International Journal of Science and Research (IJSR)
ISSN: 2319-7064
Impact Factor 2025: 7.089

Augmented Euler Sombor Indices on Lexicographic Product of Open Neighborhood Graphs

Dr. Akkilli Naresh[1], Rudrapati Bhuvaneswara Prasad[2]

Assistant Professor, Department of Mathematics & Computing, Central University of Andhra Pradesh, Janthaluru, Ananthapuramu 515701, A.P, India
Email: *akkilinaresh[at]gmail.com*

[2]Research Scholar, Department of Mathematics, Sri Krishnadevarya University, Ananthapuramu, Andhra Pradesh, India, 515 003
Email: *bhuvaneswaraprasad100[at]gmail.com*

Abstract: ***This paper introduces and investigates the Augmented Euler Sombor (AES) index and the Reciprocal Augmented Euler Sombor (RAES) index in the context of lexicographic product graphs formed from open neighborhood graphs. By merging the structural richness of Euler Sombor-type degree-based topological indices with the hierarchical complexity of lexicographic products over open neighborhood graphs, we derive exact closed-form formulas for eight novel theorems covering cycle, complete, and complete bipartite graph families and their open neighborhood counterparts. Each theorem is supported by detailed proofs and computational examples verified via MATLAB. We also apply the AES index to three prominent chemical drug structures- chloroquine, hydroxychloroquine, and remdesivir revealing quantitative correlations between molecular topology and index values. Comparative analysis with classical Sombor, Euler Sombor, and related indices demonstrates that the AES framework offers superior structural sensitivity. Our findings establish a foundational methodology bridging discrete graph theory, chemical graph theory, and network science.***

Keywords: Augmented Euler Sombor index, Open neighborhood graph, Lexicographic product, Topological indices, Chemical graph theory

1. Introduction

Graph theory serves as a fundamental pillar of discrete mathematics, offering powerful abstractions for modeling real-world systems ranging from social networks and biological pathways to communication infrastructure and chemical compounds. Among the most productive subfields is chemical graph theory, which encodes molecular structures as graphs and extracts invariant numerical descriptors- known as topological indices that correlate with physical, chemical, or biological properties of compounds.

Topological indices have been studied extensively since the introduction of the Wiener index in 1947 and the Randic connectivity index in 1975. More recently, the Sombor index defined by Gutman in 2021 as a geometry-inspired degree-based index has attracted remarkable research attention due to its discriminating power in QSPR and QSAR models. The Euler Sombor index, introduced by Gutman in 2024, extended this geometric paradigm to incorporate the product of vertex degrees, yielding a richer structural invariant.

Parallel to the development of topological indices, graph product operations have been studied as mechanisms for constructing complex graphs from simpler building blocks. Among these, the lexicographic product (also called the composition of graphs) stands out for modeling layered, hierarchical systems where one graph controls adjacency at a global level and another governs local interactions. Its non-commutative and non-associative nature makes it a particularly interesting object of mathematical study.

The open neighborhood graph N(G) of a graph G replaces each vertex with a representation of its open neighborhood, yielding a graph that encodes local adjacency patterns in a global structure. When combined with the lexicographic product, open neighborhood graphs produce intricate and computationally challenging graph families whose topological indices have not yet been systematically studied.

This paper bridges these two rich research directions. We introduce the Augmented Euler Sombor (AES) index and the Reciprocal Augmented Euler Sombor (RAES) index, then compute exact formulas for these indices over lexicographic products of open neighborhood graphs for three foundational graph families: cycles C_n, complete graphs K_n, and complete bipartite graphs $K_{n,n}$. We further compute the AES and RAES indices for three pharmacologically significant chemical drugs.

The remainder of this paper is organized as follows. Section 2 presents a literature review of relevant topological indices and graph products. Section 3 establishes preliminary definitions and notation. Section 4 contains eight original theorems with complete proofs and examples. Section 5 provides comparative analysis with established indices. Section 6 concludes with directions for future work, followed by a comprehensive reference list.

2. Literature Review

The study of topological indices emerged from the seminal work of Wiener [1] on path numbers and boiling points. Subsequently, the Randic index [2] became the most widely cited molecular descriptor, inspiring generations of connectivity-based indices. The Zagreb indices [3] introduced summation of squared degrees and products of adjacent degrees, setting the paradigm for degree-based descriptors.

The Sombor index $SO(G) = \Sigma\_\{uv \in E(G)\} \sqrt{(d(u)^2 + d(v)^2)}$, introduced by Gutman [4] in 2021, draws inspiration from Euclidean geometry and has been studied extensively for trees, unicyclic graphs, chemical graphs, and various graph operations.

Its extremal properties, spectral aspects, and chemical applications have been documented in numerous works [5–8].

The Euler Sombor index $EU(G) = Σ\_\{uv \in E(G)\} \sqrt{(d(u)^2 + d(v)^2 + d(u)d(v))}$, introduced by Gutman [9] in 2024, extended the Sombor framework by incorporating the product of endpoint degrees. This index was shown to be equivalent to the Nirmala alpha Gourava index [10] under certain parameterizations, highlighting deep connections among classes of topological descriptors.

Graph products have long been recognized as fundamental constructions in combinatorics and algebra. The Cartesian product, tensor product, strong product, and lexicographic product each impose different adjacency rules on the vertex set V(G) × V(H). The lexicographic product G[H] was studied algebraically by Sabidussi [11] and has found applications in coding theory, network design, and combinatorial optimization.

Open neighborhood graphs were formally studied in the context of domination theory by Haynes, Hedetniemi, and Slater [12], who examined how neighborhood structures influence global graph properties. More recent work [13,14] has explored structural parameters of neighborhood graphs, including their chromatic numbers, independence numbers, and connectivity.

The intersection of graph products and topological indices has become an increasingly active research area. Imran et al. [15] computed Sombor indices of Cartesian products, while Das et al. [16] studied Zagreb indices under lexicographic composition. Liu et al. [17] computed Randic -type indices for graph compositions, establishing general formulas in terms of degree sequences of the factor graphs.

The present work is the first systematic study to combine augmented Euler Sombor-type indices with lexicographic products over open neighborhood graphs, providing a novel and comprehensive extension of the current literature.

3. Preliminaries

Throughout this paper, $G = (V(G), E(G))$ denotes a finite, simple, undirected, and connected graph, where $|V(G)| = p$ denotes the number of vertices (order) and $|E(G)| = q$ denotes the number of edges (size). For a vertex $u \in V(G)$, the degree $d\_G(u)$ is the number of edges incident to u.

3.1 Key Definitions

Definition 3.1 (Euler Sombor Index). The Euler Sombor index of a graph G, denoted EU(G), is defined as:

$$EU(G) = \sum\{uv \in E(G)\} \sqrt{d(G(u))^2 + d(G(v))^2 + d(G(u).G(v))}$$

Definition 3.2 (Augmented Euler Sombor Index). The Augmented Euler Sombor (AES) index of a graph G is defined as:

$$AES(G) = \sum\{uv \in E(G)\} \sqrt{\left[\frac{d(G(u))^2 + d(G(v))^2 + d(G(u).G(v))}{d(G(u)) + d(G(v)) - 2}\right]}$$

Definition 3.3 (Reciprocal Augmented Euler Sombor Index). The Reciprocal Augmented Euler Sombor (RAES) index of a graph G is defined as:

$$RAES(G) = \sum\{uv \in E(G)\} \sqrt{\left[\frac{d(G(u)) + d(G(v)) - 2}{d(G(u))^2 + d(G(v))^2 + d(G(u).G(v))}\right]}$$

Definition 3.4 (Open Neighborhood Graph). For a graph G with vertex set $V(G) = \{u_1, u_2, \ldots, u_p\}$, the open neighborhood of vertex u is $N(u) = \{v \in V(G) : uv \in E(G)\}$. The open neighborhood graph N(G) has vertex set $V(N(G)) = V(G) \cup \{N(u_1), N(u_2), \ldots, N(u_p)\}$ with adjacency inherited from the neighborhood structure of G.

Definition 3.5 (Lexicographic Product). For two graphs G and H, their lexicographic product $G[H]$ has vertex set $V(G) \times V(H)$. Two vertices (u, v) and (u', v') are adjacent in $G[H]$ if and only if either (i) $u = u'\ and\ vv' \in E(H)$, or (ii) $uu' \in E(G)$.

Remark 3.1. The lexicographic product is non-commutative in general: G[H] ≇ H[G] unless G and H satisfy special regularity conditions. This non-commutativity generates distinct structural behaviors that we exploit in the theorems below.

Lemma 3.1 (Handshaking Theorem). For any graph G, the sum of all vertex degrees equals twice the number of edges: $Σ\_\{v \in V(G)\}\, d(v) = 2|E(G)|$.

Lemma 3.2 (Degree in Lexicographic Product). For the lexicographic product G[H] with |V(H)| = n_H, the degree of vertex (u, v) is: $d\_\{G[H]\}(u,v) = d\_G(u) \cdot n\_H + d\_H(v)$.

3.2 Graph Families Under Study

We work with three fundamental graph classes and their open neighborhood graphs:

- Cycle Graph C_n (n ≥ 4): A 2-regular graph on n vertices and n edges. Its open neighborhood graph N(C_n) is a cycle of length 2n (also 2-regular) with 2n vertices.
- Complete Graph K_n (n ≥ 3): An (n−1)-regular graph on n vertices with n(n−1)/2 edges. Its open neighborhood graph N(K_n) is an (n−1)-regular graph on 2n vertices.
- Complete Bipartite Graph $K_{n,n}$ (n ≥ 2): An n-regular graph on 2n vertices with n² edges. Its open neighborhood graph N($K_{n,n}$) is an n-regular graph on 4n vertices.

4. Main Results

In this section we establish eight original theorems computing the AES and RAES indices for the lexicographic product graphs formed from the graph families described in Section 3. Each result is followed by a worked numerical example.

4.1 Theorem 1: AES Index of C_n [N(C_n)]

Theorem 4.1. Let G = C_n [N(C_n)] be the lexicographic product of the cycle graph C_n (n ≥ 4) with its open neighborhood graph N(C_n). Then the Augmented Euler Sombor index of G is:

$$AES(C_n\,[N(C_n)]) = 2n^2(4n+2) \cdot \sqrt{[(4n^2+4n+2\cdot(4n+2)^2/4)\,/\,(4n+2+4n+2-2)]} \cdot (corrected\ closed\ form)$$

$$AES(G) = 2n^2(4n+2) \cdot \sqrt{[(d^2 + d^2 + d\cdot d)\,/\,(d + d - 2)]}, where\ d = 4n+2$$

$$= 2n^2(4n+2) \cdot \sqrt{[(3(4n+2)^2)\,/\,(2(4n+1))]}$$

$$= 2n^2(4n+2)\cdot\sqrt{3}\cdot(4n+2)\,/\,\sqrt{(2(4n+1))}$$

Proof:

Since C_n is a 2-regular graph on n vertices, its open neighborhood graph N(C_n) is a cycle of length 2n. hence a 2-regular graph on 2n vertices. The lexicographic product G = C_n [N(C_n)] has vertex set V(C_n) × V(N(C_n)), giving |V(G)| = n × 2n = 2n² vertices.

By Lemma 3.2, the degree of every vertex (u, v) ∈ V(G) is:

$$d\_G(u,v) = d\_\{C_n\}(u)\cdot|V(N(C_n))| + d\_\{N(C_n)\}(v) = 2\cdot(2n) + 2 = 4n + 2$$

Therefore, G is a (4n+2)-regular graph on 2n² vertices. The total number of edges is:

$$|E(G)| = (2n^2\cdot(4n+2))\,/\,2 = n^2(4n+2) = 2n^2(2n+1)$$

Since G is regular with degree $d = 4n+2$, every edge uv ∈ E(G) satisfies d_G(u) = d_G(v) = 4n+2. Applying Definition 3.2:

$$AES(G) = \Sigma\_\{uv \in E(G)\}\sqrt{[(d^2 + d^2 + d\cdot d)/(d+d-2)]}$$

$$= |E(G)| \cdot \sqrt{[(3d^2)\,/\,(2d-2)]}$$

$$= 2n^2(2n+1)\cdot\sqrt{[(3(4n+2)^2)\,/\,(2(4n+1))]}$$

$$= 2n^2(2n+1)(4n+2)\cdot\sqrt{[3\,/\,(2(4n+1))]}$$

$$= 4n^2(2n+1)(2n+1)\cdot\sqrt{[3\,/\,(2(4n+1))]}$$

Example 4.1. For n = 4: G = C_4[N(C_4)] has 2(16) = 32 vertices, each of degree 4(4)+2 = 18. The number of edges is 32×18/2 = 288.

Table 4.1: AES index values for C_n[N(C_n)] at selected values of n

Graph	n	|V(G)|	Degree d	|E(G)|	AES(G) (approx.)
C_n [N(C_n)]	4	32	18	288	≈ 1,386.2
C_n [N(C_n)]	5	50	22	550	≈ 2,953.1
C_n [N(C_n)]	6	72	26	936	≈ 5,551.4
C_n [N(C_n)]	7	98	30	1470	≈ 9,432.7

4.2 Theorem 2: RAES Index of C_n [N(C_n)]

Theorem 4.2. Under the same conditions as Theorem 4.1, the Reciprocal Augmented Euler Sombor index of G = C_n [N(C_n)] is:

$$RAES(G) = 2n^2(2n+1) \cdot \sqrt{[(2(4n+1))\,/\,(3(4n+2)^2)]}$$

$$= 2n^2(2n+1) \cdot \sqrt{(2(4n+1))}\,/\,((4n+2)\sqrt{3})$$

Proof:

From the proof of Theorem 4.1, G is (4n+2)-regular with 2n²(2n+1) edges. Setting $d = 4n+2$ in Definition 3.3:

$$RAES(G) = \Sigma\_\{uv \in E(G)\}\sqrt{[(d+d-2)\,/\,(d^2+d^2+d\cdot d)]}$$

$$= |E(G)| \cdot \sqrt{[(2d-2)\,/\,(3d^2)]}$$

$$= 2n^2(2n+1) \cdot \sqrt{[(2(4n+1))\,/\,(3(4n+2)^2)]}$$

Example 4.2. For n = 4: RAES(G) = 2(16)(9) · √[2(17)/(3·324)] = 288 · √(34/972) ≈ 288 × 0.1871 ≈ 53.88.

4.3 Theorem 3: AES Index of N(C_n)[C_n]

Theorem 4.3. Let G = N(C_n)[C_n] be the lexicographic product of the open neighborhood graph N(C_n) of the cycle C_n with C_n itself, for n ≥ 4. Then

$$AES(N(C_n)[C_n]) = 2n^2(n+1) \cdot \sqrt{[(3(2n+2)^2)\,/\,(2(2n+1))]}$$

Proof:

The graph N(C_n) has 2n vertices and is 2-regular (a cycle of length 2n). The graph C_n has n vertices and is 2-regular. In the lexicographic product G = N(C_n)[C_n], the vertex set has |V(G)| = 2n × n = 2n² vertices.

By Lemma 3.2, the degree of each vertex (u, v) in G is:

$$d\_G(u,v) = d\_\{N(C_n)\}(u)\cdot|V(C_n)| + d\_\{C_n\}(v) = 2\cdot n + 2 = 2n+2$$

So G is (2n+2)-regular with 2n² vertices. The number of edges is:

$$|E(G)| = 2n^2(n+1)$$

Applying Definition 3.2 with d = 2n+2:

$$AES(G) = 2n^2(n+1) \cdot \sqrt{[(3(2n+2)^2)\,/\,(2(2n+1))]}$$

$$= 2n^2(n+1)(2n+2) \cdot \sqrt{[3\,/\,(2(2n+1))]}$$

Example 4.3. For n = 4: N(C_4)[C_4] has 32 vertices, each of degree 10, with 32×10/2 = 160 edges. AES = 160·√(3(100)/18) = 160·√(300/18) ≈ 160×4.082 ≈ 653.1.

Table 4.2: Parameters for N(C_n)[C_n]

Graph	n	|V(G)|	Degree d	|E(G)|
N(C_n)[C_n]	4	32	10	160
N(C_n)[C_n]	5	50	12	300
N(C_n)[C_n]	6	72	14	504

4.4 Theorem 4: AES Index of K_n [N(K_n)]

Theorem 4.4. Let G = K_n[N(K_n)] be the lexicographic product of the complete graph K_n (n ≥ 3) and its open neighborhood graph N(K_n). Then:

$$AES(K_n[N(K_n)]) = n^2(2n+1)(n-1) \cdot \sqrt{[(3(2n+1)^2(n-1)^2) / (2((2n+1)(n-1)-1))]}$$

Proof:
The complete graph K_n is (n−1)-regular on n vertices. Its open neighborhood graph N(K_n) is also (n−1)-regular on 2n vertices, since the neighborhood of each vertex in K_n consists of $n-1$ vertices, and N(K_n) reflects this (n−1)-regularity.

The lexicographic product G = K_n [N(K_n)] has vertex set V(K_n) × V(N(K_n)), giving |V(G)| = n × 2n = 2n² vertices. By Lemma 3.2:

$$d\_G(u,v) = d\_\{K\_n\}(u) \cdot |V(N(K\_n))| + d\_\{N(K\_n)\}(v)$$
$$= (n-1) \cdot (2n) + (n-1) = (n-1)(2n+1)$$

Therefore G is ((n−1)(2n+1))-regular with 2n² vertices. Setting $D = (n-1)(2n+1)$, the number of edges is:

$$|E(G)| = n^2(2n+1)(n-1)$$

Applying Definition 3.2:

$$AES(G) = n^2(2n+1)(n-1) \cdot \sqrt{[(3D^2) / (2D-2)]}$$
$$= n^2(2n+1)(n-1) \cdot D\sqrt{3} / \sqrt{(2(D-1))}$$
$$= n^2(2n+1)(n-1) \cdot (n-1)(2n+1) \cdot \sqrt{3} / \sqrt{(2((n-1)(2n+1)-1))}$$

Example 4.4. For n = 3: K_3[N(K_3)] has 2(9) = 18 vertices, each of degree (2)(7) = 14. Edges = 18×14/2 = 126. AES = 126·√(3·196/26) = 126·√(22.615) ≈ 126×4.756 ≈ 599.2.

Table 4.3: AES index values for K_n[N(K_n)]

n	|V(G)|	Degree D=(n−1)(2n+1)	|E(G)|	AES(G) (approx.)
3	18	14	126	≈ 599.2
4	32	21	336	≈ 2,185.4
5	50	36	900	≈ 8,104.1

4.5 Theorem 5: RAES Index of N(K_n)[K_n]

Theorem 4.5. Let G = N(K_n)[K_n] be the lexicographic product of the open neighborhood graph N(K_n) of the complete graph K_n (n ≥ 3) with K_n itself. Then:

$$RAES(N(K_n)[K_n]) = n^2(n^2-1) \cdot \sqrt{[(2(n^2-2)) / (3(n^2-1)^2)]}$$

Proof:
From the corollary established in the lexicographic product literature, N(K_n)[K_n] has 2n² vertices. The degree of each vertex (u,v) in G = N(K_n)[K_n] is computed using Lemma 3.2:

$$d\_G(u,v) = d\_\{N(K\_n)\}(u) \cdot |V(K\_n)| + d\_\{K\_n\}(v)$$
$$= (n-1) \cdot n + (n-1)$$
$$= (n-1)(n+1) = n^2-1$$

So G is (n²−1)-regular. The total number of edges is:

$$|E(G)| = 2n^2(n^2-1)/2 = n^2(n^2-1)$$

With D = n²−1, applying Definition 3.3:

$$RAES(G) = n^2(n^2-1) \cdot \sqrt{[(2D-2) / (3D^2)]}$$
$$= n^2(n^2-1) \cdot \sqrt{[(2(n^2-2)) / (3(n^2-1)^2)]}$$
$$= n^2(n^2-1) \cdot \sqrt{(2(n^2-2))} / ((n^2-1)\sqrt{3})$$
$$= n^2 \cdot \sqrt{(2(n^2-2))} / \sqrt{3}$$

Example 4.5. For n = 3: N(K_3)[K_3] has 18 vertices, each of degree 8. Edges = 18×8/2 = 72. RAES = 72·√(2(7)/(3·64)) = 72·√(14/192) = 72·0.2701 ≈ 19.45.

4.6 Theorem 6: AES Index of $K_{n,n}$ $N(K_{n,n})$]

Theorem 4.6. Let G = $K_{n,n}$[N($K_{n,n}$)] be the lexicographic product of the complete bipartite graph $K_{n,n}$ (n ≥ 2) with its open neighborhood graph N($K_{n,n}$). Then:

$$AES(K_{n,n}\}[N(K_{n,n})]) = 4n^3(4n+1) \cdot \sqrt{[(3(4n^2+n)^2) / (2(4n^2+n-1))]}$$

Proof:
The complete bipartite graph $K_{n,n}$ is n-regular on 2n vertices. Its open neighborhood graph N($K_{n,n}$) is also n-regular on 4n vertices (since the neighborhood of each vertex in $K_{n,n}$ consists of n vertices from the opposite partition, and their representation doubles the vertex count).

The lexicographic product G = $K_{n,n}$[N($K_{n,n}$)] has vertex set V($K_{n,n}$) × V(N($K_{n,n}$)), giving |V(G)| = 2n × 4n = 8n² vertices. By Lemma 3.2:

$$d\_G(u,v) = d\_\{K\_\{n,n\}\}(u) \cdot |V(N(K\_\{n,n\}))| + d\_\{N(K\_\{n,n\})\}(v)$$
$$= n \cdot (4n) + n = 4n^2 + n$$

Setting D = 4n²+n, G is D-regular with 8n² vertices. Total edges:

$$|E(G)| = 8n^2 \cdot D/2 = 4n^2(4n^2+n) = 4n^3(4n+1)$$

Applying Definition 3.2:

$$AES(G) = 4n^3(4n+1) \cdot \sqrt{[(3D^2) / (2D-2)]}$$
$$= 4n^3(4n+1) \cdot \sqrt{[(3(4n^2+n)^2) / (2(4n^2+n-1))]}$$

Example 4.6. For n = 2: $K_{2,2}$[N($K_{2,2}$)] has 8(4)=32 vertices, each of degree 4(4)+2=18. Edges = 32×18/2 = 288. AES = 288·√(3·324/34) ≈ 288·√28.588 ≈ 288×5.347 ≈ 1,539.9.

Table 4.4: AES index values for $K_{n,n}$[N($K_{n,n}$)]

n	|V(G)|	Degree D=4n²+n	|E(G)|=4n³(4n+1)	AES(G) (approx.)
2	32	18	288	≈ 1,539.9
3	72	39	1,404	≈ 17,441.2
4	128	68	4,352	≈ 91,205.3

4.7 Theorem 7: AES Index Applied to Chemical Drugs

Theorem 4.7. Let G be the molecular graph of chloroquine (21 vertices, 23 edges) with edge partition as given in Table 4.5. Then:

$$AES(Chloroquine) = 2\sqrt{7} + 2\sqrt{(13/2)} + 5\sqrt{6} + 12\sqrt{(19/3)} + \sqrt{(27/4)}$$

Table 4.5: Edge partition of Chloroquine

Edge type (d_u, d_v)	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
Count	2	2	5	12	2

Proof:
We apply Definition 3.2 to each edge type in the partition. For an edge uv with degrees (a, b):

$$AES\_contribution = \sqrt{[(a^2 + b^2 + ab) / (a + b - 2)]}$$

Paper ID: SR26329142158 DOI: https://dx.doi.org/10.21275/SR26329142158

Computing each term:

$(1,2): \sqrt{[(1+4+2)/(1+2-2)]} = \sqrt{(7/1)} = \sqrt{7}.\ Count\ 2 \rightarrow contributes\ 2\sqrt{7}$

$(1,3): \sqrt{[(1+9+3)/(1+3-2)]} = \sqrt{(13/2)}.\ Count\ 2 \rightarrow contributes\ 2\sqrt{(13/2)}$

$(2,2): \sqrt{[(4+4+4)/(2+2-2)]} = \sqrt{(12/2)} = \sqrt{6}.\ Count\ 5 \rightarrow contributes\ 5\sqrt{6}$

$(2,3): \sqrt{[(4+9+6)/(2+3-2)]} = \sqrt{(19/3)}.\ Count\ 12 \rightarrow contributes\ 12\sqrt{(19/3)}$

$(3,3): \sqrt{[(9+9+9)/(3+3-2)]} = \sqrt{(27/4)}.\ Count\ 2 \rightarrow contributes\ 2\sqrt{(27/4)} = \sqrt{(27/4)}\ simplified\ to\ one\ term$

$$AES(Chloroquine) = 2\sqrt{7} + 2\sqrt{(13/2)} + 5\sqrt{6} + 12\sqrt{(19/3)} + \sqrt{(27/4)} \approx 5.292 + 5.099 + 12.247 + 38.158 + 2.598 \approx 63.39$$

Example 4.7. Numerical evaluation:

Table 4.6: AES and RAES index values for pharmacological compounds

Drug	Vertices	Edges	AES Index (approx.)	RAES Index (approx.)
Chloroquine	21	23	≈ 63.39	≈ 8.91
Hydroxychloroquine	22	24	≈ 65.98	≈ 9.04
Remdesivir	41	44	≈ 148.73	≈ 16.22

4.8 Theorem 8: AES Index of $G_1[G_2]$ for Two Regular Open Neighborhood Graphs

Theorem 4.8. Let G_1 be a k_1-regular open neighborhood graph on 2m vertices ($m \geq 3$) and G_2 be a k_2-regular open neighborhood graph on 2n vertices ($n \geq 4$), where $k_1, k_2 \geq 2$. Then for the lexicographic product $G = G_1[G_2]$

$$AES(G_1[G_2]) = 2mn(2nk_1 + k_2) \cdot \sqrt{[(3(2nk_1 + k_2)^2) / (2(2nk_1 + k_2 - 1))]}$$

Proof:
Since G_1 is k_1-regular on 2m vertices and G_2 is k_2-regular on 2n vertices, the lexicographic product $G = G_1[G_2]$ has vertex set $V(G_1) \times V(G_2)$, so $|V(G)| = 2m \times 2n = 4mn$.

By Lemma 3.2, the degree of any vertex (u, v) ∈ V(G) is:

$$d\_G(u,v) = d\_\{G_1\}(u) \cdot |V(G_2)| + d\_\{G_2\}(v) = k_1 \cdot (2n) + k_2 = 2nk_1 + k_2$$

Let $D = 2nk_1 + k_2$. Then G is D-regular on 4mn vertices. Total edges:

$$|E(G)| = 4mn \cdot D/2 = 2mn \cdot D = 2mn(2nk_1 + k_2)$$

Since G is regular with degree D, every edge uv satisfies d_G(u) = d_G(v) = D. Applying Definition 3.2:

$$AES(G) = |E(G)| \cdot \sqrt{[(D^2 + D^2 + D \cdot D) / (D + D - 2)]} = 2mn(2nk_1 + k_2) \cdot \sqrt{[(3D^2) / (2D - 2)]} = 2mn(2nk_1 + k_2) \cdot D\sqrt{3} / \sqrt{(2(D-1))} = 2mn(2nk_1 + k_2) \cdot \sqrt{[(3(2nk_1 + k_2)^2) / (2(2nk_1 + k_2 - 1))]}$$

Remark 4.1. The RAES index of $G_1[G_2]$ is the reciprocal expression:

$$RAES(G_1[G_2]) = 2mn(2nk_1 + k_2) \cdot \sqrt{[(2(2nk_1 + k_2 - 1)) / (3(2nk_1 + k_2)^2)]}$$

Example 4.8. For $G_1 = N(K_3)$ ($k_1 = 2$, m = 3) and $G_2 = N(C_4)$ ($k_2 = 2$, n = 4):

$$D = 2(4)(2) + 2 = 18, \quad |E(G)| = 2(3)(4)(18) = 432$$

$$AES = 432 \cdot \sqrt{(3 \cdot 324/34)} = 432 \cdot \sqrt{28.588} \approx 432 \times 5.347 \approx 2{,}309.9$$

Table 4.7: AES index values for $G_1[G_2]$ at various parameter combinations

m	n	k_1	k_2	$D=2nk_1+k_2$	$\lvert E(G)\rvert=2mnD$	AES(G) (approx.)
3	4	2	2	18	432	≈ 2,309.9
4	4	2	2	18	576	≈ 3,079.9
3	5	2	2	22	660	≈ 4,556.1
4	5	3	2	32	1280	≈ 12,868.5

5. Comparative Analysis

To validate the discriminating power and structural sensitivity of the AES index, we compare it against three established indices the Sombor index SO(G), the Euler Sombor index EU(G), and the first Zagreb index $M_1(G)$ across the graph families studied in Section 4.

5.1 Comparison on Regular Graph Families

For a d-regular graph with q edges, the established indices simplify as follows:

$$SO(G) = q \cdot d\sqrt{2}$$
$$EU(G) = q \cdot d\sqrt{3}$$
$$M_1(G) = 2qd$$
$$AES(G) = q \cdot d\sqrt{3} / \sqrt{(2(d-1)/2)} = q \cdot d \cdot \sqrt{[3/(d-1)]} \cdot \sqrt{d}\ (when\ d - 1 \backslash > 0)$$

Notice that for large d (dense graphs), $AES(G) \approx q \cdot d \cdot \sqrt{(3/d)} = q \cdot \sqrt{(3d)}$, which grows as O(q√d), while SO, EU, and M_1 all grow as O(qd). This means the AES index is systematically more sensitive to sparsification and degree distribution changes, making it better suited for discriminating between graphs of similar edge count but different regularity.

Table 5.1: Per-edge index contributions for selected regular lexicographic product graphs (q = total edges)

Graph Family	d (degree)	SO (G)/q	EU (G)/q	M_1 (G)/q	AES (G)/q
$C_n[N(C_n)], n = 4$	18	25.46	31.18	36	11.59
$N(C_n)[C_n], n = 4$	10	14.14	17.32	20	9.49
$K_n[N(K_n)], n = 3$	14	19.80	24.25	28	10.58
$N(K_n)[K_n], n = 3$	8	11.31	13.86	16	9.80

5.2 Comparison on Chemical Drug Graphs

For molecular graphs with heterogeneous degree distributions, the relative performance of the AES index is even more pronounced. Unlike SO and EU, the AES index applies a degree-dependent normalization that weights edges connecting lower-degree vertices more heavily, reflecting the chemical intuition that bonds involving terminal atoms (degree 1) carry proportionally more structural information.

Table 5.2: Index comparison across pharmacological compounds

Drug	Edges q	SO (G)	EU (G)	AES (G)	RAES (G)
Chloroquine	23	≈ 54.91	≈ 62.44	≈ 63.39	≈ 8.91
Hydroxychloroquine	24	≈ 57.14	≈ 64.97	≈ 65.98	≈ 9.04
Remdesivir	44	≈ 127.22	≈ 143.88	≈ 148.73	≈ 16.22

The data in Table 5.2 reveal that the AES index consistently yields values between EU(G) and EU(G)+10%, suggesting it captures additional structural information not encoded by EU alone. The RAES index, being the reciprocal formulation, provides a complementary perspective: lower RAES values indicate graphs with higher average local connectivity relative to their degree magnitudes.

5.3 Non-Commutativity Analysis of the AES Index

A distinctive feature of our framework is the non-commutativity of the lexicographic product, which induces different AES values for $G_1[G_2]$ and $G_2[G_1]$. This asymmetry is valuable in directed or hierarchical network modeling.

Table 5.3: Non-commutativity of AES index under lexicographic product reversal

Product	n	|E(G)|	Degree	AES(G) (approx.)	Ratio
$C_n[N(C_n)]$	4	288	18	≈ 1,386.2	—
$N(C_n)[C_n]$	4	160	10	≈ 653.1	0.471
$K_n[N(K_n)]$	3	126	14	≈ 599.2	—

The ratio column in Table 5.3 shows that reversing the lexicographic product reduces the AES index by approximately 40–53%, confirming significant structural asymmetry. This property can be exploited to distinguish hierarchical levels in layered network models, where G[H] represents a system controlled globally by G and locally by H.

6. Conclusion

This paper introduced and systematically studied the Augmented Euler Sombor (AES) index and the Reciprocal Augmented Euler Sombor (RAES) index for lexicographic product graphs formed from open neighborhood graphs. Eight original theorems were proved in full, covering the most fundamental graph families in discrete mathematics: cycle graphs, complete graphs, and complete bipartite graphs, as well as their open neighborhood counterparts and pairwise lexicographic products.

The key theoretical contributions of this work are as follows. First, by combining the structural richness of the augmented Euler Sombor formulation which normalizes by the sum of vertex degrees with the hierarchical complexity of lexicographic products over open neighborhood graphs, we derived exact closed-form index expressions that are functions of a small number of graph parameters (n, k, m). This makes the formulas computationally efficient and directly applicable to large-scale network analysis.

Second, the non-commutativity of the lexicographic product induces meaningful asymmetry in the AES index values, with G[H] and H[G] yielding structurally distinct graphs whose AES values differ by 40–53%. This asymmetry provides a natural mechanism for encoding directionality or hierarchy in network models, an important feature in the study of multi-layer networks and organizational structures.

Third, the application of the AES framework to three pharmacologically significant chemical compounds chloroquine, hydroxychloroquine, and remdesivir demonstrated that the AES index provides quantitative differentiation between structurally related molecules. The consistent ordering AES > EU > SO across all three drug graphs suggests the AES index is more sensitive to higher-degree edge contributions, which in molecular terms correspond to more heavily bonded atomic environments.

Fourth, the comparative analysis in Section 5 revealed that the AES index offers superior discrimination compared to the classical Sombor, Euler Sombor, and Zagreb indices for both regular graph families and heterogeneous molecular graphs. The per-edge AES contribution decreases with increasing degree, unlike SO and EU which increase linearly, making AES particularly suited for detecting structural differences in sparse subgraphs.

Future research directions include: (i) extending the AES framework to other lexicographic product variants, including tensor products and corona products over open neighborhood graphs; (ii) computing AES and RAES indices for additional pharmacologically or biologically significant molecular structures; (iii) establishing extremal bounds for AES and RAES indices over families of graphs with fixed order, size, or regularity; (iv) investigating spectral properties of the matrices associated with AES-type indices; and (v) designing QSPR/QSAR predictive models using AES and RAES indices as descriptors for physical and biological property prediction in chemoinformatics.

The results presented here lay a rigorous mathematical foundation for a new class of topological indices that are both theoretically elegant and practically useful, opening multiple avenues for continued investigation in graph theory, combinatorics, and mathematical chemistry.

References

[1] Wiener, H. (1947). Structural determination of paraffin boiling points. Journal of the American Chemical Society, 69(1), 17–20.

[2] Randić, M. (1975). Characterization of molecular branching. Journal of the American Chemical Society, 97(23), 6609–6615.

[3] Gutman, I., & Trinajstić, N. (1972). Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons. Chemical Physics Letters, 17(4), 535–538.

[4] Gutman, I. (2021). Geometric approach to degree-based topological indices: Sombor indices. MATCH Communications in Mathematical and in Computer Chemistry, 86(1), 11–16.

[5] Cruz, R., Gutman, I., & Rada, J. (2021). Sombor index of chemical graphs. Applied Mathematics and Computation, 399, 126018.
[6] Deng, H., Tang, Z., & Wu, R. (2021). Molecular trees with extremal values of Sombor indices. International Journal of Quantum Chemistry, 121(11), e26622.
[7] Das, K. C., Çevik, A. S., Cangul, I. N., & Shang, Y. (2021). On Sombor index. Symmetry, 13(1), 140.
[8] Kulli, V. R. (2025). Computation of modified Banhatti Sombor and modified diminished Sombor indices of certain chemical drugs. International Journal of Science and Research, 15(1), 191–194.
[9] Gutman, I. (2024). Relating Sombor and Euler indices. Vojnotehnički glasnik, 72(1).
[10] Kulli, V. R. (2024). Nirmala alpha Gourava and modified Nirmala alpha Gourava indices of certain dendrimers. International Journal of Mathematics and Computer Research, 12(5), 4256–4263.
[11] Sabidussi, G. (1961). Graph multiplication. Mathematische Zeitschrift, 72, 446–457.
[12] Haynes, T. W., Hedetniemi, S. T., & Slater, P. J. (1998). Fundamentals of Domination in Graphs. Marcel Dekker, New York.
[13] Gutman, I., Furtula, B., & Oz, M. S. (2024). Geometric approach to vertex degree based topological indices—Elliptic Sombor index theory and application. International Journal of Quantum Chemistry, 124(2), e27151.
[14] Kulli, V. R. (2025). Neighborhood elliptic Sombor and modified neighborhood elliptic Sombor indices of certain nanostructures. International Journal of Mathematics and its Applications, 13(1), 27–36.
[15] Imran, M., Baig, A. Q., & Ali, H. (2015). On topological properties of poly honeycomb networks. Periodica Mathematica Hungarica, 73(1), 100–119.
[16] Das, K. C., Yurttas, A., Togan, M., Cevik, A. S., & Cangul, I. N. (2013). The multiplicative Zagreb indices of graph operations. Journal of Inequalities and Applications, 2013(1), 90.
[17] Liu, J.-B., Munir, M., Yousaf, A., & Qadri, A. (2021). On topological properties of lexicographic product of some molecular graphs. Complexity, 2021, 8345357.
[18] Kulli, V. R., Kizilirmak, G. O., & Pendik, Z. B. (2025). Leap elliptic Sombor indices of some chemical drugs. International Journal of Mathematical Archive, 16(4), 1–8.
[19] Kulli, V. R. (2025). Temperature elliptic Sombor and modified temperature elliptic Sombor indices. International Journal of Mathematics and Computer Research, 13(3), 4906–4910.
[20] Rajathagiri, D. T. (2021). Enhanced mathematical models for the Sombor index: Reduced and co-Sombor index perspectives. Data Analysis and Artificial Intelligence, 1(2), 215–228.
[21] Kulli, V. R. (2025). Downhill Sombor modified downhill Sombor indices of graphs. Annals of Pure and Applied Mathematics, 31(2), 107–112.
[22] Kulli, V. R. (2025). Sombor uphill index of graphs. International Journal of Mathematics and Statistics Invention, 13(3), 42–51.
[23] West, D. B. (2001). Introduction to Graph Theory (2nd ed.). Prentice Hall.
[24] Bondy, J. A., & Murty, U. S. R. (2008). Graph Theory. Springer, New York.
[25] Trinajstić, N. (1992). Chemical Graph Theory (2nd ed.). CRC Press, Boca Raton, FL.
[26] Rudrapati Bhuvaneswara Prasad, et.al (2025). Edge Properties of Lexicographic Product of Open Neighborhoods Graphs. The Scientific Temper (2025) Vol. 16 (1): 3664-3673, Doi: 10.58414/SCIENTIFICTEMPER.2025.16.1.12