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Topological Descriptor Analysis of Periodic Supramolecular Star Lattices *

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ABSTRACT: This study presents a comprehensive topological analysis of periodic molecular graphs derived from supramolecular star lattices. By leveraging the inherent symmetry and periodicity of the lattice, we derive closed-form expressions for a range of distance-based and degree-based topological indices. These descriptors quantitatively capture the connectivity and structural complexity of the supramolecular framework, offering insights that support future exploration in nanomaterials design. The results strengthen the theoretical understanding of extended molecular networks and lay the groundwork for potential applications in materials modeling and computational chemistry.

Keywords: Molecular graphs, topological indices, distance, degree.

Contents

1. Introduction

The study of molecular graphs as a mathematical representation of chemical structures has long been a foundational aspect of theoretical chemistry and nanomaterials science [1,2]. Molecular graphs abstract molecules into vertices representing atoms (or groups of atoms) and edges representing chemical bonds or interactions. This abstraction enables the application of graph-theoretic techniques to quantitatively analyze molecular structures, predict their physicochemical properties, and design new materials with targeted functionalities [3]. Among the various graph invariants developed, distance-based and degree-based topological indices have proven to be particularly insightful. Distance-based indices capture the spatial relationships within a molecular graph by quantifying distances between vertices and edges [4,5], while degree-based indices characterize local structural features by incorporating vertex degrees, reflecting atomic connectivity and branching patterns [2,5]. The mathematical formulations for the most commonly used distance-based and degree-based topological indices are listed in Table 1 and Table 2, respectively. These definitions form the basis for our analytical derivations in the subsequent sections.

Distance-based topological indices such as the Wiener index, Szeged index, and their variants provide numerical summaries of how molecular components are interconnected through shortest paths or weighted distances. These indices correlate strongly with diverse molecular properties, including stability, reactivity, boiling points, and biological activity [6]. Consequently, their computation is not only of theoretical interest but also of practical importance in cheminformatics, materials science, and drug design [7,8].

In recent years, the rapid development of nanotechnology and supramolecular chemistry has introduced new classes of extended molecular frameworks, often exhibiting periodic structures with remarkable physical and chemical properties. Among these, supramolecular lattices have garnered significant attention [9]. Unlike conventional covalent networks, supramolecular lattices arise from the self-assembly of

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molecular or supramolecular building blocks through non-covalent interactions such as hydrogen bonding, metal coordination and $\pi - \pi$ stacking. These lattices exhibit a high degree of order and periodicity, forming complex architectures that can be effectively modeled as infinite periodic molecular graphs [10].

One particular supramolecular motif of interest is the star lattice, a repetitive pattern wherein each unit cell consists of a central vertex connected radially to peripheral vertices, resembling a star. When such star motifs are periodically arranged to form a lattice, they generate intricate networks that present unique challenges and opportunities for topological analysis. The inherent symmetry and periodicity of these supramolecular star lattices can be exploited to develop generalized and scalable mathematical expressions for topological indices, facilitating efficient characterization of large or infinite frameworks [11,12].

Despite their growing significance, systematic studies focusing on the computation of distance-based and degree-based topological indices for molecular graphs modeled on supramolecular star lattices remain limited. This gap is mainly due to the complexity introduced by the infinite periodicity and the rich connectivity patterns of these lattices. Hence, there is a strong motivation to develop rigorous graph-theoretic methods and analytical tools to address this challenge [12].

In this paper, we aim to fill this gap by presenting a comprehensive methodology for computing several key distance-based and degree-based topological indices for periodic molecular graphs derived from supramolecular star lattices. By leveraging the periodic structure and the symmetry properties of the lattice, we derive closed-form analytical expressions that capture essential topological features related to vertex and edge distances. These expressions not only simplify the computation of indices for infinite or large-scale lattices but also provide deeper insights into the connectivity and spatial organization of the lattice components.

The significance of this work extends beyond theoretical interest. Accurate topological characterization of supramolecular star lattices has potential applications in the rational design of nanomaterials with tailor-made properties, including enhanced mechanical strength, optimized electronic behavior, and selective chemical reactivity [9,11,12]. Furthermore, understanding the topological relationship within these lattices can aid in modeling transport phenomena, energy transfer processes, and interaction pathways relevant to catalysis and sensor design.

The structure of the paper is as follows. We begin by formalizing the construction of the periodic molecular graph representing the supramolecular star lattice. Next, we introduce the selected family of distance-based and degree-based topological indices and outline the methodology for their computation, emphasizing the exploitation of lattice symmetry and cut techniques. We then present the derived analytical expressions and illustrate their significance through numerical examples. Finally, we conclude by summarizing the main contributions and proposing directions for future research.

2. Graph-Theoretical Terminology

Let $G = (V, E)$ be a molecular graph, where V represents the set of vertices (atoms), and E denotes the set of edges (bonds). The degree of a vertex $v \in V$ is denoted by $d_G(v)$, and the shortest-path distance between any two vertices $u, v \in V$ is denoted by $d_G(u, v)$. For simplicity, we may drop the subscript and write $d(v)$ instead of $d_G(v)$, and $d(u, v)$ instead of $d_G(u, v)$, wherever the context makes it clear. The distance from a vertex u to an edge $e = xy \in E$ is defined as $d(u, e) = \min\{d(u, x), d(u, y)\}$. Similarly, for edges $e = uv$ and $f = xy$, the edge-to-edge distance is defined by $D(e, f) = \min\{d(u, f), d(v, f)\}, \quad \text{where} \quad d(u, f) = \min\{d(u, x), d(u, y)\}$.

For an edge $e = uv \in E(G)$, define:

- $N_u(e \mid G)$: the set of vertices closer to u than to v,
- $M_u(e \mid G)$: the set of edges closer to u than to v,

with corresponding cardinalities given by $n_u(e|G) = |N_u(e|G)|$, and $m_u(e|G) = |M_u(e|G)|$. Analogous definitions apply for $n_v(e|G)$ and $m_v(e|G)$, considering proximity to v over u.

The cut method has proven to be highly effective in the study of distance-based graph invariants, which are among the fundamental concepts in chemical graph theory [13,14]. This approach partitions the edge set according to the Djoković–Winkler relation Θ, defined as follows: for any two edges $e = uv$

and $f = xy$ in $E(G)$, the condition $d_G(u,x) + d_G(v,y) \neq d_G(u,y) + d_G(v,x)$ holds. The relation Θ is always reflexive and symmetric, but in general it is not transitive. For partial cubes, however, Θ is transitive, and it partitions $E(G)$ into subsets $F_1, F_2, \ldots, F_r$ known as Θ-classes or cuts. The transitive closure Θ^* forms an equivalence relation, and removing any Θ^*-class from G produces two or more convex components. A partition $\mathscr{E} = \{E_1, E_2, \ldots, E_k\}$ of $E(G)$ is said to be *coarser* than the partition $\mathscr{F}$ if each E_i is the union of one or more Θ^*-classes of G. For any class E_i, the *quotient graph* G/E_i is obtained from the disconnected graph $G \setminus E_i$ by treating each connected component as a vertex; two such components C_j^i and C_k^i are adjacent whenever there exist $x \in C_j^i$ and $y \in C_k^i$ such that $xy \in E_i$.

Table 1: Mathematical expressions of selected distance-based topological indices commonly used in molecular graph analysis.

Topological Index	**Mathematical Expression**
Wiener	$W(G_{sw}) = \sum_{u,v \in V(G_{sw})} w_v(u) w_v(v) d_{G_{sw}}(u,v)$
Edge–Wiener	$W_e(G_{sw}) = \sum_{u,v \in V(G_{sw})} s_v(u) s_v(v) d_{G_{sw}}(u,v) + \sum_{e,f \in E(G_{sw})} s_e(e) s_e(f) D_{G_{sw}}(e,f) + \sum_{u \in V(G_{sw})} \sum_{f \in E(G_{sw})} s_v(u) s_e(f) d_{G_{sw}}(u,f)$
Vertex–Edge–Wiener	$W_{ve}(G_{sw}) = \frac{1}{2}\Big[\sum_{u,v \in V(G_{sw})} (w_v(u) s_v(v) + w_v(v) s_v(u)) d_{G_{sw}}(u,v) + \sum_{u \in V(G_{sw})} \sum_{f \in E(G_{sw})} w_v(u) s_e(f) d_{G_{sw}}(u,f)\Big]$
Vertex–Szeged	$Sz_v(G_{sw}) = \sum_{e=uv \in E(G_{sw})} s_e(e) n_u(e\|G_{sw}) n_v(e\|G_{sw})$
Edge–Szeged	$Sz_e(G_{sw}) = \sum_{e=uv \in E(G_{sw})} s_e(e) m_u(e\|G_{sw}) m_v(e\|G_{sw})$
Edge–Vertex–Szeged	$Sz_{ev}(G_{sw}) = \frac{1}{2} \sum_{e=uv \in E(G_{sw})} s_e(e) \big[n_u(e\|G_{sw}) m_v(e\|G_{sw}) + n_v(e\|G_{sw}) m_u(e\|G_{sw})\big]$
Padmakar–Ivan	$PI(G_{sw}) = \sum_{e=uv \in E(G_{sw})} s_e(e) \big[m_u(e\|G_{sw}) + m_v(e\|G_{sw})\big]$
Schultz	$S(G_{sw}) = \sum_{u,v \in V(G_{sw})} \big[w_v(v) d_{G_{sw}}(u) + w_v(u) d_{G_{sw}}(v)\big] d_{G_{sw}}(u,v)$
Gutman	$Gut(G_{sw}) = \sum_{u,v \in V(G_{sw})} d_{G_{sw}}(u) d_{G_{sw}}(v) d_{G_{sw}}(u,v)$

The concept of a strength-weighted graph was initially introduced in [15] and further explored in [16,17,18,19,20,21]. Such a graph is denoted by $G_{sw} = (G, (w_v, s_v), s_e)$, where the vertex-weight function $w_v : V(G_{sw}) \to \mathbb{R}_0^+$ assigns non-negative real weights to the vertices, the vertex-strength function $s_v : V(G_{sw}) \to \mathbb{R}_0^+$ assigns non-negative real strengths to the vertices, and the edge-strength function $s_e : E(G_{sw}) \to \mathbb{R}_0^+$ assigns non-negative real strengths to the edges. In a strength-weighted graph, the distances satisfy $d_{G_{sw}}(u,v) = d_G(u,v)$, $d_{G_{sw}}(u,f) = d_G(u,f)$, and $D_{G_{sw}}(e,f) = D_G(e,f)$. Moreover, the neighbor and mutual neighbor sets satisfy $N_u(e \mid G_{sw}) = N_u(e \mid G)$ and $M_u(e \mid G_{sw}) = M_u(e \mid G)$. The corresponding weighted parameters are $n_u(e \mid G_{sw}) = \sum_{x \in N_u(e|G_{sw})} w_v(x)$ and $m_u(e \mid G_{sw}) = \sum_{x \in N_u(e|G_{sw})} s_v(x) + \sum_{f \in M_u(e|G_{sw})} s_e(f)$. The definitions of $n_v(e \mid G_{sw})$ and $m_v(e \mid G_{sw})$ are analogous. The degree of a vertex u in G_{sw} is given by $d_{G_{sw}}(u) = 2s_v(u) + \sum_{x \in N_{G_{sw}}(u)} s_e(ux)$. Several topological indices (TI) for strength-weighted graphs have been studied in [18] and are summarized in Table 1, with the property that $TI(G_{sw}) = TI(G)$ whenever $w_v = 1$, $s_v = 0$, and $s_e = 1$.

Theorem 2.1 *[15,18,22] Let $G_{sw} = (G,(w_v,s_v),s_e)$ be a strength-weighted graph, and let $\mathscr{E} = \{E_1, E_2, \dots, E_k\}$ be a partition of $E(G)$ that is coarser than $\mathscr{F}$. Suppose* TI *denotes a topological index such as W, W_e, W_{ve}, Sz_v, Sz_e, Sz_{ev}, Sz_t, PI, S, or* Gut. *Then*

$$\mathrm{TI}(G_{sw}) = \sum_{i=1}^{k} \mathrm{TI}\big(G/E_i, (w_v^i, s_v^i), s_e^i\big),$$

where:
(i) $w_v^i : V(G/E_i) \to \mathbb{R}_0^+$ is defined by $w_v^i(C) = \sum_{x\in C} w_v(x)$, for every connected component C of G/E_i,
(ii) $s_v^i : V(G/E_i) \to \mathbb{R}_0^+$ is defined by $s_v^i(C) = \sum_{xy\in C} s_e(xy) + \sum_{x\in C} s_v(x)$, for every connected component C of G/E_i,
(iii) $s_e^i : E(G/E_i) \to \mathbb{R}_0^+$ is defined as the number of edges in E_i having one endpoint in C and the other in D, for any two connected components C and D of G/E_i.

Table 2: Mathematical expressions of selected degree-based topological indices commonly used in molecular graph analysis.

Topological Index	**Mathematical Expression**
First Zagreb	$M_1(G) = \sum_{uv\in E(G)} \big[d(u)+d(v)\big]$
Second Zagreb	$M_2(G) = \sum_{uv\in E(G)} d(u)d(v)$
Harmonic	$H(G) = \sum_{uv\in E(G)} \frac{2}{d(u)+d(v)}$
Weighted Harmonic	$HM(G) = \sum_{uv\in E(G)} \frac{2\,d(u)d(v)}{d(u)+d(v)}$
Augmented Zagreb	$AZ(G) = \sum_{uv\in E(G)} \frac{d(u)d(v)}{d(u)+d(v)-2}$
Modified Harmonic	$I(G) = \sum_{uv\in E(G)} \frac{d(u)d(v)}{d(u)+d(v)}$
Geometric–Arithmetic	$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}$
Atom–Bond Connectivity	$ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$
Randić	$R(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$
Sum of Degree Difference	$SDD(G) = \sum_{uv\in E(G)} \lvert d(u)-d(v)\rvert$

3. Results and Discussion

We consider a novel two-dimensional supramolecular structure, modeled as a periodic molecular graph and denoted by $G_{m,n}$. This graph is constructed from repeating star-like units that reflect the underlying geometry of supramolecular star lattices. Each unit is isomorphic to the complete bipartite graph $K_{1,8}$, representing a central molecular site with eight coordinated vertices. The full lattice includes two types of stars: primary stars, arranged in a regular $m \times n$ grid, where m and n denote the number of rows and columns of primary star units, respectively, and interstitial stars, each placed between four neighboring primary stars to enhance structural cohesion. These interstitial units share peripheral vertices with

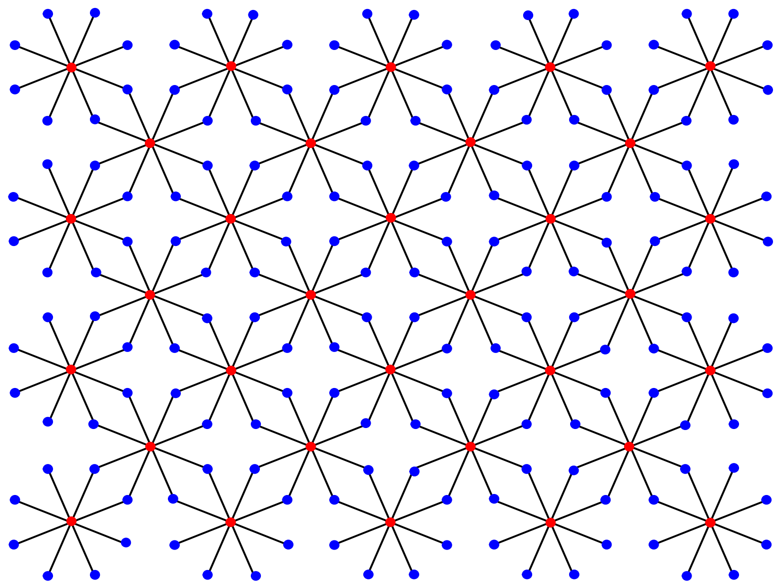

Figure 1: The supramolecular star lattice $G_{4,5}$, consisting of primary star units arranged in a 4×5 grid and interstitial star units placed between adjacent primary units. Each star unit is isomorphic to the complete bipartite graph $K_{1,8}$, forming a periodic, vertex-sharing molecular graph.

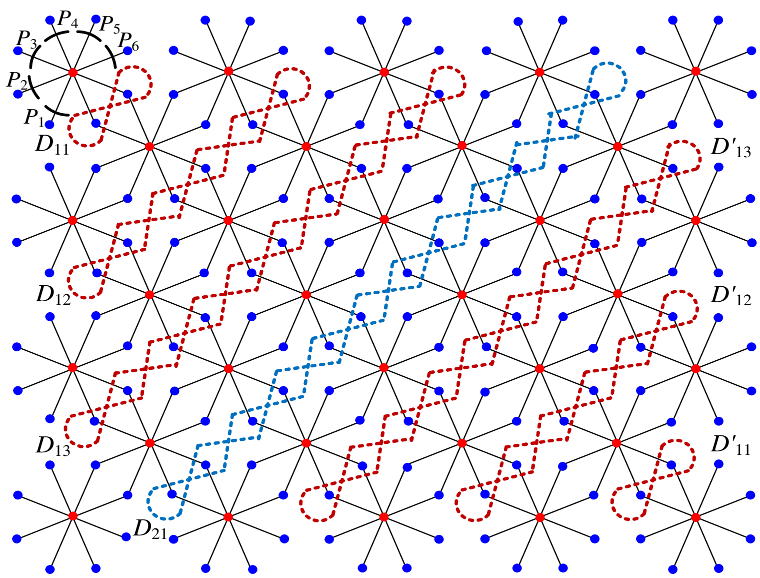

Figure 2: Edge-cut illustration on the supramolecular star lattice $G_{4,5}$. The figure highlights pendant edge cuts along the outer boundary and representative acute diagonal cuts used in the application of the cut method.

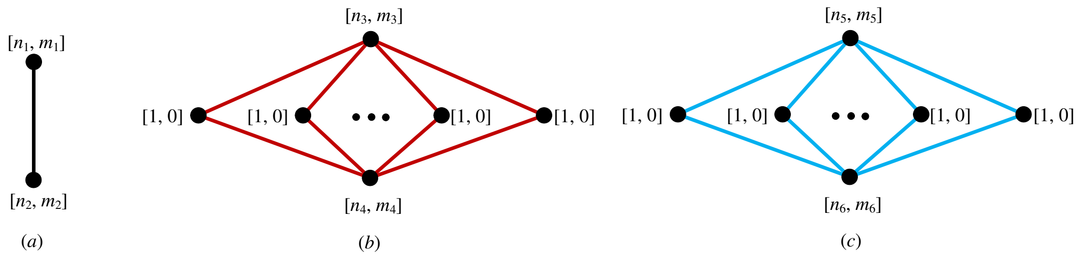

Figure 3: (a) $G_{m,n}/P_i$ (b) $G_{m,n}/D_{1t}$ (c) $G_{m,n}/D_{2t}$

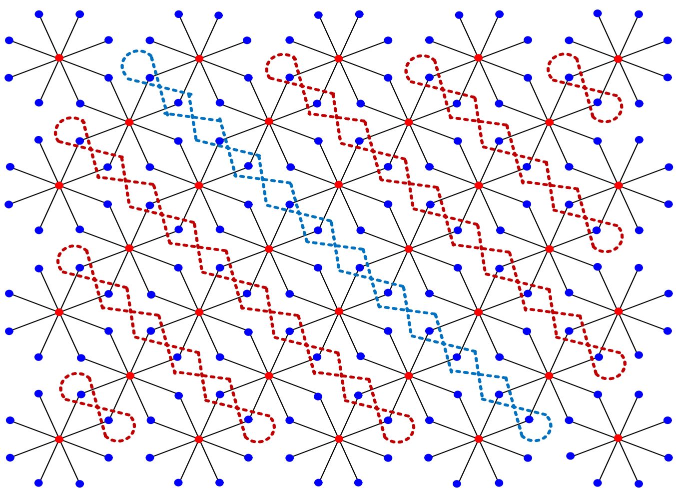

Figure 4: Edge-cut illustration on the supramolecular star lattice $G_{4,5}$. The figure highlights representative obtuse diagonal cuts, which are symmetric counterparts to the acute cuts shown in Figure 2, and are also employed in the application of the cut method.

adjacent primary stars, resulting in a highly interconnected, vertex-sharing lattice. A visual depiction of the supramolecular star lattice $G_{m,n}$ with $m = 4$ and $n = 5$ is shown in Figure 1, illustrating the arrangement of primary and interstitial star units.

The total number of star units in the lattice is $mn+(m-1)(n-1)$, and each contributes eight edges, producing a highly symmetric and robust molecular graph. This molecular graph enables the systematic derivation of closed-form expressions for several distance-based and degree-based topological indices, providing a scalable framework for analyzing the structural complexity of extended supramolecular networks.

3.1. Distance-based topological indices for $G_{m,n}$

In this section, we analyze several distance-based topological indices for the supramolecular star lattice $G_{m,n}$, including the Wiener, Szeged, PI, Schultz, and Gutman indices. These descriptors quantify the overall structural connectivity and molecular complexity of the lattice.

To derive closed-form expressions for these indices, we apply the cut method by partitioning the edge set of $G_{m,n}$ into pendant and diagonal cuts, as will be detailed in the proof of Theorem 3.1. The use of quotient graphs simplifies computation while preserving essential distance relationship.

The following theorem presents the exact formulas for each index as a function of the lattice parameters m and n.

Theorem 3.1 *Let $G_{m,n}$ be the molecular graph of a supramolecular star lattice with $m, n \geq 1$. Then*

$$(i) W(G) = \frac{1}{3}\big[-20m^5 + 100m^4n - 40m^3n + 166m^3 + 200m^2n^3 - 60m^2n^2 - 186m^2n - 30m^2 - 40mn^3 + 306mn^2 - 136mn - 116m + 2n^3 - 30n^2 + 76n\big]$$

$$(ii) W_e(G) = \frac{8}{15}\big[-32m^5 + 160m^4n - 320m^3n + 220m^3 + 320m^2n^3 - 720m^2n^2 + 660m^2n - 360m^2 - 320mn^3 + 1080mn^2 - 1055mn + 337m + 80n^3 - 360n^2 + 475n - 165\big]$$

$$(iii) W_{ve}(G) = \frac{4}{3}\big[-8m^5 + 40m^4n - 48m^3n + 56m^3 + 80m^2n^3 - 102m^2n^2 + 9m^2n - 39m^2 - 48mn^3 + 165mn^2 - 93mn + 3m + 4n^3 - 39n^2 + 53n - 12\big]$$

$$(iv) Sz_v(G) = \frac{8}{3}\big[9m^5 - 45m^4n + 92m^4 + 100m^3n^3 - 30m^3n^2 - 163m^3n - 130m^3 - 120m^2n^3 + 63m^2n^2 + 381m^2n - 80m^2 + 21mn^3 - 6mn^2 - 237mn + 145m - n^3 + 61n - 36\big]$$

$$(v) Sz_e(G) = \frac{16(m-1)}{15}\big[32m^4 + 272m^3 + 640m^2n^3 - 1440m^2n^2 + 320m^2n - 308m^2 - 640mn^3 + 2160mn^2 - 1220mn + 52m + 160n^3 - 720n^2 + 605n - 75\big]$$

$$(vi) Sz_{ev}(G) = \frac{4}{15}\big[112m^5 - 360m^4n + 1140m^4 + 1600m^3n^3 - 2040m^3n^2 - 1240m^3n - 1820m^3 - 2560m^2n^3 + 4380m^2n^2 + 2920m^2n - 810m^2 + 1040mn^3 - 1200mn^2 - 2090mn + 1933m - 80n^3 + 180n^2 + 755n - 555\big]$$

$$(vii) PI(G) = \frac{1}{3}\big[64m^3 + 768m^2n^2 - 960m^2n + 192m^2 - 768mn^2 + 1536mn - 568m + 192n^2 - 600n + 312\big]$$

$$(viii) S(G) = \frac{8}{3}\big[-16m^5 + 80m^4n - 96m^3n + 112m^3 + 160m^2n^3 - 144m^2n^2 - 18m^2n - 75m^2 - 96mn^3 + 294mn^2 - 144mn + 8n^3 - 75n^2 + 100n - 21\big]$$

$$(ix) Gut(G) = \frac{8}{15}\big[-128m^5 + 640m^4n - 1280m^3n + 920m^3 + 1280m^2n^3 - 1920m^2n^2 + 1560m^2n - 1200m^2 - 1280mn^3 + 3360mn^2 - 2540mn + 753m + 320n^3 - 1200n^2 + 1285n - 345\big]$$

Quotient Graph	**Vertex Weight** w_v	**Vertex Strength** s_v	**Edge Strength** s_e
G/P_i $1 \leq i \leq 8m+8n-8$	$n_1 = 1$ $n_2 = 10mn - m - n$	$m_1 = 0$ $m_2 = 16mn - 8m - 8n + 7$	1
G/D_{1t} $1 \leq t \leq m-1$	$n_3 = 5t^2 + 2t$ $n_4 = \lvert V(G)\rvert - n_3 - (4t-2)$	$m_3 = 8t^2 - 4t + 2$ $m_4 = \lvert E(G)\rvert - m_3 - (8t-4)$	$8t - 4$
G/D_{2t} $m \leq t \leq n-1$	$n_5 = 10mt - 5m^2 + 3m - t + 2$ $n_6 = \lvert V(G)\rvert - n_5 - (4m-4)$	$m_5 = 16mt - 8m^2 + 4m - 8t + 4$ $m_6 = \lvert E(G)\rvert - m_5 - (8m-8)$	$8m - 8$

Table 3: Weight measures associated with the quotient graphs used in the cut method for the supramolecular star lattice $G_{m,n}$. The values correspond to vertex weights, vertex strengths, and edge strengths across different edge partitions.

Proof: The graph $G_{m,n}$ consists of $10mn - m - n + 1$ vertices and $16mn - 8m - 8n + 8$ edges. A total of $8m + 8n - 8$ pendant edge cuts, denoted by $\{P_i : 1 \leq i \leq 8m + 8n - 8\}$, are identified along the outer boundary of the lattice and correspond to the removal of boundary edges. The classification of pendant edge cuts used in this method is illustrated in Figure 2. Apart from these boundary cuts, three families of internal diagonal cuts are considered: $\{D_{1t} : 1 \leq t \leq m-1\}$, $\{D'_{1t} : 1 \leq t \leq m-1\}$, and $\{D_{2t} : m \leq t \leq n-1\}$. Here, D_{1t} and D'_{1t} represent symmetric diagonal cuts. The quotient graphs resulting from $G_{m,n}/P_i$, $G_{m,n}/D_{1t}$, and $G_{m,n}/D_{2t}$ are (a) a path on two vertices (b) a complete bipartite graph $K_{2,4t-2}$ (c) a complete bipartite graph $K_{2,4m-4}$ as shown in Figure 3. The associated vertex strength weight measures for these cuts are provided in Table 3. Owing to the inherent symmetry of $G_{m,n}$, the contribution of obtuse cuts is analogous to that of the acute ones. These symmetric cuts are visualized in Figure 4. Therefore, computations are carried out only for the acute diagonal cuts, and their contributions are appropriately doubled to account for their symmetric counterparts in the overall analysis.

$$(i)\ W(G) = n_1n_2(8m+8n-8) + 2\Bigg[2\sum_{t=1}^{m-1}\big[(4t-2)(n_3+n_4) + 2n_3n_4 + (4t-2)(4t-3)\big] + \sum_{t=m}^{n-1}\big[(4m-4)(n_5+n_6) + 2n_5n_6 + (4m-4)(4m-5)\big]\Bigg].$$

$$(ii)\ W_e(G) = m_1m_2(8m+8n-8) + 2\Bigg[2\sum_{t=1}^{m-1}\big[(4t-2)(m_3+m_4) + 2m_3m_4 + (4t-2)(4t-3)\big] + \sum_{t=m}^{n-1}\big[(4m-4)(m_5+m_6) + 2m_5m_6 + (4m-4)(4m-5)\big]\Bigg].$$

$$(iii)\ W_{ve}(G) = \tfrac{1}{2}\Bigg[(n_1m_2+n_2m_1)(8m+8n-8) + 2\Bigg[2\sum_{t=1}^{m-1}\big[(4t-2)(n_3+n_4+m_3+m_4) + 2(n_3m_4+n_4m_3) + 2(4t-2)(4t-3)\big] + \sum_{t=m}^{n-1}\big[(4m-4)(n_5+n_6+m_5+m_6) + 2(n_5m_6+n_6m_5) + 2(4m-4)(4m-5)\big]\Bigg]\Bigg].$$

$$(iv)\ Sz_v(G) = n_1n_2(8m+8n-8) + 2\Bigg[2\sum_{t=1}^{m-1}(4t-2)\big[(n_3+4t-3)(n_4+1) + (n_4+4t-3)(n_3+1)\big] + \sum_{t=m}^{n-1}(4m-4)\big[(n_5+4m-5)(n_6+1) + (n_6+4m-5)(n_5+1)\big]\Bigg].$$

$$(v)\ Sz_e(G) = m_1m_2(8m+8n-8) + 2\Bigg[2\sum_{t=1}^{m-1}(4t-2)\big[(m_3+4t-3)(m_4+1) + (m_4+4t-3)(m_3+1)\big] + \sum_{t=m}^{n-1}(4m-4)\big[(m_5+4m-5)(m_6+1) + (m_6+4m-5)(m_5+1)\big]\Bigg].$$

$$(vi)\ Sz_{ev}(G) = \tfrac{1}{2}\Bigg[(n_1m_2+n_2m_1)(8m+8n-8)+2\Bigg[2\sum_{t=1}^{m-1}(4t-2)\big[(n_3+4t-3)(m_4+1) + (m_3+4t-3)(n_4+1)+(n_4+4t-3)(m_3+1)+(m_4+4t-3)(n_3+1)\big] + \sum_{t=m}^{n-1}(4m-4)\big[(n_5+4m-5)(m_6+1)+(m_5+4m-5)(n_6+1) + (n_6+4m-5)(m_5+1)+(m_6+4m-5)(n_5+1)\big]\Bigg]\Bigg].$$

$$(vii)\ PI(G) = (m_1+m_2)(8m+8n-8)+2\Bigg[2\sum_{t=1}^{m-1}\big[(4t-2)(2(m_3+m_4)+8t-4)\big] + \sum_{t=m}^{n-1}\big[(4m-4)(2(m_5+m_6)+8m-8)\big]\Bigg].$$

$$(viii)\ S(G) = \big[n_1(2m_2+1)+n_2(2m_1+1)\big](8m+8n-8)+2\Bigg[2\sum_{t=1}^{m-1}\big[(4t-2)\big[2(n_3+n_4+m_3+m_4) + (8t-4)\big]+2\big[n_3(2m_4+4t-2)+n_4(2m_3+4t-2)\big]+4(4t-2)(4t-3)\big] + \sum_{t=m}^{n-1}\big[(4m-4)\big[2(n_5+n_6+m_5+m_6)+(8m-8)\big]+2\big[n_5(2m_6+4m-4) + n_6(2m_5+4m-4)\big]+4(4m-4)(4m-5)\big]\Bigg].$$

$$(ix)\ Gut(G) = (2m_2+1)(2m_1+1)(8m+8n-8)+2\Bigg[2\sum_{t=1}^{m-1}\big[(8t-4)\big[2(m_3+m_4)+(8t-4)\big] + 2\big[(2m_3+4t-2)(2m_4+4t-2)\big]+4(4t-2)(4t-3)\big] + \sum_{t=m}^{n-1}\big[(8m-8)\big[2(m_5+m_6)+(8m-8)\big]+2\big[(2m_5+4m-4)(2m_6+4m-4)\big] + 4(4m-4)(4m-5)\big]\Bigg].$$

The proof concludes upon substitution of the expressions from Table 3 followed by direct simplification. □

The numerical values of the indices listed in Table 1 are evaluated for different $m = n$ values and presented in Table 4. A graphical comparison of the growth behavior of the distance-based topological indices is shown in Figure 5.

3.2. Degree-based topological indices for $G_{m,n}$

This subsection focuses on the computation of degree-based topological indices for the supramolecular star lattice $G_{m,n}$. These indices including the first and second Zagreb indices, harmonic, inverse sum, augmented Zagreb, geometric-arithmetic, atom–bond connectivity, and Randić-type descriptors capture the local structural features and branching complexity of the molecular graph.

Table 4: Numerical values of selected distance-based topological indices for the supramolecular star lattices $G_{m,n}$ with $m = n$ ranging from 1 to 10.

TI	$W(G)$	$W_e(G)$	$W_{ve}(G)$	$Sz_v(G)$	$Sz_e(G)$	$Sz_{ev}(G)$	$PI(G)$	$S(G)$	$Gut(G)$
(1,1)	64	0	28	64	0	56	56	184	0
(2,2)	2720	1736	2272	8288	2805.33	15368	2152	10568	8168
(3,3)	20864	20448	21052	223008	249632	484600	19672	93048	92960
(4,4)	88672	105608	97920	2040384	2675136	4703816	94472	422280	467592
(5,5)	272800	363392	317628	10878080	15340309.33	25944760	315768	1349560	1579968
(6,6)	683584	979208	824128	41852064	61749856	102110344	839080	3466824	4202792
(7,7)	1486240	2240224	1836572	129343328	196970976	320784248	1905176	7670648	9523680
(8,8)	2912064	4557896	3665312	341491328	532470485.33	857531592	3859016	15226248	19235272
(9,9)	5269632	8490496	6727900	800650944	1271587200	2030307640	7168696	27831480	35625344
(10,10)	8956000	14765640	11565088	1710849760	2757556512	4372831496	12444392	47680840	61666920

The analysis is based on a degree-partitioned edge set, where edges are grouped according to the degree pairs of their endpoints. The total number of edges in each partition is given in Table 5. By applying the respective mathematical expressions to each group and simplifying, we derive closed-form formulas for all considered indices.

The following theorem summarizes these results.

Table 5: Number of edges in each set of the partition based on vertex degree pairs $(d(u), d(v))$ for edges $uv \in E(G)$.

$(d(u), d(v))$ **where** $uv \in E(G)$	**Number of Edges**
$(1, 8)$	$8m + 8n - 8$
$(2, 8)$	$16(m - 1)(n - 1)$

Theorem 3.2 *Let $G_{m,n}$ be the molecular graph of a supramolecular star lattice with $m, n \geq 1$. Then*

$$\begin{aligned}
&\text{(i)} && M_1(G_{m,n}) &&= 160mn - 88m - 88n + 88\\
&\text{(ii)} && M_2(G_{m,n}) &&= 256mn - 192m - 192n + 192\\
&\text{(iii)} && H(G_{m,n}) &&= \frac{1}{45}(144mn - 64m - 64n + 64)\\
&\text{(iv)} && HM(G_{m,n}) &&= \frac{16}{45}(144mn - 104m - 104n + 104)\\
&\text{(v)} && AZ(G_{m,n}) &&= \frac{1}{7}(224mn - 160m - 160n + 160)\\
&\text{(vi)} && I(G_{m,n}) &&= \frac{8}{45}(144mn - 104m - 104n + 104)\\
&\text{(vii)} && GA(G_{m,n}) &&= \frac{1}{45}\Big(10\sqrt{8}(8m + 8n - 8) + 576(m-1)(n-1)\Big)\\
&\text{(viii)} && ABC(G_{m,n}) &&= \sqrt{\frac{7}{8}}(8m + 8n - 8) + 8\sqrt{2}(m-1)(n-1)\\
&\text{(ix)} && R(G_{m,n}) &&= \sqrt{\frac{1}{8}}(8m + 8n - 8) + 4(m-1)(n-1)\\
&\text{(x)} && SDD(G_{m,n}) &&= 96mn - 40m - 40n + 40
\end{aligned}$$

Proof: It is clear that $G_{m,n}$ has $8(m - 2) + 8(n - 2) + 24$ vertices of degree 1, $8(m - 1)(n - 1)$ vertices of degree 2, $mn + (m - 1)(n - 1)$ vertices of degree 8. Substituting the formulas from Table 2 along with the corresponding values from Table 5, and applying direct calculations, the proof is readily obtained. □

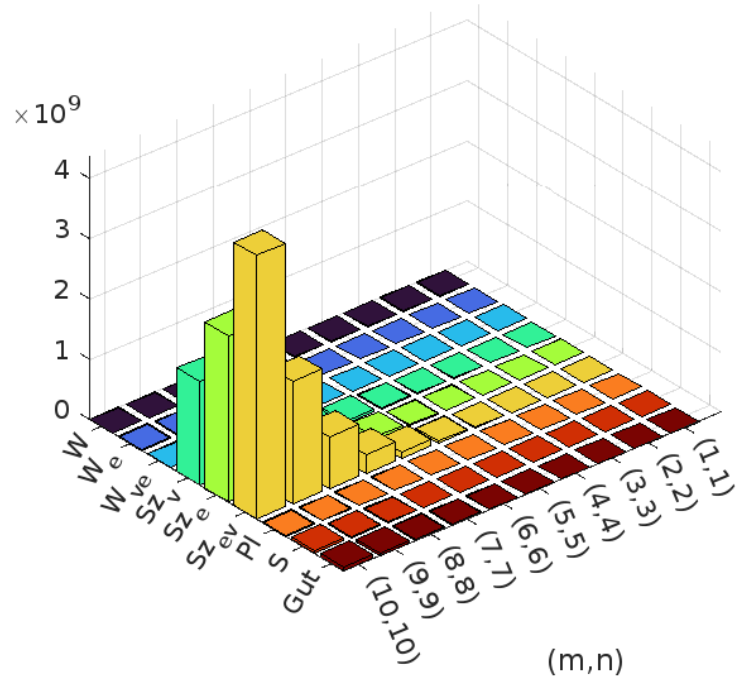

Figure 5: Graphical comparison of distance-based topological indices for the supramolecular star lattices $G_{m,n}$ with $m = n$ ranging from 1 to 10. The plots visualize the growth behavior of indices such as Wiener, Szeged, PI, Schultz, and Gutman, reflecting structural complexity as the lattice expands.

Based on the definitions from Table 2, the numerical results for varying lattice sizes are summarized in Table 6. The trends in the computed degree-based indices are summarized graphically in Figure 6.

Table 6: Numerical values of selected degree-based topological indices for the supramolecular star lattices $G_{m,n}$ with $m = n$ from 1 to 10.

TI	$M_1(G)$	$M_2(G)$	$H(G)$	$HM(G)$	$AZ(G)$	$I(G)$	$GA(G)$	$ABC(G)$	$R(G)$	$SDD(G)$
(1,1)	72	64	1.7778	28.4444	9.1429	14.2222	25.2982	0.0000	0.0000	56
(2,2)	304	448	7.1111	113.7778	36.5714	56.8889	107.1926	21.4500	13.3137	248
(3,3)	648	1024	15.1111	241.7778	78.8571	120.8889	207.0869	50.9000	31.6274	552
(4,4)	1104	1792	25.7778	412.4444	136.0000	206.2222	324.9811	87.3500	54.9411	968
(5,5)	1672	2688	39.1111	624.7778	208.0000	312.8889	460.8753	130.8000	83.2548	1496
(6,6)	2352	3712	55.1111	878.7778	294.8571	440.8889	614.7696	181.2500	116.5685	2136
(7,7)	3144	4864	73.7778	1174.4444	396.5714	590.2222	786.6638	238.7000	154.8822	2896
(8,8)	4048	6144	95.1111	1511.7778	513.1429	760.8889	976.5580	303.1500	198.1959	3776
(9,9)	5064	7552	119.1111	1889.7778	644.5714	952.8889	1184.4523	374.6000	246.5096	4776
(10,10)	6192	9088	145.7778	2309.4444	790.8571	1166.2222	1410.3465	453.0500	299.8233	5896

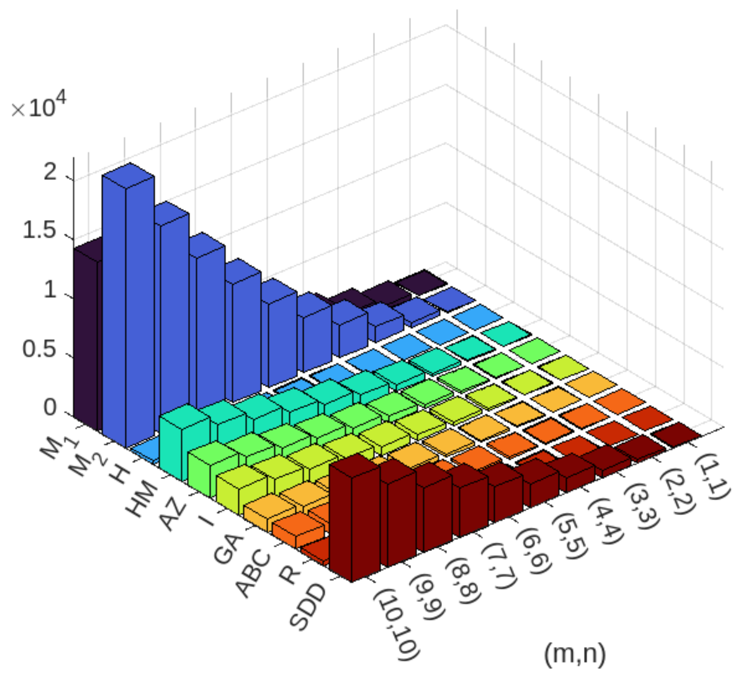

Figure 6: Graphical comparison of degree-based topological indices for the supramolecular star lattices $G_{m,n}$ with $m = n$ from 1 to 10. The figure illustrates trends in indices such as the first and second Zagreb, harmonic, ABC, and Randić indices as the lattice scales in size.

4. Conclusion

This work presents a comprehensive analytical investigation of distance-based and degree-based topological indices for periodic molecular graphs modeled on supramolecular star lattices. By exploiting the inherent symmetry and structural regularity of the lattice, we have derived closed-form expressions for a variety of well-known descriptors, including the Wiener, Szeged, Zagreb indices, and others.

The results obtained deepen the mathematical understanding of periodic supramolecular systems and provide practical tools for characterizing their structural complexity. These findings are particularly relevant in materials chemistry, where such descriptors can guide the design of nanostructures with specific topological and functional properties.

Future directions include extending this framework to three-dimensional supramolecular architectures, exploring additional classes of topological indices, and integrating these descriptors into QSPR/QSAR models to uncover correlations with experimental properties and support rational molecular design.

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