Hindawi
Journal of Mathematics
Volume 2024, Article ID 7521699, 12 pages
https://doi.org/10.1155/2024/7521699

Research Article

Mathematical Concepts and Empirical Study of Neighborhood Irregular Topological Indices of Nanostructures TUC_4C_8 $[p, q]$ and GTUC $[p, q]$

Shahid Zaman,[1] **Asad Ullah**,[2] **Rabia Naseer**,[1] **and Kavi Bahri Rasool**[3]

[1]Department of Mathematics, University of Sialkot, Sialkot 51310, Pakistan
[2]Department of Mathematical Sciences, Karakoram International University Gilgit-Baltistan, Gilgit 15100, Pakistan
[3]Faculty of Science, University of Zakho, Duhok, Kurdistan Region, Iraq

Correspondence should be addressed to Asad Ullah; dr.asadullah@kiu.edu.pk

Received 29 May 2023; Revised 3 September 2023; Accepted 6 December 2023; Published 29 January 2024

Academic Editor: Ram Jiwari

A topological index is a structural descriptor of any molecule/nanostructure that characterizes its topology. In the QSAR and QSPR research, topological indices are employed to predict the physical characteristics associated with bioactivities and chemical reactivity within specific networks. 2D nanostructured materials have many exhibit numerous chemical, mechanical, and physical features. These nanomaterials are exceptionally thin, displaying high chemical functionality and anisotropy. For applications necessitating robust surface interactions on a small scale, 2D materials stand out as the optimal choice due to their expansive surface area and status as the thinnest among all discovered materials. This paper characterized the neighborhood irregular topological invariants of nanostructures $TUC_4C_8[p, q]$ and $GTUC[p, q]$ and derived closed form expressions for them. A comparative analysis is then performed on the basis of these computed indices.

1. Introduction

Carbon nanotubes (CNTs), cylindrical molecules composed of rolled-up sheets of single-layer carbon atoms (graphene), come in two main types: single-walled and multiwalled. Single-walled nanotubes have a diameter of less than one nanometer (nm), while multiwalled nanotubes exceed one hundred nm and consist of multiple concentrically interconnected nanotubes. The discovery of multiwalled carbon nanotubes took place in 1991 by Sumio Iijima, [1]. Chemically, sp^2 bonds–a very potent type of molecular interaction–bind CNTs together. Since the direction in which the graphene layers roll up determines the electrical properties of a material, these nanotubes also inherit those characteristics. Furthermore, carbon nanotubes (CNTs) exhibit distinctive mechanical and thermal properties, including but not limited to lightweight composition, high tensile strength, low density, superior thermal conductivity, high aspect ratio, and exceptional chemical stability. Since CNTs are the ideal choices for electron field emitters, transistors, cathode ray tubes (CRTs), electronic devices, and transistors, all of these qualities make them intriguing for the development of new materials. Modeling and characterizing these carbon nanotubes (CNTs) is essential for gaining a deeper understanding of their structural topology and enhancing their physical characteristics. This becomes particularly crucial given their diverse range of applications and significance.

Mathematical chemistry involves the study of chemical structures using mathematical methods and approaches. Chemical graph theory is a discipline of chemistry that transforms chemical occurrences into mathematical models using graph theory ideas. Atoms and chemical bonds are depicted as the vertices and edges, respectively, in the straightforward linked graph often termed the chemical graph. Using the graph G and edge set E, it is possible to create a connected graph with an order of $n = |V(G)|$ and a size of $m = |E(G)|$. Research in the field of nanotechnology primarily centers on atoms and molecules. A 2D lattice is formed through the Cartesian product of a path graph with dimensions m and n.

The topological index is a class of molecular structure descriptors whose final product is based on a chemical compound's structure. In biology, as well as in the pharmaceutical and medical industries, the QSAR is a method linking biological structure and activity to specific molecular properties and is extensively employed [2, 3]. Because of its unique application in chemical sciences, carbon nanotubes play a fascinating role in the scientific community. The chemical graphic theory has a vital role in many topological indicators.

The Zagreb indices, Zagreb polynomials of some nanostar dendrimers, are obtained in [4], and an edge irregularity strength of graphs is characterized in [5]. The assembly of certain bioconjugate networks and their structural modeling through irregularity topological indices is presented in [6]. The article [7] delves into the quantitative structure-property relationship (QSPR) analysis of novel drugs employed in blood cancer treatment, utilizing degree-based topological indices and regression models. Investigating rational curve fitting between topological indices and entropy measures for graphite carbon nitride is the focus of [8]. The computation of degree-based topological indices for porphyrazine and tetrakis porphyrazine is conducted in [9].

The Albertson index (AL) [10], created by Albertson, is a degree-based index that is constructed as $AL(G) = \sum_{uv\in E}|d_u - d_v|$, and Vukicevic and Gasparov defined the irregularity index [11] as $IR(G) = \sum_{uv\in E}|\ln d_u - \ln d_v|$. Abdoo et al. defined the total irregularity index (IRRT) [12] as $IRRT(G) = (1/2)\sum_{uv\in E}|d_u - d_v|$. Gutman presented the IRF(G) irregularity index [13] as $IRF(G) = \sum_{uv\in E}(d_u - d_v)^2$. The Randić index (Li and Gutman) [14] is defined as $IRA(G) = \sum_{uv\in E}(d_u^{(-1/2)} - d_v^{(-1/2)})^2$. In 2018, Reti et al. [15] introduced the following irregularity topological indices: $IRDIF(G) = \sum_{uv\in E}|(d_u/d_v) - (d_v/d_u)|$, $IRLF(G) = \sum_{uv\in E}(|d_u - d_v|/\sqrt{d_u d_v})$, $LA(G) = 2\sum_{uv\in E}(|d_u - d_v|/(d_u + d_v))$, and $IRDI(G) = \sum_{uv\in E}\ln\{1 + |d_u - d_v|\}$. Chu et al. Abid have defined the IRGA(G) in [16] as $IRGA(G) = \sum_{uv\in E}\ln(d_u + d_v/2\sqrt{d_u d_v})$. The bond-additive index was described in [17] as $IRA(G) = \sum_{uv\in E}(d_u^{(1/2)} - d_v^{(1/2)})^2$. Very recently, Ullah et al. [18] introduced the concept of neighborhood version of irregularity topological indices. Motivated by [18], we have computed the neighborhood-based irregularity topological indices for the nanostructures $TUC_4C_8[p,q]$ and $GTUC[p,q]$. The list of those indices is given in Table 1.

There have been numerous attempts to look into the TI for different nanotubes and nanosheets in the literature. Pentaheptagonal nanosheets and $TURC_4C_8(S)$ are both explored for their topological invariants [19, 20]. The TI of nanotubes and nanotori of the V-phenylenic type have been studied in [21], and armchair polyhex type nanotubes in [22]. However, despite all of these studies, the nanostructure topology is still not fully understood. In this study, we have formulated closed expressions for key neighborhood irregular topological indices pertaining to the nanostructures $TUC_4C_8[p,q]$ and $GTCU[p,q]$, and a comparative analysis is also performed.

Table 1: The notations and formulas of various topological indices [18].

Notation	Formula
$N_{AL}(G)$	$\sum_{uv\in E}\lvert\delta_u - \delta_v\rvert$
$N_{IRL}(G)$	$\sum_{uv\in E}\lvert\ln\delta_u - \ln\delta_v\rvert$
$N_{IRRL}(G)$	$(1/2)\sum_{uv\in E}\lvert\delta_u - \delta_v\rvert$
$N_{IRF}(G)$	$\sum_{uv\in E}(\delta_u - \delta_v)^2$
$N_{IRA}(G)$	$\sum_{uv\in E}(\delta_u^{(-1/2)} - \delta_v^{(-1/2)})^2$
$N_{IRDIF}(G)$	$\sum_{uv\in E}\lvert(\delta_u/\delta_v) - (\delta_v/\delta_u)\rvert$
$N_{IRLF}(G)$	$\sum_{uv\in E}(\lvert\delta_u - \delta_v\rvert/\sqrt{\delta_u\delta_v})$
$N_{LA}(G)$	$2\sum_{uv\in E}(\lvert\delta_u - \delta_v\rvert/(\delta_u + \delta_v))$
$N_{IRDI}G)$	$\sum_{uv\in E}\ln\{1 + \lvert\delta_u - \delta_v\rvert\}$
$N_{IRGA}(G)$	$\sum_{uv\in E}\ln(\delta_u + \delta_v/2\sqrt{\delta_u\delta_v})$
$N_{IRB}(G)$	$\sum_{uv\in E}(\delta_u^{(1/2)} - \delta_v^{(1/2)})^2$

2. $TUC_4C_8[p,q]$ Nanotorus and Nanotube

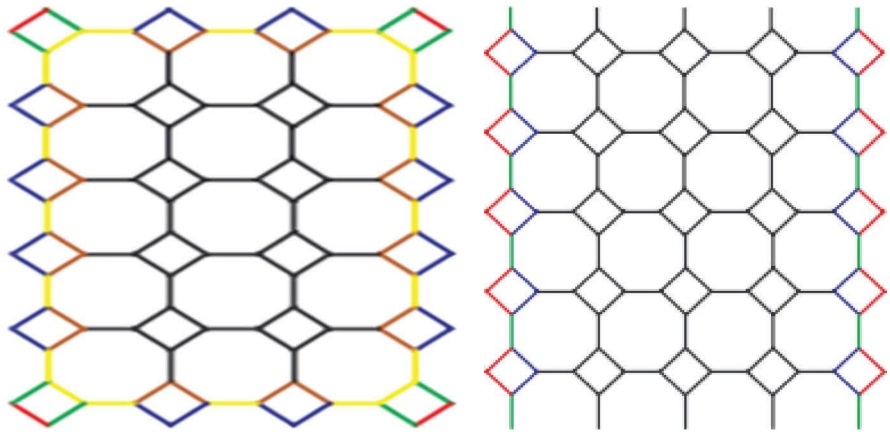
In this section, we first presented the structure of $TUC_4C_8[p,q]$. The number of octagons in row and column of nanostructure $TUC_4C_8[p,q]$ is q and p, respectively. In the $TUC_4C_8[p,q]$ nanostructure, $[p,q]$, the total number of squares and octagons is the same in each column. In 2D lattice of $TUC_4C_8[p,q]$, the total number of octagon in column and row is, respectively, p and q. In the 2D lattice of $TUC_4C_8[p,q]$, the total number of squares in a row and column are $(q+1)$ and $(p+1)$.

The number of vertices and edges of Figures 1(a) and 1(b) are $(4q^2 + 4q)(p+1)$ and $6pq + 5q + 5p + 4$, respectively. In Table 2, we have shown the edge partition of $TUC_4C_8[p,q]$. Correspondingly, for $GTUC[p,q]$, vertex set and edge set remain $4pq + 4q$ and $6pq + 5q$.

Theorem 1. *Let $G \in TUC_4C_8[p,q]$ nanotorus. Then, one has $N_{AL}(G) = 12p + 12q$.*

Proof. By definition

$$\begin{aligned}
N_{AL}(G) &= \sum_{uv\in E}\lvert\delta_u - \delta_v\rvert \\
&= (6pq - 5p - 5q + 4)\lvert 9-9\rvert + 4(p+q-2)\lvert 9-8\rvert + 2(p+q+2)\lvert 8-8\rvert + 4\lvert 8-6\rvert(p+q-2) + 8(8-5) + 4(5-5) \\
&= 4(p+q-2) + 4(2)(p+q-2) + 3(8) + 4(0) \\
&= 12p + 12q.
\end{aligned} \tag{1}$$



(a) (b)

Figure 1: The $TUC_4C_8[p, q]$ with (a) $q = 5$ and $p = 3$ and (b) $q = 5$ and $p = 5$.

Table 2: The neighborhood edge partitions of $TUC_4C_8[p, q]$.

(δ_u, δ_v)	F
(9, 9)	$6pq - 5p - 5q + 4$
(9, 8)	$4(p + q - 2)$
(8, 8)	$2(p + q + 2)$
(8, 6)	$4(p + q - 2)$
(8, 5)	8
(5, 5)	4

Theorem 2. *Let $G \in TUC_4C_8[p, q]$ nanotorus. Then, one has*

$$N_{\mathrm{IRL}}(G) = 1.62186p + 1.62186q + 0.5163088. \tag{2}$$

Proof. By definition

$$\begin{aligned} N_{\mathrm{IRL}}(G) &= \sum_{uv\epsilon E} |\ln\delta_u - \ln\delta_v| \\ &= (6\mathrm{pq} - 5p - 5q + 4)(\ln 9 - \ln 9) + 4(p + q - 2)(\ln 9 - \ln 8) + 2(p + q + 2)(\ln 8 - \ln 8) \\ &\quad + 4(p + q - 2)(\ln 8 - \ln 6) + 8(\ln 8 - \ln 5) + 4(\ln 5 - \ln 5) \\ &= (4p + 4q - 8)(0.117783) + (4p + 4q - 8)(0.287682) + 8(0.4700036) \\ &= 0.471132p + 0.4771132q - 0.942264 + 1.1507728p + 1.150728q - 2.301456 + 3.7600288 \\ N_{\mathrm{IRL}}(G) &= 1.62186p + 1.62186q + 0.5163088. \end{aligned} \tag{3}$$

□

Theorem 3. *Let $G \in TUC_4C_8[p, q]$ nanotorus. Then, one has $N_{IRRL}(G) = 6p + 6q$.*

Proof. By definition

$$\begin{aligned}
N_{\mathrm{IRRL}}(G) &= \frac{1}{2}\sum_{\mathrm{uv}\epsilon E}\left|\delta_u - \delta_v\right| \\
&= (6\mathrm{pq} - 5p - 5q + 4)\frac{1}{2}|9-9| + 4(p+q-2)\frac{1}{2}|9-8| + 2(p+q+2)\frac{1}{2}|8-8| \\
&\quad + 4(p+q-2)\frac{1}{2}|8-6| + 8\frac{1}{2}|8-5| + 4\frac{1}{2}|5-5| \\
&= 2(p+q-2)(1) + 2(p+q-2)(2) + 4(3) \\
&= 2p + 2q - 4 + 4p + 4q - 8 + 12 \\
N_{\mathrm{IRRL}}(G) &= 6p + 6q.
\end{aligned} \tag{4}$$

□

Theorem 4. *Let $G \in TUC_4C_8[p,q]$ nanotorus. Then, one has $N_{IRF}(G) = 20p + 20q + 32$.*

Proof. By definition

$$\begin{aligned}
N_{\mathrm{IRF}}(G) &= \sum_{\mathrm{uv}\epsilon E}\left(\delta_u - \delta_v\right)^2 \\
&= (6\mathrm{pq} - 5p - 5q + 4)(9-9)^2 + 4(p+q-2)(9-8)^2 + 2(p+q+2)(8-8)^2 \\
&\quad + 4(p+q-2)(8-6)^2 + 8(8-5)^2 + 4(5-5)^2 \\
&= 4\mathrm{p} + 4q - 8 + 16p + 16q - 32 + 72 \\
N_{\mathrm{IRF}}(G) &= 20p + 20q + 32.
\end{aligned} \tag{5}$$

□

Theorem 5. *Let $G \in TUC_4C_8[p,q]$ nanotorus. Then, one has*

$$N_{\mathrm{IRA}}(G) = 0.013607344p + 0.013607344q + 0.0429636. \tag{6}$$

Proof. By definition

$$\begin{aligned}
N_{\mathrm{IRA}}(G) &= \sum_{\mathrm{uv}\epsilon E}\left(\delta_u^{(-1/2)} - \delta_v^{(-1/2)}\right)^2 \\
&= 4(p+q-2)\left(9^{(-1/2)} - 8^{(-1/2)}\right)^2 + 4(p+q-2)\left(8^{(-1/2)} - 6^{(-1/2)}\right)^2 + 8\left(8^{(-1/2)} - 5^{(-1/2)}\right)^2 \\
&= 4(p+q-2)(0.33333 - 0.353553)^2 + 4(p+q-2)(0.353553 - 0.408249)^2 + 8(0.353553 - 0.4472135)^2 \\
&= 4(p+q-2)(0.0004101840) + 4(p+q-2)(0.002991652) + 8(0.0087722) \\
&= 0.001640736p + 0.001640736q - 0.003281472 + 0.011966608p + 0.011966608q - 0.023933216 + 0.0701783 \\
N_{\mathrm{IRA}}(G) &= 0.013607344p + 0.013607344q + 0.0429636.
\end{aligned} \tag{7}$$

□

Theorem 6. *Let $G \in TUC_4C_8[p,q]$ nanotorus. Then, one has*

$$N_{\text{IRDIF}}(G) = 3.27774p + 3.27774q + 1.24448. \quad (8)$$

Proof. By definition

$$\begin{aligned} N_{\text{IRDIF}}(G) &= \sum_{uv\epsilon E}\left|\frac{\delta_u}{\delta_v} - \frac{\delta_v}{\delta_u}\right| \\ &= (6\text{pq} - 5p - 5q + 4)\left(\frac{9}{9} - \frac{9}{9}\right) + 4(p + q - 2)\left(\frac{9}{8} - \frac{8}{9}\right) + 2(p + q - 2)\left(\frac{8}{8} - \frac{8}{8}\right) \\ &\quad + 4(p + q - 2)\left(\frac{8}{6} - \frac{6}{8}\right) + 8\left(\frac{8}{5} - \frac{5}{8}\right) + 4\left(\frac{5}{5} - \frac{5}{5}\right) \\ &= 4(p + q - 2)(1.125 - 0.88889) + 4(p + q - 2)(1.3333 - 0.75) + 8(1.6 - 0.625) \\ &= 0.94444p + 0.94444q - 1.88888 + 2.333332p + 2.33332q - 4.66664 + 7.8 \\ N_{\text{IRDIF}}(G) &= 3.27774p + 3.27774q + 1.24448. \end{aligned} \quad (9)$$

□

Theorem 7. *Let* $G \in TUC_4C_8[\text{p}, q]$ *nanotorus. Then, one has*

$$N_{\text{IRLF}}(G) = 1.62611045p + 1.62611045q + 0.5425231. \quad (10)$$

Proof. By definition

$$\begin{aligned} N_{\text{IRLF}}(G) &= \sum_{uv\epsilon E}\frac{|\delta_u - \delta_v|}{\sqrt{\delta_u\delta_v}} \\ &= (6\text{pq} - 5p - 5q + 4)\frac{|9 - 9|}{\sqrt{9\times 9}} + 4(p + q - 2)\frac{|9 - 8|}{\sqrt{9\times 8}} + 2(p + q + 2)\frac{|8 - 8|}{\sqrt{8\times 8}} \\ &\quad + 4(p + q - 2)\frac{|8 - 6|}{\sqrt{8\times 6}} + 8\frac{|8 - 5|}{\sqrt{8\times 5}} + 4\frac{|5 - 5|}{\sqrt{5\times 5}} \\ &= 4(p + q - 2)\frac{1}{\sqrt{72}} + 4(p + q - 2)\frac{2}{\sqrt{48}} + 8\frac{3}{\sqrt{40}} \\ &= 0.471404p + 0.471404q - 0.9428090 + 1.1547005p + 1.154700538q - 2.3094010 + 3.7947331 \\ N_{\text{IRLF}}(G) &= 1.62611045p + 1.62611045q + 0.5425231. \end{aligned} \quad (11)$$

Based on the proof of Theorem 7, it is easy to calculate the following result. □

Corollary 8. *Let* $G \in TUC_4C_8[p, q]$ *nanotorus. Then, one has*

$$N_{\mathrm{LA}}(G) = 1.61344537p + 1.61344537q + 0.46541694. \tag{12}$$

Proof. By definition

$$\begin{aligned} N_{\mathrm{LA}}(G) &= 2\sum_{uv\epsilon E}\frac{|\delta_u-\delta_v|}{(\delta_u+\delta_v)} \\ &= (6pq-5p-5q+4)2\frac{|9-9|}{(9+9)}+4(p+q-2)2\frac{|9-8|}{(9+8)}+2(p+q+2)2\frac{|8-8|}{(8+8)} \\ &\quad +4(p+q-2)2\frac{|8-6|}{(8+6)}+8(2)\frac{|8-5|}{(8+5)}+4(2)\frac{|5-5|}{(5+5)} \\ &= 0.47058823p+0.47058823q-0.94117647+1.14285714p+1.14285714q-2.28571428+3.69230769 \\ N_{LA}(G) &= 1.61344537p+1.61344537q+0.46541694. \end{aligned} \tag{13}$$

□

Theorem 9. *Let $G \in TUC_4C_8[p,q]$ nanotorus. Then, one has*

$$N_{\mathrm{IRDI}}G) = 7.167036p + 7.167036q - 3.243771. \tag{14}$$

Proof. By definition

$$\begin{aligned} N_{\mathrm{IRDI}}G) &= \sum_{uv\epsilon E}\ln\left(1+|\delta_u-\delta_v|\right) \\ &= (6pq-5p-5q+4)\ln(1+|9-9|)+4(p+q-2)\ln(1+|9-8|)+2(p+q+2)\ln(1+|8-8|) \\ &\quad +4(p+q-2)\ln(1+|8-6|)+8\ln(1+|8-5|)+4\ln(1+|5-5|) \\ &= 4(p+q-2)\ln(1+1)+4(p+q-2)\ln(1+2)+8\ln(1+3) \\ &= (4p+4q-8)(0.693147)+(4p+4q-8)(1.098612)+11.0903 \\ &= 2.772588p+2.772588q-5.545176+4.394448p+4.394448q-8.788896+11.0903 \\ N_{\mathrm{IRDI}}G) &= 7.167036p+7.167036q-3.243771. \end{aligned} \tag{15}$$

□

Theorem 10. *Let $G \in TUC_4C_8[p,q]$ nanotorus. Then, one has*

$$N_{\mathrm{IRGA}}(G) = 0.048817p + 0.04817q + 0.1255859. \tag{16}$$

Proof. By definition

$$\begin{aligned} N_{\mathrm{IRGA}}(G) &= \sum_{uv\epsilon E}\ln\frac{|\delta_u+\delta_v|}{2\sqrt{\delta_u\delta_v}} \\ &= (6pq-5p-5q+4)\ln\frac{|9+9|}{2\sqrt{9\times 9}}+4(p+q-2)\ln\frac{|9+8|}{2\sqrt{9\times 8}}+2(p+q+2)\ln\frac{|8+8|}{2\sqrt{8\times 8}} \\ &\quad +4(p+q-2)\ln\frac{|8+6|}{2\sqrt{8\times 6}}+8\ln\frac{|8+5|}{2\sqrt{8\times 5}}+4\ln\frac{|5+5|}{2\sqrt{5\times 5}} \\ &= 4(p+q-2)\ln\frac{17}{2\sqrt{72}}+4(p+q-2)\ln\frac{14}{2\sqrt{48}}+8\ln\frac{13}{2\sqrt{40}} \\ &= 0.00693241p+0.006993241q-0.013864+0.04123857p+0.041123857q-0.082477+0.21889959 \\ N_{\mathrm{IRGA}}(G) &= 0.048817p+0.04817q+0.1255859. \end{aligned} \tag{17}$$

□

Theorem 11. *Let $G \in TUC_4C_8[p,q]$ nanotorus. Then, one has*

$$N_{\mathrm{IRB}}(G) = 0.6916877p + 0.691687q + 1.42373975. \quad (18)$$

Proof. By definition

$$\begin{aligned} N_{\mathrm{IRB}}(G) &= \sum_{uv\epsilon E}\left(\delta_u^{(1/2)} - \delta_v^{(1/2)}\right)^2 \\ &= (6\mathrm{pq} - 5p - 5q + 4)\left(9^{(1/2)} - 9^{(1/2)}\right)^2 + 4(p+q-2)\left(9^{(1/2)} - 8^{(1/2)}\right)^2 + 2(p+q+2)\left(8^{(1/2)} - 8^{(1/2)}\right)^2 \\ &\quad + 4(p+q-2)\left(8^{(1/2)} - 6^{(1/2)}\right)^2 + 8\left(8^{(1/2)} - 5^{(1/2)}\right)^2 + 4\left(5^{(1/2)} - 5^{(1/2)}\right)^2 \\ &= 0.118336p + 0.118336q - 0.236672 + 0.573351p + 0.57351q - 1.146703 + 2.8071475 \\ N_{\mathrm{IRB}}(G) &= 0.6916877p + 0.691687q + 1.42373975. \end{aligned} \quad (19)$$

□

3. The GTUC $[p,q]$ Nanotube, $(p,q > 1)$

GTUC[p, q] nanotubes are carbon allotropes with a nanostructure whose length-to-diameter ratio can exceed 1,000,000. These cylindrical carbon molecules have unique features that could make them valuable in a variety of nanotechnology applications. They have remarkable mechanical characteristics, such as high toughness and high elastic modulus, and are formal derivatives of the graphene sheet. They display both semiconducting and metallic behavior, which encompasses the entire range of qualities necessary for technology. The properties of GTUC[p, q] are still being studied extensively, and scientists have only just started to explore their potential. Without a doubt, carbon nanotubes are a substance with enormous potential that may lead to advancements in a new generation of gadgets, electric machinery, and biosectors. In GTUC$[p,q]$ as shown in Figure 2, the number of vertex sets and edge sets in a nanotorus is $4\mathrm{pq} + 4q$ and $6\mathrm{pq} + 5q$. In Table 3, we have shown the neighborhood edge partitions of GTUC$[p,q]$.

Theorem 12. *Let $G \in GTUC[p,q]$ nanotorus. Then, one has $N_{AL}(G) = 12q$.*

Proof. Based on the definition given below, one has

$$\begin{aligned} N_{\mathrm{AL}}(G) &= \sum_{uv\epsilon E}\left|\delta_u - \delta_v\right| \\ &= (6\mathrm{pq} - 5q)|9-9| + 4q|9-8| \\ &\quad + 2q|8-8| + 4q|8-6| \\ &= 4q + 4q(2) \\ &= 4q + 8q \\ N_{\mathrm{AL}}(G) &= 12q. \end{aligned} \quad (20)$$

□

Theorem 13. *Let $G \in GTUC[p,q]$ nanotorus. Then, one has $N_{IRL}(G) = 1.62186029p$.*

Proof. By definition

$$\begin{aligned} N_{\mathrm{IRL}}(G) &= \sum_{uv\epsilon E}\left|\ln\delta_u - \ln\delta_v\right| \\ &= (6\mathrm{pq} - 5p)|\ln 9 - \ln 9| + 4p|\ln 9 - \ln 8| + 2p|\ln 8 - \ln 8| + +4p|\ln 8 - \ln 6| \\ &= 4p(0.117783) + 4p(0.287682) \\ &= 0.471132p + 1.15072829p \\ N_{\mathrm{IRL}}(G) &= 1.62186029p. \end{aligned} \quad (21)$$

Theorem 15. *Let $G \in GTUC[p,q]$ nanotorus. Then, one has $N_{IRRT}(G) = 6p$.*

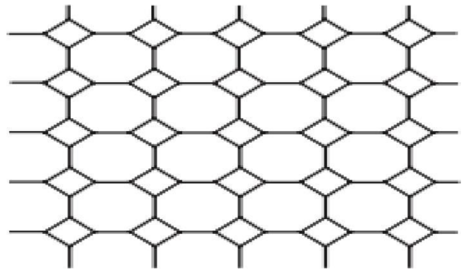


FIGURE 2: The GTUC $[p, q]$ nanotube with $q = 5$ and $p = 4$.

TABLE 3: The neighborhood edge partitions of GTUC$[p, q]$.

(δ_u, δ_v)	F
(9, 9)	$6pq - 5q$
(9, 8)	$4q$
(8, 8)	$2q$
(8, 6)	$4q$

Proof. By definition

$$\begin{aligned} N_{\mathrm{IRRT}}(G) &= \frac{1}{2}\sum_{uv\in E}\left|\delta_u - \delta_v\right| \\ &= (6pq - 5p)\frac{1}{2}|9-9| + 4p\frac{1}{2}|9-8| \\ &\quad + 2p\frac{1}{2}|8-8| + 4p\frac{1}{2}|8-6| \\ &= 2p + 4p \\ N_{\mathrm{IRRT}}(G) &= 6p. \end{aligned} \tag{22}$$

□

Theorem 16. *Let $G \in GTUC[p, q]$ nanotorus. Then, one has $N_{IRF}(G) = 20p$.*

Proof. By definition

$$\begin{aligned} N_{\mathrm{IRF}}(G) &= \sum_{uv\in E}\left(\delta_u - \delta_v\right)^2 \\ &= (6pq - 5p)(9-9)^2 + 4p(9-8)^2 \\ &\quad + 2p(8-8)^2 + 4p(8-6)^2 \\ &= 4p(1)^2 + 4p(2)^2 \\ &= 4p + 16p \\ N_{\mathrm{IRF}}(G) &= 20p. \end{aligned} \tag{23}$$

□

Theorem 17. *Let $G \in GTUC[p, q]$ nanotorus. Then, one has $N_{IRA}(G) = 0.0185096876p$.*

Proof. By definition

$$\begin{aligned} N_{\mathrm{IRA}}(G) &= \sum_{uv\in E}\left(\delta_u^{(-1/2)} - \left(\delta_v^{(-1/2)}\right)^2\right. \\ &= (6pq - 5p)\left(9^{(-1/2)} - 9^{(-1/2)}\right)^2 + 4p\left(9^{(-1/2)} - 8^{(-1/2)}\right)^2 + 2p\left(8^{(-1/2)} - 8^{(-1/2)}\right)^2 + 4p\left(8^{(-1/2)} - 6^{(-1/2)}\right)^2 \\ &= 4p(0.33333 - 0.353553)^2 + 4p(0.353553 - 0.408218)^2 \\ &= 0.0065435156p + 0.011966172p \\ N_{\mathrm{IRA}}(G) &= 0.0185096876p. \end{aligned} \tag{24}$$

□

Theorem 18. *Let $G \in GTUC[p, q]$ nanotorus. Then, one has $N_{IRDIF}(G = 3.2776p$.*

Proof. By definition

$$\begin{aligned} N_{\mathrm{IRDIF}}(G &= \sum_{uv\epsilon E}\left|\frac{\delta_u}{\delta_v}-\frac{\delta_v}{\delta_u}\right| \\ &= (6pq-5p)\left|\frac{9}{9}-\frac{9}{9}\right| + 4p\left|\frac{9}{8}-\frac{8}{9}\right| + 2p\left|\frac{8}{8}-\frac{8}{8}\right| + 4p\left|\frac{8}{6}-\frac{6}{8}\right| \\ &= 4p(1.125-0.8889)+4p(1.3333-0.75) \\ &= 0.9444p+2.33332p \\ N_{\mathrm{IRDIF}}(G &= 3.2776p. \end{aligned} \tag{25}$$

□

Theorem 19. *Let $G \in GTUC[p,q]$ nanotorus. Then, one has $N_{IRLF}(G) = 1.626105p$.*

Proof. By definition

$$\begin{aligned} N_{\mathrm{IRLF}}(G) &= \sum_{uv\epsilon E}\frac{|\delta_u-\delta_v|}{\sqrt{\delta_u\delta_v}} \\ &= (6pq-5p)\frac{|9-9|}{\sqrt{9\times 9}} + 4p\frac{|9-8|}{\sqrt{9\times 8}} \\ &\quad + 2p\frac{|8-8|}{\sqrt{8\times 8}} + 4p\frac{|8-6|}{\sqrt{8\times 6}} \\ &= 4p\frac{1}{\sqrt{72}} + 4p\frac{2}{\sqrt{48}} \\ &= 0.4714045p + 1.1547005p \\ N_{\mathrm{IRLF}}(G) &= 1.626105p. \end{aligned} \tag{26}$$

Based on the proof of Theorem 19, it is easy to calculate the following result. □

Corollary 20. *Let $G \in GTUC[p,q]$ nanotorus. Then, one has $N_{LA}(G) = 1.61344596639p$.*

Theorem 21. *Let $G \in GTUC[p,q]$ nanotorus. Then, one has $N_{IRDI}G) = 7.167037155p$.*

Proof. By definition

$$\begin{aligned} N_{\mathrm{IRDI}}G) &= \sum_{uv\epsilon E}\ln\left(1+|\delta_u-\delta_v|\right) \\ &= (6pq-5p)\ln(1+|9-9|) + 4p\ln(1+|9-8|) + 2p\ln(1+|8-6|) \\ &= 4p\ln(1+1) + 4p\ln(1+2) \\ &= 4p\ln 2 + 4p\ln 3 \\ N_{\mathrm{IRDI}}G) &= 2.772588p + 4.394449p \\ N_{\mathrm{IRDI}}G) &= 7.167037155p. \end{aligned} \tag{27}$$

□

Theorem 22. *Let $G \in GTUC[p,q]$ nanotorus. Then, one has $N_{IRGA}(G) = 8.048390284p$.*

Table 4: Comparison of the neighborhood topological indices of $TUC_4C_8[p,q]$.

$[p, q]$	N_{AL}	N_{IRL}	N_{IRRL}	N_{IRF}	N_{IRA}	N_{IRDIF}	N_{IRLF}	N_{LA}	N_{IRDI}	N_{IRGA}	N_{IRB}
[1, 1]	24	5.38	12	72	0.070	7.79	3.791	3.69	11.09	0.22	2.80
[2, 2]	48	8.62	24	112	0.097	14.35	7.04	6.91	25.42	0.318	4.15
[3, 3]	72	11.86	36	152	0.12	20.91	10.29	10.14	39.75	0.41	5.57
[4, 4]	96	15.11	48	192	0.15	27.46	13.55	13.37	54.09	0.51	6.95
[5, 5]	120	18.35	60	232	0.179	34.02	16.80	16.59	68.42	0.60	8.34
[6, 6]	144	21.600	72	272	0.20	40.57	20.05	19.82	82.76	0.70	9.72

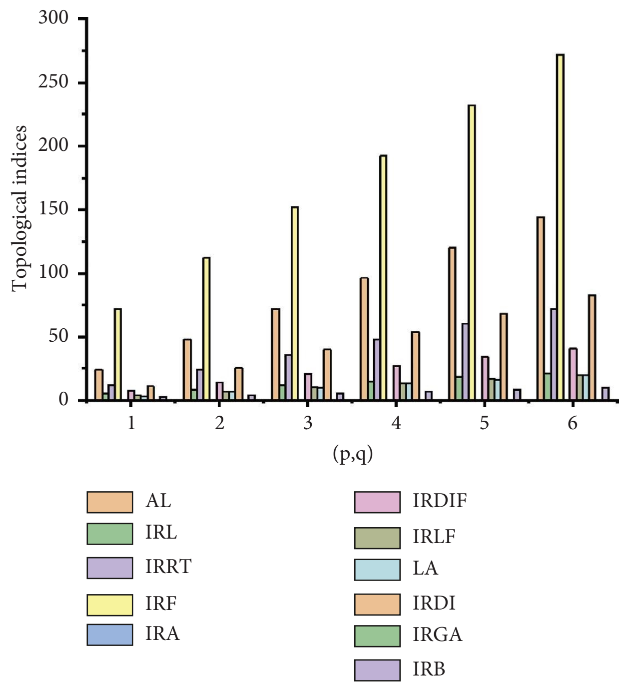


Figure 3: Comparison of the neighborhood topological indices of $TUC_4C_8[p,q]$.

Proof. By definition

$$\begin{aligned} N_{\mathrm{IRGA}}(G) &= \sum_{uv\epsilon E} \frac{\ln|\delta_u + \delta_v|}{2\sqrt{\delta_u\delta_v}} \\ &= 4p\ln\frac{17}{2\sqrt{72}} + 4p\ln\frac{14}{2\sqrt{48}} \\ &= 4.0069384p + 4.0414518p \\ N_{\mathrm{IRGA}}(G) &= 8.048390284p. \end{aligned} \tag{28}$$

□

Theorem 23. *Let $G \in GTUC[p,q]$ nanotorus. Then, one has $N_{IRB}(G) = 0.6921229p$.*

Proof. Based on the definition given below, one has

$$\begin{aligned} N_{\mathrm{IRB}}(G) &= \sum_{uv\epsilon E} \left(\delta_u^{(1/2)} - \delta_v^{(1/2)}\right)^2 \\ &= (6pq - 5p)\left(9^{(1/2)} - 9^{(1/2)}\right)^2 + 4p\left(9^{(1/2)} - 8^{(1/2)}\right)^2 + 2p\left(8^{(1/2)} - 8^{(1/2)}\right)^2 + 4p\left(8^{(1/2)} - 6^{(1/2)}\right)^2 \\ &= 4p(0.0294372) + 4p(0.14359353) \\ &= 0.1177488p + 0.5743741p \\ N_{\mathrm{IRB}}(G) &= 0.6921229p. \end{aligned} \tag{29}$$

□

Table 5: Comparison of the neighborhood topological indices of GTUC$[p, q]$.

$[p, q]$	N_{AL}	N_{IRL}	N_{IRRL}	N_{IRF}	N_{IRA}	N_{IRDIF}	N_{IRLF}	N_{LA}	N_{IRDI}	N_{IRGA}	N_{IRB}
[1, 1]	12	1.62	6	20	0.06	3.27	1.62	1.613	8.04	8.04	0.69
[2, 2]	24	3.24	12	40	0.03	6.55	3.24	3.22	14.33	16.09	1.38
[3, 3]	36	4.86	18	60	0.05	9.83	4.86	4.84	21.50	24.14	2.07
[4, 4]	48	6.48	24	80	0.07	13.11	6.48	6.45	28.66	32.19	2.76
[5, 5]	60	8.10	30	100	0.09	16.38	8.10	8.06	35.83	40.24	3.46
[6, 6]	72	9.73	36	120	0.11	19.66	9.73	9.73	43.00	48.29	4.15

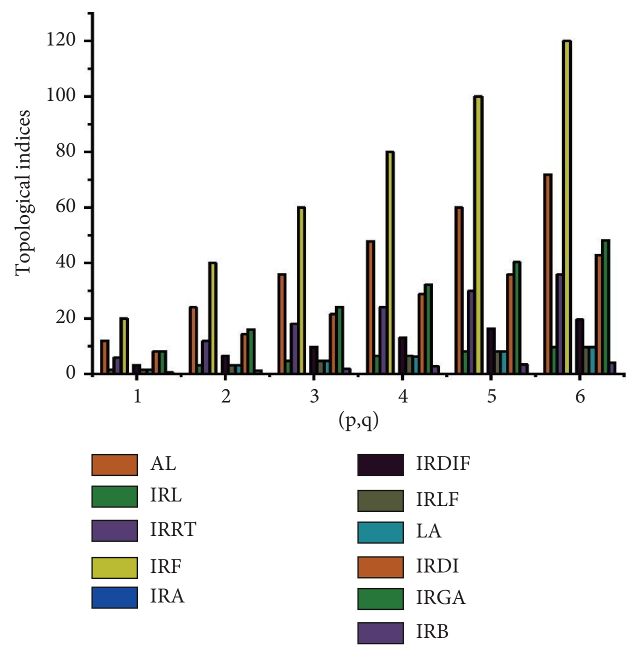


Figure 4: Comparison of the neighborhood topological indices of GTUC$[p, q]$.

4. Discussion and Conclusion

We wrap up our work in this section with a few key points. In Section 2, we created the $TUC_4C_8[p, q]$ nanotube structures for $p, q > 1$. We produced the neighborhood edge partitions indicated in Table 2 based on Figures 1(a) and 1(b). We calculated the neighborhood irregularity topological indices using these neighborhood edge partitions. Additionally, Table 4 and Figure 3 provide numerical and visual comparisons of all taken into account neighborhood topological indices which establishes a positive link between p, q, and these topological indices. In other words, topological indices rise in value as the values of p and q increase. It is clear from this comparison that the N_{IRF} index value is higher than the values of the other topological indices.

In Section 3, we built the GTUC $[p, q]$ nanotube structures for $p, q > 1$. Using Figure 2, we came up with the neighborhood edge partitions that are displayed in Table 3. These neighborhood edge partitions allowed us to calculate the irregularity of topological indices. Additionally, Table 5 and Figure 4 provide numerical and visual comparisons of all taken-in topological indices which shows that there is a positive correlation between p, q, and these topological indices; as p and q rise, the topological indices' values rise as well. It is clear from this comparison that the N_{IRF} index value is higher than the values of the other topological indices.

The application of distance-based topological indices presents increased challenges and complexity; however, they can be utilized in conjunction with existing methods. The exploration of such studies will be the focal point of future research.

Data Availability

No data were used to support this study.

Disclosure

The results in this article were produced without the use of any code.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

S.Z. conceptualized the study; A.U. curated the data; R.N. performed formal analysis; K.B.R. contributed funding acquisition; S.Z. investigated the study; A.U. and R.N. developed the methodology; S.Z. administered the project; R.N. collected resources; S.Z. performed the software analysis; A.U. supervised the study; S.Z. validated the manuscript; K.B.R. and S.Z. performed the data visualization; A.U., R.N., K.B.R., and S.Z. wrote the original draft; A.U., R.N., K.B.R., and S.Z. reviewed and edited the manuscript. All authors have read and agreed to the published version of the manuscript.

References

[1] S. Iijima, "Helical microtubules of graphitic carbon," *Nature*, vol. 354, no. 6348, pp. 56–58, 1991.
[2] V. R. Kuli, "Some topological indices of certain nanotubes," *Journal of Computer and Mathematical Sciences*, vol. 8, pp. 1–7, 2017.
[3] V. L. K. N. Parvathi, "Computation of topological indices of HA (C5c6c7) nanotube," *Annals of the Romanian Society for Cell Biology*, vol. 25, pp. 3080–3085, 2021.
[4] M. K. Siddiqui, M. Imran, and A. Ahmad, "On Zagreb indices, Zagreb polynomials of some nanostar dendrimers," *Applied Mathematics and Computation*, vol. 280, pp. 132–139, 2016.
[5] A. Ahmad, O. B. S. Al-Mushayt, and M. Bača, "On edge irregularity strength of graphs," *Applied Mathematics and Computation*, vol. 243, pp. 607–610, 2014.
[6] A. Ullah, S. Zaman, A. Hamraz, and M. Muzammal, "On the construction of some bioconjugate networks and their structural modeling via irregularity topological indices," *The European Physical Journal E*, vol. 46, no. 8, p. 72, 2023.
[7] S. Zaman, H. S. A. Yaqoob, A. Ullah, and M. Sheikh, "QSPR analysis of some novel drugs used in blood cancer treatment via degree based topological indices and regression models," *Polycyclic Aromatic Compounds*, pp. 1–17, 2023.
[8] Z.-Q. Chu, M. K. Siddiqui, S. Manzoor, S. A. K. Kirmani, M. F. Hanif, and M. H. Muhammad, "On rational curve fitting between topological indices and entropy measures for graphite carbon nitride," *Polycyclic Aromatic Compounds*, vol. 43, no. 3, pp. 2553–2570, 2023.
[9] M. Naeem, M. Atif, A. Khalid, M. Sajid, and M. A. Mustafa, "Computation of degree-based topological indices for porphyrazine and tetrakis porphyrazine," *Molecular Physics*, vol. 121, no. 13, 2023.
[10] M. O. Albertson, "The irregularity of a graph," *Ars Combinatoria*, vol. 46, pp. 219–225, 1997.
[11] D. Vukičević and A. Graovac, "Valence connectivity versus Randić, Zagreb and modified Zagreb index: a linear algorithm to check discriminative properties of indices in acyclic molecular graphs," *Croatian Chemical Journal*, vol. 77, pp. 501–508, 2004.
[12] H. Abdo, S. Brandt, and D. Dimitrov, "The total irregularity of a graph," *Discrete Mathematics and Theoretical Computer Science*, vol. 16, no. 1, 2014.
[13] I. Gutman, "Topological indices and irregularity measures," *Bulletin*, vol. 8, pp. 469–475, 2018.
[14] X. Li and I. Gutman, *Mathematical Aspects of Randic-type Molecular Structure Descriptors*, Faculty of Science, University of Kragujevac Kragujevac, Kragujevac, Serbia, 2006.
[15] T. Réti, R. Sharafdini, A. Dregelyi-Kiss, and H. Haghbin, "Graph irregularity indices used as molecular descriptors in QSPR studies, MATCH Commun," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 79, pp. 509–524, 2018.
[16] Y.-M. Chu, M. Abid, M. I. Qureshi, A. Fahad, and A. Aslam, "Irregular topological indices of certain metal organic frameworks," *Main Group Metal Chemistry*, vol. 44, no. 1, pp. 73–81, 2021.
[17] A. Avdullahu and S. Filipovski, "On certain topological indices of graphs," 2022, https://arxiv.org/abs/2210.12981.
[18] A. Ullah, S. Zaman, A. Hussain, A. Jabeen, and M. B. Belay, "Derivation of mathematical closed form expressions for certain irregular topological indices of 2D nanotubes," *Scientific Reports*, vol. 13, no. 1, Article ID 11187, 2023.
[19] Y. Y. Gao, M. S. Sardar, S. M. Hosamani, and M. R. Farahani, "Computing sanskruti index of TURC4C8 (s) nanotube," *International Journal of Pharmaceutical Sciences and Research*, vol. 8, pp. 4423–4425, 2017.
[20] F. Deng, X. Zhang, M. Alaeiyan, A. Mehboob, and M. R. Farahani, "Topological indices of the pent-heptagonal nanosheets VC5C7 and HC5C7," *Advances in Materials Science and Engineering*, vol. 2019, Article ID 9594549, 12 pages, 2019.
[21] H. Jiang, M. S. Sardar, M. R. Farahani, M. Rezaei, M. K. Siddiqui, and B. Zahra, "Computing Sanskruti index of V-phenylenic nanotubes and nanotori," *International Journal of Pure and Apllied Mathematics*, vol. 115, no. 4, pp. 859–865, 2017.
[22] M. R. Farahani, "Computing GA5 index of armchair polyhex nanotube," *Le Mathematics*, vol. 69, pp. 69–76, 2014.