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Topological Indices of Advanced Nanotube Architectures: Hexagonal, Zigzag-Edge Coronoid and Starphene Fusions

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ABSTRACT: Chemical graph theory (CGT) utilizes graph-theoretical tools to model molecular structures and predict their physicochemical properties. Topological indices (TIs), as numerical descriptors derived from molecular graphs, serve as essential tools in theoretical chemistry and nanotechnology. In this study, we investigate advanced nanotube architectures, specifically hexagonal parallelogram nanotubes, triangular benzenoids, and zigzag-edge coronoids fused with starphene units. Using a systematic algebraic approach, we derive novel neighborhood M-polynomials (NM-polynomials) for these nanostructures. From the NM-polynomials, we compute various neighborhood-based topological indices, including the second Zagreb index, harmonic index, and forgotten index. The proposed methodology simplifies the computation of TIs and provides closed-form expressions for complex fused structures. The findings have promising implications for the design and analysis of nanomaterials in fields such as drug delivery, molecular electronics, and material science.

Key Words:: Topological indices, NM-polynomials, hexagonal parallelogram nanotubes, zigzag-edge coronoids, starphene nanotubes, drug design.

Contents

1. Introduction

Chemical graph theory (CGT) is a vibrant interdisciplinary field where graph-theoretical tools are applied to study chemical and biological structures. In CGT, atoms and bonds of molecules are represented as vertices and edges of a graph, respectively, enabling mathematical analysis of molecular properties. One of the central concepts in CGT is the *topological index* (TI)—a numerical descriptor invariant under graph isomorphisms that captures the structural information of molecular graphs.

Topological indices have proven to be effective in predicting a variety of physicochemical and biological properties of chemical compounds, such as boiling point, entropy, heat of formation, and heat of combustion [1,2,3,4]. Due to their success, TIs are widely used in quantitative structure–property relationship (QSPR) and quantitative structure–activity relationship (QSAR) studies [9,10]. The earliest TI, known as the Wiener index, was introduced by Harold Wiener in 1947 [11], followed by several other important indices including the Randić index [12], Zagreb indices [15,16,17], and many others. To date, over 150 TIs have been developed, each with connections to specific molecular features or experimental properties [18,19].

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The computation of these indices, particularly for complex molecular graphs, can be highly labor-intensive. To address this challenge, researchers introduced the *M-polynomial*, an algebraic generating function that encodes degree-based edge information in a compact form [20,21,22]. From the M-polynomial, various degree-based topological indices can be derived systematically and efficiently. A further generalization, the *neighborhood M-polynomial* (NM-polynomial), was proposed in [23] to compute neighborhood degree-based TIs, which consider the degrees of neighboring vertices of each edge in a graph.

In this paper, we investigate advanced nanostructures, including the line graph of the subdivision graph of hexagonal parallelogram nanotubes (HPN), triangular benzenoids (TB), and zigzag-edge coronoids fused with starphene nanotubes (ZCST). For each of these molecular graphs, we construct the corresponding NM-polynomials and then use them to compute a suite of ten neighborhood-based topological indices. These include the third Zagreb index, second Zagreb index, neighborhood harmonic index, neighborhood inverse sum index, Sanskruti index, and several others. Our approach not only simplifies the derivation of these indices but also offers closed-form expressions useful for chemical modeling and nanomaterials research.

The derivation and application of these indices are outlined in the subsequent sections, beginning with definitions and preliminaries.

2. Preliminaries

Definition 1. The *neighborhood M-polynomial (NM-polynomial)* of a graph G was introduced in [23] and is defined as

$$NM(G;r,s) = \sum_{i \leq j} m_{i,j} r^i s^j,$$

where $m_{i,j}$ is the number of edges $pq \in E(G)$ such that the neighborhood degrees $\{\delta_p, \delta_q\} = \{i, j\}$.

Definition 2. A *neighborhood degree-based topological index* (or neighborhood TI) defined on the edge set of a graph G is given by

$$I(G) = \sum_{pq \in E(G)} f(\delta_p, \delta_q), \tag{2.1}$$

where $f(\delta_p, \delta_q)$ is a real-valued function of the neighborhood degrees of vertices p and q. Equation (2.1) can also be rewritten in terms of edge frequency as:

$$I(G) = \sum_{i \leq j} m_{i,j} f(i,j).$$

Various neighborhood-based indices can be obtained by specifying the function $f(i,j)$ as follows:

- $f(i,j) = i + j$: Neighborhood Zagreb index (third version)
- $f(i,j) = ij$: Neighborhood second Zagreb index
- $f(i,j) = i^2 + j^2$: Neighborhood Forgotten index
- $f(i,j) = \frac{1}{ij}$: Neighborhood second modified Zagreb index
- $f(i,j) = (ij)^\alpha$: Neighborhood general Randić index
- $f(i,j) = ij(i+j)$: Neighborhood ND_3 index
- $f(i,j) = \frac{i}{j} + \frac{j}{i}$: Neighborhood ND_5 index
- $f(i,j) = \frac{2}{i+j}$: Neighborhood Harmonic index

- $f(i,j) = \frac{ij}{i+j}$: Neighborhood Inverse Sum index
- $f(i,j) = \left(\frac{ij}{i+j-2}\right)^3$: Sanskruti index
- $f(i,j) = (i+j)^2$: Fifth hyper M_1 Zagreb index
- $f(i,j) = (ij)^2$: Fifth hyper M_2 Zagreb index
- $f(i,j) = \frac{i+j}{ij}$: Fifth Arithmetic-Geometric index
- $f(i,j) = \frac{2\sqrt{ij}}{i+j}$: Fifth Geometric-Arithmetic index

While the direct calculation of these indices involves extensive computation, they can be efficiently derived using the NM-polynomial. Table 1 summarizes the relationships between the NM-polynomial and various neighborhood-based topological indices.

Table 1: Neighborhood degree-based indices derived from the NM-polynomial [28]– [29].

Graphical Index	$f(u,v)$	**Derivation from** $NM(G)$
M_1'	$u+v$	$(D_u+D_v)(NM(G))\|_{u=v=1}$
M_2^*	uv	$(D_uD_v)(NM(G))\|_{u=v=1}$
F_N^*	u^2+v^2	$(D_u^2+D_v^2)(NM(G))\|_{u=v=1}$
M_2^{nm}	$\frac{1}{uv}$	$(S_uS_v)(NM(G))\|_{u=v=1}$
NR_α	$(uv)^\alpha$	$(D_u^\alpha D_v^\alpha)(NM(G))\|_{u=v=1}$
ND_3	$uv(u+v)$	$D_uD_v(D_u+D_v)(NM(G))\|_{u=v=1}$
ND_5	$\frac{u^2+v^2}{uv}$	$(D_uS_v+S_uD_v)(NM(G))\|_{u=v=1}$
NH	$\frac{2}{u+v}$	$2S_uJ(NM(G))\|_{u=v=1}$
NI	$\frac{uv}{u+v}$	$(S_uJD_uD_v)(NM(G))\|_{u=v=1}$
S	$\left(\frac{uv}{u+v-2}\right)^3$	$(S_u^3Q_{-2}JD_u^3D_v^3)(NM(G))\|_{u=v=1}$
HM_1G_5	$(u+v)^2$	$(D_u^2+D_v^2+2D_uD_v)(NM(G))\|_{u=v=1}$
HM_2G_5	$(uv)^2$	$D_uD_v(D_uD_v)(NM(G))\|_{u=v=1}$
AG_5	$\frac{u+v}{2\sqrt{uv}}$	$\frac{1}{2}S_u^{1/2}S_v^{1/2}(D_u+D_v)(NM(G))\|_{u=v=1}$
GA_5	$\frac{2\sqrt{uv}}{u+v}$	$2S_uJD_u^{1/2}D_v^{1/2}(NM(G))\|_{u=v=1}$

where the operators used are defined as follows:

- $D_u(f(u,v)) = u\frac{\partial f(u,v)}{\partial u}, \quad D_v(f(u,v)) = v\frac{\partial f(u,v)}{\partial v}$
- $S_u(f(u,v)) = \int_0^u \frac{f(t,v)}{t}\,dt, \quad S_v(f(u,v)) = \int_0^v \frac{f(u,t)}{t}\,dt$
- $J(f(u,v)) = f(u,u), \quad Q_\alpha(f(u,v)) = u^\alpha f(u,v)$

3. Methodology

The methodology begins with the construction of the line graph of the subdivision graphs corresponding to three nanostructures: hexagonal parallelogram nanotubes (HPN), triangular benzenoids (TB), and zigzag-edge coronoids fused with starphene nanotubes (ZCFN). In these molecular graphs, atoms are represented as vertices, while chemical bonds are modeled as edges.

For each structure, the following steps are performed:

1. **Graph Construction:** The subdivision graph is obtained by inserting a new vertex into each edge of the original molecular graph. Then, the line graph of this subdivision graph is constructed, where each vertex represents an edge of the subdivision graph, and two vertices are adjacent if the corresponding edges share a common vertex.

2. **Neighborhood Degree Calculation:** The neighborhood degree $\delta(v)$ of a vertex v in the line graph is computed by counting the number of vertices at a distance of one unit from v.

3. **Edge Classification:** The edges of the line graph are partitioned into distinct edge classes based on the unordered pair of neighborhood degrees (δ_p, δ_q) for each edge pq.

4. **NM-Polynomial Derivation:** The NM-polynomial for each molecular structure is then computed using the formal definition:
$$NM(G; r, s) = \sum_{i \leq j} m_{i,j} r^i s^j,$$
where $m_{i,j}$ denotes the number of edges having neighborhood degrees i and j.

5. **Computation of Topological Indices:** Finally, ten neighborhood-based topological indices are derived from the NM-polynomial using operator-based formulas summarized in Table 1.

This structured approach ensures both efficiency and accuracy in computing topological descriptors of complex molecular nanostructures.

4. Main Results

In this section, we present the NM-polynomials and corresponding neighborhood-based topological indices for three molecular nanostructures: hexagonal parallelogram nanotubes (HPN), triangular benzenoids (TB), and zigzag-edge coronoids fused with starphene nanotubes (ZCFN). These mathematical formulations provide insights into the structural characteristics and complexity of the studied graphs.

4.1. Results for Hexagonal Parallelogram Nanotube (HPN)

Let $P(k_1, k_2)$ denote a hexagonal parallelogram nanotube consisting of hexagons arranged in a parallelogram configuration, where k_1 is the number of hexagons in each row, and k_2 is the number of hexagons in each column.

- The total number of vertices in $P(k_1, k_2)$ is $2(k_1 + k_2 + k_1k_2)$.
- The number of edges in $P(k_1, k_2)$ is $3k_1k_2 + 2k_1 + 2k_2 - 1$.

Figure 1 illustrates the molecular graph of $P(k_1, k_2)$, while Figures 2 and 3 depict its subdivision graph and the corresponding line graph, respectively.

The line graph of the subdivision graph of $P(k_1, k_2)$ contains $2(3k_1k_2 + 2k_1 + 2k_2 - 1)$ vertices and $9k_1k_2 + 4k_1 + 4k_2 - 5$ edges.

The derived indices provide meaningful numerical invariants that can be used to characterize the structural and functional behavior of HPN-type molecular systems.

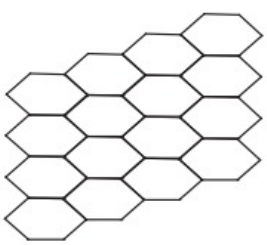

Figure 1: A hexagonal parallelogram $P(4, 4)$

Theorem 4.1 *Let Υ be the line graph of the subdivision graph of a hexagonal parallelogram nanotube (HPN) with $k_1 = 1$. Then, the following neighborhood-based topological indices hold:*

Figure 2: A Subdivision of hexagonal parallelogram $P(4,4)$

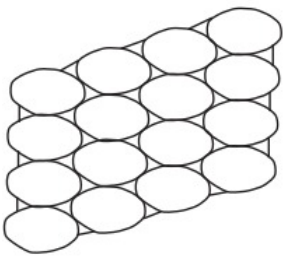

Figure 3: A line graph of subdivision graph of hexagonal parallelogram $P(4,4)$.

1. $M_1^{'}(\Upsilon) = 190k_2 - 74$,
2. $M_2^{*}(\Upsilon) = 707k_2 - 517$,
3. $F_N^{*}(\Upsilon) = 1454k_2 - 1070$,
4. ${}^{nm}M_2(\Upsilon) = 0.2785k_2 - 0.4664$,
5. $NR_\alpha(\Upsilon) = n\big[2(25)^\alpha + 4(40)^\alpha + 2(64)^\alpha + 4(72)^\alpha + (81)^\alpha\big] + \big[10(16)^\alpha + 4(20)^\alpha - 4(25)^\alpha - 4(40)^\alpha - 2(64)^\alpha - 4(72)^\alpha - (81)^\alpha\big]$,
6. $ND_3(\Upsilon) = 12842k_2 - 10842$,
7. $ND_5(\Upsilon) = 26.95k_2 - 2.75$,
8. $NH(\Upsilon) = 0.922n + 0.5678$,
9. $NI(\Upsilon) = 46.747k_2 - 22.86$,
10. $S(\Upsilon) = 1016.52k_2 - 794.64$.

Proof: Consider

$$NM(\Upsilon) = f(u,v) = 10u^4v^4 + 4u^4v^5 + 2(k_2-2)u^5v^5 + 4(k_2-1)u^5v^8 + 2(k_2-1)u^8v^8 + 4(k_2-1)u^8v^9 + (k_2-1)u^9v^9.$$

Then, using the operators given in Table 1, we have:

$$\begin{aligned}(D_u + D_v)(f(u,v)) &= 80u^4v^4 + 36u^4v^5 + 20(k_2-2)u^5v^5 + 52(k_2-1)u^5v^8 \\ &\quad + 32(k_2-1)u^8v^8 + 68(k_2-1)u^8v^9 + 18(k_2-1)u^9v^9,\end{aligned}$$

$$\begin{aligned}D_uD_v(f(u,v)) &= 160u^4v^4 + 80u^4v^5 + 50u^5v^5 + 160(k_2-1)u^5v^8 \\ &\quad + 128(k_2-1)u^8v^8 + 288(k_2-1)u^8v^9 + 81(k_2-1)u^9v^9,\end{aligned}$$

$$\begin{aligned}(D_u^2 + D_v^2)(f(u,v)) &= 320u^4v^4 + 164u^4v^5 + 100(k_2-2)u^5v^5 + 356(k_2-1)u^5v^8 \\ &\quad + 256(k_2-1)u^8v^8 + 580(k_2-1)u^8v^9 + 162(k_2-1)u^9v^9,\end{aligned}$$

$$\begin{aligned}S_uS_v(f(u,v)) &= \frac{5}{8}u^4v^4 + \frac{1}{5}u^4v^5 + \frac{2}{25}(k_2-2)u^5v^5 + \frac{1}{10}(k_2-1)u^5v^8 \\ &\quad + \frac{1}{32}(k_2-1)u^8v^8 + \frac{1}{18}(k_2-1)u^8v^9 + \frac{1}{81}(k_2-1)u^9v^9,\end{aligned}$$

$$\begin{aligned}D_u^\alpha D_v^\alpha(f(u,v)) &= 10(16)^\alpha u^4v^4 + 4(20)^\alpha u^4v^5 + 2(25)^\alpha(k_2-2)u^5v^5 \\ &\quad + 4(40)^\alpha(k_2-1)u^5v^8 + 2(64)^\alpha(k_2-1)u^8v^8 \\ &\quad + 4(72)^\alpha(k_2-1)u^8v^9 + (81)^\alpha(k_2-1)u^9v^9,\end{aligned}$$

$$\begin{aligned}D_uD_v(D_u + D_v)(f(u,v)) &= 1280u^4v^4 + 720u^4v^5 + 500(k_2-2)u^5v^5 + 3328(k_2-1)u^5v^8 \\ &\quad + 2048(k_2-1)u^8v^8 + 4896(k_2-1)u^8v^9 + 1458(k_2-1)u^9v^9,\end{aligned}$$

$$\begin{aligned}S_uD_v + D_uS_v(f(u,v)) &= 20u^4v^4 + \frac{41}{5}u^4v^5 + 4(k_2-2)u^5v^5 + \frac{89}{10}(k_2-1)u^5v^8 \\ &\quad + 4(k_2-1)u^8v^8 + \frac{145}{18}(k_2-1)u^8v^9 + 2(k_2-1)u^9v^9,\end{aligned}$$

$$\begin{aligned}S_uJ(f(u,v)) &= \frac{5}{4}u^8 + \frac{4}{9}u^9 + \frac{1}{5}(k_2-2)u^{10} + \frac{4}{13}(k_2-1)u^{13} \\ &\quad + \frac{1}{8}(k_2-1)u^{16} + \frac{4}{17}(k_2-1)u^{17} + \frac{1}{18}(k_2-1)u^{18},\end{aligned}$$

$$\begin{aligned}S_uJD_uD_v(f(u,v)) &= 20u^8 + \frac{80}{9}u^9 + 5(k_2-2)u^{10} + \frac{160}{13}(k_2-1)u^{13} \\ &\quad + 8(k_2-1)u^{16} + \frac{288}{17}(k_2-1)u^{17} + \frac{9}{2}(k_2-1)u^{18},\end{aligned}$$

$$\begin{aligned}S_u^3Q_{-2}JD_u^3D_v^3(f(u,v)) &= 189.62u^6 + 93.29u^7 + 61.03(k_2-2)u^8 + 192.33(k_2-1)u^{11} \\ &\quad + 191.03(k_2-1)u^{14} + 442.36(k_2-1)u^{15} + 129.74u^{16}.\end{aligned}$$

Now, using the definitions given in Table 1, straightforward computations lead to the required results. □

Theorem 4.2 *Let Υ be the line graph of the subdivision graph of hexagonal parallelogram nanotubes*

(HPN) for $k_1 > 1$, then the NM-polynomial of Υ is given by

$$NM(\Upsilon) = 8u^4v^4 + 8u^4v^5 + 2(k_1+k_2-4)u^5v^5 + 4(k_1+k_2-2)u^5v^8 + 2(k_1+k_2-2)u^8v^8 + 4(k_1+k_2-2)u^8v^9 + (9k_1k_2 - 8(k_1+k_2)+7)u^9v^9.$$

Proof: Based on the degree sum of the neighborhood degrees of the endpoints of each edge (as shown in Table 2) and the structure of the line graph of the subdivision graph of HPN (see Fig. 3), we determine the edge partition of the line graph.

Table 2: The edge partition table of the HPN subdivision line graph for $k_1 > 1$.

Edge Class	Count
$e_{4,4}$	8
$e_{4,5}$	8
$e_{5,5}$	$2(k_1+k_2-4)$
$e_{5,8}$	$4(k_1+k_2-2)$
$e_{8,8}$	$2(k_1+k_2-2)$
$e_{8,9}$	$4(k_1+k_2-2)$
$e_{9,9}$	$9k_1k_2 - 8(k_1+k_2)+7$

Each edge class $e_{i,j}$ contributes a term $m_{i,j}u^iv^j$ to the NM-polynomial. Therefore, summing all contributions from the edge classes, we obtain:

$$\begin{aligned} NM(\Upsilon) = {} & 8u^4v^4 + 8u^4v^5 + 2(k_1+k_2-4)u^5v^5 + 4(k_1+k_2-2)u^5v^8 \\ & + 2(k_1+k_2-2)u^8v^8 + 4(k_1+k_2-2)u^8v^9 \\ & + (9k_1k_2 - 8(k_1+k_2)+7)u^9v^9. \end{aligned}$$

This completes the proof. □

Now, using table 2 and definition of NM-polynomial, the result follows by some simple calculations.

Theorem 4.3 *Let Υ be the line graph of the subdivision graph of a hexagonal parallelogram nanotube (HPN) for $k_1 > 1$, then we have:*

1. $M_1^{'}(\Upsilon) = 162nk_1 + 28k_1 + 28k_2 - 122,$
2. $M_2^{*}(\Upsilon) = 729k_1k_2 - 22k_1 - 22k_2 - 497,$
3. $F_N^{*}(\Upsilon) = 1458k_1k_2 - 4k_1 - 4k_2 - 1066,$
4. ${}^{nm}M_2(\Upsilon) = 0.111k_1k_2 - 0.468k_1 - 0.468k_2 - 1.107,$
5. $NR_\alpha(\Upsilon) = 9(81)^\alpha nk_1 + m\left[2(25)^\alpha + 4(40)^\alpha + 2(64)^\alpha + 4(72)^\alpha - 8(81)^\alpha\right] + n\left[2(25)^\alpha + 4(40)^\alpha + 2(64)^\alpha + 4(72)^\alpha - 8(81)^\alpha\right] + 8(16)^\alpha + 8(20)^\alpha - 8(25)^\alpha - 8(40)^\alpha - 4(64)^\alpha - 8(72)^\alpha + 7(81)^\alpha,$

6. $ND_3(\Upsilon) = 13122k_1k_2 - 2148k_1 - 2148k_2 - 7362$,

7. $ND_5(\Upsilon) = 18k_1k_2 - 16k_1 - 16k_2 + 14$,

8. $NH(\Upsilon) = 18nk_1 + 8.955k_1 - 8.955k_2 - 11.51$,

9. $NI(\Upsilon) = 40.5nk_1 + 6.248k_1 + 6.248k_2 - 29.225$,

10. $S(\Upsilon) = 1167.71k_1k_2 - 151.94k_1 - 151.94k_2 - 647.67$.

Proof: Consider the NM-polynomial of Υ:

$$\begin{aligned} NM(\Upsilon) = f(u,v) = {} & 8u^4v^4 + 8u^4v^5 + 2(k_1+k_2-4)u^5v^5 + 4(k_1+k_2-2)u^5v^8 \\ & + 2(k_1+k_2-2)u^8v^8 + 4(k_1+k_2-2)u^8v^9 + (9k_1k_2 - 8(k_1+k_2)+7)u^9v^9. \end{aligned}$$

Using the definitions and differential operators listed in Table 1, we apply each operator to $f(u,v)$:

$$\begin{aligned} (D_u + D_v)(f(u,v)) = {} & 64u^4v^4 + 72u^4v^5 + 20(k_1+k_2-4)u^5v^5 + 52(k_1+k_2-2)u^5v^8 \\ & + 32(k_1+k_2-2)u^8v^8 + 68(k_1+k_2-2)u^8v^9 \\ & + [162k_1k_2 - 144(k_1+k_2) + 126]u^9v^9, \\ D_uD_v(f(u,v)) = {} & 128u^4v^4 + 160u^4v^5 + 50(k_1+k_2-4)u^5v^5 + 160(k_1+k_2-2)u^5v^8 \\ & + 128(k_1+k_2-2)u^8v^8 + 288(k_1+k_2-2)u^8v^9 \\ & + [729k_1k_2 - 648(k_1+k_2) + 567]u^9v^9, \\ (D_u^2 + D_v^2)(f(u,v)) = {} & 256u^4v^4 + 328u^4v^5 + 100(k_1+k_2-4)u^5v^5 + 356(k_1+k_2-2)u^5v^8 \\ & + 256(k_1+k_2-2)u^8v^8 + 580(k_1+k_2-2)u^8v^9 \\ & + [1458k_1k_2 - 1296(k_1+k_2) + 1134]u^9v^9, \\ S_uS_v(f(u,v)) = {} & \tfrac{1}{2}u^4v^4 + \tfrac{2}{5}u^4v^5 + \tfrac{2}{25}(k_1+k_2-4)u^5v^5 + \tfrac{4}{10}(k_1+k_2-2)u^5v^8 \\ & + \tfrac{1}{32}(k_1+k_2-2)u^8v^8 + \tfrac{1}{18}(k_1+k_2-2)u^8v^9 \\ & + \tfrac{1}{81}[9k_1k_2 - 8(k_1+k_2)+7]u^9v^9, \\ D_u^\alpha D_v^\alpha(f(u,v)) = {} & 8(16)^\alpha u^4v^4 + 8(20)^\alpha u^4v^5 + 2(25)^\alpha(k_1+k_2-4)u^5v^5 \\ & + 4(40)^\alpha(k_1+k_2-2)u^5v^8 + 2(64)^\alpha(k_1+k_2-2)u^8v^8 \\ & + 4(72)^\alpha(k_1+k_2-2)u^8v^9 + (81)^\alpha[9k_1k_2 - 8(k_1+k_2)+7]u^9v^9, \\ D_uD_v(D_u+D_v)(f(u,v)) = {} & \ldots \text{(continue similarly)}. \end{aligned}$$

Using the operator definitions from Table 1, we compute each index according to its respective operator. This leads to the closed-form expressions presented in the theorem. □

4.2. Results of Triangular Benzenoid (TB)

Let G_n denote the triangular benzenoid (TB) family, which can be viewed as a generalization of the benzene molecule C_6H_6, where all benzene rings are arranged in a triangular configuration. The TB structure is generated by incrementally adding one hexagon in each new row, as illustrated in Fig. 4.

The graph G_n has $k_2^2 + 4n + 1$ vertices and $\frac{3}{2}n(n+3)$ edges.

The subdivision graph of G_n is shown in Fig. 5, while the **line graph** of this subdivision graph is depicted in Fig. 6. The line graph of the subdivision graph of G_n contains $3n(n+3)$ vertices and $\frac{3}{2}(3k_2^2 + 7n - 2)$ edges.

In this section, we compute the neighborhood metric polynomial (NM-polynomial) for the TB structure and derive ten corresponding neighborhood-based topological indices.

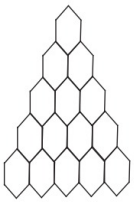

Figure 4: A subdivision of TB

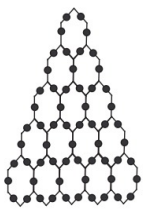

Figure 5: A Subdivision of TB

Theorem 4.4 *Let Υ be the line graph of the subdivision graph of the triangular benzenoid (TB). Then, the NM-polynomial of Υ is given by:*

$$\begin{aligned} NM(\Upsilon) &= 9u^4v^4 + 6u^4v^5 + 3(k_2-2)u^5v^5 + 6(k_2-1)u^5v^8 \\ &\quad +3(k_2-1)u^8v^8 + 6(k_2-1)u^8v^9 + \frac{3}{2}(3k_2^2-5k_2+2)u^9v^9. \end{aligned}$$

Proof: From Fig. 6, and by applying a vertex-degree-based edge-counting method, we obtain the edge partition of the line graph of the subdivision graph of TB. This is based on the degree sum of the neighboring vertices of the endpoints of each edge and is summarized in Table 3.

Edge Type (s_u, s_v)	**Number of Edges**
$(4,4)$	9
$(4,5)$	6
$(5,5)$	$3(k_2-2)$
$(5,8)$	$6(k_2-1)$
$(8,8)$	$3(k_2-1)$
$(8,9)$	$6(k_2-1)$
$(9,9)$	$\frac{3}{2}(3k_2^2-5k_2+2)$

Table 3: Edge partition of the line graph of the subdivision graph of TB.

Using the above partition data and the definition of the NM-polynomial, we directly compute:

$$NM(\Upsilon) = \sum_{uv \in E(\Upsilon)} u^{\deg(u)} v^{\deg(v)} = \text{(as shown above)}.$$

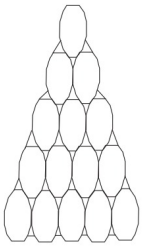

Figure 6: A line graph of subdivision graph of TB

This completes the proof. □

Theorem 4.5 *Let Υ be the line graph of the subdivision graph of the triangular benzenoid (TB). Then, the following neighborhood-based indices hold:*

1. $M_1(\Upsilon) = 81k_2^2 + 123k_2 - 108$,
2. $M_2^*(\Upsilon) = 364.5k_2^2 + 331.5k_2 - 507$,
3. $F_N^*(\Upsilon) = 729k_2^2 - 1215k_2 + 46$,
4. $M_2^{nm}(\Upsilon) = 0.057k_2^2 + 0.0497k_2 + 0.31$,
5. $NR_\alpha(\Upsilon) = 9(16)^\alpha + 6(20)^\alpha + 3(k_2-2)(25)^\alpha + 6(k_2-1)(40)^\alpha + 3(k_2-1)(64)^\alpha$
   $+6(k_2-1)(72)^\alpha + \frac{3}{2}(3k_2^2 - 5k_2 + 2)(81)^\alpha$,
6. $ND_3(\Upsilon) = 6561k_2^2 + 3351k_2 - 8430$,
7. $ND_5(\Upsilon) = 9k_2^2 + 22.43k_2 - 7.13$,
8. $NH(\Upsilon) = 0.25k_2^2 + 0.881k_2 + 0.36$,
9. $NI(\Upsilon) = 364.5k_2^2 + 331.5k_2 - 507$,
10. $S(\Upsilon) = 583.8k_2^2 + 357.15k_2 - 721.9$.

Proof: Consider the NM-polynomial of the line graph of the subdivision graph of TB:

$$f(u,v) = 9u^4v^4 + 6u^4v^5 + 3(k_2-2)u^5v^5 + 6(k_2-1)u^5v^8 + 3(k_2-1)u^8v^8 + 6(k_2-1)u^8v^9 + \tfrac{3}{2}(3k_2^2 - 5n + 2)u^9v^9.$$

Now, applying the corresponding differential and neighborhood operators (as defined in Table 1), we obtain:

$$(D_u + D_v)(f(u,v)) = 72u^4v^4 + 54u^4v^5 + 30(k_2-2)u^5v^5 + 78(k_2-1)u^5v^8 + 48(k_2-1)u^8v^8 + 102(k_2-1)u^8v^9 + 27(3k_2^2 - 5n + 2)u^9v^9,$$

$$D_uD_v(f(u,v)) = 144u^4v^4 + 120u^4v^5 + 75(k_2-2)u^5v^5 + 240(k_2-1)u^5v^8 + 192(k_2-1)u^8v^8 + 432(k_2-1)u^8v^9 + \tfrac{243}{2}(3k_2^2-5n+2)u^9v^9,$$

$$(D_u^2+D_v^2)(f(u,v)) = 288u^4v^4 + 246u^4v^5 + 150(k_2-2)u^5v^5 + 534(k_2-1)u^5v^8 + 384(k_2-1)u^8v^8 + 870(k_2-1)u^8v^9 + 243(3k_2^2-5n+2)u^9v^9,$$

$$S_uS_v(f(u,v)) = \tfrac{9}{16}u^4v^4 + \tfrac{6}{20}u^4v^5 + \tfrac{3}{25}(k_2-2)u^5v^5 + \tfrac{6}{40}(k_2-1)u^5v^8 + \tfrac{3}{64}(k_2-1)u^8v^8 + \tfrac{6}{72}(k_2-1)u^8v^9 + \tfrac{1}{54}(3k_2^2-5n+2)u^9v^9,$$

$$D_u^\alpha D_v^\alpha(f(u,v)) = 9(16)^\alpha u^4v^4 + 6(20)^\alpha u^4v^5 + 3(25)^\alpha(k_2-2)u^5v^5 + 6(40)^\alpha(k_2-1)u^5v^8 + 3(64)^\alpha(k_2-1)u^8v^8 + 6(72)^\alpha(k_2-1)u^8v^9 + \tfrac{3}{2}(81)^\alpha(3k_2^2-5n+2)u^9v^9,$$

$$D_uD_v(D_u+D_v)(f(u,v)) = 1152u^4v^4 + 1080u^4v^5 + 750(k_2-2)u^5v^5 + 3120(k_2-1)u^5v^8 + 3072(k_2-1)u^8v^8 + 7344(k_2-1)u^8v^9 + 2187(3k_2^2-5n+2)u^9v^9,$$

$$D_uS_v + S_uD_v(f(u,v)) = 18u^4v^4 + \tfrac{123}{10}u^4v^5 + 6(k_2-2)u^5v^5 + \tfrac{267}{20}(k_2-1)u^5v^8 + 6(k_2-1)u^8v^8 + \tfrac{435}{36}(k_2-1)u^8v^9 + 3(3k_2^2-5n+2)u^9v^9,$$

$$S_uJ(f(u,v)) = \tfrac{9}{8}u^8 + \tfrac{2}{3}u^9 + \tfrac{3}{10}(k_2-2)u^{10} + \tfrac{6}{13}(k_2-1)u^{13} + \tfrac{3}{16}(k_2-1)u^{16} + \tfrac{6}{17}(k_2-1)u^{17} + \tfrac{1}{12}(3k_2^2-5n+2)u^{18},$$

$$S_uJD_uD_v(f(u,v)) = 18u^8 + \tfrac{120}{9}u^9 + \tfrac{15}{2}(k_2-2)u^{10} + \tfrac{240}{13}(k_2-1)u^{13} + 12(k_2-1)u^{16} + \tfrac{432}{17}(k_2-1)u^{17} + \tfrac{243}{36}(3k_2^2-5n+2)u^{18},$$

$$S_u^3Q_{-2}JD_u^3D_v^3(f(u,v)) = \tfrac{36864}{216}u^6 + \tfrac{48000}{343}u^7 + \tfrac{46875}{512}(k_2-2)u^8 + \tfrac{384000}{1331}(k_2-1)u^{11} + \tfrac{786432}{2744}(k_2-1)u^{14} + \tfrac{2239488}{3375}(k_2-1)u^{15} + \tfrac{1594323}{8192}(3k_2^2-5n+2)u^{16}.$$

Finally, using the definitions in Table 1, we compute the desired topological indices from the above expressions.

□

4.3. Results of Zigzag-Edge Coronoid Fused with Starphene Nanotubes (ZCFN)

The ZCFN structure is a composite benzenoid system formed by fusing the zigzag-edge coronoid (ZC) with the starphene (St). The molecular graph of ZCFN, as shown in Fig. 7, contains $36k - 54$ vertices and $15(j + k + k_1) - 63$ edges.

The subdivision graph of ZCFN is illustrated in Fig. 8, while its line graph, derived from the subdivision graph, is shown in Fig. 9. This line graph of the subdivision graph of ZCFN consists of $30(j + k + k_1) - 126$ vertices and $39(j + k + k_1) - 153$ edges.

This subsection presents the Neighborhood M-polynomial (NM-polynomial) for the ZCFN structure, followed by the computation of ten first-order neighborhood degree-based topological indices (TIs).

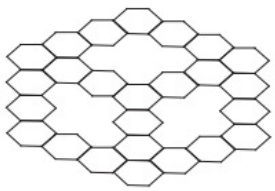

Figure 7: ZCFN

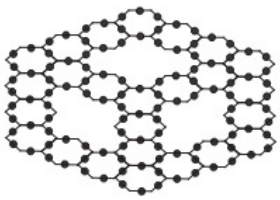

Figure 8: A subdivision of ZCFN

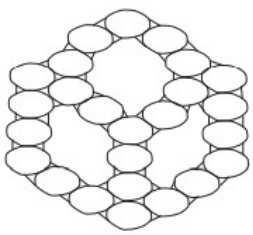

Figure 9: A line graph of the subdivision graph of ZCFN

Theorem 4.6 *Let Υ be the line graph of the subdivision graph of ZCFN. Then, we have*

$$\begin{aligned} NM(\Upsilon) &= 6u^4v^4 + 12u^4v^5 + 6(k+l+k_1-8)u^5v^5 + 12(k+l+k_1-7)u^5v^8 \\ &\quad +6(k+l+k_1-9)u^8v^8 + 12(k+l+k_1-5)u^8v^9 + 3(k+l+k_1+25)u^9v^9. \end{aligned}$$

Proof: From Fig. 9, by a counting method, we obtain the edge partition of the line graph of the subdivision graph of ZCFN, based on the degree sum of the neighboring vertices of the end vertices of each edge, as shown in Table 4.

m_{s_u,s_v}	$e_{4,4}$	$e_{4,5}$	$e_{5,5}$	$e_{5,8}$	$e_{8,8}$	$e_{8,9}$	$e_{9,9}$
# of Edges	6	12	$6(k+l+k_1-8)$	$12(k+l+k_1-7)$	$6(k+l+k_1-9)$	$12(k+l+k_1-5)$	$3(k+l+k_1+25)$

Table 4: Edge partition for the line graph of the subdivision graph of ZCFN.

Now, using Table 4 and the definition of the NM-polynomial, the result follows through straightforward computation. □

Theorem 4.7 *Let Υ be the line graph of the subdivision graph of ZCFN. Then, the following neighborhood-based topological indices hold:*

1. $M_1^{'}(\Upsilon) = 570(j+k+k_1) - 1950$,
2. $M_2^{*}(\Upsilon) = 2229(j+k+k_1) - 6465$,
3. $F_N^{*}(\Upsilon) = 4362(j+k+k_1) - 12654$,
4. $M^{nm}(\Upsilon) = 0.837(j+k+k_1) - 3.796$,
5. $NR_\alpha(\Upsilon) = 6(16)^\alpha + 12(20)^\alpha + 6(25)^\alpha(k+l+k_1-8) + 12(40)^\alpha(k+l+k_1-7)$
   $+6(64)^\alpha(k+l+k_1-9) + 12(72)^\alpha(k+l+k_1-5) + 3(81)^\alpha(k+l+k_1+25)$,
6. $ND_3(\Upsilon) = 33306(j+k+k_1) - 74654$,
7. $ND_5(\Upsilon) = 80.86(j+k+k_1) - 332.3$,
8. $NH(\Upsilon) = 2.761(j+k+k_1) - 11.909$,
9. $NI(\Upsilon) = 146.59(j+k+k_1) - 504.13$,
10. $S(\Upsilon) = 3049.63(j+k+k_1) - 7173.7$.

Proof: Consider

$$\begin{aligned} f(u,v) &= 6u^4v^4 + 12u^4v^5 + 6(k+l+k_1-8)u^5v^5 \\ &\quad +12(k+l+k_1-7)u^5v^8 + 6(k+l+k_1-9)u^8v^8 \\ &\quad +12(k+l+k_1-5)u^8v^9 + 3(k+l+k_1+25)u^9v^9. \end{aligned}$$

Now, using the operators given below Table 1, we obtain:

$$\begin{aligned} (D_u+D_v)(f(u,v)) &= 48u^4v^4 + 108u^4v^5 + 60(k+l+k_1-8)u^5v^5 \\ &\quad +156(k+l+k_1-7)u^5v^8 + 96(k+l+k_1-9)u^8v^8 \\ &\quad +204(k+l+k_1-5)u^8v^9 + 54(k+l+k_1+25)u^9v^9, \end{aligned}$$

$$\begin{aligned} D_uD_v(f(u,v)) &= 96u^4v^4 + 240u^4v^5 + 150(k+l+k_1-8)u^5v^5 \\ &\quad +480(k+l+k_1-7)u^5v^8 + 384(k+l+k_1-9)u^8v^8 \\ &\quad +972(k+l+k_1-5)u^8v^9 + 243(k+l+k_1+25)u^9v^9, \end{aligned}$$

$$\begin{aligned} (D_u^2+D_v^2)(f(u,v)) &= 192u^4v^4 + 492u^4v^5 + 300(k+l+k_1-8)u^5v^5 \\ &\quad +1068(k+l+k_1-7)u^5v^8 + 768(k+l+k_1-9)u^8v^8 \\ &\quad +1740(k+l+k_1-5)u^8v^9 + 486(k+l+k_1+25)u^9v^9, \end{aligned}$$

$$\begin{aligned} S_uS_v(f(u,v)) &= \frac{3}{8}u^4v^4 + \frac{3}{5}u^4v^5 + \frac{6}{25}(k+l+k_1-8)u^5v^5 \\ &\quad +\frac{3}{10}(k+l+k_1-7)u^5v^8 + \frac{3}{32}(k+l+k_1-9)u^8v^8 \\ &\quad +\frac{1}{6}(k+l+k_1-5)u^8v^9 + \frac{3}{81}(k+l+k_1+25)u^9v^9, \end{aligned}$$

$$\begin{aligned} D_u^{\alpha}D_v^{\alpha}(f(u,v)) &= 6(16)^{\alpha}u^4v^4 + 12(20)^{\alpha}u^4v^5 + 6(25)^{\alpha}(k+l+k_1-8)u^5v^5 \\ &\quad +12(40)^{\alpha}(k+l+k_1-7)u^5v^8 + 6(64)^{\alpha}(k+l+k_1-9)u^8v^8 \\ &\quad +12(72)^{\alpha}(k+l+k_1-5)u^8v^9 + 3(81)^{\alpha}(k+l+k_1+25)u^9v^9, \end{aligned}$$

$$\begin{aligned} D_uD_v(D_u+D_v)(f(u,v)) &= 768u^4v^4 + 2160u^4v^5 + 1500(k+l+k_1-8)u^5v^5 \\ &\quad +6600(k+l+k_1-7)u^5v^8 + 6144(k+l+k_1-9)u^8v^8 \\ &\quad +14688(k+l+k_1-5)u^8v^9 + 4374(k+l+k_1+25)u^9v^9, \end{aligned}$$

$$\begin{aligned} (D_uS_v+S_uD_v)(f(u,v)) &= 12u^4v^4 + \frac{87}{5}u^4v^5 + 12(k+l+k_1-8)u^5v^5 \\ &\quad +\frac{267}{10}(k+l+k_1-7)u^5v^8 + 12(k+l+k_1-9)u^8v^8 \\ &\quad +\frac{145}{6}(k+l+k_1-5)u^8v^9 + 6(k+l+k_1+25)u^9v^9, \end{aligned}$$

$$\begin{aligned} S_uJ(f(u,v)) &= \frac{3}{4}u^8 + \frac{4}{3}u^9 + \frac{3}{5}(k+l+k_1-8)u^{10} \\ &\quad +\frac{12}{13}(k+l+k_1-7)u^{13} + \frac{3}{8}(k+l+k_1-9)u^{16} \\ &\quad +\frac{12}{17}(k+l+k_1-5)u^{17} + \frac{1}{6}(k+l+k_1+25)u^{18}, \end{aligned}$$

$$\begin{aligned} S_uJD_uD_v(f(u,v)) &= 12u^8 + \frac{80}{3}u^9 + 15(k+l+k_1-8)u^{10} \\ &\quad +\frac{480}{13}(k+l+k_1-7)u^{13} + \frac{384}{16}(k+l+k_1-9)u^{16} \\ &\quad +\frac{972}{17}(k+l+k_1-5)u^{17} + \frac{243}{18}(k+l+k_1+25)u^{18}, \end{aligned}$$

$$\begin{aligned} S_u^3 Q_{-2} J D_u^3 D_v^3(f(u,v)) &= \frac{24576}{216}u^6 + \frac{96000}{343}u^7 + \frac{93750}{512}(k+l+k_1-8)u^8 \\ &+\frac{768000}{1331}(k+l+k_1-7)u^{11} + \frac{1572864}{2744}(k+l+k_1-9)u^{14} \\ &+\frac{4478976}{3375}(k+l+k_1-5)u^{15} + \frac{1594323}{4096}(k+l+k_1+25)u^{16}. \end{aligned}$$

Now, it is straightforward to compute the desired indices using the definitions provided in Table 1. □

5. Conclusion

Topological indices (TIs) serve as essential tools in understanding and predicting the physicochemical properties of nanotubes, molecular structures, and chemical compounds. Their significance spans various domains, including chemical information processing, structural uniqueness determination, chiral center identification, isomer enumeration, and the prediction of nuclear magnetic resonance (NMR) spectra.

In this study, we derived NM-polynomials for the line graph of the subdivision graph of three notable nanostructures: hexagonal parallelogram nanotubes (HCN), triangular benzenoids (TB), and zigzag-edge coronoids fused with starphene nanotubes (ZCFN). Based on these NM-polynomials, we computed ten neighborhood-based topological indices for each structure. The methodology adopted here for computing neighborhood-based TIs is both effective and computationally efficient, thus holding potential for wide applicability in quantitative structure–property relationships (QSPR) and quantitative structure–activity relationships (QSAR) modeling.

Future work could explore the formulation of eccentricity-based M-polynomials and the derivation of corresponding eccentricity-based TIs. This direction remains largely untapped and could offer new insights into molecular topology and its relationship to chemical properties.

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