

Entire Neighborhood Topological Indices: Theory and Applications in Predicting Physico-Chemical Properties

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Abstract. Topological indices are numerical descriptors that describe the chemical structures of chemical compounds using their molecular graphs. Recent advancements in topological indices have seen the emergence of neighborhood indices and entire topological indices, offering distinct perspectives on molecular structure. Neighborhood indices emphasize local atomic environments, while entire indices provide a comprehensive view by considering interactions between atoms, bonds, and their combinations. To achieve a more balanced and informative representation, we introduce 'entire neighborhood indices'. By integrating the localized focus of neighborhood indices within the framework of entire indices, these new descriptors offer a more complete picture of molecular structure and are expected to significantly enhance the accuracy of predictions for various molecular properties. In this paper, we introduce a new version of Zagreb topological indices named first, second, and modified entire neighborhood topological indices; denoted by NM_1^e , NM_2^e , and MNM_1^e , respectively. The structure-property regression analysis is used to investigate and compute the chemical significant of these newly introduced indices for the prediction of the physico-chemical properties of octane isomers and benzenoid hydrocarbons benchmark datasets. We analyze and calculate the specific formulae of the entire neighborhood indices for several important graph families such as path, regular, cycle, complete, bipartite, book, gear and helm graph. Furthermore, we determine the exact value of these new indices for some types of bridge graphs and Sierpiński graphs.

1. INTRODUCTION

Let $\Gamma(V, E)$ be a finite, undirected, and simple graph, where V and E denote the vertex and edge sets respectively. The number of vertices [edges] is called the order [size] of the graph. Two

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vertices v and u are adjacent, or neighbors, if there is an edge between them and the set of all neighbors of v is called an open neighborhood of v , $N(v)$. For any vertex $v \in V$, the degree $d(v)$ of the vertex v is defined to be the number of edges that incident to it; that is $d(v) = |N(v)|$. Also, for any edge $e \in E$, the degree $d(e)$ of the edge e is the number of edges adjacent to e in the graph; that is, $d(e) = d(u) + d(v) - 2$, where u and v are endpoints of e . The symbols P_n , K_n , W_n , C_n , S_n , and $K_{a,b}$ denote the path, complete, wheel, cycle, star, and complete bipartite graph of order n , respectively. The line graph $L(\Gamma)$ of a simple graph Γ is the graph whose vertices are in one-to-one correspondence with edges of Γ , and two vertices of $L(\Gamma)$ are adjacent if and only if the corresponding edges of Γ are adjacent. The number of the edges in the line graph $L(\Gamma)$ is equal

$$m(L(\Gamma)) = \frac{1}{2} \left[\sum_{i=1}^n d_i^2 \right] - m,$$

where, $|V(\Gamma)| = n$, $|E(\Gamma)| = m$, and $d_i = d(v_i)$, for all $1 \leq i \leq n$. A subdivision of Γ is a graph obtained from the graph Γ by subdivision some or all of its edges by adding new vertices on those edges. The Cartesian product of two graphs Γ and Λ , $\Gamma \times \Lambda$ or $\Gamma \square \Lambda$, is a graph has vertex set $V(\Gamma \times \Lambda) = V(\Gamma) \times V(\Lambda)$ in which two vertices (u_1, v_1) and (u_2, v_2) are adjacent in $\Gamma \times \Lambda$ if and only if either $u_1 = u_2$ and v_1 is adjacent to v_2 in Λ or u_1 is adjacent to u_2 in Γ and $v_1 = v_2$. For more details about definitions and terminologies, we refer the reader to [1–3].

Topological indices are numerical values that correspond to chemical structures using their molecular graph. These invariants present the most useful tools to study and predict the physico-chemical properties and biological activities of the chemical compounds that are used directly in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) [4].

The journey of exploring topological indices begins in 1947 when H. Wiener introduced the Wiener index [5]. This index is a distance based topological index defined to be the sum of the distance between all pairs of vertices of a graph which has applicability to predict the boiling points of paraffin. Then, several other distance-based indices were proposed such as Harary [6], Szeged [7], hyper wiener [8], and Mostar [9].

One of the most widely used topological descriptors in QSPR/QSAR analysis and play a crucial role is degree-based topological indices which is another important branch in this field. The earliest indices based on degrees were presented in 1972 by I. Gutman and Trinajstić [10], namely the first and second Zagreb topological indices defined as

$$M_1(\Gamma) = \sum_{v \in V(\Gamma)} d^2(v) = \sum_{uv \in E(\Gamma)} [d(u) + d(v)],$$

and

$$M_2(\Gamma) = \sum_{uv \in E(\Gamma)} [d(u) \cdot d(v)].$$

The Zagreb indices have applicability to relate the π -electron energy of molecules. The Randić index was introduced by Randić in 1975 [11], and is useful to capture the branching structure of

carbon skeletons and exhibit correlations with numerous chemical characteristics. An alternative index to Randić one was then presented, named as harmonic index [12]. In 1998, Estrada et al. [13], defined the atom-bond connectivity index (ABC). This index became an efficient resource to examine the thermodynamic properties of organic chemical compounds. In 2015, B. Furtula and I. Gutman introduced the forgotten index [14]. Subsequently, numerous researchers have introduced and proposed several versions and developed multiple topological indices, see for example [15–18].

The concept of neighborhood indices was started in 2018 when S. Mondal, N. De, and A. Pal [19] introduced first and second neighborhood Zagreb indices defined as:

$$NM_1(\Gamma) = \sum_{v \in V(\Gamma)} \delta^2(v),$$

$$NM_2(\Gamma) = \sum_{uv \in E(\Gamma)} [\delta(u) \cdot \delta(v)],$$

where, $\delta(v) = \sum_{u \in N(v)} d(u)$ is the neighborhood degree of a vertex v in the graph Γ . The neighborhood indices have significant applications in various areas of computational chemistry and drug discovery. There are numerous studies in this field, along with a wide range of applications, which can be explored through many published articles, for more details, see [20–23]

The initial appearance of the entire topological indices was in 2018 by A. Alwardi et al. [24]. The first and second entire indices are defined as follows

$$M_1^e(\Gamma) = \sum_{x \in V(\Gamma) \cup E(\Gamma)} d^2(x),$$

and

$$M_2^e(\Gamma) = \sum_{\substack{x \text{ is either adjacent} \\ \text{or incident to } y}} d(x)d(y).$$

Subsequently, the entire indices was proposed for several known indices such as the entire forgotten index [25], the entire ABC index [26], the entire Randić index [27], the entire Sombor index [28], the entire harmonic index [29], and the recently introduced, the entire Albertson index and the entire sigma index [30]. Additionally, the literature is rich with research on this type of topological indices.

Now, the entire indices, provide a comprehensive view by incorporating interactions between the vertices, edges, and their combinations; that is, the incident and the adjacency relations between the elements of the graph are considered, and the word element means either a vertex or an edge. on the other hand, neighborhood indices are centered on capturing the specifics of local atomic environments. To achieve a more balanced and informative representation, and based on the fact that the neighborhood and the entire indices have highly significant and good applications, we are motivated to introduce new indices named the first, second, and modified entire neighborhood topological indices. By combining both approaches, these new descriptors offer a

more comprehensive understanding of the molecular structures and are expected to significantly enhance the accuracy of predictions for various molecular properties. We investigate the applicability of their prediction of the physico-chemical properties of molecules through the quantitative structure-property relationships (QSPR) methodology. Using the (SPSS software, 25), we find the correlation coefficients of the newly introduced indices with some physical and chemical characteristics for octan isomers and benzenoid hydrocarbons. These new indices exhibit a strong and excellent Correlations, ranging between (0.815-0.989) with octan isomers and between (0.932-0.991) with benzenoid hydrocarbons. Later, the general formulae for the entire neighborhood indices is obtained for some families of graphs such as path, k -regular, cycle complete, complete bipartite, star, book, gear, and helm graph. Furthermore, we determine the exact value of the newly defined indices for certain types of bridge graphs and Sierpiński graphs.

Definition 1.1. Let Γ be a graph with vertex set V and edge set E . For an element $x \in V(\Gamma) \cup E(\Gamma)$, consider the neighborhood degree of x ,

$\delta(x) = \sum_{y \in N(x)} d(y)$. Then, the first and second entire neighborhood indices are defined as follows,

$$NM_1^e(\Gamma) = \sum_{x \in V(\Gamma) \cup E(\Gamma)} \delta^2(x),$$

and,

$$\begin{aligned} NM_2^e(\Gamma) &= \sum_{\substack{x \text{ is either adjacent} \\ \text{or incident to } y}} \delta(x)\delta(y) \\ &= \sum_{uv \in E(\Gamma)} [\delta(u)\delta(v)] + \sum_{ef \in E(L(\Gamma))} [\delta(e)\delta(f)] + \sum_{\substack{v \text{ incident} \\ \text{to } e \text{ in } \Gamma}} [\delta(v)\delta(e)]. \end{aligned}$$

The modified entire neighborhood index is defined as follows

$$\begin{aligned} MNM_1^e(\Gamma) &= \sum_{\substack{x \text{ is either adjacent} \\ \text{or incident to } y}} [\delta(x) + \delta(y)] \\ &= \sum_{uv \in E(\Gamma)} [\delta(u) + \delta(v)] + \sum_{ef \in E(L(\Gamma))} [\delta(e) + \delta(f)] + \sum_{\substack{v \text{ incident} \\ \text{to } e \text{ in } \Gamma}} [\delta(v) + \delta(e)]. \end{aligned}$$

2. COMPARATIVE ANALYZES OF ENTIRE NEIGHBORHOOD INDICES FOR PREDICTING MOLECULAR PROPERTIES

The mathematical exploration of a new topological index can be evaluated by its potential applications and prediction power. The significance of the topological indices can be assessed through regression analysis, specifically by its ability to correlate the physical and chemical properties of a benchmark dataset. In this section, we use the octan isomers and benzenoid hydrocarbons as benchmark datasets. Since the number of these compounds is large enough to create statistical accuracy and reliability, the choice of these two sets is advantageous for these studies. Also, these

molecules have well-defined structures that make it possible to present different types of graphs, including cyclic and acyclic chemical systems, for this research, which is particularly beneficial if the predictive value of this new index is high, as it provides evidence of its significant effectiveness. The newly defined indices will be investigated in this section to elucidate the structural features of molecules using the quantitative structure-property relationship QSPR methodology. The (SPSS software, 25) is used for this modeling and for graphical analysis and plotting the scientific results. The molecular graphs are obtained by considering the atoms as vertices and the bonds as edges and, deleting the hydrogen atoms, Figure 1 shows the molecular graphs for octane isomers.

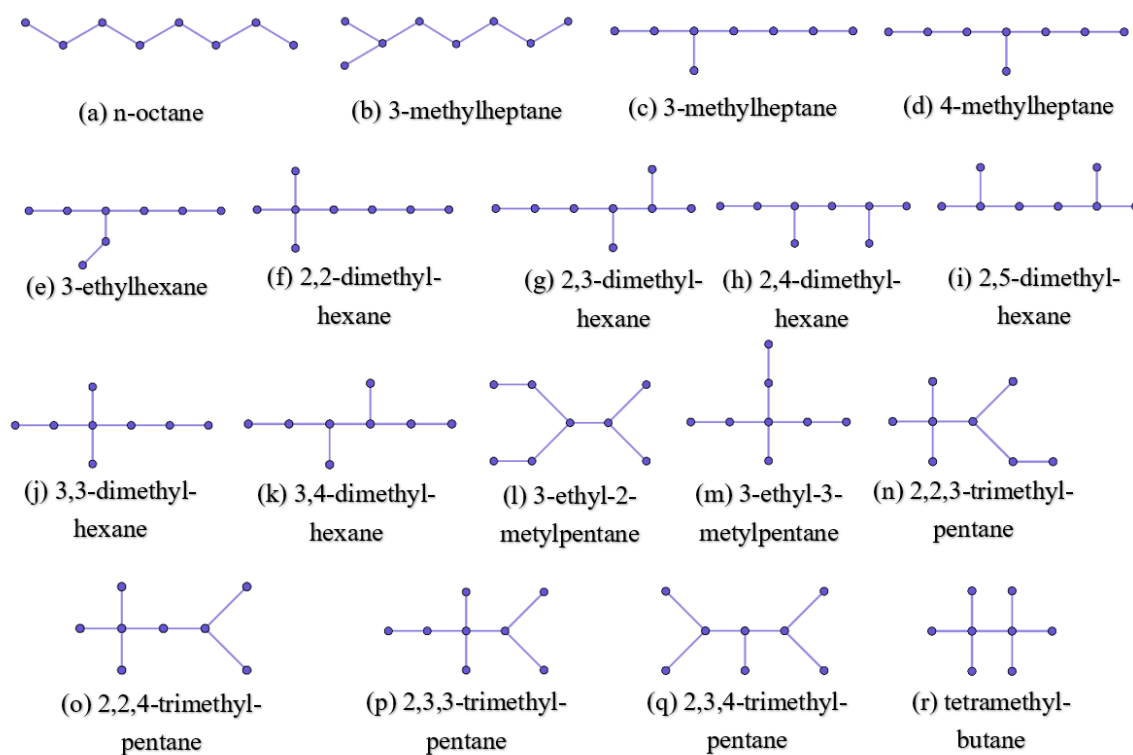


FIGURE 1. Molecular graph of octane isomers.

The theoretical indices of these graphs are reported in tables 3 and 4, represents the approximate values of the properties acentric factor (AF), entropy (S), enthalpy of vaporization (HVAP), and standard enthalpy of vaporization (DHVAP) which are taken from NIST databases [31] and retrieved from [18]. The values of NM_1^ϵ , MNM_1^ϵ , and NM_2^ϵ are computed using a mathematical formation which defined in Definition 1.1. We use the partition method for the calculation of the adjacent vertices and edges and for the incident vertices and edges. For example, the partitions for molecular graph Γ of n-octane molecule are as shown in Tables 1 and 2.

TABLE 1. Partition of the vertices and the edges in Γ .

$\delta(v)$	Frequency	$\delta(e)$	Frequency
2	2	2	2
3	2	3	2
4	4	4	3

TABLE 2. The hole partition of Γ

$\delta(v), \delta(u)$	Frequency	$\delta(e), \delta(f)$	Frequency	$\delta(v), \delta(e)$	Frequency
2,3	2	2,3	2	2,2	2
3,4	2	3,4	2	2,3	2
4,4	3	4,4	2	3,3	2
-	-	-	-	3,4	2
-	-	-	-	4,4	6

Then, the value of the indices are calculated as the following

$$\begin{aligned}
 NM_1^e(\Gamma) &= 2(2^2) + 2(3^2) + 4(4^2) + 2(2^2) + 2(3^2) + 3(4^2) \\
 &= 164,
 \end{aligned}$$

$$\begin{aligned}
 MNM_1^e(\Gamma) &= 2(6) + 2(12) + 3(16) + 2(6) + 2(12) + 2(16) + 2(4) + 2(6) + 2(9) + 2(12) + 6(16) \\
 &= 180,
 \end{aligned}$$

$$\begin{aligned}
 NM_2^e(\Gamma) &= 2(5) + 2(7) + 3(8) + 2(5) + 2(7) + 2(8) + 2(4) + 2(5) + 2(6) + 2(7) + 6(8) \\
 &= 310.
 \end{aligned}$$

The newly introduced indices for the rest of molecular graphs are computed in a similar manner.

TABLE 3. Octan isomers and its value of NM_1 , MNM_1 , NM_2 , NM_1^ϵ , MNM_1^ϵ , and NM_2^ϵ .

Molecular name	NM_1	MNM_1	NM_2	NM_1^ϵ	MNM_1^ϵ	NM_2^ϵ
(a)	90	48	84	164	180	310
(b)	104	52	98	244	228	483
(c)	108	54	106	276	244	566
(d)	110	54	107	284	246	584
(e)	114	56	115	314	262	664
(f)	138	60	132	608	378	1334
(g)	126	60	129	412	312	892
(h)	124	58	121	368	294	770
(i)	118	56	113	326	276	663
(j)	146	64	148	698	414	1589
(k)	130	62	136	444	328	978
(l)	132	62	137	450	330	993
(m)	152	68	163	776	454	1819
(n)	162	70	171	858	484	2006
(o)	156	64	147	714	430	1580
(p)	164	72	179	906	502	2152
(q)	144	66	151	552	380	1235
(r)	194	80	217	1832	664	3421

TABLE 4. The experimental values of AF, S, HVAP, and DHVAP for octan isomers.

Molecular name	AF	S	HVAP	DHVAP
(a)	0.397898	111.67	73.19	9.915
(b)	0.377916	109.84	70.3	9.484
(c)	0.371002	111.26	71.3	9.521
(d)	0.371504	109.32	70.91	9.483
(e)	0.362472	109.43	71.7	9.476
(f)	0.339426	103.42	67.7	8.915
(g)	0.348247	108.02	70.2	9.272
(h)	0.344223	106.98	68.5	9.029
(i)	0.35683	105.72	68.6	9.051
(j)	0.322596	104.74	68.5	8.973
(k)	0.340345	106.59	70.2	9.316
(l)	0.332433	106.06	69.7	9.209
(m)	0.306899	101.48	69.3	9.081
(n)	0.300816	101.31	67.3	8.826
(o)	0.30537	104.09	64.87	8.402
(p)	0.293177	102.06	68.1	8.897
(q)	0.317422	102.39	68.37	9.014
(r)	0.255294	93.06	66.2	8.41

The illustrated data in Table 3 shows that entire neighborhood indices are an effective and promising tool for describing physico-chemical properties. Cubic models constructed in SPSS show statistically significant correlations with the properties as illustrated in Table 5.

TABLE 5. Correlation coefficient of NM_1 , MNM_1 , NM_2 , NM_1^ϵ , MNM_1^ϵ , and NM_2^ϵ with AF, S, HVAP, and DHVAP.

Indices	AF	S	HVAP	DHVAP
NM_1	0.994556963	0.952614387	0.826047189	0.893552603
MNM_1	0.98642	0.94169	0.72815	0.81182
NM_2	0.98533	0.94809	0.72522	0.81179
NM_1^ϵ	0.983	0.964	0.826	0.892
MNM_1^ϵ	0.982	0.963	0.815	0.883
NM_2^ϵ	0.989	0.966	0.829	0.895

The correlation of these indices can be represented in Figure 2.

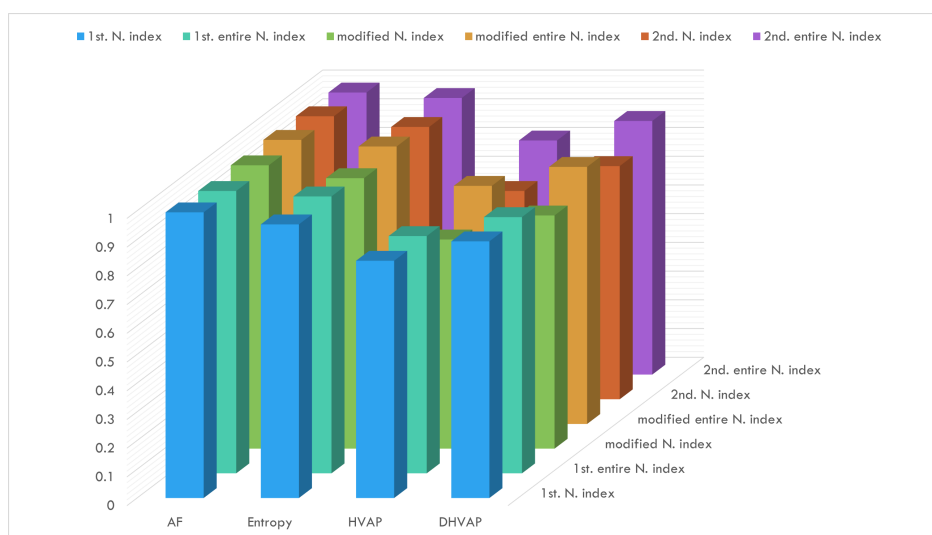


FIGURE 2. Graphical representation of the correlations between the indices and the properties of octan isomers.

The entire neighborhood indices showed a strong correlation with entropy and EF, which achieved 0.98 and 0.96, respectively. as indicated in this table. The other properties have good correlation values with these indices ranging between 0.81 - 0.89. The following figs. 3 to 5 depicts the correlations argued above.

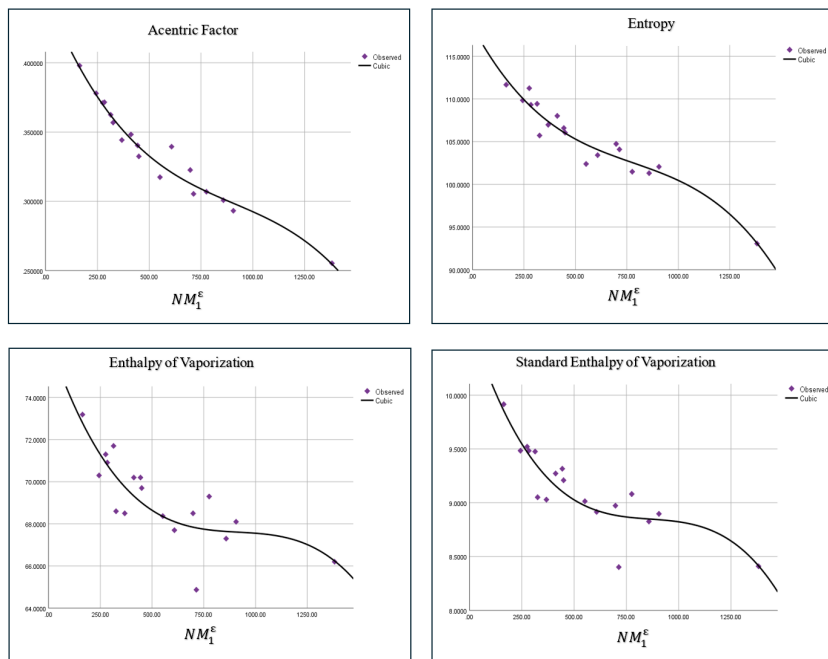


FIGURE 3. Correlations of AF, S, HVAP, and DHVAP with first entire neighborhood index for octane isomers.

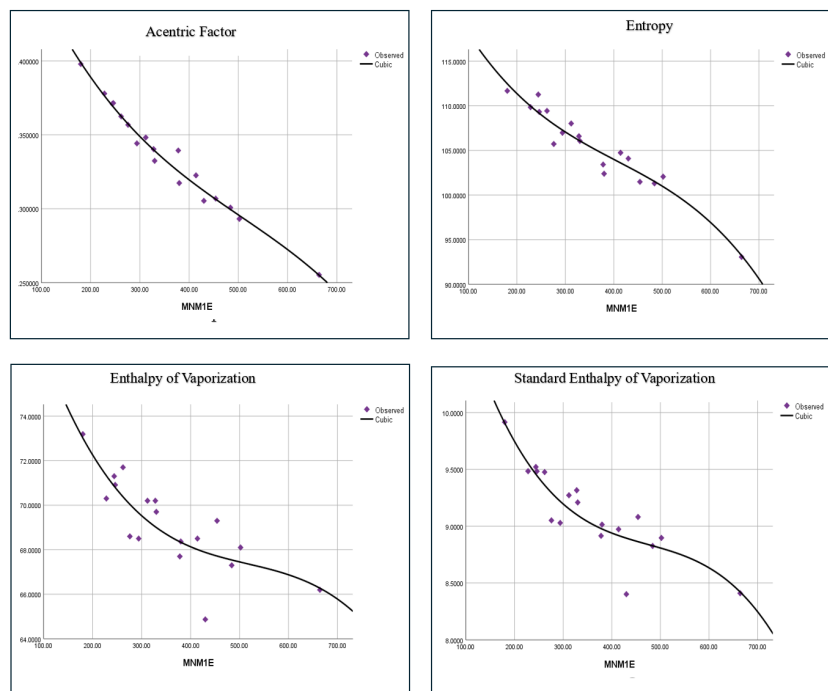


FIGURE 4. Correlations of AF, S, HVAP, and DHVAP with modified entire neighborhood index for octane isomers.

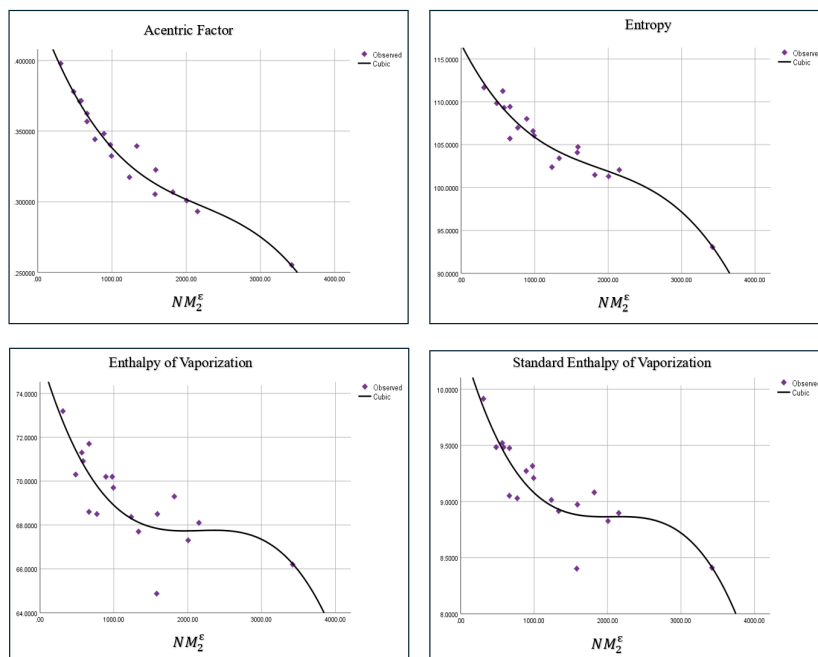


FIGURE 5. Correlations of AF, S, HVAP, and DHVAP with second entire neighborhood index for octane isomers.

The next predictive regression equations are produced through the cubic QSPR modeling, which establishes a relationship between the newly defined indices and the physico-chemical properties of octane isomers.

(1) For the first entire neighborhood index

$$AF = 3.407 \times 10^{-7}(NM_1^E)^2 - 1.256 \times 10^{-10}(NM_1^E)^3 + 0.449$$

$$S = -0.045(NM_1^E) + 4.655 \times 10^{-5}(NM_1^E)^2 - 1.991 \times 10^{-8}(NM_1^E)^3 + 118.495$$

$$HVAP = -0.029(NM_1^E) + 3.073 \times 10^{-5}(NM_1^E)^2 - 1.116 \times 10^{-8}(NM_1^E)^3 + 76.731$$

$$DHVAP = -0.006(NM_1^E) + 6.850 \times 10^{-6}(NM_1^E)^2 - 2.637 \times 10^{-9}(NM_1^E)^3 + 10.679$$

(2) For the modified entire neighborhood index

$$AF = -0.001(MNM_1^E) + 1.335 \times 10^{-6}(MNM_1^E)^2 - 8.810 \times 10^{-10}(MNM_1^E)^3 + 0.523$$

$$S = -0.124(MNM_1^E) - 1.924 \times 10^{-7}(MNM_1^E)^3 + 128.252$$

$$HVAP = -0.087(MNM_1^E) - 1.026 \times 10^{-7}(MNM_1^E)^3 + 84.173$$

$$DHVAP = -0.02(MNM_1^E) + 4.005 \times 10^{-5}(MNM_1^E)^2 - 2.815 \times 10^{-8}(MNM_1^E)^3 + 12.407$$

(3) For the second entire neighborhood index

$$AF = 5.533 \times 10^{-8} (NM_2^\varepsilon)^2 - 8.395 \times 10^{-12} (NM_2^\varepsilon)^3 + 0.435$$

$$S = -0.017 (NM_2^\varepsilon) + 7.233 \times 10^{-6} (NM_2^\varepsilon)^2 - 1.269 \times 10^{-9} (NM_2^\varepsilon)^3 + 116.706$$

$$HVAP = -0.011 (NM_2^\varepsilon) + 5.280 \times 10^{-6} (NM_2^\varepsilon)^2 - 8.152 \times 10^{-10} (NM_2^\varepsilon)^3 + 75.734$$

$$DHVAP = -0.002 (NM_2^\varepsilon) + 1.132 \times 10^{-6} (NM_2^\varepsilon)^2 - 1.831 \times 10^{-10} (NM_2^\varepsilon)^3 + 10.456$$

In order to confirm the predictive power of these new novel indices, we expanded our analysis to include benzenoid hydrocarbons dataset and Figure 6 depicts the chemical graphs for these compounds.

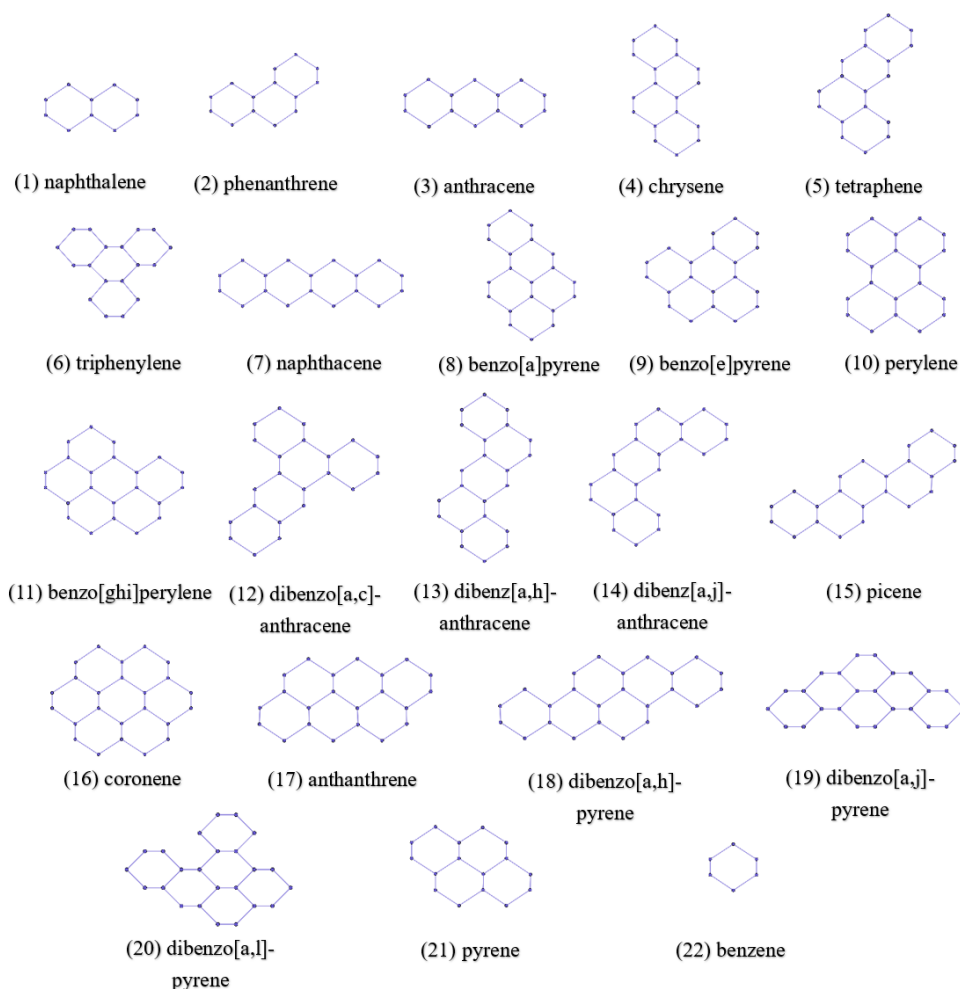


FIGURE 6. Molecular graphs of benzenoid hydrocarbon compounds.

The values of the neighborhood and entire neighborhood indices of these graphs are explained in Table 6 with their properties π -electronic energy (E_π), enthalpy of formation (EF), and boiling point (BP), which are taken from NIST databases [31] and retrieved from [32].

TABLE 6. Theoretical indices for benzenoid hydrocarbons and their experimental value of π -electronic energy (E_π), enthalpy of formation (EF), and boiling point (BP).

Compounds	NM_1	MNM_1	NM_2	NM_1^ϵ	MNM_1^ϵ	NM_2^ϵ	E_π	EF	BP
(1)	262	114	301	862	592	199	13.6832	141	218
(2)	440	182	533	1666	1020	4055	19.4483	202.7	338
(3)	432	180	518	1576	996	3782	19.3137	222.6	340
(4)	618	250	766	2472	1448	6128	25.1922	271.1	431
(5)	610	248	751	2382	1424	5853	25.1012	277.1	425
(6)	630	252	792	2604	1476	6558	25.2745	275.1	429
(7)	602	246	735	2290	1400	5567	24.9308	310.5	440
(8)	770	302	982	3278	1818	8317	28.222	296	496
(9)	780	304	1004	3392	1844	8690	28.3361	289.9	493
(10)	780	304	1002	3388	1844	8666	28.2453	319.2	497
(11)	930	356	1218	4184	2212	10848	31.4251	301.2	542
(12)	800	318	1011	3322	1880	8371	30.9418	348	535
(13)	788	316	984	3188	1852	7924	30.8805	335	536
(14)	788	316	984	3188	1852	7925	30.8795	336.3	531
(15)	796	318	999	3278	1876	8201	30.9432	336.9	519
(16)	1080	408	1434	4980	2580	13032	34.5718	296.7	590
(17)	922	354	1199	4086	2188	10523	31.253	323	547
(18)	950	370	1221	4106	2248	10477	33.928	375.6	596
(19)	950	370	1221	4106	2248	10477	33.954	366	594
(20)	962	372	1249	4244	2276	10950	34.031	393.3	595
(21)	590	234	743	2450	1388	6157	22.506	221.3	393
(22)	96	48	96	192	192	384	8	75.2	80.1

The represented data in Table 6 underscores once again that these new indices are both reliable and have significant potential as indicators. Additionally, a cubic model designed to improve the predictive ability of these newly defined indices which shows good correlations with the properties of the benzenoid hydrocarbon compounds in Table 7.

TABLE 7. Correlation coefficient of NM_1 , MNM_1 , NM_2 , NM_1^ε , MNM_1^ε , and NM_2^ε with E_π , EF, and BP.

Indices	E_π	EF	BP
NM_1	0.983503	0.895749	0.977581
MNM_1	0.991016	0.913259	0.98594
NM_2	0.974563	0.877489	0.967496
NM_1^ε	0.983	0.932	0.985
MNM_1^ε	0.990	0.940	0.991
NM_2^ε	0.980	0.928	0.983

The graphical representation for the correlations of these indices with the properties of benzenoid hydrocarbons is displayed in Figure 7.

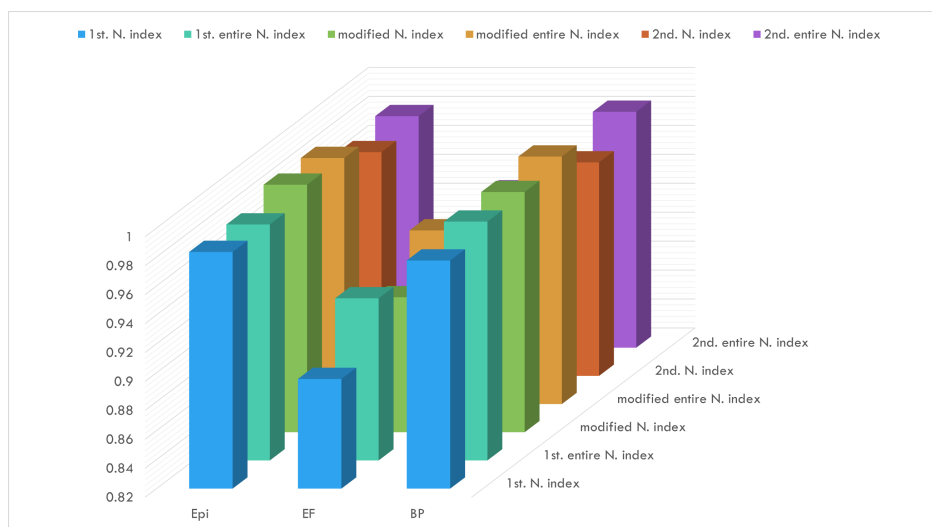


FIGURE 7. Graphical representation of the correlations between the indices and the properties of benzenoid hydrocarbons.

As highlighted, the modified entire neighborhood index demonstrates strong and significant correlations with E_π and BP, with a correlation value equal to 0.99. A significant correlation of the first and second entire neighborhood indices appears with these properties where it takes values ranging between 0.98 and 0.985. Also, the entire neighborhood indices depict a good correlation with EF having values of 0.92, 0.93, and 0.94.

Since these new indices have demonstrated a high correlation rate, they are therefore considered a valuable tool for modeling and estimating physical and chemical properties, and they possess a greater level of predictive ability. Subsequently, they are expected to have valuable applications in various fields, such as therapies and different types of networks including social, biological, and technological networks. The following figs. 8 to 10 illustrate these discussed correlations.

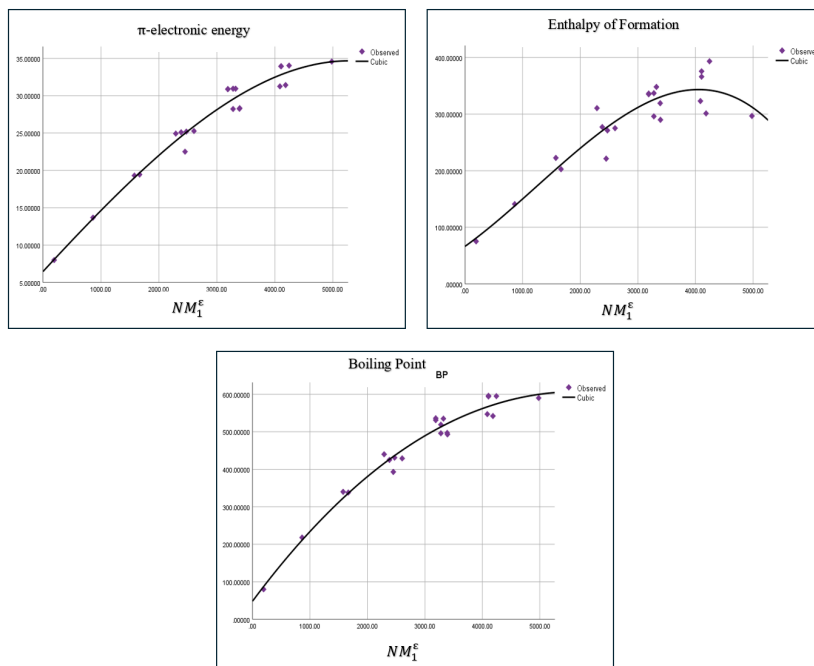


FIGURE 8. Correlations of E_{π} , EF, and BP with first entire neighborhood index for benzenoid hydrocarbon compounds.

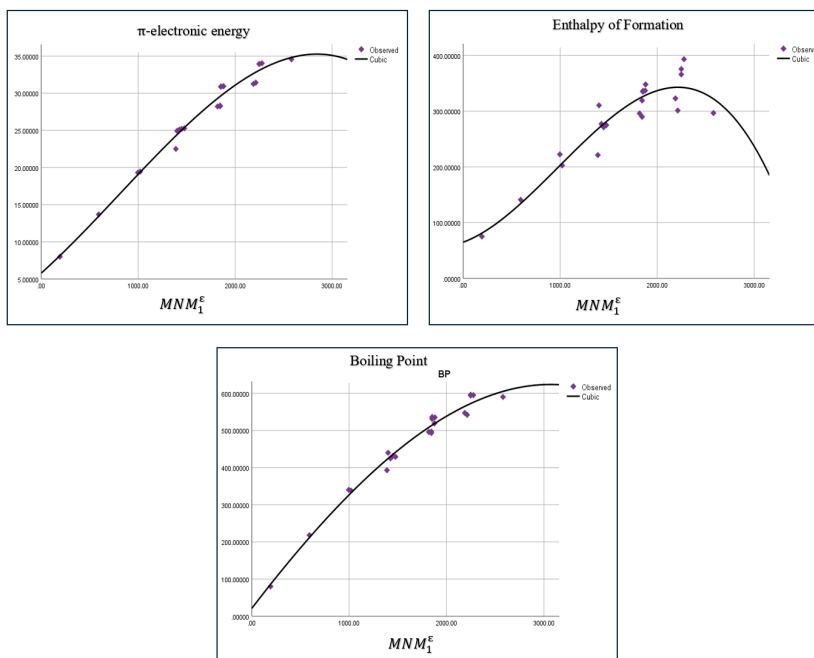


FIGURE 9. Correlations of E_{π} , EF, and BP with modified entire neighborhood index for benzenoid hydrocarbon compounds.

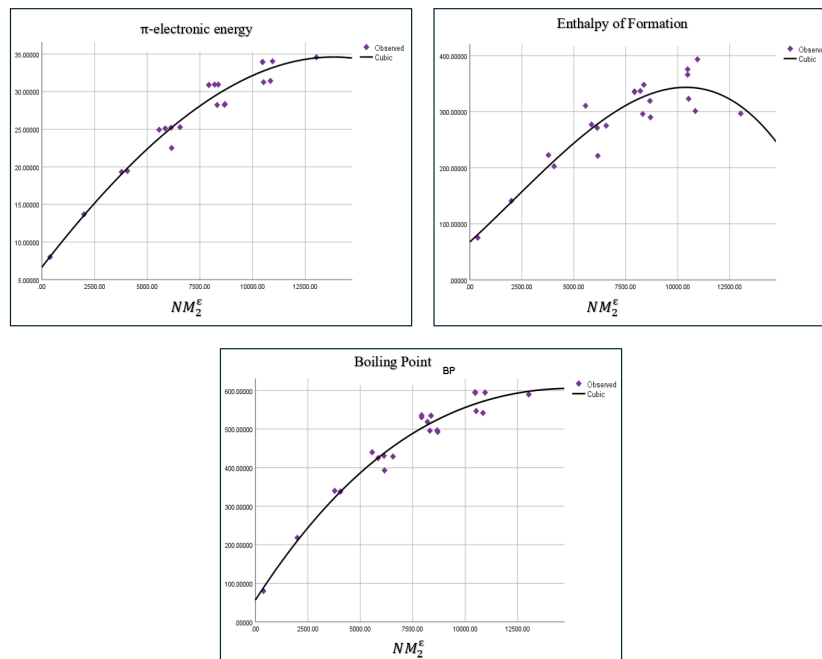


FIGURE 10. Correlations of E_{π} , EF, and BP with second entire neighborhood index for benzenoid hydrocarbon compounds.

The cubic QSPR modeling produced the following predictive regression equations, effectively linking the entire neighborhood indices to the physico-chemical properties of benzenoid hydrocarbon compounds.

(1) For the first entire neighborhood index

$$E_{\pi} = 0.008(NM_1^{\epsilon}) - 1.421 \times 10^{-7}(NM_1^{\epsilon})^2 - 8.248 \times 10^{-11}(NM_1^{\epsilon})^3 + 6.469$$

$$EF = 0.073(NM_1^{\epsilon}) + 1.444 \times 10^{-5}(NM_1^{\epsilon})^2 - 3.859 \times 10^{-9}(NM_1^{\epsilon})^3 + 66.344$$

$$BP = 0.206(NM_1^{\epsilon}) - 2.046 \times 10^{-5}(NM_1^{\epsilon})^2 + 2.685 \times 10^{-10}(NM_1^{\epsilon})^3 + 48.488$$

(2) For the modified entire neighborhood index

$$E_{\pi} = 0.012(MNM_1^{\epsilon}) + 2.690 \times 10^{-6}(MNM_1^{\epsilon})^2 - 1.114 \times 10^{-9}(MNM_1^{\epsilon})^3 + 5.799$$

$$EF = 0.064(MNM_1^{\epsilon}) - 3.821 \times 10^{-8}(MNM_1^{\epsilon})^3 + 65.089$$

$$BP = 0.342(MNM_1^{\epsilon}) - 3.116 \times 10^{-5}(MNM_1^{\epsilon})^2 - 5.329 \times 10^{-9}(MNM_1^{\epsilon})^3 + 21.173$$

(3) For the second entire neighborhood index

$$E_{\pi} = 0.004(NM_2^{\epsilon}) - 8.694 \times 10^{-8}(NM_2^{\epsilon})^2 - 2.121 \times 10^{-12}(NM_2^{\epsilon})^3 + 6.670$$

$$EF = 0.034(NM_2^{\epsilon}) + 1.097 \times 10^{-6}(NM_2^{\epsilon})^2 - 1.757 \times 10^{-10}(NM_2^{\epsilon})^3 + 67.628$$

$$BP = 0.085(NM_2^{\epsilon}) - 4.015 \times 10^{-6}(NM_2^{\epsilon})^2 + 5.387 \times 10^{-11}(NM_2^{\epsilon})^3 + 56.366$$

3. ENTIRE NEIGHBORHOOD INDICES FOR SOME GRAPH FAMILIES

In this section, we determine the first, second, and modified entire neighborhood indices for variety types of graphs. In, addition, we identify these indices for some types of bridge graphs and Sierpiński graphs.

3.1. Some Standard Graphs.

Proposition 3.1. *Let n be a positive integer and consider the path graph P_n , $n > 2$. Then,*

$$(1) \quad NM_1^\varepsilon(P_n) = \begin{cases} 14, & \text{if } n = 3; \\ 38, & \text{if } n = 4; \\ 4(8n - 23), & \text{otherwise.} \end{cases}$$

$$(2) \quad NM_2^\varepsilon(P_n) = \begin{cases} 17, & \text{if } n = 3; \\ 61, & \text{if } n = 4; \\ 119, & \text{if } n = 5; \\ 2(32n - 101), & \text{otherwise.} \end{cases}$$

$$(3) \quad MNM_1^\varepsilon(P_n) = \begin{cases} 22, & \text{if } n = 3; \\ 52, & \text{if } n = 4; \\ 84, & \text{if } n = 5; \\ 4(8n - 19), & \text{otherwise.} \end{cases}$$

Proof. Let n be a positive integer and consider the path graph P_n , $n > 2$. Then, P_n has $V(P_n) = \{v_1, v_2, v_3, \dots, v_{n-1}, v_n\}$ and $E(P_n) = \{e_1, e_2, \dots, e_{n-2}, e_{n-1}\}$. It is clear for $n = 3, 4$, or 5 . Let $n > 5$, the neighborhood degree of all elements of P_n is 4 except for the elements $\delta(v_1) = \delta(v_n) = \delta(e_1) = \delta(e_{n-1}) = 2$ and $\delta(v_2) = \delta(v_{n-1}) = \delta(e_2) = \delta(e_{n-2}) = 3$. Now, according to the definition we have

$$\begin{aligned} NM_1^\varepsilon(P_n) &= \sum_{v \in V(P_n)} \delta^2(v) + \sum_{e \in E(P_n)} \delta^2(e) \\ &= 2(2^2) + 2(3^2) + (n-4)(4^2) + 2(2^2) + 2(3^2) + (n-5)(4^2) \\ &= 4(8n - 23). \end{aligned}$$

Let $V_{a,b}$ denote the set of all adjacent vertices uv such that $\delta(u) = a$ and $\delta(v) = b$, $E_{a,b}$ denote the set of all adjacent edges ef where $\delta(e) = a$ and $\delta(f) = b$, and $A_{a,b}$ be the set of all pairs (v, e) in which the vertex v is incident to the edge e such that $\delta(v) = a$ and $\delta(e) = b$. Now, tables 8 to 10 represent the partitions for the graph P_n as follows,

TABLE 8. Partition of the vertices in path graphs

Type	$V_{2,3}$	$V_{3,4}$	$V_{4,4}$
Frequency	2	2	$n - 5$

TABLE 9. Partition of the edges in path graphs

Type	$E_{2,3}$	$E_{3,4}$	$E_{4,4}$
Frequency	2	2	$n - 6$

TABLE 10. Partition of vertices incident with edges in path graphs

Type	$A_{2,2}$	$A_{3,2}$	$A_{3,3}$	$A_{4,3}$	$A_{4,4}$
Frequency	2	2	2	2	$2n - 10$

Then, we have

$$\begin{aligned}
 NM_2^\varepsilon(P_n) &= 2(6 + 12) + (n - 5)(16) + 2(6 + 12) + (n - 6)(16) + 2(4 + 6 + 9 + 12) \\
 &\quad + (2n - 10)(16) = 64n - 202, \\
 MNM_1^\varepsilon(P_n) &= 2(5 + 7) + (n - 5)(8) + 2(5 + 7) + (n - 6)(8) + 2(4 + 5 + 6 + 7) \\
 &\quad + (2n - 10)(8) = 32n - 76.
 \end{aligned}$$

□

Note that, $\sum_{a,b} |V_{a,b}| = |E(\Gamma)|$, $\sum_{a,b} |E_{a,b}| = |E(L(\Gamma))|$, and $\sum_{a,b} |A_{a,b}| = 2|E(\Gamma)|$.

Proposition 3.2. *Let Γ be a k -regular graph of order n . Then, the first and second neighborhood indices of Γ are as follows*

- (1) $NM_1^\varepsilon(\Gamma) = nk[k^3 + 8(k - 1)^4]$.
- (2) $NM_2^\varepsilon(\Gamma) = nk[\frac{1}{2}k^4 + (2k - 2)^2(2k^3 - 5k^2 + 6k - 2)]$.
- (3) $MNM_1^\varepsilon(\Gamma) = nk[2k^2 + k(2k - 2)^2]$.

Proof. Let Γ be a k -regular graph of order n . Then, Γ has $m = \frac{nk}{2}$ edges and each edge has degree $d(e) = 2k - 2$. Thus, the neighborhood degree of each vertex and each edge in this graph are $\delta(v) = \sum_{u \in N(v)} d(u) = k^2$ and $\delta(e) = \sum_{f \in N(e)} d(f) = (2k - 2)^2$, respectively. Thus,

$$NM_1^\varepsilon(\Gamma) = \sum_{v \in V(\Gamma)} \delta^2(v) + \sum_{e \in E(\Gamma)} \delta^2(e) = nk^4 + \frac{nk}{2}(2k - 2)^4 = nk[k^3 + 8(k - 1)^4].$$

Now, the graph Γ has $|V_{k^2,k^2}| = \frac{1}{2}nk$, $|E_{(2k-2)^2,(2k-2)^2}| = \frac{1}{2}nk(k - 1)$, and $|A_{k^2,(2k-2)^2}| = nk$. Then, we have

$$\begin{aligned}
 NM_2^\varepsilon(\Gamma) &= \frac{nk}{2}k^4 + \frac{nk}{2}(k - 1)(2k - 2)^4 + nk[k^2(2k - 2)^2] \\
 &= nk[\frac{1}{2}k^4 + (2k - 2)^2(2k^3 - 5k^2 + 6k - 2)].
 \end{aligned}$$

and

$$\begin{aligned} MNM_1^\varepsilon(\Gamma) &= \frac{1}{2}nk(2k^2) + \frac{1}{2}nk(k-1)[2(2k-2)^2] + nk[k^2 + (2k-2)^2] \\ &= nk[k^2 + (k-1)(2k-2)^2 + k^2 + (2k-2)^2]. \end{aligned}$$

□

Corollary 3.1. For the cycle graph C_n , and the complete graph K_n , $n \geq 3$, we have

- (1) $NM_1^\varepsilon(C_n) = MNM_1^\varepsilon(C_n) = 32n$.
- (2) $NM_2^\varepsilon(C_n) = 2NM_1^\varepsilon(C_n)$.
- (3) $NM_1^\varepsilon(K_n) = n^3(3n-10)^2 + 5n(10n^2+13) - 164n^2$.
- (4) $NM_2^\varepsilon(K_n) = n^3(8n^4 - 879n + 1175) - \frac{n}{2}(167n^5 - 739n^4 + 1659n - 479)$.
- (5) $MNM_1^\varepsilon(K_n) = 2n(2n^4 - 11n^3 + 23n^2 - 21n + 7)$.

Proposition 3.3. For any complete bipartite graph $K_{a,b}$,

- (1) $NM_1^\varepsilon(K_{a,b}) = ab[(a+b)^4 + 24(a+b)^2 - 8(a^3+b^3) - (a+b)(23ab+32) + 16]$.
- (2) $NM_2^\varepsilon(K_{a,b}) = ab[(ab)^2 + \frac{(a+b-2)^2}{2}((a+b)^3 - 2(a+b)^2 - (2a-2)^2 - (2b-2)^2 + 4(a+b-ab))]$.
- (3) $MNM_1^\varepsilon(K_{a,b}) = ab[(a+b)^3 - 2(a+b)^2 + 4(a+b) - 2(a^2+b^2)]$.

Proof. Consider the complete bipartite graph $K_{a,b}$ with $a+b$ vertices and ab edges. The neighborhood degree of every vertex v in $V(K_{a,b})$ is $\delta(v) = ab$ and $\delta(e) = (a+b-2)^2$ for any edge e in $E(K_{a,b})$. Therefore

$$\begin{aligned} NM_1^\varepsilon(K_{a,b}) &= (a+b)(ab)^2 + ab(a+b-2)^4 \\ &= ab[a^4 + 4a^3b - 8a^3 + 6a^2b^2 - 23a^2b + 24a^2 + 4ab^3 \\ &\quad - 23ab^2 + 48ab - 32a + b^4 - 8b^3 + 24b^2 - 32b + 16]. \end{aligned}$$

Now, for the second and modified entire neighborhood indices, the graph has the following partitions,

$|V_{ab,ab}| = ab$, $|E_{(a+b-2)^2, (a+b-2)^2}| = \frac{1}{2}(ab^2 + a^2b) - ab$, and $|A_{ab, (a+b-2)^2}| = 2ab$. Hence, by [1.1] we get that

$$\begin{aligned} NM_2^\varepsilon(K_{a,b}) &= ab(ab)^2 + [\frac{1}{2}(ab^2 + a^2b) - ab](a+b-2)^4 + 2ab[ab(a+b-2)^2] \\ &= ab[(ab)^2 + \frac{a+b-2}{2}(a+b-2)^4 + 2ab(a+b-2)^2] \\ &= ab[(ab)^2 + \frac{(a+b-2)^2}{2}(a^3 - 6a^2 - 8ab + 3ab^2 + 3a^2b + 12a + b^3 - 6b^2 + 12b - 8)], \end{aligned}$$

and

$$\begin{aligned} MNM_1^\epsilon(K_{a,b}) &= ab(2ab) + \left[\frac{1}{2}(ab^2 + a^2b) - ab\right](2(a + b - 2)^2) + 2ab[ab + (a + b - 2)^2] \\ &= 4(ab)^2 + (ab^2 + a^2b)(a^2 + 2ab + b^2 - 4a - 4b + 4) \\ &= ab[a^3 - 4a^2 - 4ab + 3ab^2 + 3a^2b + 4a + b^3 - 4b^2 + 4b]. \end{aligned}$$

□

Corollary 3.2. For the star graph S_b , we have

- (1) $NM_1^\epsilon(S_b) = (b - 1)[b^4 - 8b^3 + 25b^2 - 33b + 16]$.
- (2) $NM_2^\epsilon(S_b) = (b - 1)\left[\frac{1}{2}b^5 - 5b^4 + 22b^3 - 49b^2 + 54b - 23\right]$.
- (3) $MNM_1^\epsilon(S_b) = (b - 1)[b^3 - 4b^2 + 8b - 4]$.

A book graph B_n is defined to be a Cartesian product of the star graph S_{n+1} and the path graph P_2 , that is $B_n = S_{n+1} \square P_2$. It has $2n + 2$ vertices and $3n + 1$ edges. The graph B_n is a biregular graph with two possible vertex degrees which are 2 and $m + 1$.

Proposition 3.4. For the book graph B_n , we have

- (1) $NM_1^\epsilon(B_n) = 2[n^5 + 6n^4 + 13n^3 + 25n^2 + 18n + 1]$.
- (2) $NM_2^\epsilon(B_n) = n^6 + 7n^5 + 26n^4 + 69n^3 + 104n^2 + 48n + 1$.
- (3) $MNM_1^\epsilon(B_n) = 2[n^4 + 7n^3 + 25n^2 + 30n + 2]$.

Proof. Consider the book graph B_n . Then, according to the neighborhood degree of each element in this graph, there are $2n$ vertices with $\delta(v) = n + 3$ and 2 with $\delta(v) = 3n + 1$. Also, B_n has n edges with $\delta(e) = 2n + 2$, $2n$ edges with $\delta(e) = (n + 1)^2$, and one edge with $\delta(e) = 2n(n + 1)$. Hence, we have that

$$\begin{aligned} NM_1^\epsilon(B_n) &= 2n(n + 3)^2 + 2(3n + 1)^2 + n(2n + 2)^2 + 2n(n + 1)^4 + (2n^2 + 2n)^2 \\ &= 2n(n^2 + 6n + 9) + 2(9n^2 + 6n + 1) + 4n(n^2 + 2n + 1) + 2n(n^2 + 2n + 1)^2 \\ &\quad + 4n^2(n + 1)^2 = 2(n^3 + 15n^2 + 15n + 1) + 2n(n + 1)^2[n^2 + 4n + 3]. \end{aligned}$$

Now, tables 11 to 13 depict the partitons of the vertices and edges in this graph as follows

TABLE 11. Partition of the vertices in book graphs.

Type	$V_{n+3,n+3}$	$V_{n+3,3n+1}$	$V_{3n+1,3n+1}$
Frequency	n	$2n$	1

TABLE 12. Partition of the edges in book graphs.

Type	$E_{2n+2,(n+1)^2}$	$E_{(n+1)^2,2n^2+2n}$	$E_{(n+1)^2,(n+1)^2}$
Frequency	$2n$	$2n$	$n^2 - n$

TABLE 13. Partition of the vertices incident with edges in book graphs.

Type	$A_{n+3,2n+2}$	$A_{n+3,(n+1)^2}$	$V_{3n+1,(n+1)^2}$	$A_{3n+1,2n^2+2n}$
Frequency	$2n$	$2n$	$2n$	2

Therefore, we get that

$$\begin{aligned}
 NM_2^\varepsilon(B_n) &= n(n+3)^2 + 2n[(n+3)(3n+1)] + (3n+1)^2 + 2n[(2n+2)(n+1)^2] \\
 &\quad + 2n[(n+1)^2(2n^2+2n)] + (n^2-n)(n+1)^4 + 2n[(n+3)(2n+2)] \\
 &\quad + 2n[(n+3)(n+1)^2] + 2n[(3n+1)(n+1)^2] + 2[(3n+1)(2n^2+2n)] \\
 &= n(n+3)[2n^2+15n+11] + (n+1)^2[n^2(n^2+13)+5n(n^2+1)] \\
 &\quad + (3n+1)[4n^2+7n+1],
 \end{aligned}$$

and

$$\begin{aligned}
 MNM_1^\varepsilon(B_n) &= n[2(n+3)] + 2n[n+3+3n+1] + 2[3n+1] + 2n[2n+2+(n+1)^2] \\
 &\quad + 2n[(n+1)^2+2n^2+2n] + (n^2-n)[2(n+1)^2] + 2n[n+3+2n+2] \\
 &\quad + 2n[n+3+(n+1)^2] + 2n[3n+1+(n+1)^2] + 2[3n+1+2n^2+2n] \\
 &= 2n[6n^2+23n+20] + 2n^4 + 2n^3 + 4n^2 + 20n + 4.
 \end{aligned}$$

□

The gear graph G_n is obtained from a wheel graph W_n by adding a new vertex between each pair of adjacent vertices in the cycle. On the other hand, a helm graph H_n is obtained from a wheel graph W_n by joining a pendent vertex to every vertex in the cycle. Each of these two graphs has $2n+1$ vertices and $3n$ edges.

Proposition 3.5. For any gear graph G_n , we have

- (1) $NM_1^\varepsilon(G_n) = n^3(n^2+13) + 5n(9n+35)$.
- (2) $NM_2^\varepsilon(G_n) = 11n^4 + 20n^3 + \frac{1}{2}n[n^5 - n^4 + 257n + 727]$.
- (3) $MNM_1^\varepsilon(G_n) = n^4 + 3n^3 + 25n^2 + 131n$.

Proof. For any gear graph G_n , let $V_{(i)}$ and $E_{(i)}$ denote the subset of vertices and edges in which all of its element has neighborhood degrees equal i , respectively. Then, G_n has $|V_{(6)}| = n$, $|V_{(n+4)}| = n$, $|V_{(3n)}| = 1$, $|E_{(n+7)}| = 2n$, and $|E_{(n^2+5)}| = n$. The first entire neighborhood index can be computed as the following

$$\begin{aligned}
 NM_1^\varepsilon(G_n) &= n(6^2) + n(n+4)^2 + (3n)^2 + 2n(n+7)^2 + n(n^2+5)^2 \\
 &= n[n^4 + 13n^2 + 45n + 175].
 \end{aligned}$$

Additionally, G_n has the partitions that can be shown in tables 14 to 16.

TABLE 14. Partition of the vertices in gear graphs.

Type	$V_{6,n+4}$	$V_{n+4,3n}$
Frequency	$2n$	n

TABLE 15. Partition of the edges in gear graphs.

Type	$E_{n+7,n+7}$	E_{n+7,n^2+5}	E_{n^2+5,n^2+5}
Frequency	$2n$	$2n$	$\frac{1}{2}n(n-1)$

TABLE 16. Partition of vertices incident with edges in gear graphs.

Type	$A_{6,n+7}$	$A_{n+4,n+7}$	A_{n+4,n^2+5}	A_{3n,n^2+5}
Frequency	$2n$	$2n$	n	n

Thus, the second and modified entire neighborhood indices will be obtained by using [1.1],

$$\begin{aligned}
 NM_2^\varepsilon(G_n) &= 2n[6(n+4)] + n[3n(n+4)] + 2n(n+7)^2 + 2n[(n+7)(n^2+5)] \\
 &\quad + \frac{n(n-1)}{2}(n^2+5)^2 + 2n[6(n+7)] + 2n[(n+4)(n+7)] + n[(n+4)(n^2+5)] \\
 &\quad + n[3n(n^2+5)] \\
 &= 2n[n^3 + 9n^2 + 42n + 178] + n[4n^3 + 7n^2 + 32n + 20 + \frac{n-1}{2}(n^4 + 10n^2 + 25)],
 \end{aligned}$$

Similarly, we have

$$\begin{aligned}
 MNM_1^\varepsilon(G_n) &= 2n[n+10] + n[4n+4] + 2n[2n+14] + 2n[n^2+n+12] + n(n-1)[n^2+5] \\
 &\quad + 2n[n+13] + 2n[2n+11] + n[n^2+n+9] + n[n^2+3n+5] \\
 &= 2n[n^2+8n+61] + n[n^3+n^2+9n+9].
 \end{aligned}$$

□

Proposition 3.6. For the helm graph H_n , we have

- (1) $NM_1^\varepsilon(H_n) = n[n^4 + 2n^3 + 27n^2 + 170n + 877]$.
- (2) $NM_2^\varepsilon(H_n) = \frac{1}{2}n^3[n(n^2+13) + (n+13)^2] + 2n[(2n+34)^2 + (n+4)^2 + 119n+3]$.
- (3) $MNM_1^\varepsilon(H_n) = n^3(n+5) + 3n(17n+117)$.

Proof. Consider the helm graph, then we have $|V_{(4)}| = n, |V_{(n+9)}| = n, |V_{(4n)}| = 1, |E_{(2n+22)}| = n, |E_{(n+14)}| = n,$ and $|E_{(n^2+n+10)}| = n$. Thus, the first entire neighborhood index can be obtained by calculating the following equation.

$$\begin{aligned}
 NM_1^\varepsilon(H_n) &= n(4^2) + n(n+9)^2 + (4n)^2 + n(2n+22)^2 + n(n+14)^2 + n(n^2+n+10)^2 \\
 &= 6n^3 + 150n^2 + 777n + n(n^4 + 2n^3 + 21n^2 + 20n + 100).
 \end{aligned}$$

Now, for the two remaining indices we consider the partitions for the helm graph represented in tables 17 to 19.

TABLE 17. Partition of the vertices in helm graphs.

Type	$V_{4,n+9}$	$V_{n+9,n+9}$	$V_{n+9,4n}$
Frequency	n	n	n

TABLE 18. Partition of the edges in helm graphs.

Type	$E_{2n+22,2n+22}$	$E_{2n+22,n+14}$	E_{n+14,n^2+n+10}	E_{2n+22,n^2+n+10}	E_{n^2+n+10,n^2+n+10}
Frequency	n	$2n$	n	$2n$	$\frac{1}{2}(n^2 - n)$

TABLE 19. Partition of the vertices incident with edges in helm graphs.

Type	$A_{4,n+14}$	$A_{n+9,n+14}$	$A_{n+9,2n+22}$	A_{n+9,n^2+n+10}	A_{4n,n^2+n+10}
Frequency	n	n	$2n$	n	n

Consequently, we get that

$$\begin{aligned}
 NM_2^\varepsilon(H_n) &= n[4(n+9)] + n(n+4)^2 + n[4n(n+4)] + n(2n+22)^2 + 2n[(2n+22)(n+14)] \\
 &\quad + n[(n+14)(n^2+n+10)] + 2n[(2n+22)(n^2+n+10)] + \frac{n^2-n}{2}(n^2+n+10)^2 \\
 &\quad + n[4(n+14)] + n[(n+9)(n+14)] + 2n[(n+9)(2n+22)] + n[(n+9)(n^2+n+10)] \\
 &\quad + n[4n(n^2+n+10)] \\
 &= n[6n^3 + 39n^2 + 222n + 948] + 2n[2n^3 + 28n^2 + 132n + 726] \\
 &\quad + \frac{n^2-n}{2}[n^4 + 2n^3 + 21n^2 + 20n + 100] \\
 &= \frac{1}{2}n^3[n^3 + n^2 + 39n + 189] + 526n^2 + 2350n.
 \end{aligned}$$

Also, the modified one can be computed through the following equation

$$\begin{aligned}
 MNM_1^\varepsilon(H_n) &= n[n+13] + n[2(n+4)] + n[5n+4] + n[4n+44] + 2n[3n+36] \\
 &\quad + n[n^2+2n+24] + 2n[n^2+3n+32] + \frac{n^2-n}{2}[2(n^2+n+10)] \\
 &\quad + n[n+18] + n[2n+23] + 2n[3n+31] + n[n^2+2n+19] + n[n^2+5n+10] \\
 &= n[3n^2+24n+163] + 2n[n^2+9n+99] + n^4+9n^2-10n \\
 &= n^4+5n^3+51n^2+351n.
 \end{aligned}$$

□

3.2. The Bridge graph. Bridge graphs are valuable tools for identifying essential connections within a network that are important for maintaining its connectivity. They have vast applications in various fields such as communication, transportation, and chemistry, providing to understand and improve the structure and accuracy of these systems. By considering these crucial links, bridge graphs simplify the analysis and resolution of problems in complex networks.

Let Γ_1 and Γ_2 be two connected graphs, and let $u \in V(\Gamma_1), v \in V(\Gamma_2)$. The bridge graph is obtained by joining $u \in V(\Gamma_1)$ with $v \in V(\Gamma_2)$, for more detailed information see [33]. Through this section, we compute the defining topological indices for three cases of bridge graphs.

Bridge graph over path P_n . Let P_n be the path graph of order n . The bridge graph $G_m(P_n; v)$ has mn vertices and $mn - 1$ edges. For instance, the bridge graph over the path P_4 can be shown in Figure 11.

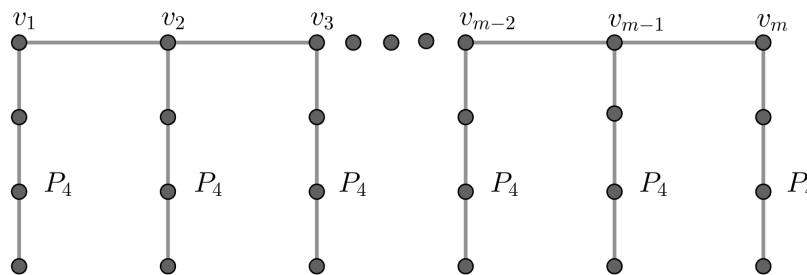


FIGURE 11. Bridge graph over path P_4 .

Proposition 3.7. Let m and n be positive integers greater than 4, and consider the bridge graph $G_m(P_n; v)$ over path. Then,

- (1) $NM_1^\epsilon(G_m(P_n; v)) = 4(73m + 8mn - 203)$.
- (2) $NM_2^\epsilon(G_m(P_n; v)) = 32m(2n + 25) - 2260$.
- (3) $MNM_1^\epsilon(G_m(P_n; v)) = 16m(2n + 7) - 328$.

Proof. Let m and n be positive integers greater than 4, and consider the bridge graph $G_m(P_n; v)$ over path. Then, $G_m(P_n; v)$ contains $|V_{(2)}| = |V_{(3)}| = |V_{(5)}| = m, |V_{(4)}| = m(n - 4) + 2, |V_{(7)}| = 2, |V_{(8)}| = m - 4, |E_{(2)}| = |E_{(3)}| = |E_{(5)}| = m, |E_{(4)}| = m(n - 5) + 2, |E_{(9)}| = 4, |E_{(10)}| = m - 4, |E_{(13)}| = 2,$ and $|E_{(14)}| = m - 5$.

Then, the first entire neighborhood index can be calculated from the following

$$NM_1^\epsilon(G_m(P_n; v)) = m[4 + 9 + 25] + [m(n - 4) + 2](16) + 2(49) + (m - 4)(64) + m(4 + 9 + 25) + [m(n - 5) + 2](16) + 4(81) + (m - 4)(100) + 2(169) + (m - 5)(196).$$

Moreover, we can see that $G_m(P_n; v)$ has the following partitions as demonstrated in tables 20 to 22,

TABLE 20. Partition of the vertices in bridge graphs over path.

Type	$V_{2,3}$	$V_{3,4}$	$V_{4,4}$	$V_{4,5}$	$V_{5,7}$	$V_{7,8}$	$V_{8,8}$	$V_{5,8}$
Frequency	m	m	$m(n-5)+2$	m	4	2	$m-5$	$m-4$

TABLE 21. Partition of the edges in bridge graphs over path.

Type	$E_{2,3}$	$E_{3,4}$	$E_{4,4}$	$E_{4,5}$	$E_{5,9}$	$E_{9,9}$
Frequency	m	m	$m(n-6)+2$	m	4	2

Type	$E_{10,14}$	$E_{13,14}$	$E_{14,14}$	$E_{10,13}$	$E_{5,10}$	$E_{9,13}$
Frequency	$2(m-6)+2$	2	$m-6$	2	$m-4$	4

TABLE 22. Partition of the vertices incident with edges in bridge graphs over path.

Type	$A_{2,2}$	$A_{3,2}$	$A_{3,3}$	$A_{4,3}$	$A_{4,4}$	$A_{4,5}$	$A_{5,5}$
Frequency	m	m	m	m	$2mn-10m+4$	m	m

Type	$A_{5,9}$	$A_{7,9}$	$A_{7,13}$	$A_{5,10}$	$A_{8,10}$	$A_{8,13}$	$A_{8,14}$
Frequency	4	4	2	$m-4$	$m-4$	2	$2(m-6)+2$

Therefore, the second entire neighborhood index can be obtained from the following

$$\begin{aligned}
 NM_2^e(G_m(P_n;v)) &= 2m[6+12+20] + [m(n-5)+2]16 + 4[35+45+117+63+45] \\
 &\quad + 2[56+81+182+130+91+104] + (m-4)[40+50+50+80] \\
 &\quad + (m-5)[64] + (m-6)[196] + m[4+6+9+12+20+25] \\
 &\quad + [m(n-6)+2]16 + [2(m-6)+2](140+112) + [2mn-10m+4]16 \\
 &= 64mn + 800m - 2260.
 \end{aligned}$$

In a similar manner, we can get the modified entire neighborhood index

$$\begin{aligned}
 MNM_1^e(G_m(P_n;v)) &= m[83] + 2[124] + 4[78] + (m-4)[61] + (m-5)[16] \\
 &\quad + (m-6)[28] + [m(n-5)+2]8 + [m(n-6)+2]8 \\
 &\quad + [2(m-6)+2]46 + [2mn-10m+4]8 \\
 &= 112m + 32mn - 328.
 \end{aligned}$$

□

Bridge graph over cycle C_n . Let C_n be the cycle graph of order n . The bridge graph $G_m(C_n;v)$ has mn vertices and $mn+m-1$ edges. Figure 12 illustrates the graph $G_m(C_6;v)$.

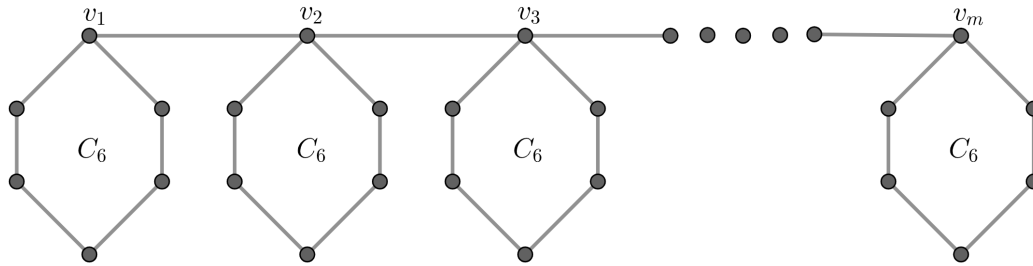


FIGURE 12. Bridge graph over cycle C_6 .

Proposition 3.8. Consider the bridge graph $G_m(C_n; v)$ over cycle, where $m > 5$ and $n > 4$. Then,

- (1) $NM_1^\epsilon(G_m(C_n; v)) = 8m(4n + 201) - 3022$.
- (2) $NM_2^\epsilon(G_m(C_n; v)) = 4m(16n + 1223) - 9946$.
- (3) $MNM_1^\epsilon(G_m(C_n; v)) = 8m(4n + 65) - 380$.

Proof. Consider the bridge graph $G_m(C_n; v)$ over cycle, where $m > 5$ and $n > 4$. Then, the vertices and edges of this graph are distributed as detailed below,

$$|V_{(4)}| = m(n - 3), |V_{(5)}| = 4, |V_{(6)}| = 2(m - 2), |V_{(7)}| = |V_{(11)}| = 2, |V_{(12)}| = m - 4, |E_{(4)}| = m(n - 4),$$

$$|E_{(5)}| = |E_{(10)}| = |E_{(17)}| = 4, |E_{(6)}| = 2(m - 2),$$

$$|E_{(18)}| = 2(m - 4), |E_{(20)}| = |E_{(27)}| = 2, \text{ and } |E_{(28)}| = m - 5. \text{ Hence, get that}$$

$$NM_1^\epsilon(G_m(C_n; v)) = [mn - 3m]16 + 2[4(25) + (2m - 4)36] + 2[49 + 121 + 400 + 729]$$

$$+ 4[100 + 289] + (m - 4)144 + (2m - 8)324 + [mn - 4m]16 + (m - 5)784$$

$$= 32mn + 1608m - 3022.$$

The graph $G_m(C_n; v)$ can be dividing to several partitions as it shown in tables 23 to 25.

TABLE 23. Partition of the vertices in bridge graphs over cycle.

Type	$V_{4,4}$	$V_{4,5}$	$V_{4,6}$	$V_{5,7}$	$V_{6,11}$	$V_{6,12}$	$V_{11,12}$	$V_{7,11}$	$V_{12,12}$
Frequency	$m(n - 4)$	4	$2(m - 2)$	4	4	$2(m - 4)$	2	2	$m - 5$

TABLE 24. Partition of the edges in bridge graphs over cycle.

Type	$E_{4,4}$	$E_{4,5}$	$E_{5,10}$	$E_{10,10}$	$E_{10,20}$	$E_{4,6}$
Frequency	$m(n - 5)$	4	4	2	4	$2(m - 2)$
Type	$E_{6,17}$	$E_{17,17}$	$E_{20,17}$	$E_{20,27}$	$E_{17,27}$	$E_{27,18}$
Frequency	4	2	4	2	4	4
Type	$E_{6,18}$	$E_{18,18}$	$E_{18,28}$	$E_{27,28}$	$E_{28,28}$	–
Frequency	$2(m - 4)$	$m - 4$	$4(m - 4) - 4$	2	$m - 6$	–

TABLE 25. Partition of the vertices incident with edges in bridge graphs over cycle.

Type	$A_{4,4}$	$A_{4,5}$	$A_{5,5}$	$A_{5,10}$	$A_{7,10}$	$A_{7,20}$
Frequency	$2m(n-4)$	4	4	4	4	2
Type	$A_{4,6}$	$A_{6,6}$	$A_{6,17}$	$A_{11,17}$	$A_{11,20}$	$A_{11,27}$
Frequency	$2(m-2)$	$2(m-2)$	4	4	2	2
Type	$A_{12,27}$	$A_{12,28}$	$A_{6,18}$	$A_{12,18}$	-	-
Frequency	2	$2(m-4)-2$	$2(m-4)$	$2(m-4)$	-	-

Therefore, the remaining two neighborhood indices can be computed as the following

$$\begin{aligned}
 NM_2^\varepsilon(G_m(C_n;v)) &= 4[2232] + 2[2875] + (2m-4)[108] + (2m-8)[504] + (m-4)[324] \\
 &\quad + (m-5)[144] + (m-6)[784] + (4mn-17m)[16] + (2m-10)[1344] \\
 &= 64mn + 4892m - 9946.
 \end{aligned}$$

Furthermore, by a similar criteria, we have

$$\begin{aligned}
 MNM_1^\varepsilon(G_m(C_n;v)) &= 4[397] + 2[302] + (2m-4)[42] + (2m-8)[96] + (m-4)[36] \\
 &\quad + (m-5)[24] + (m-6)[56] + (2m-10)[132] + (4mn-17m)[8] \\
 &= 32mn + 520m - 380.
 \end{aligned}$$

□

Bridge graph over complete graph K_n . Let K_n be a complete graph of order n . Then, $G_m(K_n;v)$ has mn vertices and $\frac{mn(n-1)+2m-2}{2}$ edges. For example, the bridge graph over K_6 ; $G_m(K_6;v)$ can be depicted in Figure 13.

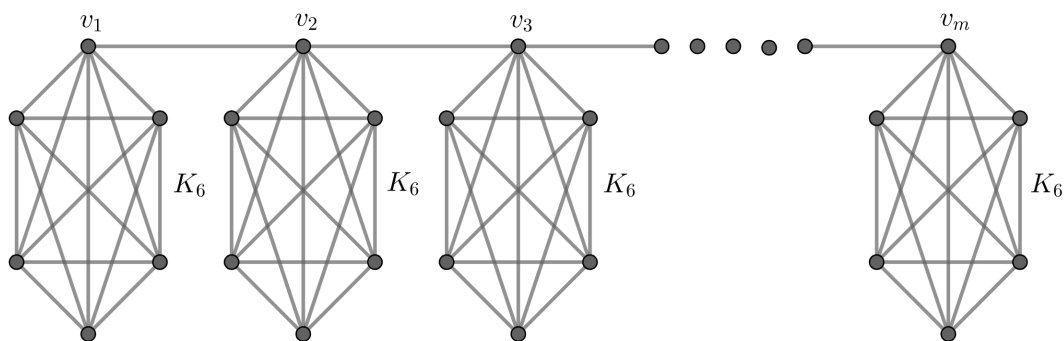


FIGURE 13. Bridge graph over complete graph K_6 .

Proposition 3.9. Let $m > 4$ and $n > 2$ be positive integers and consider the bridge graph $G_m(K_n;v)$ over complete graph. Then, we have

- (1) $NM_1^\epsilon(G_m(K_n; v)) = m[8n^2(n^4 + 141) + 4(79n^4 + 65) - n(71n^4 + 782n^2 + 839)] + 2[57n^3 - 175n^2 + 161n - 59]$.
- (2) $NM_2^\epsilon(G_m(K_n; v)) = m[n^3(8n^4 - 1456n + 2865) - \frac{1}{2}n(167n^5 - 931n^4 + 6651n - 4331) - 575] - 96n^5 + 528n^4 - 1513n^3 + 1961n^2 - 1467n + 385$.
- (3) $MNM_1^\epsilon(G_m(K_n; v)) = 2m[2n^5 - 11n^4 + 39n^3 - 53n^2 + 49n - 10] - 32n^3 + 30n^2 - 70n - 4$.

Proof. Let $m > 4$ and $n > 2$ be positive integers and consider the bridge graph $G_m(K_n; v)$ over a complete graph. Then, the bridge graph in this case has

$$|V_{(n(n-2)+2)}| = 2(n-1), |V_{(n(n-2)+3)}| = (m-2)(n-1), |V_{(n(n-1)+2)}| = |V_{(n^2+2)}| = 2, |V_{(n^2+3)}| = m-4, |E_{([2n-4]^2+2)}| = n(n-3) + 2, |E_{(4n^2-16n+20)}| = \frac{1}{2}[m(n^2 - 3n + 2) - n^2 + 3n - 2], |E_{(4n^2-10n+12)}| = (m-4)(n-1), |E_{(4n^2-13n+13)}| = |E_{(4n^2-10n+11)}| = 2(n-1), |E_{(4n^2-7n+5)}| = |E_{(4n^2-4n+3)}| = 2, and |E_{(4n^2-4n+4)}| = m-5.$$

Thus, we have

$$\begin{aligned} NM_1^\epsilon(G_m(K_n; v)) &= (2n-2)[(n^2 - 2n + 2)^2 + (4n^2 - 13n + 13)^2 + (4n^2 - 10n + 11)^2] \\ &\quad + 2[(n^2 - n + 2)^2 + (n^2 + 2)^2 + (4n^2 - 7n + 5)^2 + (4n^2 - 4n + 3)^2] \\ &\quad + (n-1)[(m-2)(n^2 - 2n + 3)^2 + (m-4)(4n^2 - 10n + 12)^2] \\ &\quad + (m-4)[(n^2 + 3)^2] + (m-5)[(4n^2 - 4n + 4)^2] \\ &\quad + (n^2 - 3n + 2)[(2n-4)^2 + 2]^2 \\ &\quad + \left[\frac{m(n^2 - 3n + 2)}{2} - n^2 + 3n - 2 \right] [(4n^2 - 16n + 20)^2] \\ &= (2n-2)[33n^4 - 188n^3 + 469n^2 - 566n + 294] - 66n^5 + 374n^4 - 1020n^3 \\ &\quad + 2[34n^4 - 90n^3 + 138n^2 - 98n + 42] + 1444n^2 - 1202n + 386 \\ &\quad + m[8n^6 - 71n^5 + 316n^4 - 782n^3 + 1128n^2 - 839n + 260]. \end{aligned}$$

Now, to determine the second and modified entire neighborhood indices, we consider the partitions of the bridge graph over complete graph which represented in tables 26 to 28.

TABLE 26. Partition of the vertices in bridge graphs over complete graphs.

Type	V_{n^2-2n+2, n^2-2n+2}	V_{n^2-2n+2, n^2-n+2}	V_{n^2-2n+3, n^2-2n+3}	V_{n^2-2n+3, n^2+2}
Frequency	$n^2 - 3n + 2$	$2(n-1)$	$\frac{1}{2}(m-2)(n^2 - 3n + 2)$	$2(n-1)$
Type	V_{n^2-2n+3, n^2+3}	V_{n^2-n+2, n^2+2}	V_{n^2+2, n^2+3}	V_{n^2+3, n^2+3}
Frequency	$(m-4)(n-1)$	2	2	$m-5$

TABLE 27. Partition of the edges in bridge graphs over complete graph.

Type	$E_{(2n-4)^2+2,(2n-4)^2+2}$	$E_{(2n-4)^2+2,4n^2-13n+13}$
Frequency	$n^3 - 6n^2 + 11n - 6$	$2n^2 - 6n + 4$
Type	$E_{4n^2-16n+20,4n^2-16n+20}$	$E_{4n^2-16n+20,4n^2-10n+11}$
Frequency	$\frac{1}{2}(m-2)(n^3 - 6n^2 + 11n - 6)$	$2n^2 - 6n + 4$
Type	$E_{4n^2-13n+13,4n^2-13n+13}$	$E_{4n^2-13n+13,4n^2-7n+5}$
Frequency	$n^2 - 3n + 2$	$2(n-1)$
Type	$E_{4n^2-10n+11,4n^2-10n+11}$	$E_{4n^2-10n+11,4n^2-7n+5}$
Frequency	$n^2 - 3n + 2$	$2(n-1)$
Type	$E_{4n^2-10n+11,4n^2-4n+3}$	$E_{4n^2-16n+20,4n^2-10n+12}$
Frequency	$2(n-1)$	$(m-4)(n^2 - 3n + 2)$
Type	$E_{4n^2-10n+12,4n^2-10n+12}$	$E_{4n^2-10n+12,4n^2-4n+3}$
Frequency	$\frac{1}{2}(m-4)(n^2 - 3n + 2)$	$2(n-1)$
Type	$E_{4n^2-10n+12,4n^2-4n+4}$	$E_{4n^2-7n+5,4n^2-4n+3}$
Frequency	$(m-4)(2n-2) - 2n + 2$	2
Type	$E_{4n^2-4n+3,4n^2-4n+4}$	$E_{4n^2-4n+4,4n^2-4n+4}$
Frequency	2	$m-6$

TABLE 28. Partition of the vertices incident with edges in bridge graphs over complete graph.

Type	$A_{n^2-2n+2,(2n-4)^2+2}$	$A_{n^2-2n+2,4n^2-13n+13}$	$A_{n^2-n+2,4n^2-13n+13}$
Frequency	$2n^2 - 6n + 4$	$2(n-1)$	$2(n-1)$
Type	$A_{n^2-n+2,4n^2-7n+5}$	$A_{n^2+2,4n^2-7n+5}$	$A_{n^2-2n+3,4n^2-16n+20}$
Frequency	2	2	$(m-2)(n^2 - 3n + 2)$
Type	$A_{n^2-2n+3,4n^2-10n+11}$	$A_{n^2+2,4n^2-10n+11}$	$A_{n^2+2,4n^2-4n+3}$
Frequency	$2(n-1)$	2	2
Type	$A_{n^2+3,4n^2-4n+3}$	$A_{n^2+3,4n^2-4n+4}$	$A_{n^2-2n+3,4n^2-10n+12}$
Frequency	$2(n-1)$	$2m-10$	$(m-4)(n-1)$
Type	$A_{n^2+3,4n^2-10n+12}$	-	-
Frequency	$(m-4)(n-1)$	-	-

Then, according to [1.1], we have

$$\begin{aligned}
 NM_2^\varepsilon(G_m(K_n; v)) &= (2n-2)[(n^2-2n+2)(n^2-n+2) + (n^2-2n+3)(n^2+2) \\
 &\quad + (4n^2-13n+13)(4n^2-7n+5) + (4n^2-10n+11)(4n^2-7n+5) \\
 &\quad + (4n^2-10n+11)(4n^2-4n+3) + (4n^2-10n+12)(4n^2-4n+3) \\
 &\quad + (n^2-2n+2)(4n^2-13n+13) + (n^2-n+2)(4n^2-13n+13) \\
 &\quad + (n^2-2n+3)(4n^2-10n+11) + (n^2+2)(4n^2-10n+11)] \\
 &\quad + 2[50n^4 - 103n^3 + 172n^2 - 124n + 72] + 16n^7 - 119n^6 + 353n^5 - 425n^4 \\
 &\quad - 193n^3 + 1242n^2 - 1478n + 604 + \frac{1}{2}[238n^6 - 167mn^6 - 1226n^5 \\
 &\quad + 931mn^5 - 2912mn^4 - 1150m + 3198n^4 - 5660n^3 + 5730mn^3 - 6651mn^2 \\
 &\quad + 5170n^2 - 2738n + 4331mn + 16mn^7 - 32n^7 + 378] \\
 &= -96n^5 + 528n^4 - 1513n^3 + 1961n^2 - 1467n + 385 \\
 &\quad + \frac{1}{2}m[16n^7 - 167n^6 + 931n^5 - 2912n^4 + 5730n^3 - 6651n^2 + 4331n - 1150].
 \end{aligned}$$

Analogously, we get that

$$\begin{aligned}
 MNM_1^\varepsilon(G_m(K_n; v)) &= (2n-2)[56n^2 - 121n + 129] + 8n^5 - 20n^4 - 60n^3 + 388n^2 \\
 &\quad - 538n + 314 + 20n^4 - 84n^3 - 4n^2 - 32n - 8n^5 - 60 \\
 &\quad + m[4n^5 - 22n^4 + 78n^3 - 106n^2 + 98n - 20] \\
 &= 2m[2n^5 - 11n^4 + 39n^3 - 53n^2 + 49n - 10] - 32n^3 + 30n^2 - 70n - 4.
 \end{aligned}$$

□

3.3. Sierpiński graphs. The Sierpiński type's graph has been observed in different branches of mathematics and many other scientific fields. The Sierpiński graphs \hat{S}_n are one of the most significant families of these graphs, generated by a finite number of iterations that reach the Sierpiński gasket at the limit. In short, \hat{S}_{n+1} is made up of three copies of \hat{S}_n that are attached, known as the top, bottom left, and bottom right components of \hat{S}_{n+1} . The introduction of these graphs was made by Scorer, Grundy, and Smith in 1944. They are crucial in dynamic systems and probability, as well as in psychology [34].

The generalized Sierpiński graph, denoted by $\hat{S}(n, G)$ and the process of constructing it involves copying $|G|$ multiple times $\hat{S}(n-1, G)$ and adding an edge between copies x and y of $\hat{S}(n-1, G)$ whenever xy is an edge of G . The Sierpiński graphs $\hat{S}(n, k)$ and $\hat{S}(n, G)$ are defined as follows

$\hat{S}(n, k)$ is a graph with vertex set $\{1, 2, \dots, n\}$, and there is an edge between two vertices $u = (u_1, u_2, \dots, u_n)$ and $v = (v_1, v_2, \dots, v_n)$ if and only if there exist an $\alpha \in \{1, 2, \dots, n\}$ such that

- $u_i = v_i$ for all $i = 1, 2, \dots, \alpha - 1$,
- $u_\alpha \neq v_\alpha$, and

- $u_i = v_\alpha, v_i = u_\alpha$ for all $i = \alpha + 1, \dots, n$.

The generalized Sierpiński graph of dimension n , $\hat{S}(n, G)$ is the graph with vertex set $\{1, 2, \dots, k\}^n$ and uv is an edge if and only if there exists $\beta \in \{1, 2, \dots, n\}$ such that

- $u_i = v_i$, for all $i < \beta$.
- $u_\beta \neq v_\beta$ and $(u_\beta, v_\beta) \in E(G)$.
- $u_i = v_\beta$ and $v_i = u_\beta$, for all $i > \beta$.

3.3.1. *Uniform subdivision of Sierpiński gasket graphs $SD(\hat{S}_n)$.* The uniform subdivision of Sierpiński gasket graphs $SD(\hat{S}_n)$ has order $\frac{1}{2}(3^n + 3) + 3^n$ and size equal $2(3^n)$. These graphs are shown in Figure 14 for $n = 1, 2, 3$.

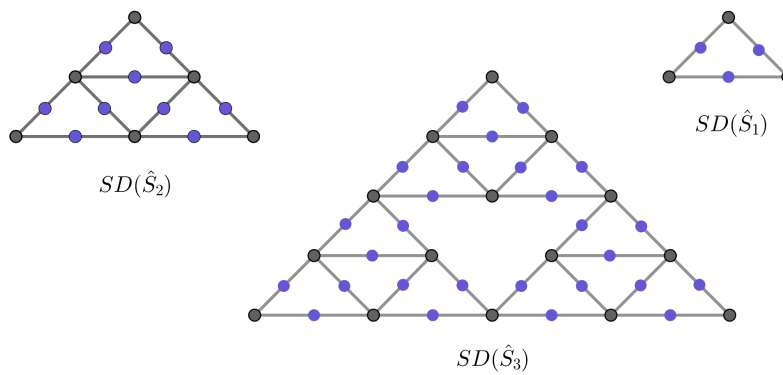


FIGURE 14. Uniform subdivision of Sierpiński gasket graph $SD(\hat{S}_1)$, $SD(\hat{S}_2)$ and $SD(\hat{S}_3)$.

Proposition 3.10. Let Γ be the graph $SD(\hat{S}_n)$, Then,

- (1) $NM_1^\epsilon(\Gamma) = 8[76(3^n) - 237]$.
- (2) $NM_2^\epsilon(\Gamma) = \begin{cases} 9312, & \text{if } n = 2; \\ 4[416(3^n) - 1419], & n > 2. \end{cases}$
- (3) $MNM_1^\epsilon(\Gamma) = \begin{cases} 1704, & \text{if } n = 2; \\ 8[32(3^n) - 75], & n > 2. \end{cases}$

Proof. Let Γ be the graph $SD(\hat{S}_n)$, Then, this graph has

$$|V_{(4)}| = 3, |V_{(6)}| = 6, |V_{(8)}| = \frac{3}{2}(3^n - 5), |E_{(6)}| = |E_{(14)}| = 6, \text{ and } |E_{(16)}| = 2(3^n) - 12.$$

Hence, we have

$$\begin{aligned} NM_1^\epsilon(\Gamma) &= 3(4^2) + 6(6^2) + \frac{3}{2}(3^n - 5)(8^2) + 6(6^2) + 6(14^2) + 2(3^n - 6)(16^2) \\ &= 1656 + 96(3^n) + 512(3^n) - 480 - 3072 \\ &= 608(3^n) - 1896. \end{aligned}$$

The uniform subdivision of Sierpiński gasket graphs $SD(\hat{S}_n)$ has the following partitions which illustrated in Tables 29 to 32.

TABLE 29. The partition of the vertices in $SD(\hat{S}_n)$.

Type	$V_{4,6}$	$V_{6,8}$	$V_{8,8}$
Frequency	6	6	$2(3^n) - 12$

For $n > 2$, we have,

TABLE 30. The partition of the edges in $SD(\hat{S}_n), n > 2$.

Type	$E_{6,6}$	$E_{6,14}$	$E_{14,16}$	$E_{16,16}$
Frequency	3	6	18	$4(3^n) - 33$

and, if $n = 2$, we have

TABLE 31. The partition of the edges in $SD(\hat{S}_n), n = 2$.

Type	$E_{6,6}$	$E_{6,14}$	$E_{14,14}$	$E_{14,16}$	$E_{16,16}$
Frequency	3	6	3	12	$4(3^n) - 30$

TABLE 32. The partition of the vertices incident with edges in $SD(\hat{S}_n)$.

Type	$A_{4,6}$	$A_{6,6}$	$A_{6,14}$	$8,14$	$A_{8,16}$
Frequency	6	6	6	6	$4(3^n) - 24$

Therefore, the second and modified entire neighborhood indices, for $n > 2$, can be determined through the following equations

$$\begin{aligned}
 NM_2^e(\Gamma) &= 6(24) + 6(48) + 2(3^n - 6)(64) + 3(36) + 6(6)(14) + 18(14)(16) \\
 &\quad + (4(3^n) - 33)(16^2) + 6(24) + 6(36) + 6(6)(14) + 6(8)(14) + 4(3^n - 6)(8)(16) \\
 &= 6612 + 128(3^n) + 1024(3^n) + 512(3^n) - 768 - 8448 - 3072 \\
 &= 1664(3^n) - 5676,
 \end{aligned}$$

and

$$\begin{aligned}
 MNM_1^e(\Gamma) &= 6(10) + 6(14) + 2(3^n - 6)(16) + 3(12) + 6(20) + 18(30) \\
 &\quad + (4(3^n) - 33)(32) + 6(10) + 6(12) + 6(20) + 6(22) + 4(3^n - 6)(24) \\
 &= 256(3^n) - 600.
 \end{aligned}$$

It is clear for $n = 2$.

□

3.3.2. *Uniform subdivision of the generalized Sierpiński graphs $SD(\hat{S}(n, C_3))$.* The generalized Sierpiński graphs $SD(\hat{S}(n, C_3))$ has order $\frac{3}{2}(3^n - 1) + 3^n$ and size equal to $3(3^n - 1)$. These graphs are depicted in Figure 15 for $n = 1, 2, 3$.

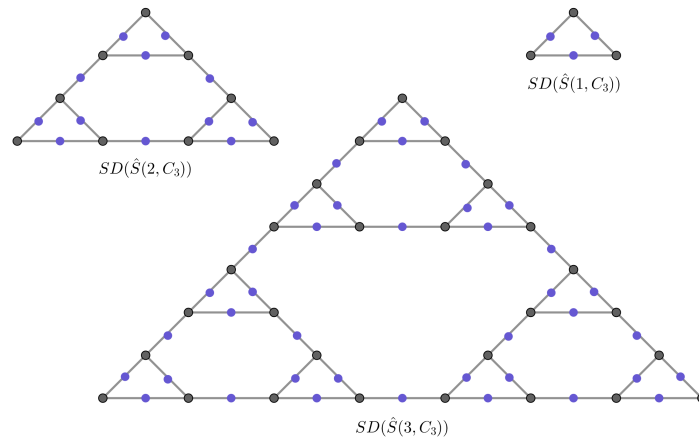


FIGURE 15. The generalized Sierpiński graphs for $SD(\hat{S}(1, C_3))$, $SD(\hat{S}(2, C_3))$ and $SD(\hat{S}(3, C_3))$.

Proposition 3.11. *Let Γ be the graph $SD(\hat{S}(n, C_3))$. Then,*

- (1) $NM_1^\varepsilon(\Gamma) = 3[111(3^n) - 287]$.
- (2) $NM_2^\varepsilon(\Gamma) = \frac{9}{2}[177(3^n) - 487]$.
- (3) $MNM_1^\varepsilon(\Gamma) = 3[69(3^n) - 145]$.

Proof. Let Γ be the graph $SD(\hat{S}(n, C_3))$. Then, the distribution of the elements of this graph is as follows

$$|V_{(4)}| = 3, |V_{(5)}| = 6, |V_{(6)}| = \frac{1}{2}[5(3^n) - 21], |E_{(5)}| = |E_{(8)}| = 6,$$

and $|E_{(9)}| = 3[3^n - 5]$.

Thus, we have the following result

$$\begin{aligned} NM_1^\varepsilon(\Gamma) &= 3(4^2) + 6(5^2) + \frac{1}{2}[5(3^n) - 21](6^2) + 6(5^2) + 6(8^2) + 3[3^n - 5](9^2) \\ &= 333(3^n) + 732 - 1593. \end{aligned}$$

The partitions of the uniform subdivision of the generalized Sierpiński graphs $SD(\hat{S}(n, C_3))$ are depicted in Tables 33 to 35.

TABLE 33. The partition of the vertices in $SD(\hat{S}(n, C_3))$.

Type	$V_{4,5}$	$V_{5,6}$	$V_{6,6}$
Frequency	6	6	$3[3^n - 5]$

TABLE 34. The partition of the edges in $SD(\hat{S}(n, C_3))$.

Type	$E_{5,5}$	$E_{5,8}$	$E_{8,9}$	$E_{9,9}$
Frequency	3	6	12	$\frac{1}{2}[3^{n+2} - 57]$

TABLE 35. The partition of the vertices incident with edges in $SD(\hat{S}(n, C_3))$.

Type	$A_{4,5}$	$A_{5,5}$	$A_{5,8}$	$A_{6,8}$	$A_{6,9}$
Frequency	6	6	6	6	$6[3^n - 5]$

Then, utility Definition 1.1, we get that

$$\begin{aligned}
 NM_2^\epsilon(\Gamma) &= 6(20) + 6(30) + [3(3^n) - 15](36) + 3(25) + 6(40) + 12(72) \\
 &+ \frac{1}{2}[3^{n+2} - 57](81) + 6(20) + 6(25) + 6(40) + 6(48) + 6[3^n - 5](54) \\
 &= \frac{1593}{2}(3^n) - \frac{4383}{2}.
 \end{aligned}$$

Also, by applying a similar procedure, we have

$$\begin{aligned}
 MNM_1^\epsilon(\Gamma) &= 6(9) + 6(11) + [3(3^n) - 15](12) + 3(10) + 6(13) + 12(7) \\
 &+ \frac{1}{2}[3^{n+2} - 57](18) + 6(9) + 6(10) + 6(13) + 6(14) + [6(3^n) - 30](15) \\
 &= 708 - 1143 + 126(3^n) + 9(3^{n+2}) \\
 &= 207(3^n) - 435.
 \end{aligned}$$

□

CONCLUSION

In this research, we introduced some new topological indices named the first, second and modified entire neighborhood indices. We investigated the prediction power of these indices through regression analysis. The new indices exhibit a significant correlation with acentric factor (AF), entropy (S), enthalpy of vaporization (HVAP), and standard enthalpy of vaporization (DHVAP) for octan isomers showed in Table 5, and with π -electronic energy (E_π), enthalpy of formation (EF), and boiling point (BP) for benzenoid hydrocarbon compounds showed in Table 7. Furthermore, we computed the new proposed topological indices for various standard graphs such as path, cycle, regular, complete, and book graphs. In addition, we determined the value of the entire neighborhood indices for some types of bridge graphs and Sierpiński graphs. Thus, according to the high correlation which is demonstrated by these indices, this is evidence of the potential for future use in various applications, such as designing medicines and obtaining new materials through changes in the properties of the graph.

Finally, as this is the initial representation of the first, second, and modified entire neighborhood indices, many open problems and potential research areas require more investigation. This includes computing these new indices for various graph operations, examining their vast applicability in many network types, such as social, biological, and technological networks, and exploring their potential in several fields, such as drug discovery in medicine and material design in engineering.

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