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Computational Principles and Experimental Investigation of Local Non-Regular Topological Indices of TUC4C8 [p, q] and GTUC [p, q] Nanostructures

K R Girish[1], Dr N Prabhudeva[2], Jayashree D N[3]

Asst. Professor[1], Professor & HOD[2], Assoc. Professor[3]

girishhspt@gmail.com[1], drnprabhudeva@gmail.com[2] , jayashreedn12@gmail.com[3]

Department of Mathematics, Proudhadevaraya Institute of Technology, T.B. Dam Road, Hosapete,

Karnataka-583225

Abstract:

which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited. Any molecular or nanostructure may have its topology described by a topological index. To forecast the physical properties linked to bioactivities and chemical reactivity in certain networks, topological indices are used in QSAR and QSPR studies. A wide variety of physical, mechanical, and chemical properties are shown by 2D nanostructured materials. These very thin nanoparticles exhibit anisotropy and great chemical functionality. Because of their thin profile and large surface area, 2D materials are the best option for applications that need strong surface interactions at a microscopic scale. In this work we obtain closed form formulas for the neighbourhood irregular topological invariants of the nanostructures TUC4C8[p, q] and GTUC[p, q]. Following the computation of these indices, a comparison analysis is carried out.

Keywords; Principles and Experimental, Investigation of Local, Non-Regular, Topological, Indices of TUC4C8.

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 inter- connected nanotubes. The discovery of multiwalled carbon nanotubes took place in 1991 by Sumio Iijima, [1]. Chem- ically, sp^2 bonds–a very potent type of molecular inter- action–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 charac- teristics. 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 un- derstanding 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

certain bioconjugate networks and their structural modeling through irregularity topological indices is presented in [6]. The article [7] delves into the quantitative structure-property re- lationship (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 $IRF(G) = \sum_{uv \in E}(d_u - d_v)^2$.

$$N_{IRB}(G) \quad \sum_{uv \in E}(\delta_u^{(1/2)} - \delta_v^{(1/2)})^2$$

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 ir- regular topological indices pertaining to the nanostructures TUC_4C_8 p, q and GTCU p, q , and a comparative analysis is also performed

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
The Randic´ index (Li and Gutman) [14] is defined as
of nanostructure $TUC_4C_8[p, q]$ is q and p, respectively. In
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($G$) � $\sum_{uv\in E}$
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
$(|d_u - d_v|/\sqrt{d_u d_v})$, LA($G$) � $2\sum_{uv\in E}(|d_u - d_v|/(d_u + d_v))$,
column and row is, respectively, p and q. In the 2D lattice of

and IRDI(G) � $\sum_{uv\in E} \ln(1 + |d_u - d_v|)$. Chu et al. Abid have defined the IR GA(G) in [16] as IRGA(G) � $\sum_{uv\in E} \ln$
$TUC_4C_8[p, q]$, the total number of squares in a row and column are $(q + 1)$ and $(p + 1)$.
$((d_u + d_v)/2\sqrt{d_u d_v})$. The bond-additive index was described
are The number of vertices and edges of Figures 1(a) and 1(b)

in [17] as IRA(G) � $\sum_{uv\in E}(d_u^{(1/2)} - d_v^{(1/2)})^2$. Very recently,
$(4q^2 + 4q)(p + 1)$ and $6pq + 5q + 5p + 4$, respectively. In Table 2, we have shown the edge partition of $TUC_4C_8[p, q]$.
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
Correspondingly, for GTUC$[p, q]$, vertex set and edge set remain $4pq + 4q$ and $6pq + 5q$.

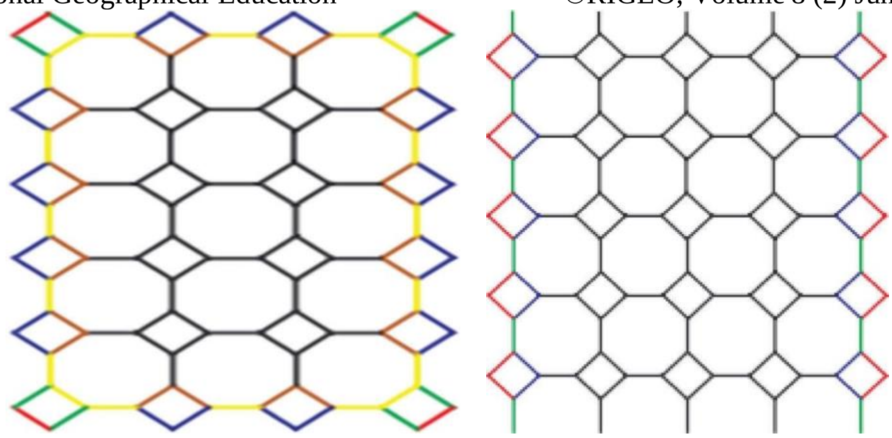
Theorem 1. Let G ∈ $TUC_4C_8[p, q]$ nanotorus. Then, one
GTUC$[p, q]$. The list of those indices is given in Table 1.
There have been numerous attempts to look into the TI for different nanotubes and nanosheets in the literature.

has $N_{AL}(G)$ � $12p + 12q$.

Pentaheptagonal nanosheets and $TURC_4C_8(S)$ are both

Proof. By definition

$$N_{AL}(G) � \sum_{uv\in E} |\delta_u - \delta_v|$$
$$� (6pq - 5p - 5q + 4)|9 - 9| + 4(p + q - 2)|9 - 8| + 2(p + q + 2)|8 - 8| + 4|8 - 6|(p + q - 2) + 8(8 - 5) + 4(5 - 5)$$
$$� 4(p + q - 2) + 4(2)(p + q - 2) + 3(8) + 4(0)$$
$$� 12p + 12q.$$



(a) (b)

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

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

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

Proof. By definition

$$N_{IRL}(G) = \sum_{uv\epsilon E} |\ln \delta_u - \ln \delta_v|$$

$$= (6pq - 5p - 5q + 4)(\ln 9 - \ln 9) + 4(p + q - 2)(\ln 9 - \ln 8) + 2(p + q + 2)(\ln 8 - \ln 8)$$
$$+ 4(p + q - 2)(\ln 8 - \ln 6) + 8(\ln 8 - \ln 5) + 4(\ln 5 - \ln 5)$$
$$= (4p + 4q - 8)(0.117783) + (4p + 4q - 8)(0.287682) + 8(0.4700036)$$
$$= 0.471132p + 0.4771132q - 0.942264 + 1.1507728p + 1.150728q - 2.301456 + 3.7600288$$
$$N_{IRL}(G) = 1.62186p + 1.62186q + 0.5163088.$$

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

Proof. By definition

$$N_{IRRL}(G) = \frac{1}{2}\sum_{uv\epsilon E} |\delta_u - \delta_v|$$

$$= (6pq - 5p - 5q + 4)\frac{1}{2}|9 - 9| + 4(p + q - 2)\frac{1}{2}|9 - 8| + 2(p + q + 2)\frac{1}{2}|8 - 8|$$
$$+ 4(p + q - 2)\frac{1}{2}|8 - 6| + 8\frac{1}{2}|8 - 5| + 4\frac{1}{2}|5 - 5|$$
$$= 2(p + q - 2)(1) + 2(p + q - 2)(2) + 4(3)$$
$$= 2p + 2q - 4 + 4p + 4q - 8 + 12$$
$$N_{IRRL}(G) = 6p + 6q.$$

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

Proof. By definition

$$N_{IRF}(G) = \sum_{uv\epsilon E} (\delta_u - \delta_v)^2$$

$$= (6pq - 5p - 5q + 4)(9 - 9)^2 + 4(p + q - 2)(9 - 8)^2$$

$+ 2(p + q + 2)(8 - 8)$

$+ 4(p + q - 2)(8 - 6)^2 + 8(8 - 5)^2 + 4(5 - 5)^2$

$= 4p + 4q - 8 + 16p + 16q - 32 + 72$

$N_{IRF}(G) = 20p + 20q + 32.$

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

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

Proof. By definition

$= 4(p + q - 2)9^{(-1/2)} - 8^{(-1/2)2} + 4(p + q - 2)8^{(-1/2)} - 6^{(-1/2)2} + 88^{(-1/2)} - 5^{(-1/2)2}$

$= 4(p + q - 2)(0.33333 - 0.353553)^2 + 4(p + q - 2)(0.353553 - 0.408249)^2 + 8(0.353553 - 0.447213 5)^2$

$= 4(p + q - 2)(0.0004101840) + 4(p + q - 2)(0.002991652) + 8(0.0087722)$

$= 0.001640736p + 0.001640736q - 0.003281472 + 0.011966608p + 0.011966608q - 0.023933216 + 0.0701783$

$N_{IRA}(G) = 0.013607344p + 0.013607344q + 0.0429636.$

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

□

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

Proof. By definition

$N_{IRDIF}(G) = \frac{\delta_u}{} - \frac{\delta_v}{}$ $_{uv\in E}\delta_v$

$= (6pq - 5p - 5q + 4)_9 -$

$_9 + 4(p + q - 2)_8 -$

$_9 + 2(p + q - 2)_8 -$

$+ 4(p + q - 2)_6 - _8 + 8_5 - _8 + 4_5 - _5$

$= 4(p + q - 2)(1.125 - 0.88889) + 4(p + q - 2)(1.3333 - 0.75) + 8(1.6 - 0.625)$

$= 0.94444p + 0.94444q - 1.88888 + 2.333332p + 2.33332q - 4.66664 + 7.8$

$N_{IRDIF}(G) = 3.27774p + 3.27774q + 1.24448.$

□

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

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

Proof. By definition

$N\ \ (G) = \frac{\delta_u - \delta_v}{}$

$= (6pq - 5p - 5q + 4)\sqrt{\overline{9 \times 9}} + 4(p + q - 2)\sqrt{\overline{9 \times 8}} + 2(p + q + 2)\sqrt{\overline{8 \times 8}}$

$+ 4(p + q - 2)\frac{|8-6|}{\sqrt{8 \times 6}} + 8\frac{|8-5|}{\sqrt{8 \times 5}} + 4\frac{|5-5|}{\sqrt{5 \times 5}}$ $3 = 4(p + q - 2)\sqrt{72} + 4(p + q - 2)\sqrt{48} + 8\sqrt{40}$

$= 0.471404p + 0.471404q - 0.9428090 + 1.1547005p + 1.154700538q - 2.3094010 + 3.7947331$

$N_{IRLF}(G) = 1.62611045p + 1.62611045q + 0.5425231.$

[ ]

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*

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

Proof. By definition

$$N_{LA}(G) = \sum_{uv\in E} 2\frac{|\delta_u - \delta_v|}{(\delta_u + \delta_v)}$$

$$= (6pq - 5p - 5q + 4)2\frac{|9-9|}{(9+9)} + 4(p+q-2)2\frac{|9-8|}{(9+8)} + 2(p+q+2)2\frac{|8-8|}{(8+8)} + 4(p+q-2)2\frac{|8-6|}{(8+6)} + 8(2)\frac{|8-5|}{(8+5)} + 4(2)\frac{|5-5|}{(5+5)}$$

$$= 0.47058823p + 0.47058823q - 0.94117647 + 1.14285714p + 1.14285714q - 2.28571428 + 3.69230769$$

$$N_{LA}(G) = 1.61344537p + 1.61344537q + 0.46541694.$$

□

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

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

Proof. By definition

$$N_{IRDI}(G) = \sum_{uv\in E} \ln\left(1 + |\delta_u - \delta_v|\right)$$

$$= (6pq - 5p - 5q + 4)\ln(1+|9-9|) + 4(p+q-2)\ln(1+|9-8|) + 2(p+q+2)\ln(1+|8-8|) + 4(p+q-2)\ln(1+|8-6|) + 8\ln(1+|8-5|) + 4\ln(1+|5-5|)$$

$$= 4(p+q-2)\ln(1+1) + 4(p+q-2)\ln(1+2) + 8\ln(1+3)$$

$$= (4p+4q-8)(0.693147) + (4p+4q-8)(1.098612) + 11.0903$$

$$= 2.772588p + 2.772588q - 5.545176 + 4.394448p + 4.394448q - 8.788896 + 11.0903$$

$$N_{IRDI}(G) = 7.167036p + 7.167036q - 3.243771.$$

□

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

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

Proof. By definition

$$N_{IRGA}(G) = \sum \ln\frac{\delta_u + \delta_v}{2\sqrt{\delta_u \delta_v}}$$

$$= (6pq - 5p - 5q + 4)\ln\frac{|9+9|}{2\sqrt{9\times 9}} + 4(p+q-2)\ln\frac{|9+8|}{2\sqrt{9\times 8}} + 2(p+q+2)\ln\frac{|8+8|}{2\sqrt{8\times 8}} + 4(p+q-2)\ln\frac{|8+6|}{2\sqrt{8\times 6}} + 8\ln\frac{|8+5|}{2\sqrt{8\times 5}} + 4\ln\frac{|5+5|}{2\sqrt{5\times 5}}$$

$$= 4(p+q-2)\ln\frac{17}{2\sqrt{72}} + 4(p+q-2)\ln\frac{14}{2\sqrt{48}} + 8\ln\frac{13}{2\sqrt{40}}$$

$$= 0.00693241p + 0.006993241q - 0.013864 + 0.04123857p + 0.041123857q - 0.082477 + 0.21889959$$

$N_{\text{IRGA}}(G)$ � $0.048817p + 0.04817q + 0.1255859.$

□

Theorem 11. *Let G ∈ TUC$_4$C$_8$ [p, q] nanotorus. Then, one has*

$N_{\text{IRB}}(G)$ � $0.6916877p + 0.691687q + 1.42373975.$ (18)

Proof. By definition

� $(6pq - 5p - 5q + 4)9^{(1/2)} - 9^{(1/2)2} + 4(p + q - 2)9^{(1/2)} - 8^{(1/2)2} + 2(p + q + 2)8^{(1/2)} - 8^{(1/2)2}$

$+ 4(p + q - 2)8^{(1/2)} - 6^{(1/2)^2} + 88^{(1/2)} - 5^{(1/2)^2} + 45^{(1/2)} - 5^{(1/2)^2}$

� $0.118336p + 0.118336q - 0.236672 + 0.573351p + 0.57351q - 1.146703 + 2.8071475$

$N_{\text{IRB}}(G)$ � $0.6916877p + 0.691687q + 1.42373975.$

□

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

GTUC[p, q] nanotubes are carbon allotropes with a nano- structure whose length-to-diameter ratio can exceed

Theorem 12. *Let G ∈ GTUC[p, q] nanotorus. Then, one has*

$N_{AL}(G)$ � $12q.$

Proof. Based on the definition given below, one has

1,000,000. These cylindrical carbon molecules have unique features that could make them valuable in a variety of nanotechnology applications. They have remarkable me-

N_{AL} uv∈E

(G) � δ_u

- chanical characteristics, such as high toughness and high elastic modulus, and are formal derivatives of the graphene sheet. They display both semiconducting and metallic be- havior, 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

� $(6pq - 5q)|9 - 9| + 4q|9 - 8|$

$+ 2q|8 - 8| + 4q|8 - 6|$

� $4q + 4q(2)$

� $4q + 8q$ $N_{\text{AL}}(G)$ � $12q.$

□

machinery, and biosectors. In GTUC $[p, q]$ as shown in Figure 2, the number of vertex sets and edge sets in a nanotorus is $4pq + 4q$ and $6pq + 5q$. In Table 3, we have shown the neighborhood edge partitions of GTUC[p, q].

$N_{\text{IRL}}(G)$ � $\ln\delta_u - \ln\delta_v$

Theorem 13. *Let G ∈ GTUC[p, q] nanotorus. Then, one has* uv∈E

$N_{IRL}(G)$ � $1.62186029p.$

Proof. By definition

� $(6pq - 5p)|\ln 9 - \ln 9| + 4p|\ln 9 - \ln 8| + 2p|\ln 8 - \ln 8| + +4p|\ln 8 - \ln 6|$

� $4p(0.117783) + 4p(0.287682)$

$= 0.471132p + 1.15072829p \; N_{\mathrm{IRL}}(G) = 1.62186029p.$

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

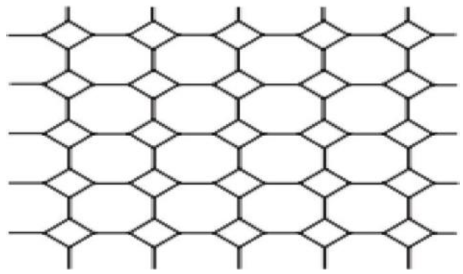


FIGURE 2: The GTUC [p, q] nanotube with $q = 5$ and $p = 4$.

$4q$

Proof. By definition

Proof. By definition

N_{IRRT}

$$N_{\mathrm{IRF}}(G) = \sum_{uv \in E} (\delta_u - \delta_v)^2$$

$$= (6pq - 5p)(9 - 9)^2 + 4p(9 - 8)^2$$

$$= (6pq - 5p)\,\frac{2}{2}|9 - 9| + 4p\,\frac{2}{2}|9 - 8| + 2p(8 - 8) + 4p(8 - 6)$$

$$= 4p(1) + 4p(2)$$

$$+ 2p\,\frac{2}{2}|8 - 8| + 4p\,\frac{2}{2}|8 - 6|$$

$$= 2p + 4p \; N_{\mathrm{IRRT}}(G) = 6p.$$

$$= 4p + 16p$$

$$N_{\mathrm{IRF}}(G) = 20p.$$

□

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

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

Proof. By definition

$$N_{IRA}(G) = \sum_{uv \in E} \left(\delta_u^{(-1/2)} - \delta_v^{(-1/2)}\right)^2$$

$$= (6pq - 5p)\left(9^{(-1/2)} - 9^{(-1/2)}\right)^2 + 4p\left(9^{(-1/2)} - 8^{(-1/2)}\right)^2 + 2p\left(8^{(-1/2)} - 8^{(-1/2)}\right)^2 + 4p\left(8^{(-1/2)} - 6^{(-1/2)}\right)^2$$

$$= 4p(0.33333 - 0.353553)^2 + 4p(0.353553 - 0.408218)^2$$

$$= 0.0065435156p + 0.011966172p \; N_{\mathrm{IRA}}(G)$$

$$= 0.0185096876p.$$

Theorem 18. *Let G ∈ GTUC[p, q] nanotorus. Then, one has*

$N_{IRDIF}(G$ � $3.2776p$.

Proof. By definition

$2p\frac{8}{}$

$4p\frac{8}{} - \frac{6}{}$

9

� $4p(1.125 - 0.8889) + 4p(1.3333 - 0.75)$

� $0.9444p +$

$2.33332p$ $N_{IRDIF}(G$ � $3.2776p$.

□

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

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

Proof. By definition

$N_{IRLF}(G)$ � $\sum_{uv \in E}$

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*
$N_{IRDI}G)$ � $7.167037155p$.

� $(6pq - 5p)\sqrt{9 \times 9} + 4p\sqrt{9 \times 8}$

Proof. By definition

$+ 2p\sqrt{\frac{|8-8|}{8 \times 8}} + 4p\sqrt{\frac{|8-6|}{8 \times 6}}$ (26)

� $4p\sqrt{\frac{1}{72}} + 4p\sqrt{\frac{2}{48}}$

� $0.4714045p + 1.1547005p$ $N_{IRLF}(G)$ � $1.626105p$.

$N_{IRDI}G)$ � $\sum_{uv \in E} \ln 1 + \delta_u - \delta_v$

� $(6pq - 5p)\ln(1 + |9 - 9|) + 4p\ln(1 + |9 - 8|) + 2p\ln(1 + |8 - 8|)$

� $4p\ln(1 + 1) + 4p\ln(1 + 2)$

� $4p\ln 2 + 4p\ln 3$ $N_{IRDI}G)$ � $2.772588p +$

$4.394449p$ $N_{IRDI}G)$ � $7.167037155p$.

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_{IRL}	N_{IRRL}	N_{IRF}	N_{IRA}	N_{IRDIF}	N_{IRLF}	N_{LA}	N_{IRDI}	N_{IRGA}	N_{IRB}	N_{AL}
[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

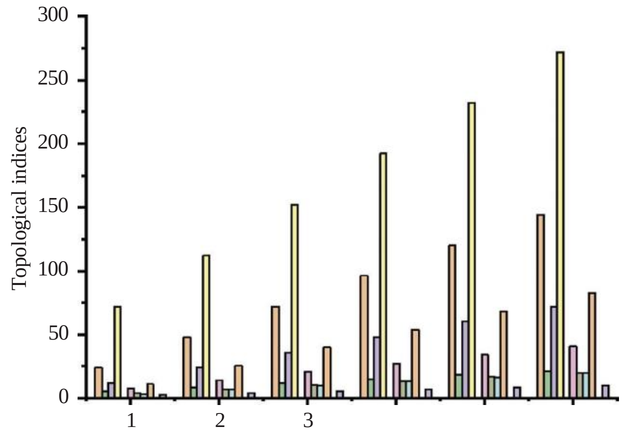


FIGURE 3: Comparison of the neighborhood topological indices of $TUC_4C_8[p, q]$.

Proof. By definition

$N_{IRGA}(G)$ � $\sum_{uv\epsilon E}$ $\ln|\delta_u + \delta_v$ $2 \; \delta_u\delta_v$

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

Proof. Based on the definition given below, one has

� $4p\ln \frac{17}{2\sqrt{72}} + 4p\ln \frac{14}{2\sqrt{48}}$

� $4.0069384p + 4.0414518p$ $N_{IRGA}(G)$ � $8.048390284p$.

� $(6pq - 5p)9^{(1/2)} - 9^{(1/2)^2} + 4p9^{(1/2)} - 8^{(1/2)^2} + 2p8^{(1/2)} - 8^{(1/2)^2} + 4p8^{(1/2)} - 6^{(1/2)^2}$

� $4p(0.0294372) + 4p(0.14359353)$

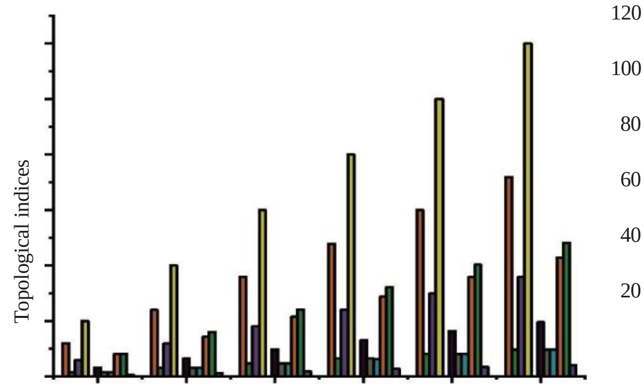
� $0.1177488p + 0.5743741p$ $N_{IRB}(G)$ �

$0.6921229p$.

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



1 2 3

AL IRL IRRT

IRF IRA

4. Discussion and Conclusion

We wrap up our work in this section with a few key points. In Section 2, we created the TUC$_4$C$_8$[*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 topo- logical 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, topo- logical 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 neighbor- hood 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 explo- ration of such studies will be the focal point of future research.

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