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Computation of certain topological indices for 2D nanotubes

A. Divya[1] · A. Manimaran[1]

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Abstract
Graph theory has various applications in chemistry and molecular structure research, and its importance has been growing continuously. In molecular graphs, points represent the atoms, and lines represent the chemical bonds between atoms. This article is about to show the precise evaluation for topological descriptors based on the degree sum of the neighbors of end vertices for some molecular structures. We derive for Sanskruti index, Neighborhood inverse sum index, Neighborhood Harmonic index, Fifth ND_e index, and Neighborhood second modified Zagreb index for two-dimensional lattice structure of certain Nanotube and Nanotorus.

Keywords Sanskruti index · Neighborhood inverse sum index · Neighborhood harmonic index · Fifth ND_e index · Neighborhood second modified Zagreb index · Nanotube and nanotorus

Mathematics Subject Classification 05C90

1 Introduction

Mathematical chemistry is the study of physical chemistry in that we use mathematical methods to analyze and estimate the molecular structure of a chemical compound. Chemical graph theory is a branch of chemistry that deals with graphs in which graph theory methods have been using to convert chemical phenomena into mathematical models. A topological index is a numerical value for chemical composition, and it

✉ A. Manimaran
marans2011@gmail.com

A. Divya
divyaarunachalam26@gmail.com

[1] Department of Mathematics, School of Advanced Sciences, Vellore Institute of Technology, Vellore 632014, India

correlates chemical structure with biological reaction or chemical reactivity. It is one of some chemical and physical characteristics. Molecular descriptors have been developed from a molecular graph for determining numbers to molecular graphs and then by using those numbers to describe the molecule [12].

A topological descriptor is a form of a molecular descriptor. Quantitative structure-property (QSPR) and structure-activity (QSAR) studies include topological descriptors. A nanostructure is a structure that lies halfway among molecular structures and microscopic in terms of dimension. It is a substance made possible by molecular engineering. It refers to something less than 100 nanometers in physical sizes, such as atom clusters to dimensional layers. Carbon nanotubes (CNTs) [19,22] are cylindrical carbon allotropes.

Recently Sanskruti index $S(G)$ is proposed by S.M. Hosamani [7,15,20] and it is defined by

$$S(G) = \sum_{uv \in E(G)} \left(\frac{\delta_G(u)\delta_G(v)}{\delta_G(u) + \delta_G(v) - 2} \right)^3$$

where $\delta_G(u) = \sum_{u' \in N(u)} d(u')$, $N(u) = \{u' : uu' \in E(G)\}$ and the same goes for $\delta_G(v)$.

The Neighborhood inverse sum index $NI(G)$, Neighborhood Harmonic index $NH(G)$ and Neighborhood second modified Zagreb index M_2^{nm} [15,16,23] is referred to as follows

$$NI(G) = \sum_{uv \in E(G)} \frac{\delta_G(u)\delta_G(v)}{\delta_G(u) + \delta_G(v)}$$

$$NH(G) = \sum_{uv \in E(G)} \frac{2}{\delta_G(u) + \delta_G(v)}$$

$$M_2^{nm}(G) = \sum_{uv \in E(G)} \frac{1}{\delta_G(u)\delta_G(v)}$$

where $\delta_G(u) = \sum_{uv \in E(G)} d_G(v)$ and $\delta_G(v) = \sum_{uv \in E(G)} d_G(u)$.

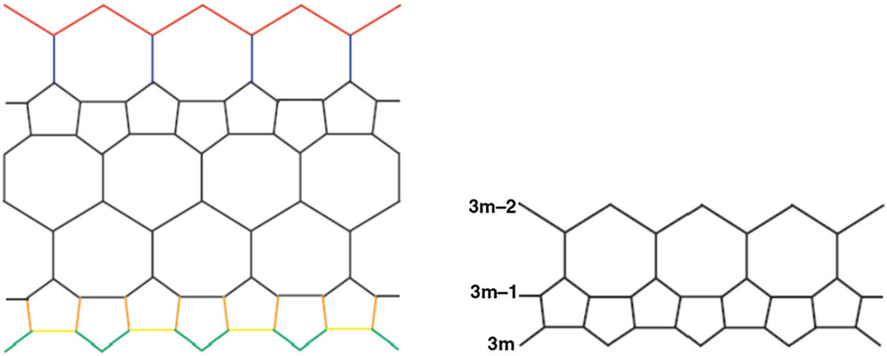
The Fifth ND_e index ND_5 [15,17] is defined as

$$ND_5(G) = \sum_{uv \in E(G)} \frac{\delta_G(u)^2 + \delta_G(v)^2}{\delta_G(u)\delta_G(v)}$$

where $\delta_G(u) = \sum_{uv \in E(G)} d_G(v)$ and $\delta_G(v) = \sum_{uv \in E(G)} d_G(u)$.

2 Applications of nanostructure

Graph theory has been commonly used to investigate the chemical and physical properties of materials over the last few decades. Chemical graph theory was proposed



(a) *The HAC_5C_7 nanotube with $p = 4$ and $q = 2$* **(b)** *The HAC_5C_7 nanotube $- m^{th}$period*

Fig. 1 $HAC_5C_7[p, q]$ nanotube

as a result of the growing interest in this area and following that, numerous topological indices were investigated and described. Chemical graph theory was also used to study nanotechnology, which is a mixture of nanoscience, mathematics, and chemistry. Quantitative structure-property relationship (QSPR) and Quantitative structure-activity relationship (QSAR) are two of these relationships that are studied to estimate nanostructure properties and biological activities. Sanskruti, Neighborhood inverse sum, Neighborhood Harmonic, Fifth ND_e, and Neighborhood second modified Zagreb index are used to estimate nanostructure bioactivity in the study of QSAR and QSPR [2,5,8,11].

3 The $HAC_5C_7[p, q]$ nanotube

A trivalent decoration has been made by combining C_5 and C_7 and is known as a C_5C_7 net. It has been using to mask both a torus and a tube. As a C_5C_7 net, the $HAC_5C_7[p, q]$ nanotube can be studied, and Fig. 1a shows an illustration. In 2007, Iranmanesh and Khormali calculated the vertex-Szeged index of HAC_5C_7 nanotube [10]. The two-dimension lattice of HAC_5C_7 has been explained consistently in [14]. In the entire lattice, the number of heptagons and periods has been represented by p and q in a row see [13]. In HAC_5C_7, there are $8pq + p$ vertices and $12pq - p$ edges, respectively [21]. The three rows of HAC_5C_7 is said to be m^{th} period, and as shown in Fig. 1b.

4 Some topological indices of $HAC_5C_7[p, q]$ nanotube, $(p, q > 1)$

The general result is determined for $HAC_5C_7[p, q]$ nanotube in this segment by above mentioned topological indices. In addition to these indices, we present a visual analogy as well as their utilization (Fig. 2).

Theorem 1 *Let G be the graph of $HAC_5C_7[p,q]$ nanotube. Then,*

1. $S(G) = 1556.956pq - 520.549p$
2. $NI(G) = 54pq - 10.773p$
3. $NH(G) = 1.333pq + 0.079p$
4. $ND_5(G) = 24pq - 1.694p$
5. $M_2^{nm}(G) = 0.148pq + 0.037p$

Proof Consider the graph of HAC_5C_7 is represented by G. The cardinality of vertex set is $8pq + p$ and the edge set is $12pq - p$ for the graph G. According to the degrees of the vertices, the vertices are divide into two groups. The collection of vertices of degree i is designated by the symbol V_i. For G, we have $|V_2| = 2p + 2$, $|V_3| = 8pq - p - 2$. The edge set is divide into the following sections corresponding to their sum of the degrees of the neighborhood, which are

$$E_1 = \{st \in E(SR_n) \mid d_u = 9 \; and \; d_v = 9\}$$
$$E_2 = \{st \in E(SR_n) \mid d_u = 9 \; and \; d_v = 8\}$$
$$E_3 = \{st \in E(SR_n) \mid d_u = 9 \; and \; d_v = 7\}$$
$$E_4 = \{st \in E(SR_n) \mid d_u = 8 \; and \; d_v = 8\}$$
$$E_5 = \{st \in E(SR_n) \mid d_u = 8 \; and \; d_v = 6\}$$
$$E_6 = \{st \in E(SR_n) \mid d_u = 7 \; and \; d_v = 6\}$$

From the graph G, we can see that | E_1 | = 12pq - 9p, | E_2 | = 2p, | E_3 | = p, | E_4 | = p, | E_5 | = 2p and | E_6 | = 2p. Then, by definition $S(G)$ index is calculated as follows by using the edge partition.

$$\begin{aligned} S(G) &= \sum_{uv \in E(G)} \left(\frac{\delta_G(u)\delta_G(v)}{\delta_G(u) + \delta_G(v) - 2} \right)^3 \\ &= (12pq - 9p)\left(\frac{9 \times 9}{9+9-2}\right)^3 + (2p)\left(\frac{9 \times 8}{9+8-2}\right)^3 \\ &+ (p)\left(\frac{9 \times 7}{9+7-2}\right)^3 + (p)\left(\frac{8 \times 8}{8+8-2}\right)^3 \\ &+ (2p)\left(\frac{8 \times 6}{8+6-2}\right)^3 + (2p)\left(\frac{7 \times 6}{7+6-2}\right)^3 \end{aligned}$$

We obtain the necessary result by reducing the above calculation,

$$S(G) = 1556.956pq - 520.549p.$$

By definition, $NI(G)$ index is calculated as follows by using the edge partition,

$$NI(G) = \sum_{uv \in E(G)} \frac{\delta_G(u)\delta_G(v)}{\delta_G(u) + \delta_G(v)}$$

$$= (12pq - 9p)\left(\frac{9\times 9}{9+9}\right) + (2p)\left(\frac{9\times 8}{9+8}\right) + (p)\left(\frac{9\times 7}{9+7}\right)$$
$$+(p)\left(\frac{8\times 8}{8+8}\right) + (2p)\left(\frac{8\times 6}{8+6}\right) + (2p)\left(\frac{7\times 6}{7+6}\right)$$

We obtain our desired outcome after simplifying the above form,

$$NI(G) = 54pq - 10.773p.$$

By definition, $NH(G)$ index is calculated as follows by using the edge partition,

$$NH(G) = \sum_{uv\in E(G)} \frac{2}{\delta_G(u) + \delta_G(v)}$$
$$= (12pq - 9p)\left(\frac{2}{9+9}\right) + (2p)\left(\frac{2}{9+8}\right) + (p)\left(\frac{2}{9+7}\right)$$
$$+ (p)\left(\frac{2}{8+8}\right) + (2p)\left(\frac{2}{8+6}\right) + (2p)\left(\frac{2}{7+6}\right)$$

We obtain the necessary result by reducing the above calculation,

$$NH(G) = 1.333pq + 0.079p.$$

By definition, $ND_5(G)$ index is calculated as follows by using the edge partition,

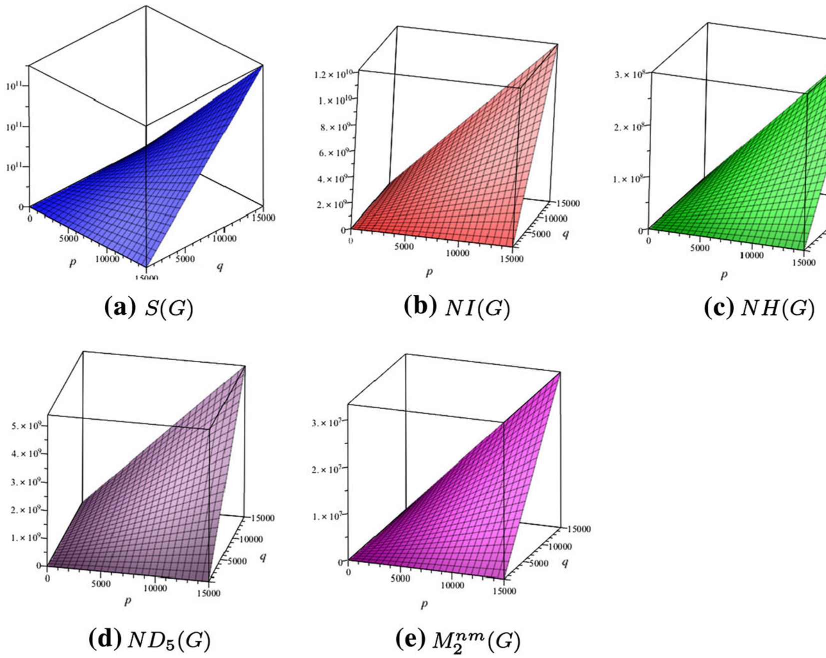
$$ND_5(G) = \sum_{uv\in E(G)} \frac{\delta_G(u)^2 + \delta_G(v)^2}{\delta_G(u)\delta_G(v)}$$
$$= (12pq - 9p)\left(\frac{9^2+9^2}{9\times 9}\right) + (2p)\left(\frac{9^2+8^2}{9\times 8}\right) + (p)\left(\frac{9^2+7^2}{9\times 7}\right)$$
$$+ (p)\left(\frac{8^2+8^2}{8\times 8}\right) + (2p)\left(\frac{8^2+6^2}{8\times 6}\right) + (2p)\left(\frac{7^2+6^2}{7\times 6}\right)$$

We obtain our desired outcome after simplifying the above form,

$$ND_5(G) = 24pq - 1.694p.$$

By definition, $M_2^{nm}(G)$ index is calculated as follows by using the edge partition,

$$M_2^{nm}(G) = \sum_{uv\in E(G)} \frac{1}{\delta_G(u)\delta_G(v)}$$
$$= (12pq - 9p)\left(\frac{1}{9\times 9}\right) + (2p)\left(\frac{1}{9\times 8}\right) + (p)\left(\frac{1}{9\times 7}\right)$$
$$+ (p)\left(\frac{1}{8\times 8}\right) + (2p)\left(\frac{1}{8\times 6}\right) + (2p)\left(\frac{1}{7\times 6}\right)$$



(a) $S(G)$ (b) $NI(G)$ (c) $NH(G)$

(d) $ND_5(G)$ (e) $M_2^{nm}(G)$

Fig. 2 Graphical representation for $HAC_5C_7[p, q]$ nanotube

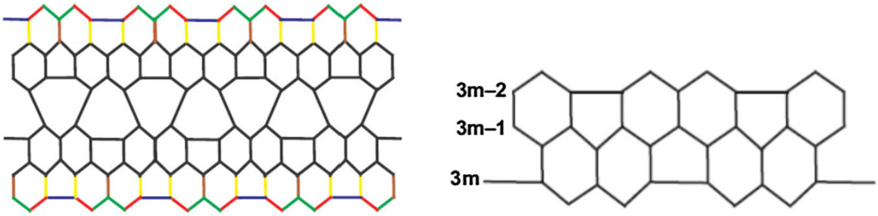
We obtain the necessary result by reducing the above calculation,

$$M_2^{nm}(G) = 0.148pq + 0.037p.$$

□

5 The $HAC_5C_6C_7[p, q]$ nanotube

A trivalent decoration has been made by combining C_5, C_6 and C_7 is known as a $C_5C_6C_7$ net see [18]. It has been using to mask a torus or a tube. As a $C_5C_6C_7$ net, the $HAC_5C_6C_7[p, q]$ nanotube can be studied, and Fig. 3a shows an illustration. The two-dimension lattice of $HAC_5C_6C_7$ has been studied consistently. In the entire lattice, the number of heptagons and periods has been represented by p and q in a row. In $HAC_5C_6C_7$, there are $8pq + p$ vertices and $12pq - p$ edges see [19]. The development of $HAC_5C_6C_7$ is discussed in [24]. The three rows of $HAC_5C_6C_7$ is said to be m^{th} period, and as shown in Fig. 3b.



(a) *The $HAC_5C_6C_7$ nanotube with $p = 4$ and $q = 2$* **(b)** *The $HAC_5C_6C_7$ nanotube – m^{th}period*

Fig. 3 $HAC_5C_6C_7[p, q]$ nanotube

6 Some topological indices of $HAC_5C_6C_7[p, q]$ nanotube, $(p, q > 1)$

The general result is determined for $HAC_5C_6C_7[p, q]$ nanotube in this segment by above mentioned topological indices. In addition to these indices, we present a visual analogy as well as their utilization (Figs. 4, 5, and 6).

Theorem 2 *Let G be the graph of $HAC_5C_6C_7[p, q]$ nanotube. Then,*

1. $S(G) = 3113.9121pq - 1063.4764p$
2. $NI(G) = 108pq - 21.955p$
3. $NH(G) = 2.667pq + 0.174p$
4. $ND_5(G) = 48pq - 3.480p$
5. $M_2^{nm}(G) = 0.296pq + 0.148p$

Proof Consider the graph of $HAC_5C_6C_7$ is represented by G. The cardinality of vertex set is $8pq + p$ and the edge set is $12pq - p$ for the graph G. The edge set is divide into the following sections corresponding to their sum of the degrees of the neighborhood, which are

$$E_1 = \{st \in E(SR_n) \mid d_u = 9 \text{ and } d_v = 9\}$$
$$E_2 = \{st \in E(SR_n) \mid d_u = 9 \text{ and } d_v = 8\}$$
$$E_3 = \{st \in E(SR_n) \mid d_u = 8 \text{ and } d_v = 8\}$$
$$E_4 = \{st \in E(SR_n) \mid d_u = 8 \text{ and } d_v = 7\}$$
$$E_5 = \{st \in E(SR_n) \mid d_u = 8 \text{ and } d_v = 6\}$$
$$E_6 = \{st \in E(SR_n) \mid d_u = 7 \text{ and } d_v = 6\}$$

From the graph G, we can see that | E_1 | = 12pq - 9p, | E_2 | = 4p, | E_3 | = 2p, | E_4 | = 2p, | E_5 | = 4p and | E_6 | = 4p. Then, by definition $S(G)$ index is calculated as follows by using the edge partition.

$$S(G) = \sum_{uv \in E(G)} \left(\frac{\delta_G(u)\delta_G(v)}{\delta_G(u) + \delta_G(v) - 2} \right)^3$$
$$= (24pq - 18p)\left(\frac{9 \times 9}{9 + 9 - 2}\right)^3 + (4p)\left(\frac{9 \times 8}{9 + 8 - 2}\right)^3$$

$$+ (2p)\left(\frac{8\times 8}{8+8-2}\right)^3 + (2p)\left(\frac{8\times 7}{8+7-2}\right)^3$$
$$+ (4p)\left(\frac{8\times 6}{8+6-2}\right)^3 + (4p)\left(\frac{7\times 6}{7+6-2}\right)^3$$

We obtain the necessary result by reducing the above calculation,

$$S(G) = 3113.9121pq - 1063.4764p.$$

By definition, $NI(G)$ index is calculated as follows by using the edge partition,

$$\begin{aligned} NI(G) &= \sum_{uv\in E(G)} \frac{\delta_G(u)\delta_G(v)}{\delta_G(u)+\delta_G(v)} \\ &= (24pq-18p)\left(\frac{9\times 9}{9+9}\right) + (4p)\left(\frac{9\times 8}{9+8}\right) + (2p)\left(\frac{8\times 8}{8+8}\right) \\ &+ (2p)\left(\frac{8\times 7}{8+7}\right) + (4p)\left(\frac{8\times 6}{8+6}\right) + (4p)\left(\frac{7\times 6}{7+6}\right) \end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$NI(G) = 108pq - 21.955p.$$

By definition, $NH(G)$ index is calculated as follows by using the edge partition,

$$\begin{aligned} NH(G) &= \sum_{uv\in E(G)} \frac{2}{\delta_G(u)+\delta_G(v)} \\ &= (24pq-18p)\left(\frac{2}{9+9}\right) + (4p)\left(\frac{2}{9+8}\right) + (2p)\left(\frac{2}{8+8}\right) \\ &+ (2p)\left(\frac{2}{8+7}\right) + (4p)\left(\frac{2}{8+6}\right) + (4p)\left(\frac{2}{7+6}\right) \end{aligned}$$

We obtain the necessary result by reducing the above calculation,

$$NH(G) = 2.667pq + 0.174p.$$

By definition, $ND_5(G)$ index is calculated as follows by using the edge partition,

$$ND_5(G) = \sum_{uv \in E(G)} \frac{\delta_G(u)^2 + \delta_G(v)^2}{\delta_G(u)\delta_G(v)}$$
$$= (24pq - 18p)\left(\frac{9^2 + 9^2}{9 \times 9}\right) + (4p)\left(\frac{9^2 + 8^2}{9 \times 8}\right) + (2p)\left(\frac{8^2 + 8^2}{8 \times 8}\right)$$
$$+ (2p)\left(\frac{8^2 + 7^2}{8 \times 7}\right) + (4p)\left(\frac{8^2 + 6^2}{8 \times 6}\right) + (4p)\left(\frac{7^2 + 6^2}{7 \times 6}\right)$$

We obtain our desired outcome after simplifying the above form,

$$ND_5(G) = 48pq - 3.480p.$$

By definition, $M_2^{nm}(G)$ index is calculated as follows by using the edge partition,

$$M_2^{nm}(G) = \sum_{uv \in E(G)} \frac{1}{\delta_G(u)\delta_G(v)}$$
$$= (24pq - 18p)\left(\frac{1}{9 \times 9}\right) + (4p)\left(\frac{1}{9 \times 8}\right) + (2p)\left(\frac{1}{8 \times 8}\right)$$
$$+ (2p)\left(\frac{1}{8 \times 7}\right) + (4p)\left(\frac{1}{8 \times 6}\right) + (4p)\left(\frac{1}{7 \times 6}\right)$$

We obtain the necessary result by reducing the above calculation,

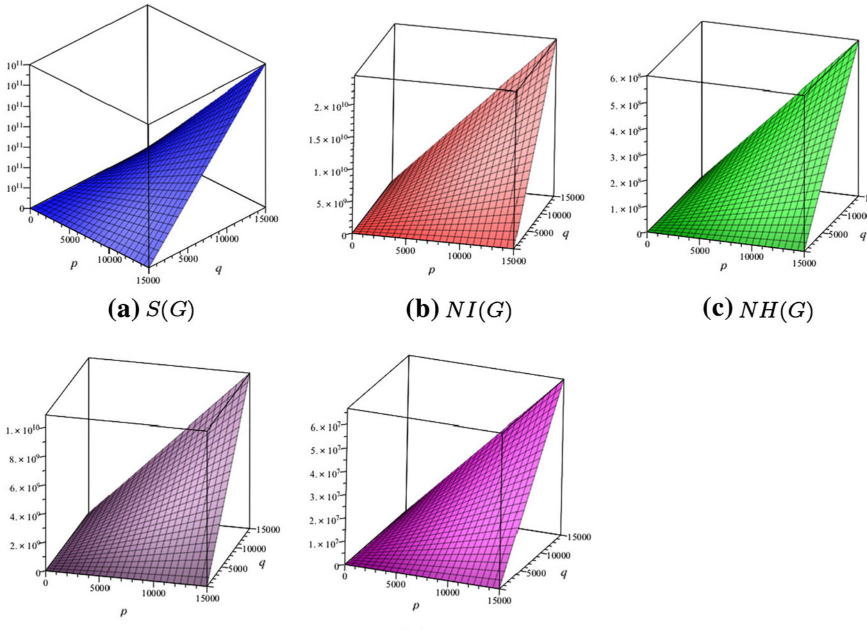
$$M_2^{nm}(G) = 0.296pq + 0.148p.$$

□

7 $TUC_4C_8[p, q]$ nanotorus and nanotube

The two-dimensional lattice and Nanotorus of $TUC_4C_8[p, q]$ has presented in Fig. 5, and we will use documentation and concept of Diudea and Graovac [19]. $GTUC[p, q]$ indicates the nanotube of $TUC_4C_8[p, q]$ see Fig. 7. The overall number of octagons in each row and column of Nanotube of $TUC_4C_8[p, q]$ is equivalent to p and q. The overall number of squares and octagons in Nanotube of $TUC_4C_8[p, q]$ is the same in each row [4,6,9]. In 2D-lattice of $TUC_4C_8[p, q]$, the overall number of octagons in each row and column is equivalent to p and q. In [1,3,19], two-dimensional lattice of $TUC_4C_8[p, q]$ nanotorus, the overall number of squares of columns and rows are (q + 1) and (p + 1).

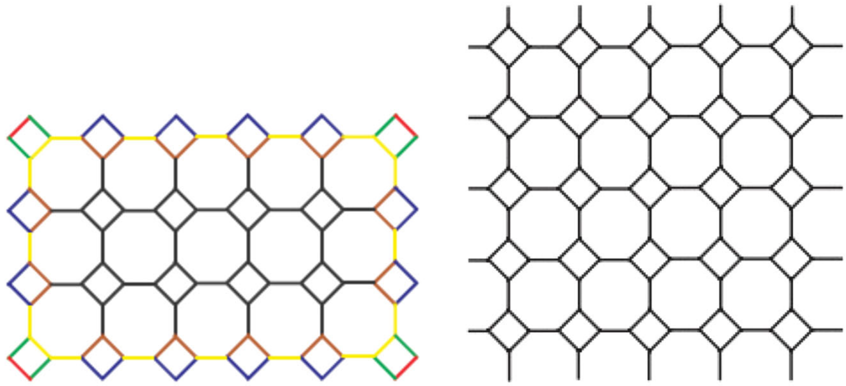
In two-dimensional lattice of $TUC_4C_8[p, q]$ nanotorus, the number of vertex set and edge set is $(4p^2 + 4p)(q + 1)$ and $6pq + 5p + 5q + 4$, similarly for $GTUC[p, q]$, vertex set and edge set is $4pq + 4p$ and $6pq + 5p$.



(a) $S(G)$ **(b)** $NI(G)$ **(c)** $NH(G)$

(d) $ND_5(G)$ **(e)** $M_2^{nm}(G)$

Fig. 4 Graphical representation for $HAC_5C_6C_7[p, q]$ nanotube



(a) $2D - lattice\ with\ p = 5\ \&\ q = 3$ **(b)** $Nanotorus\ of\ TUC_4C_8\ with\ p = 5\ \&\ q = 5$

Fig. 5 **a** 2D-lattice of $TUC_4C_8[p, q]$, **b** nanotorus of $TUC_4C_8[p, q]$

8 Some topological indices of 2D-lattice of $TUC_4C_8[p, q]$ nanotorus, $(p, q > 1)$

The general result is determined for 2D-lattice of $TUC_4C_8[p, q]$ nanotorus in this segment by above mentioned topological indices. In addition to these indices, we present a visual analogy as well as their utilization.

Theorem 3 *Let G be the graph of 2D-lattice of $TUC_4C_8[p, q]$ nanotorus. Then,*

1. $S(G) = 240.7033(p + q) + 778.4780pq + 11.1269$
2. $NI(G) = 27pq + 16.155(p + q) + 7.304$
3. $NH(G) = 0.667pq + 0.736(p + q) + 0.891$
4. $ND_5(G) = 12pq + 10.389(p + q) - 9.022$
5. $M_2^{nm}(G) = 0.074pq + 0.108(p + q) + 0.194$

Proof Consider the graph of 2D-lattice of $TUC_4C_8[p, q]$ nanotorus is represented by G. The cardinality of vertex set is $(4p^2+4p)(q+1)$ and the edge set is $6pq+5p+5q+4$ for the graph G. The edge set is divide into the following sections corresponding to their sum of the degrees of the neighborhood, which are

$$E_1 = \{st \in E(SR_n) \mid d_u = 9 \; and \; d_v = 9\}$$
$$E_2 = \{st \in E(SR_n) \mid d_u = 9 \; and \; d_v = 8\}$$
$$E_3 = \{st \in E(SR_n) \mid d_u = 8 \; and \; d_v = 8\}$$
$$E_4 = \{st \in E(SR_n) \mid d_u = 8 \; and \; d_v = 6\}$$
$$E_5 = \{st \in E(SR_n) \mid d_u = 8 \; and \; d_v = 5\}$$
$$E_6 = \{st \in E(SR_n) \mid d_u = 5 \; and \; d_v = 5\}$$

From the graph G, we can see that $\mid E_1 \mid$ = 6pq - 5p - 5q + 4, $\mid E_2 \mid$ = 4(p + q - 2), $\mid E_3 \mid$ = 2(p + q + 2), $\mid E_4 \mid$ = 4(p + q - 2), $\mid E_5 \mid$ = 8 and $\mid E_6 \mid$ = 4. Then, by definition $S(G)$ index is calculated as follows by using the edge partition,

$$\begin{aligned} S(G) = & \sum_{uv \in E(G)} \left(\frac{\delta_G(u)\delta_G(v)}{\delta_G(u) + \delta_G(v) - 2} \right)^3 \\ & = (6pq - 5p - 5q + 4)\left(\frac{9 \times 9}{9 + 9 - 2} \right)^3 + (4p + 4q - 8)\left(\frac{9 \times 8}{9 + 8 - 2} \right)^3 \\ & + (2p + 2q + 4)\left(\frac{8 \times 8}{8 + 8 - 2} \right)^3 + (4p + 4q - 8)\left(\frac{8 \times 6}{8 + 6 - 2} \right)^3 \\ & + (8)\left(\frac{8 \times 5}{8 + 5 - 2} \right)^3 + (4)\left(\frac{5 \times 5}{5 + 5 - 2} \right)^3 \end{aligned}$$

We obtain the necessary result by reducing the above calculation,

$$S(G) = 240.7033(p + q) + 778.4780pq + 11.1269.$$

By definition, $NI(G)$ index is calculated as follows by using the edge partition,

$$\begin{aligned} NI(G) = & \sum_{uv \in E(G)} \frac{\delta_G(u)\delta_G(v)}{\delta_G(u) + \delta_G(v)} \\ & = (6pq - 5p - 5q + 4)\left(\frac{9 \times 9}{9 + 9} \right) + (4p + 4q - 8)\left(\frac{9 \times 8}{9 + 8} \right) \end{aligned}$$

$$+ (2p + 2q + 4)\left(\frac{8 \times 8}{8 + 8}\right) + (4p + 4q - 8)\left(\frac{8 \times 6}{8 + 6}\right)$$
$$+ (8)\left(\frac{8 \times 5}{8 + 5}\right) + (4)\left(\frac{5 \times 5}{5 + 5}\right)$$

We obtain our desired outcome after simplifying the above form,

$$NI(G) = 27pq + 16.155(p + q) + 7.304.$$

By definition, $NH(G)$ index is calculated as follows by using the edge partition,

$$\begin{aligned} NH(G) &= \sum_{uv \in E(G)} \frac{2}{\delta_G(u) + \delta_G(v)} \\ &= (6pq - 5p - 5q + 4)\left(\frac{2}{9 + 9}\right) + (4p + 4q - 8)\left(\frac{2}{9 + 8}\right) \\ &\quad + (2p + 2q + 4)\left(\frac{2}{8 + 8}\right) + (4p + 4q - 8)\left(\frac{2}{8 + 6}\right) \\ &\quad + (8)\left(\frac{2}{8 + 5}\right) + (4)\left(\frac{2}{5 + 5}\right) \end{aligned}$$

We obtain the necessary result by reducing the above calculation,

$$NH(G) = 0.667pq + 0.736(p + q) + 0.891.$$

By definition, $ND_5(G)$ index is calculated as follows by using the edge partition,

$$\begin{aligned} ND_5(G) &= \sum_{uv \in E(G)} \frac{\delta_G(u)^2 + \delta_G(v)^2}{\delta_G(u)\delta_G(v)} \\ &= (6pq - 5p - 5q + 4)\left(\frac{9^2 + 9^2}{9 \times 9}\right) + (4p + 4q - 8)\left(\frac{9^2 + 8^2}{9 \times 8}\right) \\ &\quad + (2p + 2q + 4)\left(\frac{8^2 + 8^2}{8 \times 8}\right) + (4p + 4q - 8)\left(\frac{8^2 + 6^2}{8 \times 6}\right) \\ &\quad + (8)\left(\frac{8^2 + 5^2}{8 \times 5}\right) + (4)\left(\frac{5^2 + 5^2}{5 \times 5}\right) \end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$ND_5(G) = 12pq + 10.389(p + q) - 9.022.$$

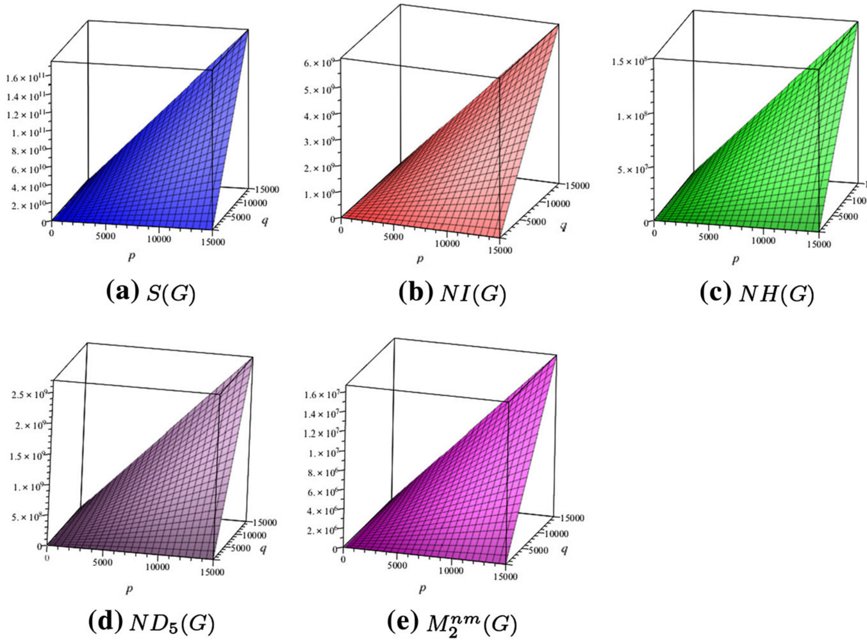


Fig. 6 Graphical representation for 2D-lattice of $TUC_4C_8[p,q]$ nanotorus

By definition, $M_2^{nm}(G)$ index is calculated as follows by using the edge partition,

$$
\begin{aligned}
M_2^{nm}(G) &= \sum_{uv\in E(G)} \frac{1}{\delta_G(u)\delta_G(v)} \\
&= (6pq-5p-5q+4)\left(\frac{1}{9\times 9}\right)+(4p+4q-8)\left(\frac{1}{9\times 8}\right) \\
&\quad +(2p+2q+4)\left(\frac{1}{8\times 8}\right)+(4p+4q-8)\left(\frac{1}{8\times 6}\right) \\
&\quad +(8)\left(\frac{1}{8\times 5}\right)+(4)\left(\frac{1}{5\times 5}\right)
\end{aligned}
$$

We obtain the necessary result by reducing the above calculation,

$$M_2^{nm}(G) = 0.074pq + 0.108(p+q) + 0.194.$$

□

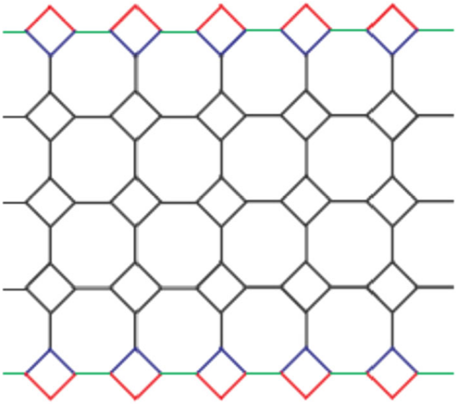


Fig. 7 $GTUC[p,q]$ nanotube with p = 5 and q = 4

9 Some topological indices of *GTUC*[*p*, *q*] nanotube, (*p*, *q* > 1)

The general result is determined for $GTUC[p,q]$ nanotube in this segment by above mentioned topological indices. In addition to these indices, we present a visual analogy as well as their utilization.

Theorem 4 *Let G be the graph of* $GTUC[p,q]$ *nanotube. Then,*

1. $S(G) = 778.4780pq + 240.70p$
2. $NI(G) = 27pq + 16.155p$
3. $NH(G) = 0.667pq + 0.736p$
4. $ND_5(G) = 12pq + 10.389p$
5. $M_2^{nm}(G) = 0.074pq + 0.108p$

Proof Consider the graph of $GTUC$ is represented by G. The cardinality of vertex set is $4pq + 4p$ and the edge set is $6pq + 5p$ for the graph G. The edge set is divide into the following sections corresponding to their sum of the degrees of the neighborhood, which are

$$E_1 = \{st \in E(SR_n) \mid d_u = 9 \; and \; d_v = 9\}$$
$$E_2 = \{st \in E(SR_n) \mid d_u = 9 \; and \; d_v = 8\}$$
$$E_3 = \{st \in E(SR_n) \mid d_u = 8 \; and \; d_v = 8\}$$
$$E_4 = \{st \in E(SR_n) \mid d_u = 8 \; and \; d_v = 6\}$$

From the graph G, we can see that $\mid E_1 \mid$ = 6pq - 5p, $\mid E_2 \mid$ = 4p, $\mid E_3 \mid$ = 2p, $\mid E_4 \mid$ = 4p. Then, by definition $S(G)$ index is calculated as follows by using the edge partition,

$$S(G) = \sum_{uv \in E(G)} \left(\frac{\delta_G(u)\delta_G(v)}{\delta_G(u) + \delta_G(v) - 2} \right)^3$$
$$= (6pq - 5p)\left(\frac{9 \times 9}{9 + 9 - 2}\right)^3 + (4p)\left(\frac{9 \times 8}{9 + 8 - 2}\right)^3$$

$$+ (2p)\left(\frac{8 \times 8}{8+8-2}\right)^3 + (4p)\left(\frac{8 \times 6}{8+6-2}\right)^3$$

We obtain the necessary result by reducing the above calculation,

$$S(G) = 778.4780pq + 240.70p.$$

By definition, $NI(G)$ index is calculated as follows by using the edge partition,

$$\begin{aligned} NI(G) &= \sum_{uv \in E(G)} \frac{\delta_G(u)\delta_G(v)}{\delta_G(u)+\delta_G(v)} \\ &= (6pq-5p)\left(\frac{9 \times 9}{9+9}\right) + (4p)\left(\frac{9 \times 8}{9+8}\right) \\ &\quad + (2p)\left(\frac{8 \times 8}{8+8}\right) + (4p)\left(\frac{8 \times 6}{8+6}\right) \end{aligned}$$

We obtain our desired outcome after simplifying the above form,

$$NI(G) = 27pq + 16.155p.$$

By definition, $NH(G)$ index is calculated as follows by using the edge partition,

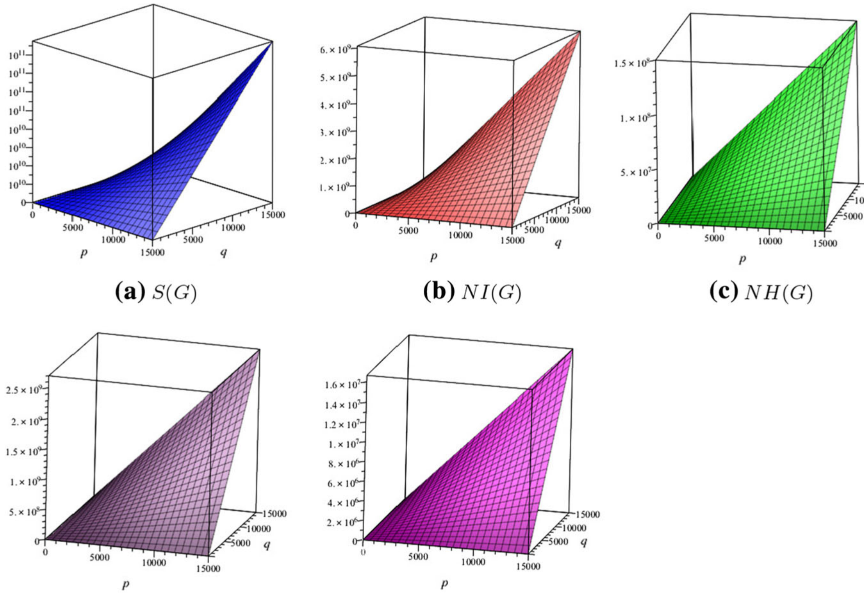
$$\begin{aligned} NH(G) &= \sum_{uv \in E(G)} \frac{2}{\delta_G(u)+\delta_G(v)} \\ &= (6pq-5p)\left(\frac{2}{9+9}\right) + (4p)\left(\frac{2}{9+8}\right) \\ &\quad + (2p)\left(\frac{2}{8+8}\right) + (4p)\left(\frac{2}{8+6}\right) \end{aligned}$$

We obtain the necessary result by reducing the above calculation,

$$NH(G) = 0.667pq + 0.736p.$$

By definition, $ND_5(G)$ index is calculated as follows by using the edge partition,

$$\begin{aligned} ND_5(G) &= \sum_{uv \in E(G)} \frac{\delta_G(u)^2+\delta_G(v)^2}{\delta_G(u)\delta_G(v)} \\ &= (6pq-5p)\left(\frac{9^2+9^2}{9 \times 9}\right) + (4p)\left(\frac{9^2+8^2}{9 \times 8}\right) \\ &\quad + (2p)\left(\frac{8^2+8^2}{8 \times 8}\right) + (4p)\left(\frac{8^2+6^2}{8 \times 6}\right) \end{aligned}$$



(a) $S(G)$ **(b)** $NI(G)$ **(c)** $NH(G)$

(d) $ND_5(G)$ **(e)** $M_2^{nm}(G)$

Fig. 8 Graphical representation for $GTUC[p, q]$ nanotube

We obtain our desired outcome after simplifying the above form,

$$ND_5(G) = 12pq + 10.389p.$$

By definition, $M_2^{nm}(G)$ index is calculated as follows by using the edge partition,

$$\begin{aligned} M_2^{nm}(G) &= \sum_{uv \in E(G)} \frac{1}{\delta_G(u)\delta_G(v)} \\ &= (6pq - 5p)\left(\frac{1}{9 \times 9}\right) + (4p)\left(\frac{1}{9 \times 8}\right) \\ &\quad + (2p)\left(\frac{1}{8 \times 8}\right) + (4p)\left(\frac{1}{8 \times 6}\right) \end{aligned}$$

We obtain the necessary result by reducing the above calculation,

$$M_2^{nm}(G) = 0.074pq + 0.108p.$$

□

Table 1 Comparison table for HAC_5C_7[p,q] nanotube

$[p, q]$	S	NI	NH	ND_5	M_2^{nm}
[1,1]	1036.4	43.23	1.41	22.30	0.19
[2,2]	5186.7	194.45	5.49	92.61	0.67
[3,3]	12,451	453.68	12.24	210.92	1.45
[4,4]	22,829	820.90	21.65	377.22	2.52
[5,5]	36,321	1296.13	33.73	591.53	3.89
[6,6]	52,927	1879.36	48.47	853.83	5.56

Table 2 Comparison table for $HAC_5C_6C_7$[p,q] nanotube

$[p, q]$	S	NI	NH	ND_5	M_2^{nm}
[1,1]	2050.4	86.05	2.84	44.52	0.38
[2,2]	10,329	388.09	11.01	185.04	1.34
[3,3]	24,835	906.14	24.52	421.56	2.90
[4,4]	45,569	1640.2	43.36	754.08	5.06
[5,5]	72,530	2590.2	67.54	1182.6	7.80
[6,6]	10,572	3756.3	97.04	1707.1	11.14

Table 3 Comparison table for 2D-lattice of $TUC_4C_8[p, q]$ nanotorus

$[p, q]$	S	NI	NH	ND_5	M_2^{nm}
[1,1]	1271	66.62	7.13	41.80	0.49
[2,2]	4087.9	179.93	10.60	98.58	0.92
[3,3]	8461.6	347.24	15.41	179.36	1.51
[4,4]	14,392	568.55	21.55	284.13	2.25
[5,5]	21,880	843.86	29.03	412.91	3.13
[6,6]	30,925	1173.2	37.83	565.69	4.16

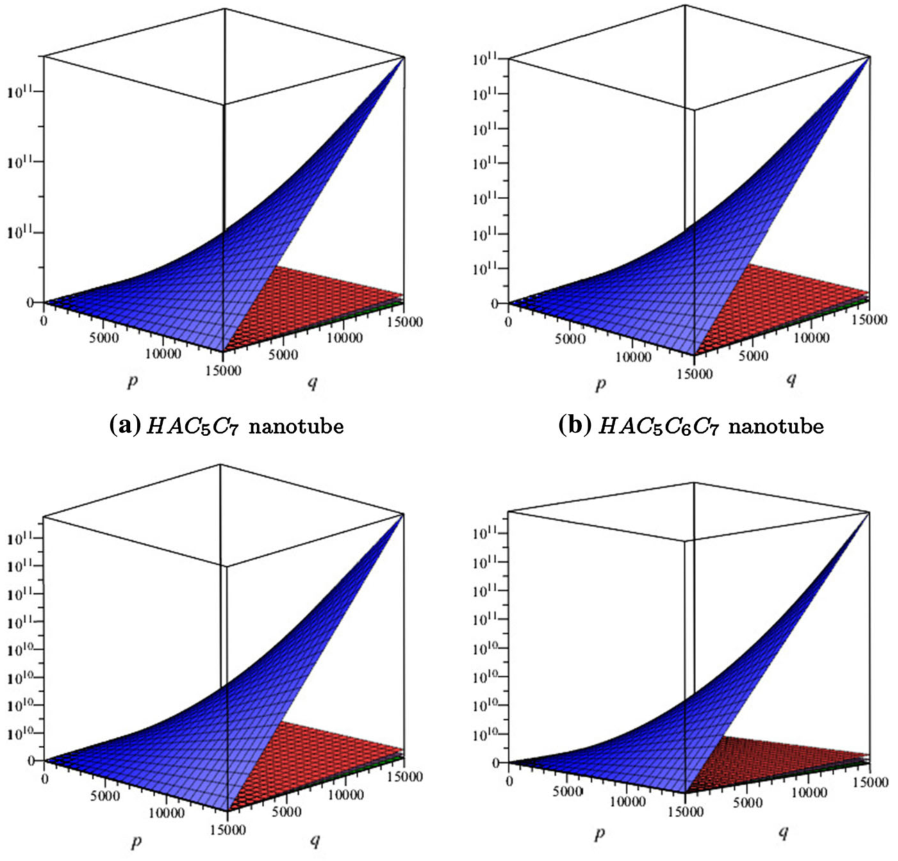
10 Graphical comparison and discussion

For the Nanotubes and Nanotorus HAC_5C_7, $HAC_5C_6C_7$, 2D-lattice of $TUC_4C_8[p, q]$ nanotorus, and $GTUC$, we have calculated mentioned topological indices for some various p and q values. We also create the following tables for small p and q values for these topological indices to HAC_5C_7, $HAC_5C_6C_7$, 2D-lattice of TUC_4C_8, and $GTUC$, respectively. Tables 1, 2, 3, and 4 show that as the values of p and q increase, the value of all the indices increases correspondingly.

The graphical representations of topological indices using the following tables for HAC_5C_7, $HAC_5C_6C_7$, 2D-lattice of TUC_4C_8 nanotorus, and $GTUC$ are shown in Figs. 2, 4, 6, and 8 for various p and q values. The comparison graphs for the 2D-lattice structure of certain nanotube and nanotorus are presented in Fig. 9 using the following tables. All the topological indices are highlighted individually in the graphs. In this paper, we derive close formulae for all topological indices, and graphically it is shown that the Sanskruti index is more rapid than all other indices.

Table 4 Comparison table for $GTUC[p, q]$ nanotube

$[p, q]$	S	NI	NH	ND_5	M_2^{nm}
[1,1]	1019.2	43.16	1.40	22.39	0.18
[2,2]	3595.3	140.31	4.14	68.78	0.51
[3,3]	7728.4	291.47	8.20	139.17	0.99
[4,4]	13418	496.62	13.61	233.56	1.62
[5,5]	20,665	755.78	20.35	351.94	2.39
[6,6]	29,469	1068.9	28.42	494.33	3.32



(a) HAC_5C_7 nanotube

(b) $HAC_5C_6C_7$ nanotube

(c) 2D-lattice TUC_4C_8 nanotorus

(d) $GTUC$ nanotube

Fig. 9 Comparison graphs of topological indices are presented for the 2D-lattice structure and individually highlighted for indices using blue, red, green, violet, and purple, respectively (color figure online)

11 Conclusion

In this paper, we have estimated the Sanskruti index, the Neighborhood inverse sum index, the Neighborhood Harmonic index, the Fifth ND_e index and the Neighborhood second modified Zagreb index for two dimensional lattice structure of certain Nanotube and Nanotorus.

Declarations

Conflict of interest The authors declare that there is no conflict of interest.

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