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ON THE REVERSE SOMBOR COINDEX OF GRAPHS AND ITS CHEMICAL APPLICABILITY

NAGENDRAPPA G[1], VENKANAGOUDA M GOUDAR[2], MANOHAR R GOMBI[3], RAJATHAGIRI D T[4]

ABSTRACT: In this paper, we introduced a new parameter, known as reverse Sombor coindex. Also, we obgtained an exact expressions for the reverse Sombor index and reverse Sombor coindex for few standard graphs like paths, cycles, complete graphs, star graphs, wheel graphs, and complete bipartite graphs. Furthermore, several bounds are established with regard to classical graph parameters and well-known topological descriptors such as the Zagreb indices and forgotten index. Bounds for these descriptors under Cartesian product and composition of graphs are also derived. In addition, the chemical applicability of revrese Sombor index and the reverse Sombor coindex are examined with the help of hetero-atom containing molecules and polycyclic aromatic hydrocarbons (PAHs) and are compared with Sombor index, first Zagreb index, and forgotten index.. The obtained correlation coefficients and coefficients of determination indicate strong linear relationships between the considered descriptors and total π-electron energy. In particular, the reverse Sombor coindex exhibited the highest predictive performance, yielding correlation coefficients of R=0.9921 for heteroatom-containing molecules and R=0.9896 for polycyclic aromatic hydrocarbons (PAHs). These results demonstrate the usefulness of reverse degree-based descriptors in chemical graph theory, QSPR/QSAR studies, and molecular structure analysis.

Key words: Correlation analysis, graph products, reverse Sombor coindex, reverse Sombor index, Sombor index, topological indices, Zagreb indices, π-electron energy.

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1 Introduction.

Topological indices (TIs) are numerical graph invariants that play a significant role, particularly in QSPR and QSAR studies. These descriptors provide important information regarding the structural and electronic characteristics of molecular graphs. Among the various TIs, the Zagreb indices, forgotten index [7], and Sombor index [8, 9] have attracted considerable attention because of their wide range of applications in chemical graph theory. Recently, Gutman introduced the Sombor index [9, 11], which stimulated extensive research concerning its mathematical properties and chemical applicability [19–24].

Later, Narahari et al. [13] proposed the reverse Sombor index by employing the concept of reverse vertex degree. Motivated by this development, we define the reverse Sombor coindex and further investigate the mathematical and chemical properties of the reverse Sombor coindex and reverse Sombor index.

The main objective of this study is to investigate the reverse Sombor index and reverse Sombor coindex of graphs. In particular, we derive explicit expressions for several standard graph classes, establish the bounds regarding the classical graph parameters and topological indices, examine

their behavior under graph operations, and analyze their chemical applicability using molecular datasets.

In theoretical chemistry, the total π-electron energy [10] is an important parameter associated with conjugated molecular systems. Since exact quantum-chemical computations are often computationally expensive, graph-theoretical descriptors are frequently employed to estimate molecular properties efficiently. Therefore, establishing strong correlations between topological indices and π-electron energy remains an important research direction.

To demonstrate the usefulness of the proposed descriptors, correlation analyses are performed using datasets of heteroatom-containing molecules and polycyclic aromatic hydrocarbons (PAHs). The obtained results indicate that the reverse Sombor index and reverse Sombor coindex possess strong predictive capability for estimating electronic properties of molecular structures.

Throughout this paper, all graphs considered are finite, simple, connected, and undirected graphs. Let $G = (V, E)$ be a graph with $|V(G)| = n$ and $|E(G) = m$. For any vertex $u \in V(G)$, its degree is denoted by $d(u)$, representing the number of edges incident to u. Let Δ and δ be the maximum and minimum vertex degrees of G respectively. Let $\overline{G}$, be the complement of G and the number of edges in $\overline{G}$ is given by $\overline{m} = \binom{n}{2} - m$.

For any undefined terminology or notation, the reader is referred to [6, 17].

2 Preliminaries

We begin this section by recapping some definitions and notations.

Definition 2.1 For any two graphs G_1 and G_2, the Cartesian product [3, 12, 14], denoted by

$G_1 \square G_2$, is a graph with vertex set $V(G_1 \square G_2) = V(G_1) \times V(G_2)$, where two vertices (u_i, v_j) and (u_k, v_ℓ) are adjacent if and only if $u_i = u_k$ and $v_j \sim v_\ell$ in G_2 or $v_j = v_\ell$ and $u_i \sim u_k$ in G_1. We notice that $|E(G_1 \square G_2)| = n_1 m_2 + m_1 n_2$, and $d_{G_1 \square G_2}(u_i, v_j) = d_{G_1}(u_i) + d_{G_2}(v_j)$.

Definition 2.2 For any two graphs G_1 and G_2, the composition (or lexico-graphic product) [3, 12, 14], denoted by $G_1[G_2]$, has a vertex set $V(G_1[G_2]) = V(G_1) \times V(G_2)$, in which (u_i, v_j) and (u_k, v_ℓ) are adjacent whenever either $u_i \sim u_k$ in G_1 or $u_i = u_k$ and $v_j \sim v_\ell$ in G_2. In the graph $G_1[G_2], |V(G_1[G_2])| = n_1 n_2, |E(G_1[G_2])| = n_1 m_2 + m_1 n_2^2$ and $d_{G_1[G_2]}(u_i, v_j) = |V(G_2)| d_{G_1}(u_i) + d_{G_2}(v_j)$.

Definition 2.3 The first Zagreb index of a graph G [10] is defined as

$$M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)]$$

whereas, the second Zagreb index is defined as

$$M_2(G) = \sum_{uv \in E(G)} d(u) d(v),$$

where $d(u)$ denotes the degree of the vertex u.

Definition 2.4 The first Zagreb coindex of a graph G [2] is defined as

$$\overline{M_1}(G) = \sum_{uv \notin E(G)} [d(u) + d(v)]$$

while the second Zagreb coindex is defined as

$$\overline{M_2}(G) = \sum_{uv \notin E(G)} d(u)d(v).$$

Definition 2.5 The forgotten index (or F-index) of a graph G [7] is

$$F(G) = \sum_{uv \in E(G)} [d(u)^2 + d(v)^2].$$

Definition 2.6 The forgotten coindex of a graph G [1] is defined by

$$\overline{F}(G) = \sum_{uv \notin E(G)} [d(u)^2 + d(v)^2].$$

Definition 2.7 The Sombor index of a graph G [9] is defined as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d(u)^2 + d(v)^2},$$

where $d(u)$ is the degree of the vertex $u \in G$.

Definition 2.8 The Sombor coindex of a graph G [15] is defined as

$$\overline{SO}(G) = \sum_{uv \notin E(G)} \sqrt{d(u)^2 + d(v)^2},$$

where $d(u)$ is the degree of the vertex u of G.

Definition 2.9 For a graph G with maximum degree Δ, the reverse vertex degree of a vertex u [18, 19, 20, 21] is

$$r(u) = \Delta + 1 - d(u).$$

Definition 2.10 The reverse Sombor index of a graph G [13], denoted by $R_eSO(G)$, is defined as

$$\begin{aligned} R_eSO(G) &= \sum_{uv \in E(G)} \sqrt{r(u)^2 + r(v)^2} \\ &= \sum_{uv \in E(G)} \sqrt{[\Delta + 1 - d(u)]^2 + [\Delta + 1 - d(v)]^2}, \end{aligned}$$

where $r(u) = \Delta + 1 - d(u)$ is the reverse vertex degree of u.

Motivated by the concept of the reverse Sombor index [12, 13], we now define a new topological descriptor called the reverse Sombor coindex of a graph.

Definition 2.11 Let G be a graph and Δ be the maximum degree of a vertex u. The reverse Sombor coindex of G, denoted by $\overline{R_eSO}(G)$, is defined as

$$\overline{R_eSO}(G) = \sum_{uv \notin E(G)} \sqrt{r(u)^2 + r(v)^2}$$

$$= \sum_{uv \notin E(G)} \sqrt{[\Delta + 1 - d(u)]^2 + [\Delta + 1 - d(v)]^2},$$

Where, $r(u) = \Delta + 1 - d(u)$ is the reverse vertex degree of u.

3. Properties of the Reverse Sombor Index

Let G be a simple connected graph with $| V(G) | > 2$. Since G contains at least three vertices, we have $\Delta \geq 2$. The following propositions provide closed-form expressions for the reverse Sombor index of some standard graphs.

Proposition 3.1 For the path $P_n, n \geq 2$,

$$R_eSO(P_n) = (n-3)\sqrt{2} + 2\sqrt{5}.$$

Proposition 3.2 For the cycle $C_n, n \geq 3$,

$$R_eSO(C_n) = n\sqrt{2}.$$

Proposition 3.3 For the complete graph $K_n, n \geq 2$,

$$R_eSO(K_n) = \frac{n(n-1)}{\sqrt{2}}.$$

Proposition 3.4 For a star graph $K_{1,n-1}, n \geq 3$,

$$R_eSO(K_{1,n-1}) = (n-1)\sqrt{n^2 - 2n + 2}.$$

Proposition 3.5 For a wheel graph $W_n, n \geq 4$,

$$R_eSO(W_n) = (n-1)(n-3)\sqrt{2} + (n-1)\sqrt{n^2 - 6n + 10}.$$

Proposition 3.6 Let $K_{m,n}, m \geq n$ be a complete bipartite graph. Then,

$$R_eSO(K_{m,n}) = mn\sqrt{(m-n+1)^2 + 1}, if\ \Delta = m,$$

$$R_eSO(K_{m,n}) = mn\sqrt{(n-m+1)^2 + 1}, if\ \Delta = n,$$

4 Extremal Properties of the Reverse Sombor Index

After deriving exact expressions for several standard graph classes, we now investigate extremal properties and general bounds of the reverse Sombor index. In particular, we characterize graphs attaining minimum and maximum values among trees and establish sharp inequalities in terms of graph parameters.

The following results establish extremal properties of the reverse Sombor index for trees.

Theorem 4.1 For all trees of order $n \geq 2$, *the path* P_n *attains the minimum reverse Sombor index.*

Proof. For the path graph $P_n, \Delta(P_n) = 2$. The two pendent vertices have degree 1, and hence their reverse degree equals $r(u) = 2 + 1 - 1 = 2$. All remaining internal vertices have degree 2, and therefore their reverse degree equals $r(u) = 2 + 1 - 2 = 1$.

Thus, every pendent edge contributes $\sqrt{2^2 + 1^2} = \sqrt{5}$,

while every internal edge contributes $\sqrt{1^2 + 1^2} = \sqrt{2}$. Since the path graph contains two pendent edges and $n - 3$ internal edges, we obtain

$$R_eSO(P_n) = 2\sqrt{5} + (n-3)\sqrt{2}$$

Now let T be any tree on n vertices distinct from P_n. Then, there is at least one vertex whose degree greater than 2. Consequently, the corresponding reverse-degree structure produces larger edge contributions compared to the path graph. Moreover, $\sqrt{r(u)^2 + r(v)^2} \geq \sqrt{2}$ for every edge $uv \in E(T)$, with equality only when r$(u) = r(v) = 1$.

Since the path graph contains the smallest possible variation among reverse degrees of adjacent vertices, it follows that

$$ReSO(T) \geq ReSO(P_n).$$

Hence, $ReSO(P_n) = 2\sqrt{5} + (n-3)\sqrt{2}$ is the minimum reverse Sombor index for all trees of order n.

Theorem 4.2 For all trees of order $n \geq 2$, the star graph $K_{1,n-1}$ attains the maximum reverse Sombor index.

Proof. For the star $K_{1,n-1}, \Delta(K_{1,n-1}) = n - 1$ and the central vertex has degree $n - 1$. Therefore its reverse degree is $r(u) = (n-1) + 1 - (n-1) = 1$. Each pendent vertex has degree 1, and thus its reverse degree becomes $r(v) = (n-1) + 1 - 1 = n - 1$.

Hence, every edge contributes $\sqrt{1^2 + (n-1)^2}$. Since the star graph has exactly $n - 1$ edges,

$$ReSO(K_{1,n-1}) = (n-1)\sqrt{(n-1)^2 + 1}$$

Now let T be any tree distinct from $K_{1,n-1}$. Then T contains at least two non-pendent vertices, which reduces the extremal difference between reverse degrees along adjacent vertices. Consequently, $ReSO(T) \leq ReSO(K_{1,n-1})$. Hence, the star graph attains the maximum reverse Sombor index for all trees of order n.

Theorem 4.3 Let G be any connected graph having m edges with maximum degree Δ,

$$\sqrt{2}m \leq R_eSO(G) \leq \sqrt{2}m\Delta.$$

Proof. For each edge $uv \in E(G), 1 \leq r(u), r(v) \leq \Delta$. Therefore, $\sqrt{2} \leq \sqrt{r(u)^2 + r(v)^2} \leq \sqrt{2\Delta^2}$ Summing over all edges of G, we obtain

$$\sum_{uv \in E(G)} \sqrt{2} \leq R_eSO(G) \leq \sum_{uv \in E(G)} \sqrt{2\Delta^2}$$

Hence, $\sqrt{2}m \leq R_eSO(G) \leq \sqrt{2}m\Delta$.

Corollary 4.4 Equality in the lower bound of Theorem 4.3 holds if and only if all reverse edge degrees are equal to 1, while equality in the upper bound holds for regular graphs.

The following examples demonstrate the extremal behavior of the reverse Sombor index for trees.

Example 4.5 For the path graph P_6,

$$ReSO(P_6) = 2\sqrt{5} + 3\sqrt{2}.$$

Example 4.6 For the star graph $K_{1,5}$,

$$ReSO(K_{1,5}) = 5\sqrt{26}.$$

Since, $2\sqrt{5} + 3\sqrt{2} < 5\sqrt{26}$, the path graph produces the minimum value while the star graph gives the maximum value among trees of order six.

Table 1: Comparison of reverse Sombor index values for extremal trees.

Graph	Reverse Sombor Index
P_6	$2\sqrt{5} + 3\sqrt{2}$
$K_{1,5}$	$5\sqrt{26}$

5 Bounds for the Reverse Sombor Index Under Graph Operations

In this section, we derive bounds for the reverse Sombor index under various graph operations using well-known degree-based properties. In particular, we consider the Cartesian product and composition of graphs.

Lower bounds on the reverse Sombor index

Theorem 5.1 Let G_1 and G_2 be graphs with vertices n_1, n_2 and edges m_1, m_2 respectively. Then

$$R_eSO(G_1 \square G_2) \geq (n_1m_2 + m_1n_2)\sqrt{2}.$$

The equality holds if and only if both G_1 and G_2 are regular graphs.

Proof. Let $G_1 \square G_2$ be the Cartesian product of G_1 and G_2. Then,

$$|V(G_1 \square G_2)| = n_1 n_2, |E(G_1 \square G_2)| = n_1 m_2 + m_1 n_2.$$

For any vertex $(u_i, v_j) \in V(G_1 \square G_2)$, its degree is given by

$$d_{G_1 \square G_2}(u_i, v_j) = d_{G_1}(u_i) + d_{G_2}(v_j).$$

Hence,

$$\Delta = \Delta(G_1) + \Delta(G_2).$$

By definition,

$$R_e SO(G) = \sum_{uv \in E(G)} \sqrt{r(u)^2 + r(v)^2}$$

For all $(u_i, v_j), (u_k, v_\ell) \in V(G_1 \square G_2)$, Since

$d_{G_1 \square G_2}(u_i, v_j) \leq \Delta$ and $d_{G_1 \square G_2}(u_k, v_\ell) \leq \Delta$, we have

$$r(u_i, v_j) = \Delta + 1 - d_{G_1 \square G_2}(u_i, v_j) \geq 1$$

$$r(u_k, v_\ell) = \Delta + 1 - d_{G_1 \square G_2}(u_k, v_\ell) \geq 1$$

Hence,

$$R_e SO(G_1 \square G_2) \geq \sum_{((u_i v_j),(u_k v_\ell)) \in E(G_1 \square G_2)} \sqrt{1^2 + 1^2}$$

Thus,

$$R_e SO(G_1 \square G_2) \geq (n_1 m_2 + m_1 n_2)\sqrt{2}$$

Equality holds if and only if $d_{G_1 \square G_2}(u_i, v_j) = \Delta$

for all $(u_i, v_j) \in V(G_1 \square G_2)$, which occurs only when both G_1 and G_2 are regular graphs.

Theorem 5.2 Let G_1 and G_2 be graphs with vertices n_1, n_2 and edges m_1, m_2 respectively, then

$$R_e SO(G_1[G_2]) \geq (n_1 m_2 + m_1 n_2^2)\sqrt{2}.$$

The equality holds if and only if both G_1 and G_2 are regular.

Proof. Let the com[osition of G_1 and G_2 be $G_1[G_2]$. Then,

$$|V(G_1[G_2])| = n_1 n_2, |E(G_1[G_2])| = n_1 m_2 + m_1 n_2^2.$$

For $(u_i, v_j) \in V(G_1[G_2])$, $d_{G_1[G_2]}(u_i, v_j) = n_2 d_{G_1}(u_i) + d_{G_2}(v_j)$.

Hence,

$$\Delta = n_2 \Delta(G_1) + \Delta(G_2).$$

By definition,

$$R_eSO(G) = \sum_{uv\in E(G)} \sqrt{r(u)^2 + r(v)^2}$$

For all $(u_i, v_j), (u_k, v_\ell) \in V(G_1[G_2])$, Since $d_{G_1[G_2]}(u_i, v_j) \leq \Delta$ and $d_{G_1[G_2]}(u_k, v_\ell) \leq \Delta$, we have,

$$r(u_i, v_j) = \Delta + 1 - d_{G_1[G_2]}(u_i, v_j) \geq 1 \text{ and } r(u_k, v_\ell) = \Delta + 1 - d_{G_1[G_2]}(u_k, v_\ell) \geq 1$$

Hence,

$$R_eSO(G_1[G_2]) \geq \sum_{((u_i,v_j),(u_k,v_\ell))\in E(G_1[G_2])} \sqrt{1^2 + 1^2}$$

Thus,

$$R_eSO(G_1[G_2]) \geq (n_1m_2 + m_1n_2^2)\sqrt{2}$$

Equality attained if and only if $d_{G_1[G_2]}(u_i, v_j) = \Delta$ for all $(u_i, v_j) \in V(G_1[G_2])$.

Upper bounds on the reverse Sombor index

Theorem 5.3 Let n_1, n_2 be the vertices and m_1, m_2 be the edges of the graphs G_1 and G_2 respectively, then

$$R_eSO(G_1\square G_2) \leq (n_1m_2 + m_1n_2)(\Delta - \delta + 1)\sqrt{2},$$

where Δ and δ denote the maximum degree and minimum degree of $G_1\square G_2$.

Equality holds if and only if G_1 and G_2 are regular graphs.

Proof. Let $G_1\square G_2$ be the Cartesian product of G_1 and G_2. Then

$$|V(G_1\square G_2)| = n_1n_2, |E(G_1\square G_2)| = n_1m_2 + m_1n_2.$$

For any vertex $(u_i, v_j) \in V(G_1\square G_2)$, $\delta = \delta(G_1) + \delta(G_2)$ and $\Delta = \Delta(G_1) + \Delta(G_2)$.

By definition,

$$R_eSO(G) = \sum_{uv\in E(G)} \sqrt{r(u)^2 + r(v)^2}$$

For any adjacent vertices (u_i, v_j) and (u_k, v_ℓ)

$$r(u_i, v_j) = \Delta + 1 - d_{G_1\square G_2}(u_i, v_j)$$

$$r(u_k, v_\ell) = \Delta + 1 - d_{G_1\square G_2}(u_k, v_\ell)$$

Since $d_{G_1\square G_2}(u_i, v_j) \geq \delta$ and $d_{G_1\square G_2}(u_k, v_\ell) \geq \delta$, we obtain

$$r(u_i, v_j) = \Delta + 1 - d_{G_1\square G_2}(u_i, v_j) \leq \Delta + 1 - \delta \text{ and}$$

$$r(u_k, v_\ell) = \Delta + 1 - d_{G_1\square G_2}(u_k, v_\ell) \leq \Delta + 1 - \delta$$

Therefore,

$$R_eSO(G_1 \square G_2) \leq \sum_{((u_i,v_j),(u_k,v_\ell))\in E(G_1\square G_2)} (\Delta + 1 - \delta)\sqrt{2}$$

$$\leq (n_1m_2 + m_1n_2)(\Delta + 1 - \delta)\sqrt{2}.$$

Equality satisfies if and only if $d(u_i, v_j) = \delta = \Delta$ for all $(u_i, v_j) \in V(G_1 \square G_2)$.

Theorem 5.4 Let n_1, n_2 be the vertices and m_1, m_2 be the edges of G_1 and G_2 respectively, then

$$R_eSO(G_1[G_2]) \leq (n_1m_2 + m_1n_2^2)(\Delta - \delta + 1)\sqrt{2},$$

where Δ and δ denote the maximum degree and minimum degree of $G_1[G_2]$. Equality holds if and only if G_1 and G_2 are regular graphs.

Proof. Let $G_1[G_2]$ denote the composition of G_1 and G_2. Then

$$|V(G_1[G_2])| = n_1n_2, |E(G_1[G_2])| = n_1m_2 + m_1n_2^2.$$

For any vertex $(u_i, v_j) \in V(G_1[G_2])$, we have, $\delta = n_2\delta(G_1) + \delta(G_2)$ and $\Delta = n_2\Delta(G_1) + \Delta(G_2)$.

By definition,

$$R_eSO(G) = \sum_{uv\in E(G)} \sqrt{r(u)^2 + r(v)^2}$$

For any adjacent vertices (u_i, v_j) and (u_k, v_ℓ)

$$r(u_i, v_j) = \Delta + 1 - d_{G_1[G_2]}(u_i, v_j)$$

$$r(u_k, v_\ell) = \Delta + 1 - d_{G_1[G_2]}(u_k, v_\ell)$$

Since $d_{G_1[G_2]}(u_i, v_j) \geq \delta$ and $d_{G_1[G_2]}(u_k, v_\ell) \geq \delta$, we obtain

$$r(u_i, v_j) = \Delta + 1 - d_{G_1[G_2]}(u_i, v_j) \leq \Delta + 1 - \delta \text{ and}$$

$$r(u_k, v_\ell) = \Delta + 1 - d_{G_1[G_2]}(u_k, v_\ell) \leq \Delta + 1 - \delta$$

Therefore,

$$R_eSO(G_1[G_2]) \leq \sum_{((u_i,v_j),(u_k,v_\ell))\in E(G_1[G_2])} (\Delta + 1 - \delta)\sqrt{2}$$

$$\leq (n_1m_2 + m_1n_2^2)(\Delta + 1 - \delta)\sqrt{2}.$$

Equality satisfies if and only if $d_{G_1[G_2]}(u_i, v_j) = \delta = \Delta$ for all $(u_i, v_j) \in V(G_1[G_2])$,

since $d_{G_1[G_2]}(u_i, v_j) = n_2d_{G_1}(u_i) + d_{G_2}(v_j)$. This occurs only when both G_1 and G_2 are regular graphs.

6. Properties of the Reverse Sombor Coindex

In the present section, we determine the reverse Sombor coindex for several standard graphs and derive several bounds in terms of graph parameters and other topological indices. Let G be a simple connected graph, with $|V(G)| > 2$ and maximum degree $\Delta \geq 2$.

Proposition 6.1 For a path P_n, where $n \geq 3$

$$\overline{R_eSO}(P_n) = (2n-6)\sqrt{5} + \frac{1}{\sqrt{2}}(n^2 - 7n + 16).$$

Proposition 6.2 For C_n, where $n \geq 3$,

$$\overline{R_eSO}(C_n) = \frac{n(n-3)}{\sqrt{2}}.$$

Proposition 6.3 For a star graph $K_{1,n-1}$, where $n \geq 3$,

$$\overline{R_eSO}(K_{1,n-1}) = \frac{(n-2)(n-1)^2}{\sqrt{2}}.$$

Proposition 6.4 For W_n, a wheel graph, where $n \geq 5$,

$$\overline{R_eSO}(W_n) = \frac{(n-1)(n-3)(n-4)}{\sqrt{2}}.$$

Proposition 6.5 For a complete bipartite graph $K_{m,n}$, where $m \geq n$

$$\overline{R_eSO}(K_{m,n}) = \frac{mn}{\sqrt{2}}[\mathrm{n}(m-1) + m(n-1)]$$

Theorem 6.6 For a regular graph G,

$$\overline{R_eSO}(G) = \overline{m}\sqrt{2}$$

Proof. Suppose that G is regular with $d(u) = \Delta = r$. Then, by definition,

$$\overline{R_eSO}(G) = \sum_{uv \notin E(G)} \sqrt{[\Delta + 1 - d(u)]^2 + [\Delta + 1 - d(v)]^2}$$

$$= \sum_{uv \notin E(G)} \sqrt{(r + 1 - r)^2 + (r + 1 - r)^2} = \overline{m}\sqrt{2}.$$

Theorem 6.7 For a non-regular graph G,

$\overline{m}\sqrt{2} < \overline{R_eSO}(G) < \overline{m}\Delta\sqrt{2}$, where $\overline{m} = \binom{n}{2} - m$ and Δ is the maximum degree of G.

Proof. Let us consider a non-regular graph G with $\Delta \geq 1$ and $d(u) \geq 1$.

For each $u \in V(G)$, $r(u) = \Delta + 1 - d(u) \geq 1$.

Also, for $d(u) \geq 1$, $r(u) = \Delta + 1 - d(u) \leq \Delta$. Thus,

$$\overline{R_eSO}(G) = \sum_{uv \notin E(G)} \sqrt{r(u)^2 + r(v)^2}$$

$$\geq \overline{m}\sqrt{1^2 + 1^2} = \overline{m}\sqrt{2}$$

For the upper bound, we have

$$\overline{R_eSO}(G) = \sum_{uv\notin E(G)} \sqrt{r(u)^2 + r(v)^2}$$

$$< \overline{m}\sqrt{\Delta^2 + \Delta^2} = \overline{m}\Delta\sqrt{2}.$$

Since G is non-regular, neither $c(u) = 1$ nor $c(u) = \Delta$ holds for all vertices u.

Hence, both inequalities are strict. Therefore,

$$\overline{m}\sqrt{2} < \overline{R_eSO}(G) < \overline{m}\Delta\sqrt{2}$$

Theorem 6.8 For any graph G on n vertices,

$$\overline{R_eSO}(G) \leq \sqrt{\overline{m}[2\overline{m}(\Delta+1)^2 - 2(\Delta+1)\overline{M_1}(G) + \overline{F}(G)]}.$$

Proof. Applying the Cauchy-Schwarz inequality, we have

$$\left[\sum_{uv\notin E(G)} \sqrt{r(u)^2 + r(v)^2}\right]^2 \leq \left(\sum_{uv\notin E(G)} 1\right)\left(\sum_{uv\notin E(G)} [r(u)^2 + r(v)^2]\right)$$

$$\left[\overline{R_eSO}(G)\right]^2 \leq \overline{m} \times \sum_{uv\notin E(G)} [r(u)^2 + r(v)^2]$$

Consider,

$$r(u)^2 + r(v)^2 = [\Delta + 1 - d(u)]^2 + [\Delta + 1 - d(v)]^2$$

$$= (\Delta+1)^2 + d(u)^2 - 2(\Delta+1)d(u) + (\Delta+1)^2 + d(v)^2 - 2(\Delta+1)d(v)$$

$$= 2(\Delta+1)^2 - 2(\Delta+1)[d(u) + d(v)] + [d(u)^2 + d(v)^2]$$

Therefore, $\sum_{uv\notin E(G)} [c(u)^2 + c(v)^2] = 2(\Delta+1)^2 \sum_{uv\notin E(G)} 1 - 2(\Delta+1)\sum_{uv\notin E(G)} [d(u) + d(v)]$

$$+ \sum_{uv\notin E(G)} [d(u)^2 + d(v)^2]$$

$$= \overline{m}2(\Delta+1)^2 - 2(\Delta+1)\overline{M_1}(G) + \overline{F}(G)$$

$$\overline{R_eSO}(G) \leq \sqrt{\overline{m}[2\overline{m}(\Delta+1)^2 - 2(\Delta+1)\overline{M_1}(G) + \overline{F}(G)]}$$

7. Bounds for the graph operations on $\overline{R_eSO}(G)$

In the present section, we derive bounds for the reverse Sombor coindex under certain graph operations, using degree-based properties. In particular, we consider the cartesian and composition products of graphs.

Lower bounds on the reverse Sombor coindex

Theorem 7.1 Let n_1, n_2 be the vertices and m_1, m_2 be the edges of G_1 and G_2 respectively, then

$\overline{R_eSO}(G_1 \square G_2) \geq \overline{m}\sqrt{2}$, Equality attains if and only if G_1 and G_2 are regular.

Proof. Let the Cartesian product of G_1 and G_2 be $G_1 \square G_2$. Then

$$|V(G_1 \square G_2)| = n_1 n_2, |E(G_1 \square G_2)| = n_1 m_2 + m_1 n_2 \text{ and } \overline{m} = \binom{n_1 n_2}{2} - (n_1 m_2 + m_1 n_2).$$

For any vertex $(u_i, v_j) \in V(G_1 \square G_2)$, we have $\Delta = \Delta(G_1) + \Delta(G_2)$.

By definition,

$$\overline{R_eSO}(G) = \sum_{uv \notin E(G)} \sqrt{r(u)^2 + r(v)^2}$$

For all $(u_i, v_j), (u_k, v_\ell) \in V(G_1 \square G_2)$

$$r(u_i, v_j) = \Delta + 1 - d_{G_1 \square G_2}(u_i, v_j) \text{ and}$$

$$r(u_k, v_\ell) = \Delta + 1 - d_{G_1 \square G_2}(u_k, v_\ell)$$

Since $d_{G_1 \square G_2}(u_i, v_j) \leq \Delta$ and $d_{G_1 \square G_2}(u_k, v_\ell) \leq \Delta$

$$r(u_i, v_j) = \Delta + 1 - d_{G_1 \square G_2}(u_i, v_j) \geq 1 \text{ and}$$

$$r(u_k, v_\ell) = \Delta + 1 - d_{G_1 \square G_2}(u_k, v_\ell) \geq 1$$

Hence,

$$\overline{R_eSO}(G_1 \square G_2) \geq \sum_{((u_i, v_j), (u_k, v_\ell)) \notin E(G_1 \square G_2)} \sqrt{1^2 + 1^2}$$

Therefore,

$$\overline{R_eSO}(G_1 \square G_2) \geq \overline{m}\sqrt{2}$$

If $d_{G_1 \square G_2}(u_i, v_j) = \delta = \Delta$ for all $(u_i, v_j) \in V(G_1 \square G_2)$,

then the equality condition is satisfied whenever both G_1 and G_2 are regular graphs.

Theorem 7.2 Let G_1 and G_2 be graphs having n_1 and n_2 vertices, m_1 and m_2 edges respectively, then

$$\overline{R_eSO}(G_1[G_2]) \geq \overline{m}\sqrt{2}.$$

Equality condition holds if and only if G_1 and G_2 are regular graphs.

Proof. Let the composition of G_1 and G_2 be $G_1[G_2]$. Then

$$|V(G_1[G_2])| = n_1 n_2, |E(G_1[G_2])| = n_1 m_2 + m_1 n_2^2 \text{ and } \overline{m} = \binom{n_1 n_2}{2} - (n_1 m_2 + m_1 n_2^2).$$

For any vertex $(u_i, v_j) \in V(G_1[G_2])$, we have, $\delta = n_2 \delta_1 + \delta_2$ and $\Delta = n_2 \Delta_1 + \Delta_2$.

By definition,

$$\overline{R_eSO}(G) = \sum_{uv \notin E(G)} \sqrt{r(u)^2 + r(v)^2}$$

Also, we have

$$r(u_i, v_j) = \Delta + 1 - d_{G_1[G_2]}(u_i, v_j) \text{ and}$$

$$r(u_k, v_\ell) = \Delta + 1 - d_{G_1[G_2]}(u_k, v_\ell)$$

Since $d_{G_1[G_2]}(u_i, v_j) \leq \Delta$ and $d_{G_1[G_2]}(u_k, v_\ell) \leq \Delta$, we obtain

$$r(u_i, v_j) = \Delta + 1 - d_{G_1[G_2]}(u_i, v_j) \geq 1 \text{ and}$$

$$r(u_k, v_\ell) = \Delta + 1 - d_{G_1[G_2]}(u_k, v_\ell) \geq 1$$

Therefore,

$$\overline{R_eSO}(G_1[G_2]) \geq \sum_{((u_i,v_j),(u_k,v_\ell))\notin E(G_1[G_2])} \sqrt{1^2 + 1^2}$$

Hence,

$$\overline{R_eSO}(G_1[G_2]) \geq \overline{m}\sqrt{2}$$

The equality condition is satisfied if and only if $d_{G_1\square G_2}(u_i, v_j) = \delta = \Delta$ for all $(u_i, v_j) \in V(G_1[G_2])$.

This condition is satisfied only if both G_1 and G_2 are regular graphs.

Upper bounds on the reverse Sombor coindex

Theorem 7.3 For any two graphs G_1 and G_2,

$$\overline{R_eSO}(G_1\square G_2) \leq \overline{m}\sqrt{2}(\Delta - \delta + 1),$$

Proof. Let $G_1\square G_2$ be the Cartesian product of G_1 and G_2. Then

$|V(G_1\square G_2)| = n_1n_2, |E(G_1\square G_2)| = n_1m_2 + m_1n_2$ and $\overline{m} = \binom{n_1n_2}{2} - (n_1m_2 + m_1n_2)$.

For any vertex $(u_i, v_j) \in V(G_1\square G_2)$, we have, $\delta = \delta(G_1) + \delta(G_2)$ and $\Delta = \Delta(G_1) + \Delta(G_2)$.

For any non-adjacent vertices (u_i, v_j) and (u_k, v_ℓ),

$$r(u_i, v_j) = \Delta + 1 - d_{G_1\square G_2}(u_i, v_j) \leq \Delta - \delta + 1 \text{ and}$$

$$r(u_k, v_\ell) = \Delta + 1 - d_{G_1\square G_2}(u_k, v_\ell) \leq \Delta - \delta + 1$$

Thus,

$$\overline{R_eSO}(G_1\square G_2) \leq \sum_{\left((u_i,v_j),(u_k,v_\ell)\right)\notin E(G_1\square G_2)} (\Delta + 1 - \delta)\sqrt{2}$$

$$\leq \overline{m}\sqrt{2}(\Delta - \delta + 1).$$

Equality is satisfied if and only if G_1 and G_2 are regular.

Theorem 7.4 For any two graphs G_1 and G_2,

$$\overline{R_eSO}(G_1[G_2]) \leq (\Delta - n_2\delta_1 - \delta_2 + 1)\overline{m}\sqrt{2}$$

where Δ denotes the maximum degree of $G_1[G_2]$ and δ_1, δ_2 denote minimum degrees of G_1 and G_2 respectively. Equality holds if the graphs are regular.

Proof. The composition $G_1[G_2]$ of G_1 and G_2 having

$$|V(G_1[G_2])| = n_1n_2 \text{ and } |E(G_1[G_2])| = n_1m_2 + m_1n_2^2.$$

For any vertex $(u_i, v_j) \in V(G_1[G_2])$, $\delta(G_1[G_2]) = n_2\delta_1 + \delta_2$ and $\Delta(G_1[G_2]) = n_2\Delta_1 + \Delta_2$.

For any non-adjacent vertices (u_i, v_j) and (u_k, v_ℓ),

$$r(u_i, v_j) = \Delta + 1 - d_{G_1[G_2]}(u_i, v_j) \leq \Delta - (n_2\delta_1 + \delta_2) + 1 \text{ and}$$

$$r(u_k, v_\ell) = \Delta + 1 - d_{G_1[G_2]}(u_k, v_\ell) \leq \Delta - (n_2\delta_1 + \delta_2) + 1$$

Thus,

$$\overline{R_eSO}(G_1[G_2]) \leq \sum_{((u_i,v_j),(u_k,v_\ell))\notin E(G_1[G_2])} (\Delta - (n_2\delta_1 + \delta_2) + 1)\sqrt{2}$$

$$\leq \overline{m}\sqrt{2}(\Delta - n_2\delta_1 - \delta_2 + 1).$$

Equality condition is satisfied if both G_1 and G_2 are regular graphs.

8. Chemical applicability of reverse Sombor index and reverse Sombor coindex of graphs

In recent years, several degree-based descriptors, including Zagreb index, forgotten index, and Sombor index have been successfully employed for predicting physicochemical and electronic properties of molecular graphs.

Motivated by the studies reported in [5] and [16, 18], we examine the chemical applicability of$R_eSO(G)$ and $\overline{R_eSO}$(G) by conducting correlation analysis with π-electron energy (E_π) values of heteroatom-containing molecules reported in [4] and polycyclic aromatic hydrocarbons (PAHs).

8.1 Comparative Analysis of Topological Indices for Molecules Containing Heteroatoms

In this section, we investigate the predictive capabilities of several degree-based topological descriptors for molecular graphs containing heteroatoms. In particular, we compare the reverse Sombor index $R_eSO(G)$, Sombor index $SO(G)$, first Zagreb index $M_1(G)$, and forgotten index $F(G)$ with the π-electron energy (E_π) of the corresponding molecular structures.

The considered molecular dataset consists of twenty-eight heteroatom-containing molecules denoted by H1-H28. The computed values of the considered topological indices together with their corresponding E_π values are presented in Table 2. To examine the chemical applicability of these descriptors, linear regression analysis was performed using the linear model

$$E_\pi = a + bI(G),$$

where E_π denotes the π-electron energy and $I(G)$ represents the corresponding topological descriptor.

For the considered heteroatom-containing molecular graphs, we computed $R_eSO(G)$, $SO(G)$, $M_1(G)$, and $F(G)$. The corresponding regression analyses are illustrated in Figures 1-4.

Table 2: Topological indices and $E_\pi$values of heteroatom-containing molecules

Code	$R_eSO(G)$	$SO(G)$	$M_1(G)$	$F(G)$	E_π
$H1$	4.47	4.47	6	10	2.23
$H2$	5.89	7.3	10	18	5.66
$H3$	5.89	7.3	10	18	5.76
$H4$	9.49	9.49	12	30	6.96
$H5$	5.89	7.3	10	18	6.82
$H6$	7.07	14.1	20	40	5.23
$H7$	8.49	17	24	48	6.69
$H8$	8.49	17	24	48	9.06
$H9$	8.49	17	24	48	9.1
$H10$	8.49	17	24	48	9.07
$H11$	8.49	17	24	48	9.65
$H12$	18.95	21.7	30	68	8.19
$H13$	20.7	26.3	36	88	12.21
$H14$	20.93	26.4	36	88	12.22
$H15$	20.93	26.4	36	88	12.21
$H16$	21.63	24.4	34	76	11

$H17$	27.3	35.6	50	118	14.23
$H18$	27.3	35.6	50	118	14.23
$H19$	29.1	40.2	56	138	16.15
$H20$	29.3	40.4	56	138	16.12
$H21$	27.3	35.6	50	118	13.46
$H22$	27.3	35.6	50	118	13.59
$H23$	38.9	47.1	66	150	20.1
$H24$	38.9	47.1	66	150	21.02
$H25$	37.7	54.3	76	188	20.56
$H26$	37.7	54.3	76	188	21.62
$H27$	40.7	63.2	88	228	24.23
$H28$	34.6	51.3	72	180	19.39

The values of the considered topological indices differ from one molecule to another due to variations in their molecular structures. These differences may influence the corresponding E_π values and indicate the potential applicability of the considered descriptors.

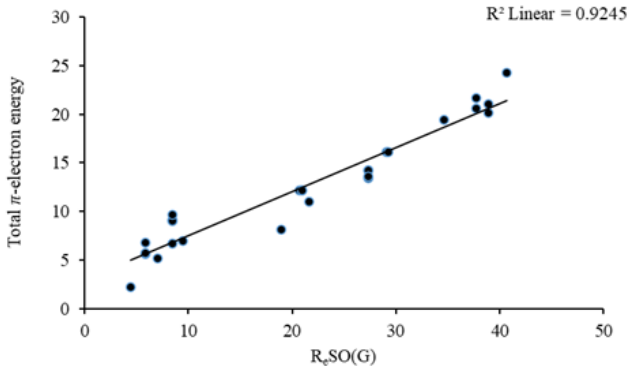

Figure 1: Correlation between $R_eSO(G)$ and E_π of heteroatom-containing molecules.

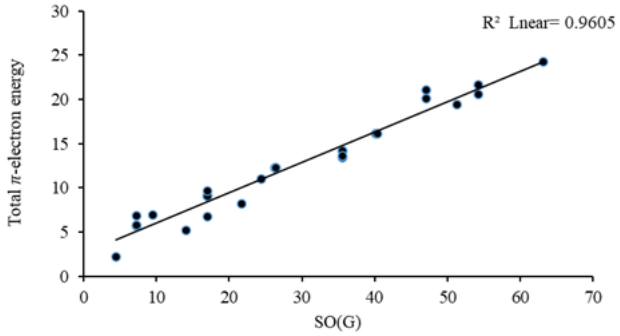

Figure 2: Correlation between $SO(G)$ and E_π of heteroatom-containing molecules.

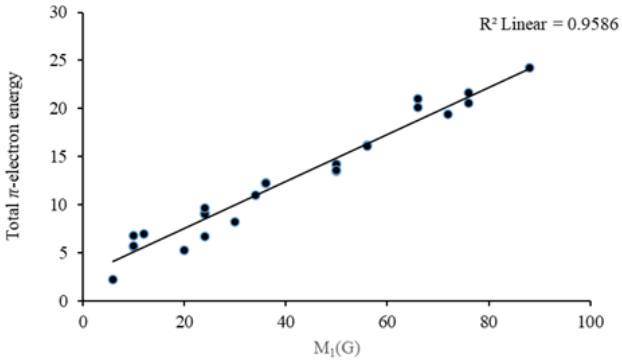

Figure 3: Correlation between $M_1(G)$ and E_π of heteroatom-containing molecules.

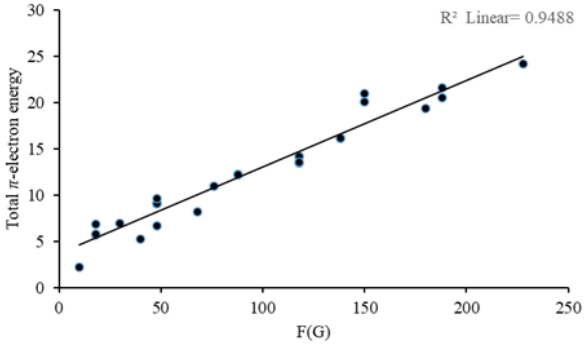

Figure 4: Correlation between $F(G)$ and E_π of heteroatom-containing molecules.

8.2 Comparative Analysis for Polycyclic Aromatic Hydrocarbons (PAHs)

Further correlation analysis was carried out for a dataset consisting of selected polycyclic aromatic hydrocarbons (PAHs). The computed values of $R_eSO(G), SO(G), M_1(G)$, and $F(G)$

together with the corresponding E_π values are presented in Tables 3. The corresponding regression analyses are illustrated in Figures 5-8. The obtained results reveal a strong linear correlation between the considered topological descriptors and E_π values of the considered PAHs.

Table 3: Topological indices and E_π values of selected PAHs

Name	$R_eSO(G)$	$SO(G)$	$M_1(G)$	$F(G)$	E_π
Benzene	8.49	16.97	24	48	8.00
Naphthalene	27.33	35.64	50	118	13.68
Phenanthrene	37.46	54.16	76	188	19.44
Anthracene	37.69	54.3	76	188	19.31
Chrysene	47.59	72.69	102	258	25.19
Benzo[a]anthracene	47.82	72.83	102	258	25.10
Benzo[a]pyrene	52.06	85.55	120	312	28.22
Triphenylene	47.36	72.54	102	258	25.27
Benzo[e]pyrene	51.83	85.41	120	312	28.33
Perylene	51.83	85.41	120	312	28.24
Anthanthrene	56.53	98.42	138	366	31.25
Dibenzo[a,c]anthracene	57.72	91.21	128	328	30.94
Dibenzo[a,h]anthracene	57.95	91.35	128	328	30.88
Dibenzo[a,j]anthracene	57.95	91.35	128	328	30.88
Picene	57.72	91.21	128	328	30.94
Dibenzo[a,h]pyrene	62.19	104.1	146	382	33.95
Pyrene	42.93	67.03	94	242	22.50
Coronene	60.77	111.1	156	420	34.57
Fluoranthene	41.7	66.89	94	242	22.50
Pentacene	58.4	91.63	128	328	30.54
Azulene	27.33	35.64	50	118	13.36

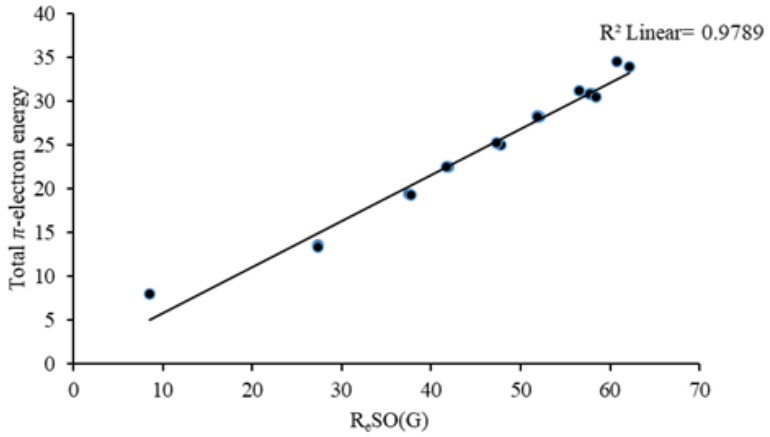

Figure 5: Correlation between $R_eSO(G)$ and E_π of selected PAHs.

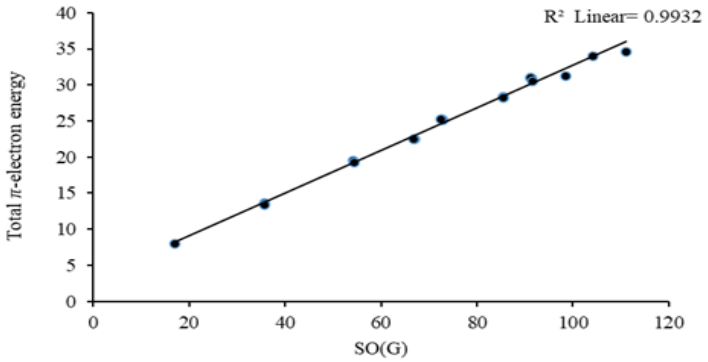

Figure 6: Correlation between $SO(G)$ and E_π of selected PAHs.

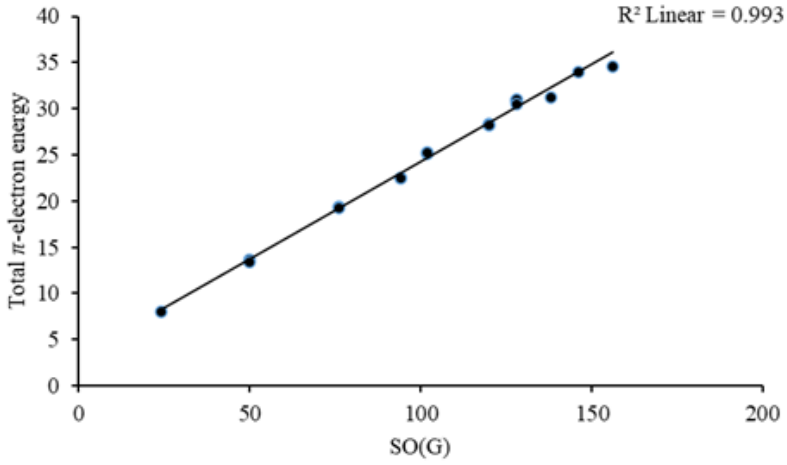

Figure 7: Correlation between $M_1(G)$ and E_π of selected PAHs.

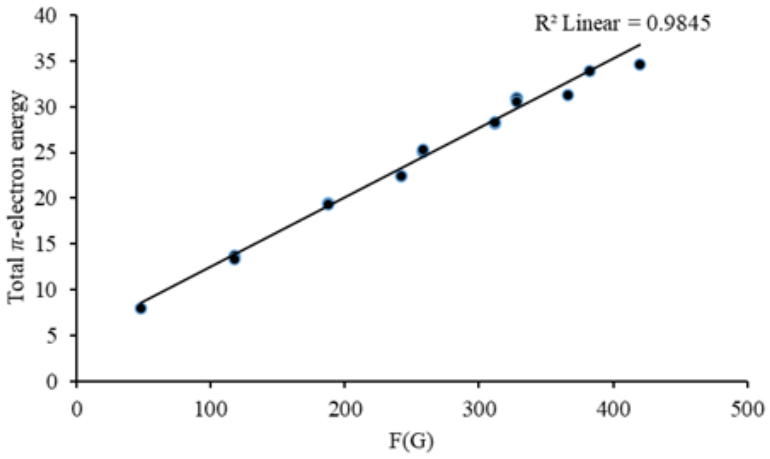

Figure 8: Correlation between $F(G)$ E_π of selected PAHs.

8.3 Comparative Analysis of the Reverse Sombor Coindex and Other Degree-Based Topological Coindices

Further, the topological coindices such as $\overline{R_eSO}(G)$, $\overline{SO}(G)$, $\overline{M_1}(G)$, and $\overline{F}(G)$ were computed for the same molecular datasets. The obtained values for heteroatom-containing molecular graphs together with the corresponding total π-electron energy values are listed in Table 4. The corresponding regression analyses are illustrated in Figures 9-12. The graphical analysis demonstrates that the reverse Sombor coindex also exhibits a strong positive linear correlation with E_π values.

Table 4: Topological coindices and $E_\pi$values of heteroatom-containing molecules

Code	$\overline{R_eSO}(G)$	$\overline{SO}(G)$	$\overline{M_1}(G)$	$\overline{F}(G)$	E_π
$H1$	2.83	1.41	2	2	2.23
$H2$	7.3	5.89	8	12	5.66
$H3$	7.3	5.89	8	12	5.76
$H4$	12.7	4.24	6	8	6.96
$H5$	7.3	5.89	8	12	6.82
$H6$	7.07	14.1	20	40	5.23
$H7$	12.7	25.5	36	72	6.69

$H8$	12.7	25.5	36	72	9.06
$H9$	12.7	25.5	36	72	9.1
$H10$	12.7	25.5	36	72	9.07
$H11$	12.7	25.5	36	72	9.65
$H12$	41.7	39	54	112	8.19
$H13$	61.3	55.7	76	164	12.21
$H14$	61.1	55.6	76	164	12.22
$H15$	61.1	55.6	76	164	12.21
$H16$	59	56.3	78	162	11
$H17$	89.1	105	148	332	14.23
$H18$	89.1	105	148	332	14.23
$H19$	116	133	184	422	16.15
$H20$	116	133	184	422	16.12
$H21$	89.1	105	148	332	13.46
$H22$	89.1	105	148	332	13.59
$H23$	203	230	324	708	20.1
$H24$	203	230	324	708	21.02
$H25$	188	243	340	800	20.56
$H26$	188	243	340	800	21.62
$H27$	267	328	452	1092	24.23
$H28$	156	206	288	684	19.39

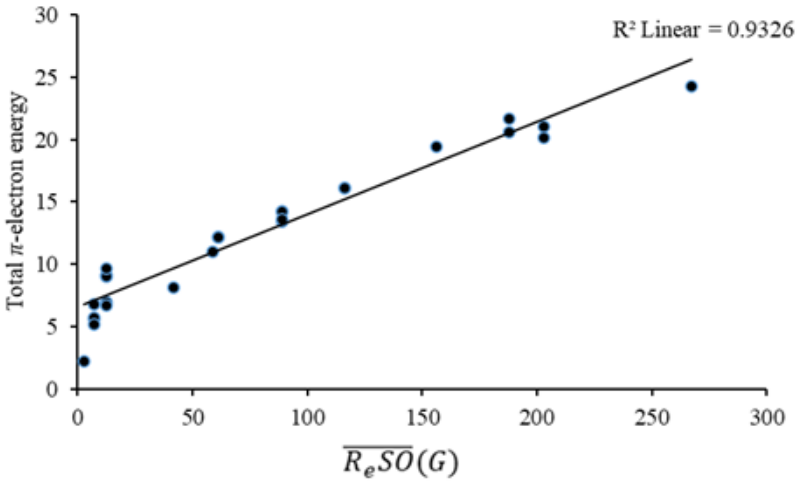

Figure 9: Correlation between $\overline{R_eSO}(G)$ and E_π of heteroatom-containing molecules.

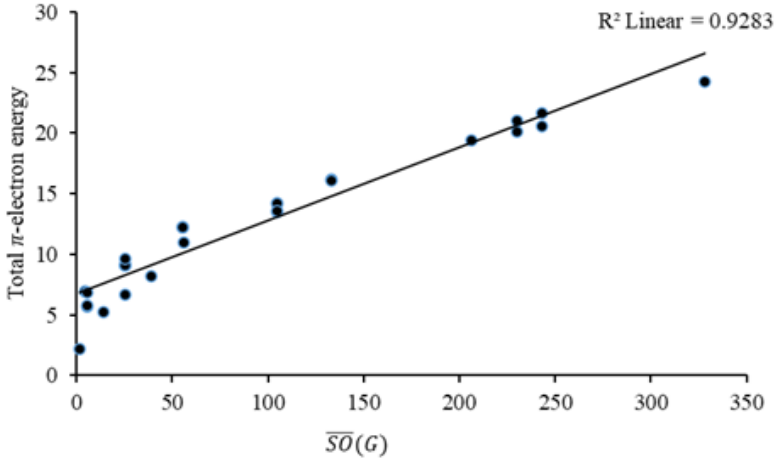

Figure 10: Correlation between $\overline{SO}(G)$ and E_π of heteroatom-containing molecules.

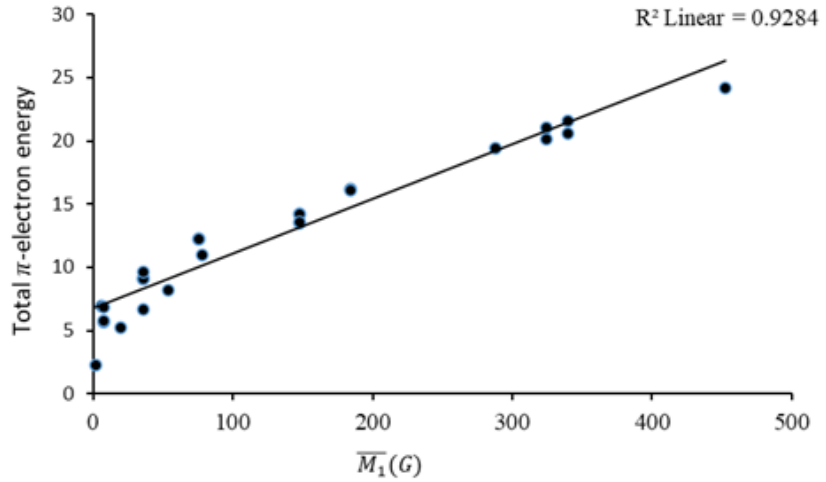

Figure 11: Correlation between $\overline{M_1}(G)$ E_π of heteroatom-containing molecules.

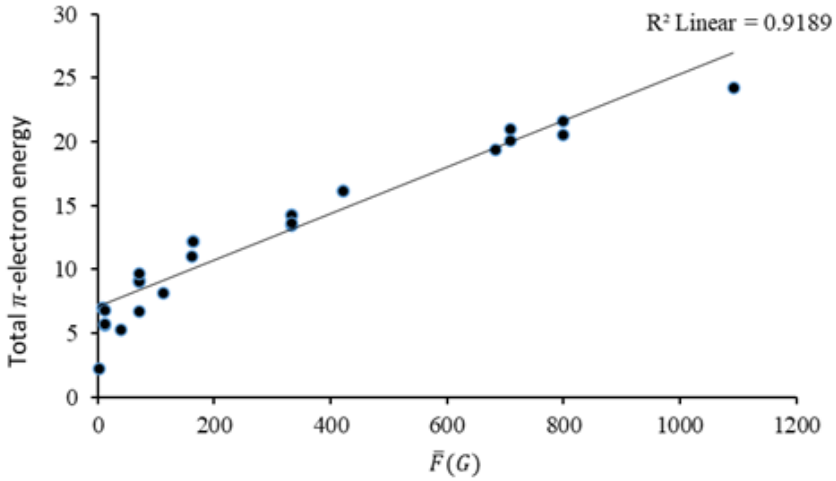

Figure 12: Correlation between $\overline{F}(G)$ and E_π of heteroatom-containing molecules.

Similarly, the reverse Sombor coindex and other coindices were computed for the selected PAHs. The obtained values together with the corresponding π-electron energy values are summarized in Tables 5. The corresponding regression analyses are illustrated in Figures 13-16. The obtained results indicate that the reverse Sombor coindex maintains a very strong linear relationship with E_π values of PAHs.

Table 5: Topological coindices and E_π values of selected PAHs

Name	$\overline{R_eSO}(G)$	$\overline{SO}(G)$	$\overline{M_1}(G)$	$\overline{F}(G)$	E_π
Benzene	12.73	25.46	36	72	8.00
Naphthalene	89.06	105.5	148	332	13.68
Phenanthrene	187.7	242.8	340	800	19.44
Anthracene	187.5	242.7	340	800	19.31
Chrysene	321.3	437.2	612	1476	25.19
Benzo[a]anthracene	321.1	437.1	612	1476	25.10
Benzo[e]pyrene	389.1	566.2	792	1968	28.22
Triphenylene	321.5	437.4	612	1476	25.27
Benzo[a]pyrene	388.9	566.1	792	1968	28.33
Perylene	389.1	566.2	792	1968	28.24
Anthanthrene	462.1	711.8	996	2532	31.25
Dibenzo[a,c]anthracene	489.7	688.8	964	2360	30.94
Dibenzo[a,h]anthracene	489.5	688.8	964	2360	30.88
Dibenzo[a,j]anthracene	489.5	688.7	964	2360	30.88
Picene	489.7	688.8	964	2360	30.94
Dibenzo[a,h]pyrene	571.9	849	1188	2976	33.95
Pyrene	240.7	340.2	476	1168	22.50
Coronene	541.2	874.7	1224	3168	34.57
Fluoranthene	241.0	340.4	476	1168	22.50
Pentacene	489.0	688.4	964	2360	30.54
Azulene	89.06	105.5	148	332	13.36

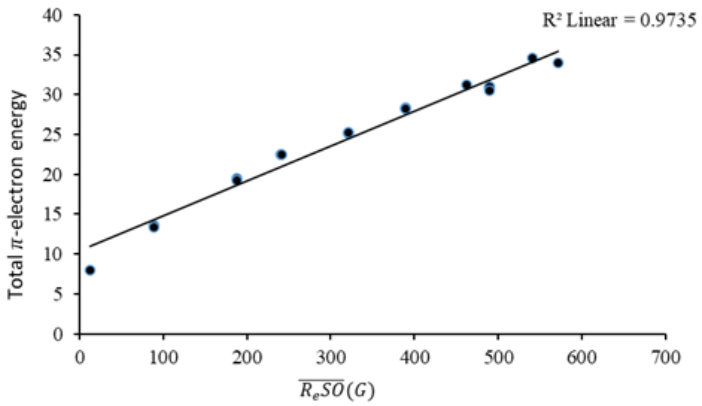

Figure 13: Correlation analysis of $\overline{R_eSO}(G)$ with E_π of selected PAHs.

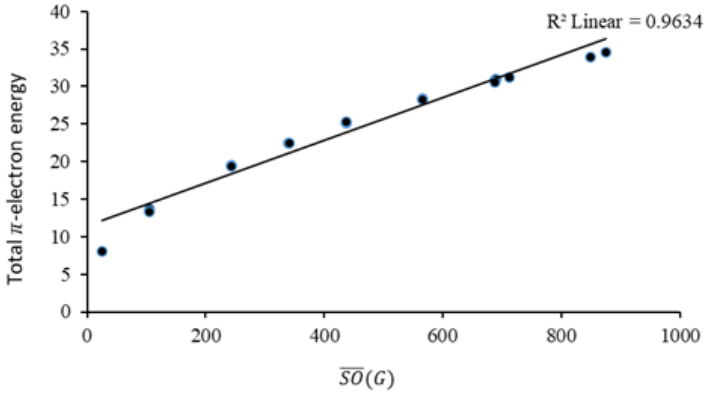

Figure 14: Correlation analysis of $\overline{SO}(G)$ with E_π of selected PAHs.

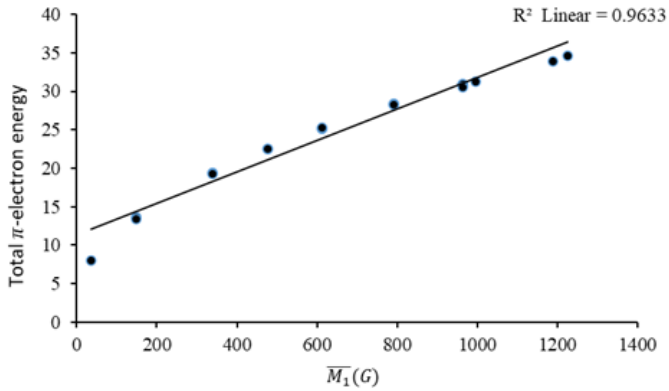

Figure 15: Correlation analysis of $\overline{M_1}(G)$ with E_π of selected PAHs.

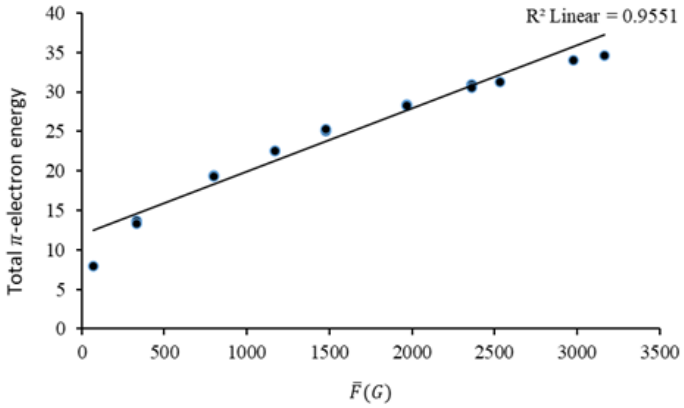

Figure 16: Correlation analysis of $\overline{F}(G)$ with E_π of selected PAHs.

8.4 Correlation Analysis

The correlation coefficients obtained between the considered topological descriptors and E_π for heteroatom-containing molecules and polycyclic aromatic hydrocarbons (PAHs) are presented in Tables 6 and Table 7, respectively. A comparative summary of the correlation coefficients is given in Table 8.

Table 6: Correlation coefficients of topological indices and coindices for heteroatom-containing molecules

Topological Index/coindex	R	R^2
$M_1(G)$	0.9412	0.8858
$F(G)$	0.9564	0.9147
$SO(G)$	0.9681	0.9372
$R_eSO(G)$	0.9783	0.9571
$\overline{M_1}(G)$	0.9726	0.9460
$\overline{F}(G)$	0.9814	0.9631
$\overline{SO}(G)$	0.9873	0.9748
$\overline{R_eSO}(G)$	0.9921	0.9843

Table 7: Correlation coefficients of topological indices and coindices for selected PAHs

Topological Index/coindex	R	R^2
$M_1(G)$	0.9348	0.8739
$F(G)$	0.9517	0.9057
$SO(G)$	0.9668	0.9347
$R_eSO(G)$	0.9754	0.9514
$\overline{M_1}(G)$	0.9792	0.9588
$\overline{F}(G)$	0.9845	0.9692
$\overline{SO}(G)$	0.9879	0.9760
$\overline{R_eSO}(G)$	0.9896	0.9793

Table 8: Comparison of correlation coefficients (R) between selected topological descriptors and total π-electron energy for heteroatom-containing molecules and polycyclic aromatic hydrocarbons (PAHs).

Topological Index/coindex	Heteroatom Molecules (R)	PAHs (R)
$M_1(G)$	0.9412	0.9348
$F(G)$	0.9564	0.9517
$SO(G)$	0.9681	0.9668
$ReSO(G)$	0.9783	0.9754
$\overline{M_1}(G)$	0.9726	0.9792
$\overline{F}(G)$	0.9814	0.9845
$\overline{SO}(G)$	0.9873	0.9879
$\overline{ReSO}(G)$	0.9921	0.9896

The obtained results indicate that all the considered degree-based descriptors exhibit positive correlation analysis with E_π values. However, the reverse Sombor index and reverse Sombor coindex show significantly stronger correlations than the classical Zagreb and forgotten indices.

Table 8 provides a direct comparison of the correlation coefficients for all the considered descriptors. In particular, for heteroatom-containing molecular graphs, the reverse Sombor coindex

yields the highest correlation coefficient, $R = 0.9921$, demonstrating excellent predictive capability. Similarly, for polycyclic aromatic hydrocarbons, the reverse Sombor coindex attains a correlation coefficient of $R = 0.9896$, which is higher than the corresponding values obtained for the Zagreb and forgotten indices.

Furthermore, the reverse Sombor index also exhibits strong correlations with the total π-electron energy, with $R = 0.9783$ for heteroatom-containing molecules and $R = 0.9754$ for PAHs. These results suggest that both the reverse Sombor index and reverse Sombor coindex are highly effective molecular descriptors for estimating total π-electron energy.

Hence, the reverse Sombor index and reverse Sombor coindex may serve as efficient molecular descriptors in QSPR modeling and chemical graph theory.

9. Conclusion

In this present paper, we proposed the reverse Sombor coindex, a new reverse degree-based topological descriptor, and investigated its mathematical and chemical properties. Exact expressions for the reverse Sombor index and reverse Sombor coindex were examined for few standard graphs, including paths, C_n, K_n, $K_{1,n-1}$, W_n, and $K_{m,n}$ graphs. Furthermore, extremal properties for trees and several upper and lower bounds involving graph parameters, $M_1(G)$, and the $F(G)$ were established. Bounds for these descriptors under Cartesian products and composition of graphs were also obtained.

To evaluate their chemical applicability, correlation analyses were performed using datasets of heteroatom-containing molecules and polycyclic aromatic hydrocarbons (PAHs). The obtained results demonstrate that both the reverse Sombor index and reverse Sombor coindex exhibit strong positive linear correlations with total π-electron energy. In particular, the reverse Sombor coindex showed the best predictive performance among all considered descriptors, yielding correlation coefficients of (R=0.9921) for heteroatom-containing molecules and (R=0.9896) for PAHs. These values are higher than those obtained for the classical Zagreb, forgotten, and Sombor descriptors and their corresponding coindices.

Therefore, the reverse Sombor coindex can be regarded as a highly effective molecular descriptor for estimating electronic properties of conjugated molecular systems. The results presented in this work contribute to the theory of reverse degree-based topological descriptors and indicate that the reverse Sombor coindex may serve as a useful tool in chemical graph theory, QSPR/QSAR modeling, molecular property prediction, and further studies involving graph operations and extremal graph problems.

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[1]**NAGENDRAPPA G:** RESEARCH SCHOLAR, SRI SIDDHARTHA ACADEMY OF HIGHER EDUCATION, TUMAKURU-572107, DEPARTMENT OF MATHEMATICS, GOVERNMENT FIRST GRADE COLLEGE, KORATAGERE-572129, KARNATAKA, INDIA (Corresponding; E-mail:nagendragmat@gmail.com).

[2]**VENKANAGOUDA M GOUDAR:** DEPARTMENT OF MATHEMATICS, SRI SIDDHARTHA INSTITUTE OF TECHNOLOGY, A CONSTITUENT COLLEGE OF SRI SIDDHARTHA ACADEMY OF HIGHER EDUCATION, TUMAKURU-572105, KARNATAKA, India, E-mail: vmgouda@gmail.com

[3]**MANOHAR R GOMBI:** DEPARTMENT OF MATHEMATICS, SRI SIDDHARTHA INSTITUTE OF TECHNOLOGY, A CONSTITUENT COLLEGE OF SRI SIDDHARTHA ACADEMY OF HIGHER EDUCATION, TUMKUR-572105, KARNATAKA, INDIA, E-mail: gombimanoj50gmail.com

[4]**RAJATHAGIRI D T**: RESEARCH SCHOLAR, SRI SIDDHARTHA ACADEMY OF HIGHER EDUCATION, TUMAKURU-572107, KARNATAKA STATE, INDIA. DEPARTMENT OF MATHEMATICS, GOVERNMENT FIRST GRADE COLLEGE, TUMAKURU, KARNATAKA STATE, INDIA-572102.Email:rajathagiridt75@gmail.com