and hence it violates one of the basic requirements for valid molecular descriptors, where as the corresponding values of F-coindex and first and second

Table 8 Few topological coindex values of $TUC_4C_8(S)[m,n]$ nanotubes

n	m	$\overline{F}$	$\overline{M}_2$	$\overline{M}_1$	$\overline{\prod}_1$	$\overline{\prod}_2$
2	2	11552	5652	4048	Inf	Inf
2	3	26928	13182	9432	Inf	Inf
2	4	48704	23848	17056	Inf	Inf
3	2	24160	11892	8336	Inf	Inf
3	3	55728	27438	19224	Inf	Inf
3	4	100288	49384	34592	Inf	Inf
4	2	41376	20436	14160	Inf	Inf
4	3	94896	46878	32472	Inf	Inf
4	4	170304	84136	58272	Inf	Inf

Table 9 Few topological coindex values of $TUC_4C_8(S)[m,n]$ nanotorus

n	m	$\overline{F}$	$\overline{M}_2$	$\overline{M}_1$	$\overline{\prod}_1$	$\overline{\prod}_2$
2	2	8064	4032	2688	Inf	Inf
2	3	19008	9504	6336	Inf	Inf
2	4	34560	17280	11520	Inf	Inf
3	2	19008	9504	6336	Inf	Inf
3	3	44064	22032	14688	Inf	Inf
3	4	79488	39744	26496	Inf	Inf
4	2	34560	17280	11520	Inf	Inf
4	3	79488	39744	26496	Inf	Inf
4	4	142848	71424	47616	Inf	Inf



(a) (b)

Fig. 5 Comparative model for different coindices of $TUC_4C_8(S)[m,n]$ (a) nanotubes and (b) nanotorus

Zagreb coindices are in the suitable numerical range. This may suggest that the F-coindex and Zagreb coindices are suitable for studying the quantitative structure-property(activity) relationships.
In Fig. 5 (a) and (b), we present a comparative model of different coindices for $TUC_4C_8(S)[m,n]$ nanotubes and nanotorus. Accordingly, in both models all the coindex values for $\overline{F}, \overline{M}_1$ and $\overline{M}_2$ are increasing with an increasing extent of the dimensions of the structures. Here also, the F-coindex is dominating over the Zagreb coindices.

4 Conclusion

In this paper, formulae for calculating certain topological coindices of graphene sheet, and $C_4C_8(S)$ nanotubes and nanotorus are derived and the final out puts of the topology are analyzed via MATLAB. The results are very important and will have significant contribution for the advancement and understanding in the topology of these important structures. We also believe that the study will attract the attention of researchers working in the area of degree based topological indices to explore more on other molecular graphs. In all the structures considered in this study, values of first and second multiplicative Zagreb coindices are found to be much higher (Inf) which violates one of the basic requirements for valid molecular descriptors, where as the corresponding values of F-coindex and Zagreb coindices are in the suitable numerical range. Thus, in future study, it would be more interesting to investigate F-coindex and Zagreb coindices from quantitative structure-property(activity) relationships.
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