

The Entire Nirmala Index: Theoretical Foundations and Applications

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Abstract. In this research work, we introduce a new entire topological index called the entire Nirmala topological index, which is based on the degrees of the graph elements (vertices and edges) along with the adjacency and incidence relations. We establish upper and lower bounds for this new index; exact expressions for some standard families of graphs are obtained, as well as closed formulae for a family of wheel related graphs along with their line graphs. Finally, we present (QSPR) analysis study on the octane isomers, which supports the significance and predictive power of this new index. In both linear and cubic regression models, the new index shows excellent correlation with the properties of the octane isomers. The comparative analysis reflects that the entire Nirmala index is more significant than the Nirmala index. We confirm the excellent predictive power of the entire Nirmala index by a comprehensive residual analysis.

1. INTRODUCTION

Graph theory represents one of the foundational frameworks in mathematical chemistry, particularly through topological indices. The topological indices have applications in many areas, including computer networks, coding theory, database systems, circuit design, and cryptographic secret sharing schemes.

In this paradigm, cheminformatics appears as an interdisciplinary area combining chemistry, graph theory, and computational technology. It connects molecular structure and physicochemical properties by using molecular graphs, which are vertex-edge representations of atoms and bonds, and their associated graph invariants. The theoretical exploration of chemical structures via these invariants constitutes a prominent research direction in mathematical chemistry, driven by critical applications in Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Property Relationship (QSPR) [1]. Quantitative estimation of molecular properties is facilitated by topological indices, which convert graphs to non-negative real values.

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The Wiener index, introduced in 1947, exemplifies this approach by correlating alkane structures with properties such as boiling points [2,3].

The first and second Zagreb indices were introduced by Gutman and Trinajstić [4] in 1972. Initially established to determine the total π -electron energy of molecular structures, these degree-based topological indices are defined as follows:

$$M_1(G) = \sum_{u \in V(G)} d_u^2,$$

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

Subsequent work has expanded this repertoire significantly [5–16]. In 2021, the Nirmala index was introduced in [17] as follows.

$$N(G) = \sum_{uv \in E(G)} \sqrt{d_u + d_v}.$$

The entire topological indices provide a full picture of molecular structure by taking into account the adjacency and incidence relationships of vertices and edges, in addition to their degrees. The idea of entire topological indices was first introduced in [18]. The first and second entire topological indices were mathematically defined as follows:

$$M_1^{\mathcal{E}}(G) = \sum_{x \in V(G) \cup E(G)} d_x^2,$$

$$M_2^{\mathcal{E}}(G) = \sum_{\substack{x \text{ adjacent to } y \\ \text{or } x \text{ incident to } y}} d_x d_y.$$

The entire indices have been the subject of great interest for a wide variety of researchers. This is supported by many studies in this area, such as [19–21], which have shown that the entire indices have attracted much attention from a wide range of researchers.

However, molecular frameworks are inherently more complex, involving interactions not only between atoms (vertices), but also atoms and bonds (edges) and even bonds themselves.

In our research, by a graph we mean a simple, finite, and undirected graph with vertex set V and edge set E . For a vertex $v \in V$, its degree is denoted by d_v . For the degree of the edge $e = uv$, we denote it by $d_e = d_u + d_v - 2$. Two edges e and f are adjacent if they have a common vertex. The notation $v \sim e$ indicates that the vertex v is incident to the edge e . The line graph of G , denoted $L(G)$, is constructed such that each vertex of $L(G)$ corresponds to an edge of G . Two vertices in $L(G)$ are adjacent if and only if their corresponding edges in G share a common vertex.

The promising applications of entire topological indices, together with the recently introduced Nirmala index, motivated us to introduce the entire Nirmala index, investigate its theoretical foundations, and demonstrate its predictive capability. In this paper, we introduce the entire Nirmala index together with the “entire partition” as a novel methodological framework for its computation. We establish upper and lower bounds for the new index and derive exact analytical

formulae for fundamental families of graphs, including paths, cycles, regular graphs, complete graphs, and complete bipartite graphs, as well as for several wheel related networks, namely wheel, gear, helm, and Jahangir graphs and their corresponding line graphs. To demonstrate the importance and applicability of this new index, we conduct (QSPR) analysis of octane isomers. Both the linear and cubic regression models show a statistically significant correlation between the experimental values of the properties and the entire Nirmala topological index. The comparative analysis shows that the new index consistently outperforms the Nirmala index in all the studied properties and the residual analysis confirms the model's accuracy and its ability to generalize across the studied properties.

2. ENTIRE NIRMALA INDEX FOR SOME STANDARD FAMILIES OF GRAPHS

Definition 2.1. For any graph G , the entire Nirmala index is defined as

$$\begin{aligned} N^{\mathcal{E}}(G) &= \sum_{\substack{x \text{ adjacent to } y \\ \text{or } x \text{ incident to } y}} \sqrt{d_x + d_y} \\ &= \sum_{uv \in E(G)} \sqrt{d_u + d_v} + \sum_{ef \in E(L(G))} \sqrt{d_e + d_f} + \sum_{u \text{ incident with } e \text{ in } G} \sqrt{d_u + d_e}. \end{aligned}$$

From the structure of the formula of the entire Nirmala index, we need to partition the elements of the graph (vertices and edges) according to their degrees and the relations between the elements, as in Definition 2.2.

Definition 2.2. By elements of the graph G we mean the vertices and edges, and by relations, we mean:

1. The adjacency between vertices and between edges. 2. The incidence relation between vertices and edges. Thus, we can define three types of partitions for the elements using the two relations and the elements of the graph as follows:

(1) Adjacent vertices based on their degrees, denoted by $\mathcal{P}_1^{(a,b)}$ and defined as:

$$\mathcal{P}_1^{(a,b)} = \{e = uv \in E(G) : \{d_u, d_v\} = \{a, b\}\}.$$

(2) Adjacent edges based on their degrees, denoted by $\mathcal{P}_2^{(a,b)}$ and defined as:

$$\mathcal{P}_2^{(a,b)} = \{\{e, f\} \subset E(G) : e \text{ and } f \text{ share a vertex, } \{d_e, d_f\} = \{a, b\}\},$$

where $d_e = d_u + d_v - 2$ for $e = uv$, and (a, b) is **unordered**.

(3) Vertices incident with edges based on their degrees, denoted by $\mathcal{P}_3^{(a,b)}$ and defined as:

$$\mathcal{P}_3^{(a,b)} = \{(v, e) \in V(G) \times E(G) : e \text{ incident to } v, d_v = a, d_e = b\},$$

where d_v is the vertex degree of v , d_e is the number of edges adjacent to edge e , and (a, b) is **ordered**.

Theorem 2.1. Let G be a connected graph with m edges, maximum degree Δ and minimum degree δ . Let m' denote the number of edges in the line graph $L(G)$. Then

$$m\sqrt{2\delta} + 2m'\sqrt{\delta-1} + 2m\sqrt{3\delta-2} \leq N^{\mathcal{E}}(G) \leq m\sqrt{2\Delta} + 2m'\sqrt{\Delta-1} + 2m\sqrt{3\Delta-2}$$

Furthermore, these bounds are sharp if and only if G is a regular graph.

Proof. Suppose that $S_1 = \sum_{uv \in E(G)} \sqrt{d_u + d_v}$, $S_2 = \sum_{ef \in E(L(G))} \sqrt{d_e + d_f}$ and $S_3 = \sum_{u \sim e} \sqrt{d_u + d_e}$.

We have $2\delta \leq d_u + d_v \leq 2\Delta$. Then

$$m\sqrt{2\delta} \leq S_1 \leq m\sqrt{2\Delta}.$$

For S_2 , we have for any edge e , $2\delta - 2 \leq d_e \leq 2\Delta - 2$, so $2(2\delta - 2) \leq d_e + d_f \leq 2(2\Delta - 2)$. Thus,

$$2m'\sqrt{\delta - 1} \leq S_2 \leq 2m'\sqrt{\Delta - 1}.$$

For S_3 , we consider the incidence pairs (u, e) . The sum is $d_u + d_e = d_u + (d_u + d_v - 2) = 2d_u + d_v - 2$. The minimum value occurs when $d_u = d_v = \delta$, giving $3\delta - 2$. The maximum occurs when $d_u = d_v = \Delta$, giving $3\Delta - 2$. There are $2m$ such incidence pairs:

$$2m\sqrt{3\delta - 2} \leq S_3 \leq 2m\sqrt{3\Delta - 2}.$$

Combining the bounds for S_1, S_2 , and S_3 , we get,

$$m\sqrt{2\delta} + 2m'\sqrt{\delta - 1} + 2m\sqrt{3\delta - 2} \leq N^{\mathcal{E}}(G) \leq m\sqrt{2\Delta} + 2m'\sqrt{\Delta - 1} + 2m\sqrt{3\Delta - 2}.$$

Equality holds if and only if $d_u = \delta = \Delta$ for all $u \in V(G)$, implying G is regular. $\square$

Theorem 2.2. Let G be a connected graph with m edges. Then

$$N^{\mathcal{E}}(G) \leq \sqrt{(3m + m')(4M_1(G) + M_1(L(G)) - 4m)}.$$

Where m' denotes the number of edges in the line graph $L(G)$ and $M_1(G), M_1(L(G))$ are the first Zagreb indices of the graphs G and $L(G)$ respectively. Equality holds if and only if G is a regular graph.

Proof. Let us denote the terms of the entire Nirmala index by $\sqrt{w_i}$, where $w_i = d_x + d_y$ for all adjacent or incident elements (x, y) in the entire graph G . The total number of terms in the summation is

$$K = m + m' + 2m = 3m + m'$$

Applying the Cauchy-Schwarz inequality $\left(\sum_{i=1}^K a_i b_i\right)^2 \leq \sum_{i=1}^K a_i^2 \sum_{i=1}^K b_i^2$, we set $a_i = 1$ and $b_i = \sqrt{w_i}$. Then

$$\left(\sum_{i=1}^K \sqrt{w_i}\right)^2 \leq K \sum_{i=1}^K w_i.$$

To evaluate $\sum w_i$, we partition the sum $S_1 = \sum_{uv \in E(G)} \sqrt{d_u + d_v}$, $S_2 = \sum_{ef \in E(L(G))} \sqrt{d_e + d_f}$ and $S_3 = \sum_{u \sim e} \sqrt{d_u + d_e}$.

Using the same method in Theorem 2.1, we get

$$\sum w_i = S_1 + S_2 + S_3 = M_1(G) + M_1(L(G)) + 3M_1(G) - 4m = 4M_1(G) + M_1(L(G)) - 4m.$$

Now, by substituting K and $\sum w_i$ into the Cauchy-Schwarz inequality, we get

$$(N^{\mathcal{E}}(G))^2 \leq (3m + m_L)(4M_1(G) + M_1(L(G)) - 4m).$$

Hence,

$$N^{\mathcal{E}}(G) \leq \sqrt{(3m + m') (4M_1(G) + M_1(L(G)) - 4m)}.$$

Clearly, the equality holds if and only if all w_i are equal, which occurs if and only if G is a regular graph. $\square$

Proposition 2.1. *Let G be the path P_t with $t \geq 4$ vertices. Then*

$$N^{\mathcal{E}}(G) = 8t + 2\sqrt{2} + 6\sqrt{3} - 26.$$

Proof. For a path graph $G \cong P_t$ with $t \geq 4$ vertices and $t - 1$ edges, apply the entire partition explained in Definition 2.2. We can summarize the results in Table 1.

TABLE 1. Path Graph Entire Partition

Partition Type	(a, b)	Cardinality
$\mathcal{P}_1^{(a,b)}$	$(1, 2)$	2
	$(2, 2)$	$t - 3$
$\mathcal{P}_2^{(a,b)}$	$(1, 2)$	2
	$(2, 2)$	$t - 4$
$\mathcal{P}_3^{(a,b)}$	$(1, 1)$	2
	$(2, 1)$	2
	$(2, 2)$	$2t - 6$

By applying the mathematical formula of the entire Nirmala index using Table 1, we get:

$$N^{\mathcal{E}}(G) = 8t + 2\sqrt{2} + 6\sqrt{3} - 26.$$

$\square$

Proposition 2.2. *For any r -regular graph G with t vertices,*

$$N^{\mathcal{E}}(G) = rt \left(\frac{\sqrt{2r}}{2} + (r-1)^{3/2} + \sqrt{3r-2} \right).$$

Proof. The degrees of the elements are either r for the vertices or $(2r-2)$ for the edges.

By applying the entire partitions as in Definition 2.2; In $\mathcal{P}_1^{(a,b)}$ there are $rt/2$ pairs of the form (r, r) . Similarly, we have $rt(r-1)/2$ pairs in $\mathcal{P}_2^{(a,b)}$ of the form $(2r-2, 2r-2)$. In the same way, there are rt pairs in $\mathcal{P}_3^{(a,b)}$ of the form $(r, 2r-2)$. By simple calculation, we get

$$N^{\mathcal{E}}(G) = rt \left(\frac{\sqrt{2r}}{2} + (r-1)^{3/2} + \sqrt{3r-2} \right).$$

$\square$

Directly, as we know that complete graph and cycle graph are special cases of regular graphs we have the results for these types of graphs.

Corollary 2.1. For any complete graph K_t and cycle graph C_t , we have

- i. $N^{\mathcal{E}}(K_t) = t(t-1) \left(\frac{\sqrt{2(t-1)}}{2} + (t-2)^{3/2} + \sqrt{3t-5} \right)$.
- ii. $N^{\mathcal{E}}(C_t) = 8t$.

Proposition 2.3. For any complete bipartite graph $G \cong K_{\alpha,\beta}$, we have,

$$N^{\mathcal{E}}(G) = \alpha\beta \left(\sqrt{\alpha+\beta} + \sqrt{2}(\alpha+\beta-2) \sqrt{\alpha+\beta-2} + \sqrt{2\alpha+\beta-2} + \sqrt{\alpha+2\beta-2} \right).$$

Proof. By using the structure of the complete bipartite graph $G \cong K_{\alpha,\beta}$ and by applying the entire partitions as in Definition 2.2; In $\mathcal{P}_1^{(a,b)}$ there are $\alpha\beta$ pairs of the form (α, β) . Similarly, we have $\alpha^2\beta + \alpha\beta^2 - 2\alpha\beta$ pairs in $\mathcal{P}_2^{(a,b)}$ of the form $(\alpha + \beta - 2, \alpha + \beta - 2)$. In the same way there are $\alpha\beta$ pairs in $\mathcal{P}_3^{(a,b)}$ of the form $(\alpha, \alpha + \beta - 2)$ and $\alpha\beta$ pairs of the form $(\beta, \alpha + \beta - 2)$. By simple calculation, we get the result. $\square$

Proposition 2.4. Let $G \cong W_t$ be a wheel graph of $t+1$ vertices. Then

$$N^{\mathcal{E}}(G) = t \left[\sqrt{t+3} + \sqrt{t+4} + 2\sqrt{t+5} + \sqrt{2t+1} + \frac{t-1}{2} \sqrt{2t+2} + (\sqrt{6} + \sqrt{8} + 2\sqrt{7}) \right]$$

Proof. By applying the entire partitions; in $\mathcal{P}_1^{(a,b)}$ there are t pairs of the form $(3, t)$ and t pairs of the form $(3, 3)$. Similarly, in $\mathcal{P}_2^{(a,b)}$, we have $t(t-1)/2$ pairs of the form $(t+1, t+1)$, also $2t$ pairs of the form $(t+1, 4)$, and t pairs of the form $(4, 4)$. In the same way, in $\mathcal{P}_3^{(a,b)}$, there are t pairs of the form $(t, t+1)$, also t pairs of the form $(3, t+1)$ and $2t$ pairs of the form $(3, 4)$. Now, applying the formula of the entire Nirmala index along with simple calculations, we get,

$$N^{\mathcal{E}}(G) = t \left[\sqrt{t+3} + \sqrt{t+4} + 2\sqrt{t+5} + \sqrt{2t+1} + \frac{t-1}{2} \sqrt{2t+2} + (\sqrt{6} + \sqrt{8} + 2\sqrt{7}) \right]$$

$\square$

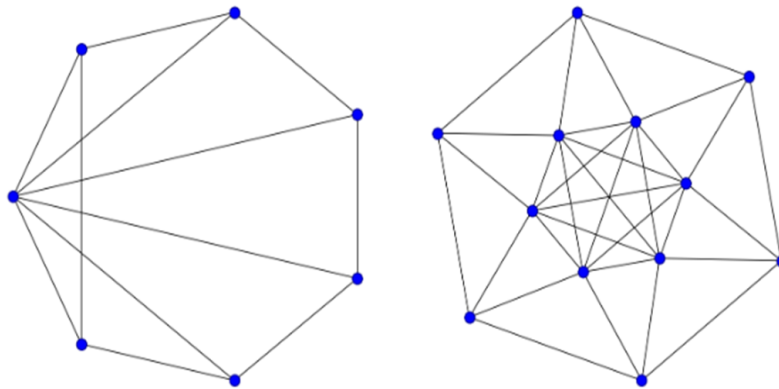


FIGURE 1. W_6 with its line graph $L(W_6)$

Proposition 2.5. Let G be the line graph of the wheel W_t ; $G \cong L(W_t)$. Then,

$$\begin{aligned} N^{\mathcal{E}}(G) = & \frac{t(t-1)}{2} \sqrt{2t+2} + 2t \sqrt{t+5} + \sqrt{8}t \\ & + \frac{t(t-1)(t-2)}{2} \sqrt{4t} + 2t(t-1) \sqrt{3t+3} + 2t \sqrt{2t+6} \\ & + 4t \sqrt{t+9} + \sqrt{12}t + t(t-1) \sqrt{3t+1} \\ & + 2t \sqrt{2t+4} + 2t \sqrt{t+7} + 2 \sqrt{10}t. \end{aligned}$$

Proof. Let G be the line graph of the wheel graph W_t (the line graph of W_6 is illustrated in Figure 1). From the definition of the line graph, clearly, G has $2t$ vertices and $3t + \frac{t(t-1)}{2}$ edges. The degrees of the vertices in G are either of degree $t+1$ or of degree 4 for the edges of G are either $2t$ or $t+3$ or 4. Utilizing the entire partition explained in Definition 2.2, we can summarize the entire partition of the line graph of the wheel graph W_t as in Table 2.

TABLE 2. The entire partition of the line graph of wheel $L(W_t)$

Partition Type	(a, b)	Cardinality
$\mathcal{P}_1^{(a,b)}$	$(t+1, t+1)$	$\frac{t(t-1)}{2}$
	$(t+1, 4)$	$2t$
	$(4, 4)$	t
$\mathcal{P}_2^{(a,b)}$	$(2t, 2t)$	$\frac{t(t-1)(t-2)}{2}$
	$(2t, t+3)$	$2t(t-1)$
	$(t+3, t+3)$	$2t$
	$(t+3, 6)$	$4t$
$\mathcal{P}_3^{(a,b)}$	$(6, 6)$	t
	$(t+1, 2t)$	$t(t-1)$
	$(t+1, t+3)$	$2t$
	$(4, t+3)$	$2t$
	$(4, 6)$	$2t$

By applying the formula of the entire Nirmala index to the entire partition explained in Table 2, we obtain,

$$\begin{aligned} N^{\mathcal{E}}(G) = & \frac{t(t-1)}{2} \sqrt{2t+2} + 2t \sqrt{t+5} + \sqrt{8}t \\ & + \frac{t(t-1)(t-2)}{2} \sqrt{4t} + 2t(t-1) \sqrt{3t+3} + 2t \sqrt{2t+6} \end{aligned}$$

$$\begin{aligned}
&+ 4t \sqrt{t+9} + \sqrt{12t} + t(t-1) \sqrt{3t+1} \\
&+ 2t \sqrt{2t+4} + 2t \sqrt{t+7} + 2 \sqrt{10t}.
\end{aligned}$$

□

Proposition 2.6. Let G be the gear graph G_t of $(2t+1)$ vertices. Then,

$$N^{\mathcal{E}}(G) = t \left[\sqrt{t+3} + 4\sqrt{5} + \frac{t-1}{2} \sqrt{2t+2} + 3\sqrt{t+4} + \sqrt{2t+1} + 4\sqrt{6} \right].$$

Proof. From the structure of the gear graph $G \cong G_t$, there are t vertices of degree two, t vertices of degree 3 and one vertex of degree one. Similarly, there are t edges of degree $t+1$ and $2t$ edges of degree 3. So by applying the entire partition, we get the partition shown in Table 3.

TABLE 3. The entire partition of the gear graph G_t

Partition Type	(a, b)	Cardinality
$\mathcal{P}_1^{(a,b)}$	$(3, t)$	t
	$(2, 3)$	$2t$
$\mathcal{P}_2^{(a,b)}$	$(t+1, t+1)$	$\frac{t(t-1)}{2}$
	$(t+1, 3)$	$2t$
	$(3, 3)$	$2t$
$\mathcal{P}_3^{(a,b)}$	$(t, t+1)$	t
	$(3, t+1)$	t
	$(3, 3)$	$2t$
	$(2, 3)$	$2t$

Using the formula of the entire Nirmala index with the entire partition explained in Table 3, we obtain the result. □

Proposition 2.7. Let G be the line graph of the gear graph G_t of $(2t+1)$ vertices. Then,

$$\begin{aligned}
N^{\mathcal{E}}(G) = t \left[\frac{t-1}{2} \sqrt{2t+2} + 2\sqrt{t+4} + (t-1)(t-2) \sqrt{t} + \sqrt{2t+4} \right. \\
+ 2(t-1) \sqrt{3t+2} + 4\sqrt{t+6} + (t-1) \sqrt{3t+1} + 2\sqrt{2t+3} \\
\left. + 2\sqrt{t+5} + 2\sqrt{6} + 4\sqrt{2} + 4\sqrt{7} \right].
\end{aligned}$$

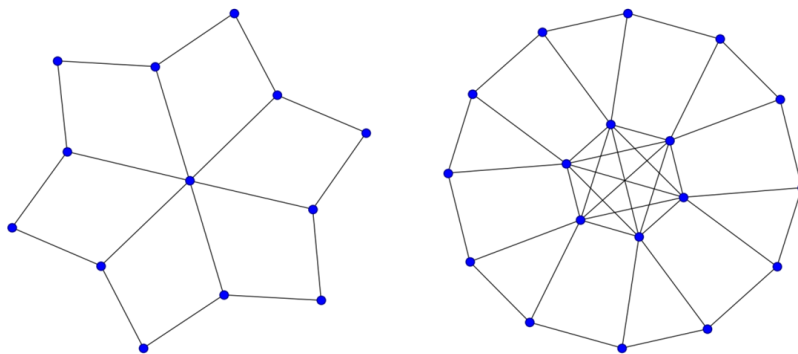
Proof. For the vertices of line graph of the gear graph $G \cong L(G_T)$ (see for illustration the line graph $L(G_6)$ in Figure 2, we have $2t$ vertices of degree 3 and t vertices of degree $t + 1$. Similarly, for the edges, we have $\frac{t(t-1)}{2}$ edges of degree $2t$, $2t$ edges of degree $t + 2$ and $2t$ edges of degree 4. Using the entire partition, we obtain the results in Table 4.

TABLE 4. The entire partition of the line graph of gear graph $L(G_t)$

Partition Type	(a, b)	Cardinality
$\mathcal{P}_1^{(a,b)}$	$(t+1, t+1)$	$\frac{t(t-1)}{2}$
	$(3, t+1)$	$2t$
	$(3, 3)$	$2t$
$\mathcal{P}_2^{(a,b)}$	$(2t, 2t)$	$\frac{t(t-1)(t-2)}{2}$
	$(t+2, 2t)$	$2t(t-1)$
	$(t+2, t+2)$	t
	$(4, t+2)$	$4t$
	$(4, 4)$	$2t$
$\mathcal{P}_3^{(a,b)}$	$(t+1, 2t)$	$t(t-1)$
	$(t+1, t+2)$	$2t$
	$(3, t+2)$	$2t$
	$(3, 4)$	$4t$

Using the formula of the entire Nirmala index with the entire partition explained in Table 4, we obtain the result.

□

FIGURE 2. The gear graph G_6 with its line graph $L(G_6)$

Proposition 2.8. Let G be the helm graph H_t of $(2t + 1)$ vertices. Then,

$$N^{\mathcal{E}}(G) = t \left[\sqrt{t+4} + \sqrt{t+5} + \sqrt{t+6} + \sqrt{t+8} + \sqrt{2t+2} + \frac{t-1}{2} \sqrt{2t+4} \right. \\ \left. + \sqrt{5} + \sqrt{7} + \sqrt{8} + \sqrt{12} + 2\sqrt{10} + 8 \right].$$

Proof. For the helm graph G , there are $2t + 1$ vertices and $3t$ edges. The vertices are either of degree t , 4 or of degree one. In the same way, the edges are either of degree $t + 2$, 6 or of degree 3. The entire partition of the helm graph is summarized in Table 5.

TABLE 5. The entire partition of the helm graph H_t

Partition Type	(a, b)	Cardinality
$\mathcal{P}_1^{(a,b)}$	$(t, 4)$	t
	$(4, 4)$	t
	$(1, 4)$	t
$\mathcal{P}_2^{(a,b)}$	$(t+2, t+2)$	$\frac{t(t-1)}{2}$
	$(t+2, 6)$	$2t$
	$(t+2, 3)$	t
	$(6, 6)$	t
	$(6, 3)$	$2t$
$\mathcal{P}_3^{(a,b)}$	$(t, t+2)$	t
	$(4, t+2)$	t
	$(4, 6)$	$2t$
	$(4, 3)$	t
	$(1, 3)$	t

By applying the formula of the entire Nirmala index to the entire partition explained in Table 5, we obtain,

$$N^{\mathcal{E}}(G) = t\sqrt{t+4} + \sqrt{8}t + \sqrt{5}t \\ + \frac{t(t-1)}{2} \sqrt{2t+4} + 2t\sqrt{t+8} + t\sqrt{t+5} \\ + t\sqrt{12} + 6t \\ + t\sqrt{2t+2} + t\sqrt{t+6} + 2t\sqrt{10} + t\sqrt{7} + 2t.$$

By simplifying, we will get the result. □

Theorem 2.3. Let G be the line graph of the helm graph H_t , where $t \geq 5$; $G \cong L(H_t)$. Then,

$$N^{\mathcal{E}}(G) = t \left[\sqrt{t+5} + 2\sqrt{t+6} + 2\sqrt{t+8} + 4\sqrt{t+10} + 2\sqrt{t+12} + 4\sqrt{t+13} + 4\sqrt{t+16} \right. \\ + 2\sqrt{2t+5} + 2\sqrt{2t+8} + 2\sqrt{2t+9} + 2\sqrt{2t+12} + \frac{t-1}{2}\sqrt{2t+4} \\ + (t-1)\sqrt{3t+4} + (t-1)\sqrt{3t+5} + 2(t-1)\sqrt{3t+8} + \frac{(t-1)(t-2)}{2}\sqrt{4t+4} \\ \left. + 2\sqrt{3} + \sqrt{20} + 2\sqrt{10} + 2\sqrt{13} + 2\sqrt{14} + 4\sqrt{17} + 14 \right].$$

Proof. The line graph G of the helm graph H_t (for understanding the structure of the line graph of the helm graph, see Figure 3) has $3t$ vertices of degree 3, 6 or of degree $(t+2)$. For the edges of G , there are $(t^2 + 11t)/2$ edges of degrees 7, 10, $(t+3)$, $(t+6)$ and $(2t+2)$. Using the entire partition method and combinatorial, we summarize the entire partition of the line graph of the helm graph in Table 6.

Table 6: The entire partition of the line graph of helm graph $L(H_t)$

Partition Type	(a, b)	Cardinality
$\mathcal{P}_1^{(a,b)}$	$(3, t+2)$	t
	$(6, t+2)$	$2t$
	$(6, 6)$	t
	$(3, 6)$	$2t$
	$(t+2, t+2)$	$\frac{t(t-1)}{2}$
$\mathcal{P}_2^{(a,b)}$	$(7, 7)$	$2t$
	$(10, 10)$	t
	$(7, 10)$	$4t$
	$(7, t+3)$	$2t$
	$(7, t+6)$	$4t$
	$(10, t+6)$	$4t$
	$(t+3, t+6)$	$2t$
	$(t+3, 2t+2)$	$t(t-1)$
	$(t+6, t+6)$	$2t$
	$(t+6, 2t+2)$	$2t(t-1)$

Partition Type	(a, b)	Cardinality
$\mathcal{P}_3^{(a,b)}$	$(2t+2, 2t+2)$	$\frac{t(t-1)(t-2)}{2}$
	$(t+2, 2t+2)$	$t(t-1)$
	$(t+2, t+6)$	$2t$
	$(t+2, t+3)$	t
	$(6, t+6)$	$2t$
	$(6, 10)$	$2t$
	$(6, 7)$	$2t$
	$(3, t+3)$	t
	$(3, 7)$	$2t$

By applying the expression of the entire Nirmala index to the entire partition explained in Table 6, we obtain the result,

$$\begin{aligned}
 N^{\mathcal{E}}(G) = t \bigg[& \sqrt{t+5} + 2\sqrt{t+6} + 2\sqrt{t+8} + 4\sqrt{t+10} + 2\sqrt{t+12} + 4\sqrt{t+13} + 4\sqrt{t+16} \\
 & + 2\sqrt{2t+5} + 2\sqrt{2t+8} + 2\sqrt{2t+9} + 2\sqrt{2t+12} + \frac{t-1}{2}\sqrt{2t+4} \\
 & + (t-1)\sqrt{3t+4} + (t-1)\sqrt{3t+5} + 2(t-1)\sqrt{3t+8} + \frac{(t-1)(t-2)}{2}\sqrt{4t+4} \\
 & + 2\sqrt{3} + \sqrt{20} + 2\sqrt{10} + 2\sqrt{13} + 2\sqrt{14} + 4\sqrt{17} + 14 \bigg].
 \end{aligned}$$

□

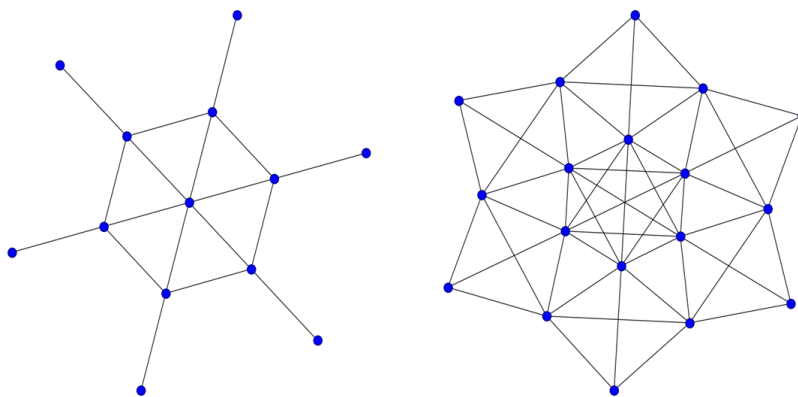


FIGURE 3. The helm graph H_6 with its line graph $L(H_6)$

For any integers $n \geq 2$ and $m \geq 3$, the Jahangir graph, denoted by $J_{n,m}$ is a graph of $(nm + 1)$ vertices and $(m(n + 1))$ edges, consisting of a cycle C_{nm} and a unique central vertex $u \notin V(C_{nm})$ that is adjacent to exactly m vertices of C_{nm} such that the distance between any two consecutive neighbors of u along the cycle is exactly n .

Theorem 2.4. Let G be the Jahangir graph $J_{n,m}$, where $n, m \geq 3$. Then

$$N^{\mathcal{E}}(G) = m \left[8n - 18 + 6\sqrt{5} + 3\sqrt{6} + \sqrt{m+3} + 3\sqrt{m+4} + \frac{m-1}{2}\sqrt{2m+2} + \sqrt{2m+1} \right].$$

Proof. For the Jahangir graph $G \cong J_{n,m}$, where $n, m \geq 3$, see Figure 4, there are m vertices of degree 3, $(m(n - 2))$ vertices of degree two and one vertex of degree m . Also for the edges, there are m edges of degree $(m + 1)$, $2m$ edges of degree 3 and $m(n - 2)$ edges of degree two. Applying the entire partition, we get the results in Table 7.

TABLE 7. The entire partition of the Jahangir graph $J_{n,m}$

Partition Type	(a, b)	Cardinality
$\mathcal{P}_1^{(a,b)}$	$(2, 2)$	$m(n - 2)$
	$(2, 3)$	$2m$
	$(3, m)$	m
$\mathcal{P}_2^{(a,b)}$	$(2, 2)$	$m(n - 3)$
	$(2, 3)$	$2m$
	$(3, 3)$	m
	$(m + 1, 3)$	$2m$
	$(m + 1, m + 1)$	$\frac{m(m - 1)}{2}$
$\mathcal{P}_3^{(a,b)}$	$(2, 2)$	$2m(n - 2)$
	$(2, 3)$	$2m$
	$(3, 3)$	$2m$
	$(3, m + 1)$	m
	$(m, m + 1)$	m

Now, by substituting in the formula of Nirmala index, we get

$$\begin{aligned} N^{\mathcal{E}}(G) = & m(n - 2)\sqrt{4} + 2m\sqrt{5} + m\sqrt{m+3} \\ & + m(n - 3)\sqrt{4} + 2m\sqrt{5} + m\sqrt{6} + 2m\sqrt{m+4} + \frac{m(m - 1)}{2}\sqrt{2m+2} \end{aligned}$$

$$+ 2m(n-2)\sqrt{4} + 2m\sqrt{5} + 2m\sqrt{6} + m\sqrt{m+4} + m\sqrt{2m+1}.$$

By simplification, the result is:

$$N^{\mathcal{E}}(G) = m \left[8n - 18 + 6\sqrt{5} + 3\sqrt{6} + \sqrt{m+3} + 3\sqrt{m+4} \right. \\ \left. + \frac{m-1}{2}\sqrt{2m+2} + \sqrt{2m+1} \right].$$

□

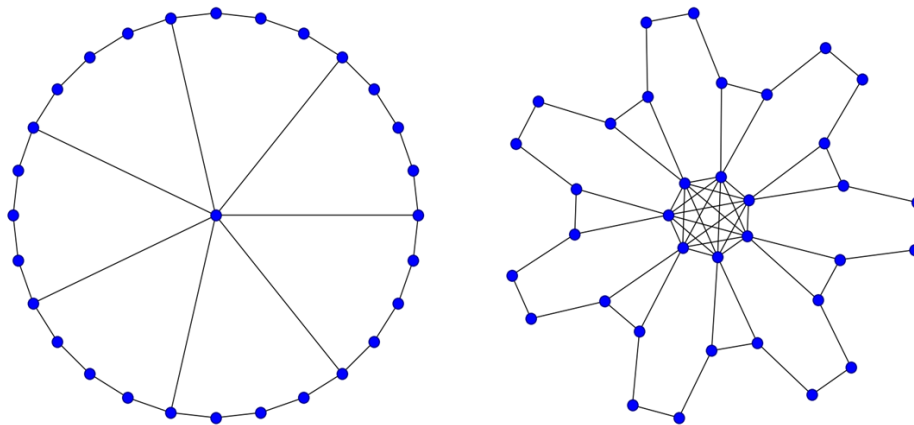


FIGURE 4. Jahangir graph $J_{4,7}$ with its line graph $L(J_{4,7})$

Theorem 2.5. Let G be the line graph of the Jahangir graph; $G \cong L(J_{n,m})$ where $n \geq 4$ and $m \geq 3$. Then

$$N^{\mathcal{E}}(G) = m \left[\frac{m-1}{2}\sqrt{2m+2} + 2\sqrt{m+4} + \sqrt{6} + 2\sqrt{5} + 2(n-3) \right. \\ + \frac{(m-1)(m-2)}{2}\sqrt{4m} + \sqrt{2m+4} + 2(m-1)\sqrt{3m+2} \\ + 2\sqrt{m+6} + 2\sqrt{m+5} + 2\sqrt{7} + 2\sqrt{5} + 2(n-4) \\ + (m-1)\sqrt{3m+1} + 2\sqrt{2m+3} + 2\sqrt{m+5} + 2\sqrt{7} + 2\sqrt{6} \\ \left. + 2\sqrt{5} + 4(n-3) \right].$$

Proof. Let $G \cong L(J_{n,m})$ be the line graph of the Jahangir graph, where $n \geq 4$ and $m \geq 3$ (the line graph of $J_{4,7}$ is shown in Figure 4). From the structure of $L(J_{n,m})$, there are $m(n-2)$ vertices of degree two, $2m$ vertices of degree three and m vertices of degree $(m+1)$. For the edge classification, there are $\frac{m(m-1)}{2}$ of degree $2m$, $2m$ edges of degree $(m+2)$, m edges of degree four, $2m$ edges of degree three and $m(m-3)$ edges of degree two. By applying the entire partition, we have the results of the partition in Table 8

TABLE 8. The entire partition of $L(J_{n,m})$

Partition Type	(a, b)	Cardinality
$\mathcal{P}_1^{(a,b)}$	$(m+1, m+1)$	$\frac{m(m-1)}{2}$
	$(m+1, 3)$	$2m$
	$(3, 3)$	m
	$(3, 2)$	$2m$
	$(2, 2)$	$m(n-3)$
$\mathcal{P}_2^{(a,b)}$	$(2m, 2m)$	$\frac{m(m-1)(m-2)}{2}$
	$(m+2, m+2)$	m
	$(2m, m+2)$	$2m(m-1)$
	$(m+2, 4)$	$2m$
	$(m+2, 3)$	$2m$
	$(4, 3)$	$2m$
	$(3, 2)$	$2m$
$\mathcal{P}_3^{(a,b)}$	$(2, 2)$	$m(n-4)$
	$(m+1, 2m)$	$m(m-1)$
	$(m+1, m+2)$	$2m$
	$(3, m+2)$	$2m$
	$(3, 4)$	$2m$
	$(3, 3)$	$2m$
	$(2, 3)$	$2m$
	$(2, 2)$	$2m(n-3)$

Now, using the results of the entire partition given by Table 8 in the formula of the entire Nirmala index, we get

$$\begin{aligned} N^{\mathcal{E}}(G) = & \frac{m(m-1)}{2} \sqrt{2m+2} + 2m \sqrt{m+4} + m \sqrt{6} + 2m \sqrt{5} + m(n-3) \sqrt{4} \\ & + \frac{m(m-1)(m-2)}{2} \sqrt{4m} + m \sqrt{2m+4} + 2m(m-1) \sqrt{3m+2} \\ & + 2m \sqrt{m+6} + 2m \sqrt{m+5} + 2m \sqrt{7} + 2m \sqrt{5} + m(n-4) \sqrt{4} \\ & + m(m-1) \sqrt{3m+1} + 2m \sqrt{2m+3} + 2m \sqrt{m+5} + 2m \sqrt{7} + 2m \sqrt{6} \\ & + 2m \sqrt{5} + 2m(n-3) \sqrt{4}. \end{aligned}$$

Then, by simplifying, we obtain the result. □

3. PREDICTIVE CAPACITY OF THE ENTIRE NIRMALA INDEX

Usually, the predictive power and chemical significance of a graph invariant are tested by regression against known molecular properties. We chose octane isomers as our benchmark molecular set, applying the comparative approach proposed by Randić and Trinajstić [22]. This dataset is ideal for this validation because the molecules within it possess well-characterized molecular topologies, significant structural diversity, and extensive experimental property records.

The isomers form a homologous series with a high degree of structural complexity regarding different branching patterns and conformations. In our comparative study, we use the octane isomers (18 octane isomers and two of their properties; the entropy (S) and the acentric factor (AF)). The experimental physicochemical properties of octane isomers in Table 9 and their molecular structures in Figure 5 were obtained from PubChem (National Center for Biotechnology Information, accessed via <http://pubchem.ncbi.nlm.nih.gov/>), ChemSpider (Royal Society of Chemistry, accessed via <http://www.chemspider.com/Search.aspx>) and [21].

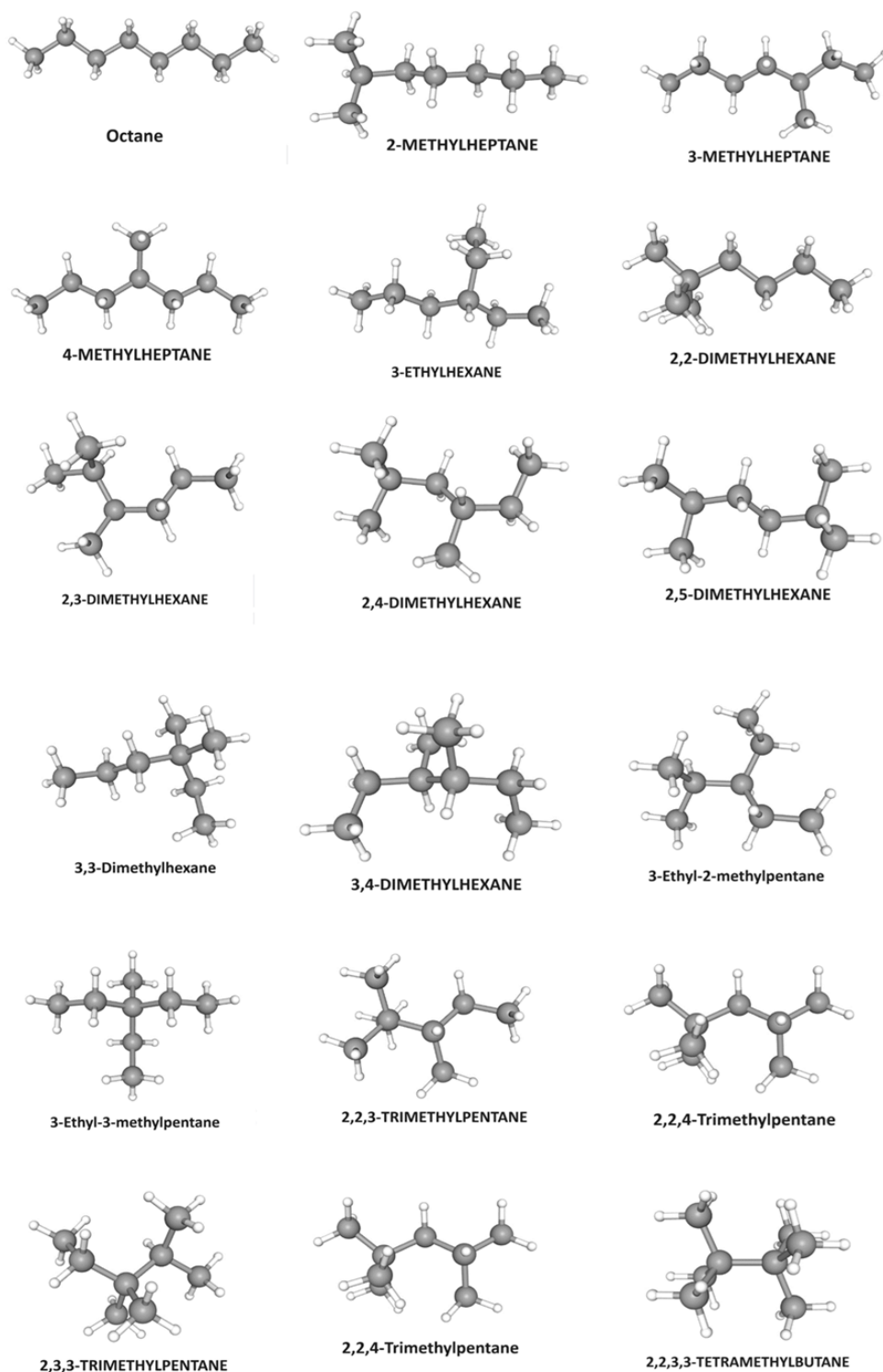


FIGURE 5. Chemical structures of 18 isomers of octane.

TABLE 9. The topological indices ($N(G)$, $N^{\mathcal{E}}(G)$) and experimental physicochemical properties (S , AF) of octane isomers.

Compound Name	$N(G)$	$N^{\mathcal{E}}(G)$	S (J/mol · K)	AF
octane	13.4641	51.2207	111.67	0.397898
2-methylheptane	13.9681	56.1764	109.84	0.377916
3-methylheptane	13.9362	56.4577	111.26	0.371002
4-methylheptane	13.9362	56.4259	109.32	0.371504
3-ethylheptane	13.9044	56.7164	109.43	0.362472
2,2-dimethylhexane	14.8897	66.7184	103.42	0.339426
2,3-dimethylhexane	14.4176	61.6437	108.02	0.348247
2,4-dimethylhexane	14.4403	61.3908	106.98	0.344223
2,5-dimethylhexane	14.4721	61.1321	105.72	0.356830
3,3-dimethylhexane	14.8352	67.2536	104.74	0.322596
3,4-dimethylhexane	14.3857	61.9397	106.59	0.340345
3-ethyl-2-methylpentane	14.3857	61.9171	106.06	0.332433
3-ethyl-3-methylpentane	14.7807	67.8297	101.48	0.306899
2,2,3-trimethylpentane	15.3221	72.4317	101.31	0.300816
2,2,4-trimethylpentane	15.3938	71.6343	104.09	0.305370
2,3,3-trimethylpentane	15.2994	72.7052	102.06	0.293177
2,3,4-trimethylpentane	14.8990	66.8479	102.39	0.317422
2,2,3,3-tetramethylbutane	16.2448	83.1408	93.06	0.255294

3.1. Linear Regression Analysis. Linear regression models were constructed to evaluate and validate the predictive capacity of the entire Nirmala index $N^{\mathcal{E}}(G)$, alongside the standard Nirmala index $N(G)$, against the experimental physicochemical properties of the octane isomers.

The statistical metrics and optimal regression equations for both properties are consolidated in Table 10. To highlight the superior predictive power for each property, the model yielding the higher correlation coefficient (R) and coefficient of determination (R^2) has been highlighted in bold.

TABLE 10. Consolidated linear regression models and statistical metrics for Nirmala and entire Nirmala indices.

Property	Index	Regression Equation	R	R^2	Adj. R^2	S.E.	F	p -value
Entropy	$N^{\mathcal{E}}(G)$	$S = -0.55563 N^{\mathcal{E}}(G) + 141.0225$	-0.959	0.919	0.914	1.323	182.329	0.0000
	$N(G)$	$S = -6.305613 N(G) + 197.536621$	-0.947	0.897	0.891	1.494	139.396	0.0000
Acentric Factor	$N^{\mathcal{E}}(G)$	$AF = -0.00446 N^{\mathcal{E}}(G) + 0.6213$	-0.980	0.960	0.957	0.007	381.824	0.0000
	$N(G)$	$AF = -0.050303 N(G) + 1.070686$	-0.963	0.927	0.923	0.010	203.489	0.0000

The linear regression models show a highly significant relationship between the topological indices and the target physicochemical properties, where the newly developed entire Nirmala index $N^{\mathcal{E}}(G)$ consistently outperforms the Nirmala index $N(G)$ across all evaluated parameters by yielding higher correlation coefficients (R) and coefficients of determination (R^2) alongside reduced standard errors (S.E.). For entropy (S) modeling, $N^{\mathcal{E}}(G)$ establishes a robust correlation ($R = -0.959$), accounting for 91.9% of the total thermodynamic variance ($R^2 = 0.919$) and reducing the standard error to 1.323, whereas the Nirmala index $N(G)$ explains only 89.7% of the variance, with a higher standard error of 1.494. This predictive advantage is even more pronounced in acentric factor (AF) modeling; while $N(G)$ performs adequately ($R^2 = 0.927$), $N^{\mathcal{E}}(G)$ provides an exceptional near-linear fit, explaining 96.0% of the variance ($R^2 = 0.960$, Adj. $R^2 = 0.957$, $F = 381.824$, S.E. = 0.007).

The excellent results of prediction for the entire Nirmala index stem from the ability of this index to capture a complete picture of the graph, as it is based not only on the degrees of the vertices and their connections but also takes into account the degrees of the edges and the two essential relations: the adjacency and incidence. The predictive performance of the entire Nirmala index, $N^{\mathcal{E}}(G)$, is illustrated in Figure 6, which depicts the linear regression models for Entropy (S) and Acentric Factor (AF) against the experimental values of octane isomers.

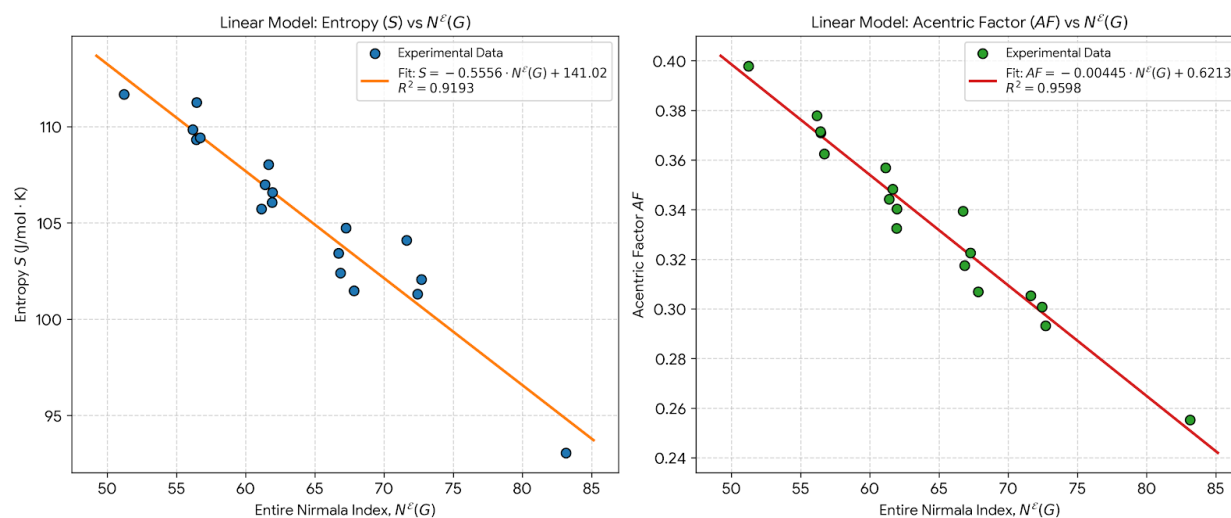


FIGURE 6. Linear regression of entire Nirmala index with S and AF

To assess the predictive accuracy of our model, we compare the experimental and predicted thermodynamic properties (Entropy (S) and the acentric factor (AF)) for eighteen octane isomers. We calculate these properties using both the Nirmala index $N(G)$ and our newly proposed Entire Nirmala index $N^{\mathcal{E}}(G)$. Table 11 presents the individual isomer predictions, and Table 12 summarizes the comparative residual metrics.

TABLE 11. The experimental and predicted entropy (S) and acentric factor (AF) values for octane isomers using linear regression model.

Compound	Entropy (S)			Acentric Factor (AF)		
	Exp.	Predicted		Exp.	Predicted	
		$N(G)$	$N^E(G)$		$N(G)$	$N^E(G)$
octane	111.67	112.64	112.56	0.3979	0.3934	0.3931
2-methylheptane	109.84	109.46	109.81	0.3779	0.3680	0.3710
3-methylheptane	111.26	109.66	109.65	0.3710	0.3697	0.3698
4-methylheptane	109.32	109.66	109.67	0.3715	0.3697	0.3699
3-ethylheptane	109.43	109.86	109.51	0.3625	0.3713	0.3686
2,2-dimethylhexane	103.42	103.65	103.95	0.3394	0.3217	0.3241
2,3-dimethylhexane	108.02	106.62	106.77	0.3482	0.3454	0.3467
2,4-dimethylhexane	106.98	106.48	106.91	0.3442	0.3443	0.3478
2,5-dimethylhexane	105.72	106.28	107.06	0.3568	0.3427	0.3489
3,3-dimethylhexane	104.74	103.99	103.65	0.3226	0.3244	0.3217
3,4-dimethylhexane	106.59	106.83	106.61	0.3403	0.3470	0.3453
3-ethyl-2-methylpentane	106.06	106.83	106.62	0.3324	0.3470	0.3454
3-ethyl-3-methylpentane	101.48	104.34	103.33	0.3069	0.3272	0.3191
2,2,3-trimethylpentane	101.31	100.92	100.78	0.3008	0.2999	0.2986
2,2,4-trimethylpentane	104.09	100.47	101.22	0.3054	0.2963	0.3022
2,3,3-trimethylpentane	102.06	101.06	100.63	0.2932	0.3011	0.2974
2,3,4-trimethylpentane	102.39	103.59	103.88	0.3174	0.3212	0.3235
2,2,3,3-tetramethylbutane	93.06	95.10	94.83	0.2553	0.2535	0.2509

TABLE 12. Residual analysis for entropy (S) and acentric factor (AF) using $N(G)$ and $N^E(G)$.

Model	Entropy (S)		Acentric Factor (AF)	
	MAE	RMSE	MAE	RMSE
$N(G)$	1.0697	1.4087	0.007106	0.009302
$N^E(G)$	0.9864	1.2470	0.005574	0.006909

Table 12 presents a comparative residual analysis evaluating the predictive accuracy of the standard Nirmala index $N(G)$ against the newly proposed Entire Nirmala index $N^E(G)$ for both entropy (S) and acentric factor (AF).

The results in Tables 11 and 12 demonstrate that the entire Nirmala index $N^E(G)$ consistently outperforms the Nirmala index $N(G)$ through all metrics. For entropy (S), $N^E(G)$ reduced the RMSE from 1.4087 to 1.2470. In the same way for the acentric factor (AF), the entire Nirmala index $N^E(G)$ reduced the MAE from 0.007106 to 0.005574 and the RMSE from 0.009302 to 0.006909.

3.2. Cubic Regression Analysis. In this subsection, we study cubic regression analysis to show the predictive performance of the Nirmala and the entire Nirmala indices. We present full statistical parameters to test the regression quality (see Tables 13 and 14). We derive the cubic regression

equations for each property and visualizations of index-property relationships (Figure 7). Employing the cubic models of the general form:

$$P = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3$$

where P represents the physicochemical property, X represents the index, and $\beta_0, \beta_1, \beta_2, \beta_3$ are the regression coefficients and the constant term, respectively.

TABLE 13. Cubic regression models for Nirmala indices predicting physicochemical properties.

Property	Index	Regression Equation
Entropy	$N^{\mathcal{E}}(G)$	$S = -0.000468 N^{\mathcal{E}}(G)^3 + 0.090374 N^{\mathcal{E}}(G)^2 - 6.289912 N^{\mathcal{E}}(G) + 260.618551$
	$N(G)$	$S = -0.772815 N(G)^3 + 33.898839 N(G)^2 - 500.917567 N(G) + 2598.199668$
Acentric Factor	$N^{\mathcal{E}}(G)$	$AF = 0.000199 N^{\mathcal{E}}(G)^2 - 0.019280 N^{\mathcal{E}}(G) + 0.980393$
	$N(G)$	$AF = -0.001980 N(G)^3 + 0.090548 N(G)^2 - 1.426669 N(G) + 8.026162$

TABLE 14. Statistical evaluation metrics for the Nirmala index cubic regression models.

Property	Index	R	R^2	Adj. R^2	S.E.	F	p -value
Entropy	$N^{\mathcal{E}}(G)$	0.964	0.930	0.915	1.315	62.243	0.0001
	$N(G)$	0.954	0.909	0.890	1.499	46.800	0.0001
Acentric Factor	$N^{\mathcal{E}}(G)$	0.981	0.963	0.955	0.008	121.276	0.0001
	$N(G)$	0.964	0.929	0.914	0.010	61.286	0.0001

The results of the cubic regression analysis in Tables 13 and 14 confirm the excellent predictive capacity of the entire Nirmala index over the Nirmala index. For entropy (S), the cubic model based on $N^{\mathcal{E}}(G)$ (Table 13) achieves $R = 0.964$ and $R^2 = 0.930$, with an adjusted $R^2 = 0.915$ and a reduced standard error of 1.315; however, the results of $N(G)$ are ($R^2 = 0.909$, Adj. $R^2 = 0.890$) with a standard error of 1.499 (Table 14). The F -statistic reinforces this advantage, with $N^{\mathcal{E}}(G)$ yielding $F = 62.243$ versus $F = 46.800$ for $N(G)$, reflecting greater overall model significance and regression efficiency. For the acentric factor (AF), the performance gap widens considerably: as reported in Table 14, $N^{\mathcal{E}}(G)$ delivers an exceptional fit with $R = 0.981$, $R^2 = 0.963$, Adj. $R^2 = 0.955$, $F = 121.276$, and a remarkably low standard error of 0.008, while for $N(G)$ $R^2 = 0.929$, Adj. $R^2 = 0.914$, and a standard error of 0.010. Overall, the transition from linear to cubic modeling yields consistent, measurable gains in explained variance and statistical significance for both indices; however, $N^{\mathcal{E}}(G)$ extracts substantially greater predictive benefit from this added flexibility, as evidenced by the metrics in Table 14. Consequently, the cubic regression presented in Tables 13 and 14 shows that $N^{\mathcal{E}}(G)$ is an exceptionally reliable, structurally informed descriptor for nonlinear (QSPR) modeling of branched alkane systems.

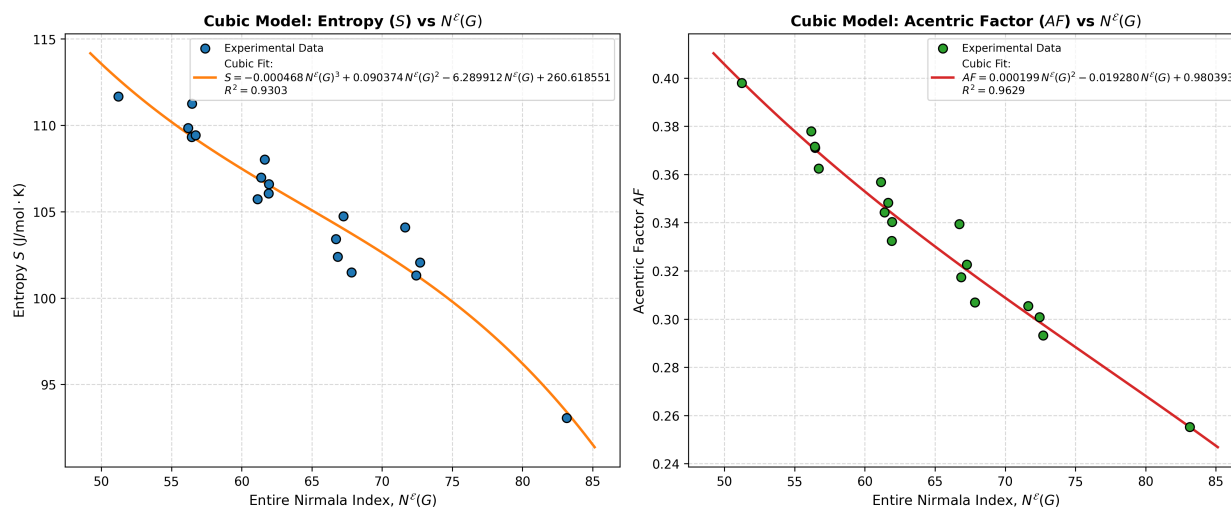


FIGURE 7. Cubic regression of entire Nirmala index with S and AF

To confirm the predictive accuracy of the cubic model, we compare the experimental and predicted values of the entropy (S) and acentric factor (AF) using the Nirmala index and the entire Nirmala index; see Table 15. Also, we summarize the comparative residual metrics in Table 16.

TABLE 15. The experimental and predicted entropy (S) and acentric factor (AF) values for octane isomers using cubic regression model.

Compound	Entropy (S)			Acentric Factor (AF)		
	Exp.	Predicted (Cubic)		Exp.	Predicted (Cubic)	
		$N(G)$	$N^E(G)$		$N(G)$	$N^E(G)$
octane	111.67	112.76	112.66	0.3979	0.3985	0.3986
2-methylheptane	109.84	109.12	109.51	0.3779	0.3679	0.3718
3-methylheptane	111.26	109.32	109.35	0.3710	0.3698	0.3703
4-methylheptane	109.32	109.32	109.37	0.3715	0.3698	0.3705
3-ethylheptane	109.43	109.53	109.21	0.3625	0.3716	0.3690
2,2-dimethylhexane	103.42	104.03	104.26	0.3394	0.3210	0.3226
2,3-dimethylhexane	108.02	106.54	106.68	0.3482	0.3440	0.3452
2,4-dimethylhexane	106.98	106.42	106.80	0.3442	0.3429	0.3464
3,4-dimethylhexane	105.72	106.25	106.93	0.3568	0.3413	0.3476
3,3-dimethylhexane	104.74	104.33	104.01	0.3226	0.3236	0.3204
2,2,4-trimethylpentane	106.59	106.71	106.53	0.3403	0.3456	0.3438
3-ethyl-2-methylpentane	106.06	106.71	106.55	0.3324	0.3456	0.3439
2,5-dimethylhexane	101.48	104.62	103.72	0.3069	0.3262	0.3179
2,2,3-trimethylpentane	101.31	101.50	101.32	0.3008	0.3007	0.2988
2,2,4-trimethylpentane	104.09	101.04	101.77	0.3054	0.2974	0.3021
2,3,3-trimethylpentane	102.06	101.65	101.17	0.2932	0.3018	0.2977
2,3,4-trimethylpentane	102.39	103.98	104.20	0.3174	0.3205	0.3221
2,2,3,3-tetramethylbutane	93.06	93.60	93.41	0.2553	0.2557	0.2552

TABLE 16. Residual analysis for entropy (S) and acentric factor (AF) using cubic regression with $N(G)$ and $N^E(G)$.

Model	Entropy (S)		Acentric Factor (AF)	
	MAE	RMSE	MAE	RMSE
$N(G)$	0.9526	1.3220	0.006733	0.009164
$N^E(G)$	0.8881	1.1594	0.004949	0.006632

The summary results of the residual analysis in Table 16 provide strong confirmation of the cubic model's ability to predict. For entropy, the cubic model based on the entire Nirmala index achieves 0.8881 for the mean absolute error and 1.1594 for the root mean square error, both markedly lower than the corresponding values for the classical $N(G)$ cubic model (MAE = 0.9526, RMSE = 1.3220).

4. CONCLUSION

In this work, we introduce a novel topological index called the entire Nirmala index, which is based on the degree and connections between all the elements of the graphs (vertices and edges). Mathematically, we establish upper and lower bounds for this new index and obtain closed form expressions for some standard families of graphs with specific focus on wheel related graphs and their line graphs. From the applied view, the (QSPR) analysis of octane isomers shows an excellent predictive power and significance of the entire Nirmala. Both linear and cubic models revealed a statistically significant correlation between the index and the experimental physicochemical properties of the isomers. Also, the comparative analysis confirmed that the entire Nirmala index consistently outperforms the Nirmala index across all studied metrics. The excellent predictive power of the entire Nirmala index draws a clear pathway for future research, not just as a robust tool for current (QSPR) studies but as a descriptor for future applications in chemical graph theory and molecular design.

Conflicts of Interest: The authors declare that there are no conflicts of interest regarding the publication of this paper.

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