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Reverse Sombor Energy of a Graph

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Abstract: The reverse Sombor index is a natural variation of the recently introduced Sombor index, a degree-based topological index found to have nice mathematical properties and very useful applications. In this article, the associated matrix of the reverse Sombor index of a graph G, called the reverse Sombor matrix $\mathcal{R}(G)$, is introduced. Also, some mathematical properties of this matrix and bounds on its eigenvalues are presented and established. The reverse Sombor energy $\mathcal{ER}(G)$ of G, the sum of the absolute values of the eigenvalues of $\mathcal{R}(G)$, is introduced, and certain bounds are established. The chemical applicability of this parameter is discussed by comparing it with the π-electron energy of some polyaromatic hydrocarbons. Further, a computational analysis of the relation between the energy and reverse Sombor energy of trees of order $n = 8,9,\cdots,14$ is presented.

Keywords: topological indices; graph energy; Sombor index; reverse Sombor index; reverse Sombor energy.

1. Introduction

A topological index/molecular descriptor is a graph invariant, which is very useful in understanding the physical, chemical, and structural properties of chemical/molecular graphs. Various topological indices are found in literature and are mainly categorized based on the degree and distance in graphs. Very commonly, vertex-degree-based(VDB) topological indices in the form

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

have been studied, Zagreb index [1], Randi$c$ index [2], and harmonic index [3] being some of them.

One of the recently introduced VDB indices, named the Sombor index [4], has found a central place in literature, owing to some of its interesting mathematical properties and its applicability to studying the chemical properties of molecular graphs. Different variations of the Sombor index have since been proposed and studied [5-17].

As introduced by Gutman [18], a graph G's energy is equal to the total of the absolute values of $A(G)$, and is denoted $E(G)$. It is worth noting that eigenvalues play a crucial role in the fundamental understanding of graphs since they are intimately linked to nearly every significant graph invariant, establishing a connection with each extreme property. Thus, graph energy, though a particular form of matrix norm, has drawn the interest of both pure and applied mathematicians. Spectral graph theory studies matrices associated with graphs, eigenvalues,

and graph energies and plays an essential role in analyzing graph matrices using matrix theory and linear algebra.

Different graph energies associated with topological indices have been introduced and extensively studied in the literature. For related work and applications of graph energy, we cite [19-25]. In particular, the Sombor energy $ESO(G)$ [26], based on the Sombor index of a graph G, is defined as the sum of the absolute values of the eigenvalues of the Sombor matrix.

In [17], Swamy *et al*. have introduced a variation of the Sombor index, namely the reverse Sombor index of G, denoted $RSO(G)$, and have studied some of its mathematical properties.

In this article, we introduce the reverse Sombor matrix of a graph G, and based on its eigenvalues, we define the reverse Sombor energy $\mathcal{ER}(G)$ of G. Further, we establish some bounds on $\mathcal{ER}(G)$for other graph invariants. Further, we study the correlation of the reverse Sombor energy of some molecules containing hetero atoms with the respective π-electron energy. Also, we make a computational analysis of the relation between the energy and reverse Sombor energy of trees of specific order and present respective regularities.

2. Materials and Methods

Based on the dataset of all trees with n unlabeled nodes available in [27], the computational analysis on the relation between the energy and reverse Sombor energy of all trees of order $n = 8,9,\cdots,14$ is made using Microsoft Excel. In particular, the correlation analysis between the π-electron energy and the reverse Sombor energy is made. Also, the correlation between the graph energy and the reverse Sombor energy is computed, and the corresponding analysis is made.

3. Preliminaries

We consider simple finite undirected graphs in this article. Given a graph G with vertex set $V(G)$ and edge set $E(G)$, two vertices $u, v \in V(G)$ are said to be adjacent if they share a common edge. The degree of a vertex $u \in V(G)$, denoted $deg(u)$, or simply $d(u)$, is the number of vertices adjacent with u in G. A vertex u with degree zero is called an isolated vertex, and that of degree one is called a pendant vertex. The maximum degree of any vertex in G is denoted by $\Delta(G)$.

The Sombor index [4] of a graph G is defined as

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

The adjacency matrix of a graph G with $V(G) = \{v_1, v_2, \cdots, v_n\}$ is defined as $A(G) = (a_{ij})$ where, $a_{ij} = \begin{cases} 1 \; if \;\; v_i v_j \in E(G) \\ 0 \quad \text{otherwise} \end{cases}$.

The reverse Sombor index of G [17] is defined as

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

where $c(u) = \Delta(G) - d(u) + 1$ is called the reverse vertex degree of u [29, 30].

The Sombor matrix [26] of a graph G with $V(G) = \{v_1, v_2, \cdots, v_n\}$ is defined as $A_{SO}(G) = ((a_{SO})_{ij})$ where,

$$(a_{SO})_{ij} = \begin{cases} \sqrt{d(v_i)^2 + d(v_j)^2} \; if \;\; v_i v_j \in E(G) \\ 0 \qquad\qquad\qquad\quad \text{otherwise} \end{cases}.$$

The total of the absolute values of the eigenvalues of $A_{SO}(G)$ is the Sombor energy of G. .

4. Reverse the Sombor energy of a graph.

Definition 4.1 The reverse Sombor matrix of a graph G with $V(G) = \{v_1, v_2, \cdots, v_n\}$ is defined as $\mathcal{R}(G) = (r_{ij})$ where, $r_{ij} = \begin{cases} \sqrt{c(v_i)^2 + c(v_j)^2} & \text{if } v_i v_j \in E(G) \\ 0 & \text{otherwise} \end{cases}$.

The reverse Sombor polynomial of G is defined as $\mathcal{P}(G)(\lambda) = |\lambda I - \mathcal{R}(G)|$with I being the identity matrix of order $n \times n$. It is to be observed that the eigenvalues of $\mathcal{R}(G)$ are all real as it is symmetric. If $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of $\mathcal{R}(G)$, then the reverse Sombor energy of G is defined as $\mathcal{ER}(G) = \sum_{i=1}^{n} |\lambda_i|$.

Observation 4.2 For the complete graph K_n, $spec(\mathcal{R}(K_n)) = \begin{pmatrix} -\sqrt{2} & (n-1)\sqrt{2} \\ (n-1) & 1 \end{pmatrix}$.

Observation 4.3 For the totally disconnected graph $\overline{K_n}$, $spec(\mathcal{R}(\overline{K_n})) = \begin{pmatrix} 0 \\ n \end{pmatrix}$.

Observation 4.4 For the graph $G = \frac{n}{2}K_2$, $spec(\mathcal{R}(G)) = \begin{pmatrix} -\sqrt{2} & \sqrt{2} \\ n/2 & n/2 \end{pmatrix}$.

Lemma 4.5 [29] If A and B are square matrices of order n, then

$$\sum_{1 \leq i \leq n} \lambda_i(A + B) \leq \sum_{1 \leq i \leq n} \lambda_i(A) + \sum_{1 \leq i \leq n} \lambda_i(B)$$

where $\lambda_i(M_j)$ corresponds to the i^{th} eigenvalue of $M_j, j = 1,2$ with $\lambda_i \geq \lambda_{i+1}$.

Theorem 4.6 For a path P_n of order $n \geq 4$,

$$\mathcal{ER}(P_n) \leq \sqrt{2}\left(2\csc\left(\frac{\pi}{n+1}\right)\sin\left(\frac{\left(2\lfloor\frac{n}{2}\rfloor + 1\right)\pi}{2(n+1)}\right)\right) + 2\left(2\sqrt{5} - 3\sqrt{2}\right).$$

Proof. It is easy to observe that, for $n \geq 4$,

$$\mathcal{R}(P_n) = \begin{pmatrix} 0 & \sqrt{5} & 0 & 0 & \cdots & 0 \\ \sqrt{5} & 0 & \sqrt{2} & 0 & \cdots & 0 \\ 0 & \sqrt{2} & 0 & \sqrt{2} & \cdots & 0 \\ 0 & 0 & \sqrt{2} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \sqrt{5} \\ 0 & 0 & 0 & 0 & \sqrt{5} & 0 \end{pmatrix}$$

$$= \sqrt{2}\begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} + \left(\sqrt{5} - \sqrt{2}\right)\begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$= \sqrt{2}A(P_n) + B$$

where

$$B = \left(\sqrt{5}-\sqrt{2}\right)\begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

has the spectrum

$$\text{spec}(B) = \begin{pmatrix} -(\sqrt{5}-\sqrt{2}) & 0 & (\sqrt{5}-\sqrt{2}) \\ 2 & (n-4) & 2 \end{pmatrix}$$

so that $E(B) = 4\left(\sqrt{5}-\sqrt{2}\right)$.

Thus, by Lemma 4.5, we have

$$\mathcal{ER}(P_n) \le \sqrt{2}E(P_n) + E(B)$$

$$= \sqrt{2}\left(4\sum_{i=1}^{\lfloor \frac{n}{2} \rfloor} \cos\left(\frac{\pi\ i}{n+1}\right)\right) + 4\left(\sqrt{5}-\sqrt{2}\right)$$

$$= \sqrt{2}\left(2\csc\left(\frac{\pi}{n+1}\right)\sin\left(\frac{\left(2\lfloor \frac{n}{2} \rfloor + 1\right)\pi}{2(n+1)}\right) - 2\right) + 4(\sqrt{5}-\sqrt{2})$$

$$= \sqrt{2}\left(2\csc\left(\frac{\pi}{n+1}\right)\sin\left(\frac{\left(2\lfloor \frac{n}{2} \rfloor + 1\right)\pi}{2(n+1)}\right)\right) + 2\left(2\sqrt{5}-3\sqrt{2}\right)$$

Theorem 4.7 Let $G = (V, E)$ be a graph with

$$\mathcal{P}_{RSO}(G) = \lambda^n + c_1\lambda^{n-1} + \cdots + c_n$$

Being the characteristic polynomial of $\mathcal{R}(G)$. Then

(i) $c_1 = 0$,

(ii) $c_2 = -RF(G)$,

(iii) $c_3 = -2\sum_{\Delta}\prod_{uv\in E(\Delta)}\sqrt{c_u^2 + c_v^2}$ where the summation is taken over all cycles Δ of length 3 in G.

Proof. Since each coefficient $c_i, i = 1,2,\cdots,n$, $(-1)^i c_i$ corresponds to the sum of all the principal minors of $A_{RSO}(G)$ with i rows and i columns, we have the following:

(i) $c_1 = 0$ as all the principal diagonal elements of $\mathcal{R}(G)$ are zero.

(ii) $c_2 = \sum_{1\le i<j\le n}\begin{vmatrix} 0 & r_{ij} \\ r_{ji} & 0 \end{vmatrix} = -\sum_{1\le i<j\le n} r_{ij}^2 = -\sum_{1\le i<j\le n}\left(c(v_i)^2 + c(v_j)^2\right) = -RF(G)$

(iii)

$$c_3 = -\sum_{1\le i<j<k\le n}\begin{vmatrix} 0 & r_{ij} & r_{ik} \\ r_{ji} & 0 & r_{jk} \\ r_{ki} & r_{kj} & 0 \end{vmatrix}$$

$$= -2\sum_{1\le i<j<k\le n} r_{ij}r_{jk}r_{ik} = -2\sum_{\Delta}\prod_{v_iv_j\in E(\Delta)}\sqrt{c(v_i)^2 + c(v_j)^2}.$$

Lemma 4.8 [Newton's identity] Given an $n \times n$ matrix A, the coefficient c_3 in the expansion of $|\lambda I - A| = \lambda^n + c_1\lambda^{n-1} + \cdots + c_n$ is given by

$$c_3 = \frac{1}{6}(-(\mathrm{tr}(A))^3 + 3\mathrm{tr}(A)\mathrm{tr}(A^2) - 2\mathrm{tr}(A^3))$$

where $\mathrm{tr}(A)$ is the trace of A.

We have the following result as a direct consequence of Theorem 4.7 and Lemma 4.8.

Theorem 4.9 Let $\mathcal{R}(G)$ be the reverse Sombor matrix of G with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Then,

(i) $\sum \lambda_i = 0$,

(ii) $\sum \lambda_i^2 = 2RF(G)$,

(iii) $\sum \lambda_i^3 = 6\sum_{\Delta} \prod_{v_iv_j \in E(\Delta)} \sqrt{c(v_i)^2 + c(v_j)^2}$.

Theorem 4.9 can be generalized as follows.

Lemma 4.10 Let p be the length of the smallest odd cycle contained in G and $\sum_{C_p}$ denote the summation over all cycles of size p contained in G. Then, for $q = 1,3,\cdots,p-2$,

(i)$\sum_{i=1}^{n} \lambda_i^q = 0$,

(ii) $\sum_{i=1}^{n} \lambda_i^p = 2p\sum_{C_p} \prod_{v_iv_j \in E(C_p)} \sqrt{c(v_i)^2 + c(v_j)^2}$.

5. Bounds for reverse Sombor energy

In this section, we have obtained some bounds on the $\mathcal{ER}(G)$ reverse Sombor energy..

Lemma 5.1 [DiazâMetcalf Inequality] Let $(a_1, a_2, \ldots, a_n)$ and $(b_1, b_2, \ldots, b_n)$ be positive real numbers, satisfying the condition $ra_i \leq b_i \leq Ra_i$ for $1 \leq i \leq n$. Then

$$\sum_{i=1}^{n} b_i^2 + rR\sum_{i=1}^{n} a_i^2 \leq (r+R)\sum_{i=1}^{n} a_ib_i.$$

In the above expression, equality holds if and only if $b_i = Ra_i$ or $b_i = ra_i$ for $1 \leq i \leq n$.

Lemma 5.2[31] Let $a_1 \leq a_2 \leq \cdots \leq a_n \leq 0$isa sequence of non-negative real numbers. Then

$$\sum_{i=1}^{n} a_i + n(n-1)\left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}} \leq n\left(\sum_{i=1}^{n} \sqrt{a_i}\right)^2 \leq (n-1)\sum_{i=1}^{n} a_i + n\left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}}.$$

Lemma 5.3 If a_i and b_i are non-negative real numbers for $1 \leq i \leq n$, then

$$\left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right) - \left(\sum_{i=1}^{n} a_ib_i\right)^2 \leq \frac{n^2}{4}(AB-ab)^2,$$

where $A = \max_{1\leq i\leq n} a_i, B = \max_{1\leq i\leq n} b_i, \quad a = \min_{1\leq i\leq n} a_i$ and $b = \min_{1\leq i\leq n} b_i$.

Lemma 5.4 [Polya-Szego inequality] Suppose a_i and b_i are positive real numbers for $i = 1,2,\ldots,m$, such that $a \leq a_i \leq A$ and $b \leq b_i \leq B$. Then,

$$\sum_{i=1}^{m} b_i^2 \sum_{i=1}^{m} a_i^2 \leq \frac{1}{4}\left(\sqrt{\frac{AB}{ab}} + \sqrt{\frac{ab}{AB}}\right)^2 \left(\sum_{i=1}^{m} a_ib_i\right)^2$$

5.1.Lower bounds for the Sombor energy.

Theorem 5.5 Let G be any graph of order n and let Φ be the absolute value of the determinant of reverse Sombor matrix $\mathcal{R}(G)$, then

$$\sqrt{2\mathrm{RF(G)} + \mathrm{n(n-1)}\Phi^{\frac{2}{\mathrm{n}}}} \leq \mathcal{ER}(\mathrm{G}).$$

Proof.

$$[\mathcal{ER}(G)]^2 = \left(\sum_{i=1}^{n} |\lambda_i|\right)^2 = \sum_{i=1}^{n} |\lambda_i|^2 + \sum_{i\neq j} |\lambda_i||\lambda_j| = 2RF(G) + \sum_{i\neq j} |\lambda_i||\lambda_j|$$

Clearly we have,

$$\frac{1}{n(n-1)}\sum_{i\neq j} |\lambda_i||\lambda_j| \geq \prod_{i\neq j} \left(|\lambda_i||\lambda_j|\right)^{\frac{1}{n(n-1)}} = \left|\prod_{i=1}^{n} \lambda_i\right|^{\frac{2}{n}} = \Phi^{\frac{2}{n}} \sum_{i\neq j} |\lambda_i||\lambda_j| \geq n(n-1)\Phi^{\frac{2}{n}}$$

so that

$$\sqrt{2RF(G) + n(n-1)\Phi^{\frac{2}{n}}} \leq \mathcal{ER}(G).$$

Theorem 5.6 Let G be a graph with order n. Then

$$\sqrt{2\mathrm{nRF(G)} - \frac{\mathrm{n}^2}{4}(\lambda_1 - \lambda_\mathrm{n})^2} \leq \mathcal{ER}(\mathrm{G}).$$

Proof. Setting $a_i = |\lambda_i|$, $b_i = 1$, $A = \lambda_1$, $B = 1$, $a = \lambda_n$, and $b = 1$ in Lemma 4.3.

$$\left(\sum_{i=1}^{n} |\lambda_i|^2\right)\left(\sum_{i=1}^{n} 1\right) - \left(\sum_{i=1}^{n} |\lambda_i|\right)^2 \leq \frac{n^2}{4}(\lambda_1 - \lambda_n)^2$$

so that

$$2\mathrm{nRF(G)} - \mathcal{ER}(\mathrm{G})^2 \leq \frac{\mathrm{n}^2}{4}(\lambda_1 - \lambda_\mathrm{n})^2.$$

After rearranging the terms, we get the required result.

Theorem 5.7 Let G be a graph of order n. Then, $\frac{2\mathrm{RF(G)} + \mathrm{n}|\lambda_1||\lambda_n|}{|\lambda_n| + |\lambda_1|} \leq \mathcal{ER}(\mathrm{G})$where $|\lambda_1|$ and $|\lambda_n|$ are the maximum and minimum of the absolute value of eigenvalues of $\mathcal{R}(\mathrm{G})$. Equality will be attained if and only if for each $1 \leq i \leq n$, either $|\lambda_i| = |\lambda_1|$ or $|\lambda_i| = |\lambda_n|$.

Proof. Substituting $b_i = |\lambda_i|$, $a_i = 1$, $r = |\lambda_n|$ and $R = |\lambda_1|$ in Lemma 5.1, we have

$$\sum_{i=1}^{n} |\lambda_i|^2 + |\lambda_n||\lambda_1| \sum_{i=1}^{n} 1 \leq (|\lambda_1| + |\lambda_n|)\mathcal{ER}(\mathrm{G})$$

so that

$$\frac{2\mathrm{RF(G)} + \mathrm{n}|\lambda_1||\lambda_n|}{|\lambda_1| + |\lambda_n|} \leq \mathcal{ER}(\mathrm{G})$$

5.2.Upper bounds for Sombor energy.

Theorem 5.8 If G is a graph of order n, then $\mathcal{ER}(\mathrm{G}) \leq \sqrt{2\mathrm{nRF(G)}}$.

Proof. Put $a_i = 1$ and $b_i = |\lambda_i|$ in Cauchy-Schwarz inequality, we get

$$[\mathcal{ER}(\mathrm{G})]^2 \leq \mathrm{n}\sum_{i=1}^{n} |\lambda_i|^2 = 2\mathrm{nRF(G)}$$

Simplifying the above equation, we get the required result.

Theorem 5.9 Let G be a non-trivial graph. Then,

$$\mathcal{ER}(G) \geq \sqrt{\frac{Tr(\mathcal{R}(G)^2)^3}{Tr(\mathcal{R}(G)^4}}.$$

Proof. Taking $a_i = |\lambda_i|^{2/3}$, $b_i = |\lambda_i|^{4/3}$, $p = \frac{3}{2}$, and $q = 3$ in the Hölder inequality

$$\sum_{i=1}^{n} a_i b_i \leq \left(\sum_{i=1}^{n} a_i^p\right)^{\frac{1}{p}} \left(\sum_{i=1}^{n} b_i^q\right)^{\frac{1}{q}},$$

$$\sum_{i=1}^{n} |\lambda_i|^2 = \sum_{i=1}^{n} |\lambda_i|^{\frac{2}{3}} (|\lambda_i|^4)^{\frac{1}{3}} \leq \left(\sum_{i=1}^{n} |\lambda_i|\right)^{\frac{2}{3}} \left(\sum_{i=1}^{n} |\lambda_i|^4\right)^{\frac{1}{3}}$$

or

$$\mathcal{ER}(G) \geq \left(\frac{\sum_{i=1}^{n} |\lambda_i|^2}{(\sum_{i=1}^{n} |\lambda_i|^4)^{\frac{1}{3}}}\right)^{\frac{3}{2}} = \sqrt{\frac{Tr(\mathcal{R}(G)^2)^3}{Tr(\mathcal{R}(G)^4)}}.$$

Theorem 5.10 Let G be a graph with order n. Then,

$$\sqrt{\frac{2RF(G) + n(n-1)\Phi^{\frac{2}{n}}}{n}} \leq \mathcal{ER}(G) \leq \sqrt{\frac{2(n-1)RF(G) + n\Phi^{\frac{2}{n}}}{n}}.$$

Proof. Setting $a_i = \lambda_i^2$ in Lemma 4.2, we get

$$\sum_{i=1}^{n} \lambda_i^2 + n(n-1)\left(\prod_{i=1}^{n} \lambda_i^2\right)^{\frac{1}{n}} \leq n\left(\sum_{i=1}^{n} |\lambda_i|\right)^2 \leq (n-1)\sum_{i=1}^{n} \lambda_i^2 + n\left(\prod_{i=1}^{n} \lambda_i^2\right)^{\frac{1}{n}}$$

so that

$$2RF(G) + n(n-1)\Phi^{\frac{2}{n}} \leq n\mathcal{ER}(G)^2 \leq 2(n-1)RF(G) + n\Phi^{\frac{2}{n}}.$$

On simplifying, we arrive at the result.

Theorem 5.11 Let G be a graph of order n. Then

$$nRF(G) \leq \frac{1}{4}\left(\sqrt{\frac{\lambda_1}{\lambda_n}} + \sqrt{\frac{\lambda_n}{\lambda_1}}\right)\mathcal{ER}(G)^2.$$

Proof. Setting $a_i = |\lambda_i|$ and $b_i = 1$ in Lemma 4.4, we get

$$\sum_{i=1}^{n} 1 \sum_{i=1}^{n} |\lambda_i|^2 \leq \frac{1}{4}\left(\sqrt{\frac{AB}{ab}} + \sqrt{\frac{ab}{AB}}\right)^2 \left(\sum_{i=1}^{n} |\lambda_i|\right)^2.$$

Clearly, $\lambda_n \leq \lambda_i \leq \lambda_1$. Choosing $A = \lambda_1$, $a = \lambda_n$, and $B = b = 1$, we have

$$nRF(G) \leq \frac{1}{4}\left(\sqrt{\frac{\lambda_1}{\lambda_n}} + \sqrt{\frac{\lambda_n}{\lambda_1}}\right)\mathcal{ER}(G)^2.$$

6. Chemical applicability of $\mathcal{ER}(G)$

In this section, we make a computational analysis of the reverse Sombor energy $\mathcal{ER}(G)$ and π-electron energy of hetero atoms. Further, we compare the graph energy $E(G)$) with $\mathcal{ER}(G)$ taking graphs G to be trees with fixed order $n = 8,9,\cdots,14$, which is very relevant as a

study of correlation within classes of graphs with fixed order and size provides a better understanding of the invariant.

6.1.Correlation analysis of π-electron energy with $\mathcal{ER}(G)$.

The Hückel molecular orbital(HOM) theory is largely concentrated on conjugated, all-carbon compounds. When considering hetero atoms, one can compare the energy values of hetero compounds to determine the range of such compounds. For hetero atoms, we must thus modify the Coulomb (α) and resonance integral (β) values (see [32, 33, 34] for specifics). We have calculated $\mathcal{ER}(G)$ with a dataset of total π-electron energy values of hetero atoms, which are found in [35]. The molecules containing hetero atoms with the total π-electron energy and the reverse Sombor energy have been tabulated in Table 1. Further, we have found that $\mathcal{ER}(G)$ has a strong correlation with that of hetero atoms with correlation coefficient $r = 0.964$ and $r^2(adjusted) = 0.930$ (see Figure 1).

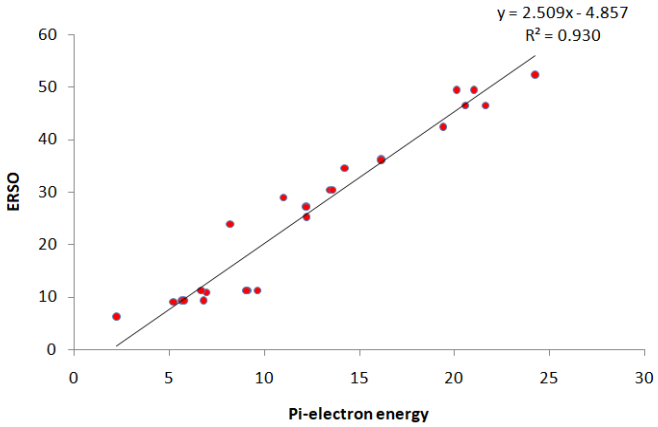


Figure 1. Correlation of $\mathcal{ER}(G)$ with the total π-electron energy of molecules containing hetero atoms.

Table 1. Molecules containing hetero atoms with total π-electron energy [35] and the reverse Sombor energy.

Molecule	Code	Total π-electron energy	$\mathcal{ER}(G)$
Vinyl chloride-like systems	H1	2.23	6.32
Butadiene perturbed at C2	H2	5.66	9.3
Acrolein like systems	H3	5.76	9.38
1, 1-Dichloro-ethylene like systems	H4	6.96	10.95
Glyoxal-like and 1,2-Dichloro-ethylene systems	H5	6.82	9.38
Pyrrole like systems	H6	5.23	9.15
Pyridine like systems	H7	6.69	11.31
Pyridazine like systems	H8	9.06	11.31
Pyrimidine like systems	H9	9.10	11.31
Pyrazine like systems	H10	9.07	11.31
S-Triazene like systems	H11	9.65	11.31
Aniline like systems	H12	8.19	23.98
O-Phenylene-diamine like systems	H13	12.21	27.23
m-Phenylene-diamine like systems	H14	12.22	25.27
p-Phenylene-diamine like systems	H15	12.21	27.23
Benzaldehyde like systems	H16	11	29.02
Quinoline like systems	H17	14.23	34.64
Iso-quinoline like systems	H18	14.23	34.64
1-Naphthalein like systems	H19	16.15	36.37
2-Naphthalein like systems	H20	16.12	36.17
Iso-indole like systems	H21	13.46	30.45
Indole like systems	H22	13.59	30.45
Benzylidine-aniline-like systems	H23	20.10	49.55
Azobenzene like systems	H24	21.02	49.55

Molecule	Code	Total π-electron energy	$\mathcal{ER}(G)$
Acridine like systems	H25	20.56	46.58
Phenazine like systems	H26	21.62	46.58
9,10-Anthraquinoline like structures	H27	24.23	52.45
Cabazole like structures	H28	19.39	42.52

6.2.Comparing E(G) and $\mathcal{ER}(G)$of trees.

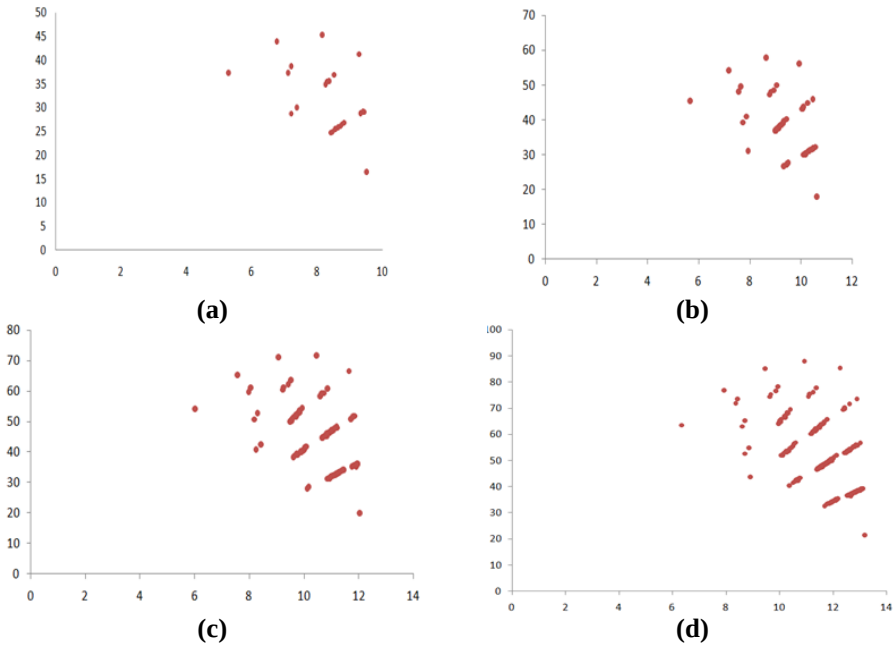
The correlation analysis of $E(G)$ and $\mathcal{ER}(G)$ has been done, taking graphs G to be trees with fixed order $n = 8,9, \dots,14$. Based on these calculations and from Figure 2 we have observed the following regularities without any exception:

- The data points in each cluster nearly form a straight line with a positive slope.
- These lines are almost parallel to each other, with the distance between them being nearly equal.
- The reverse Sombor energy and graph energy increases as the order of the tree increases.
- $\mathcal{ER}(\mathrm{G})$ is observed to be minimum for path graphs.

The correlation coefficient R between the graph energy and $\mathcal{ER}$ energy for all trees of order $\mathrm{n} = 8,9, \dots,14$ has been tabulated in Table 2.

Table 2. Correlation between graph energy and $\mathcal{ER}$ energy for all trees of order $n = 8,9,10, \dots,14$.

n	Number of trees	R
8	23	-0.479059835
9	47	-0.490346429
10	106	-0.50306039
11	235	-0.514487292
12	551	-0.525680684
13	1301	-0.530061711
14	3160	-0.5344958



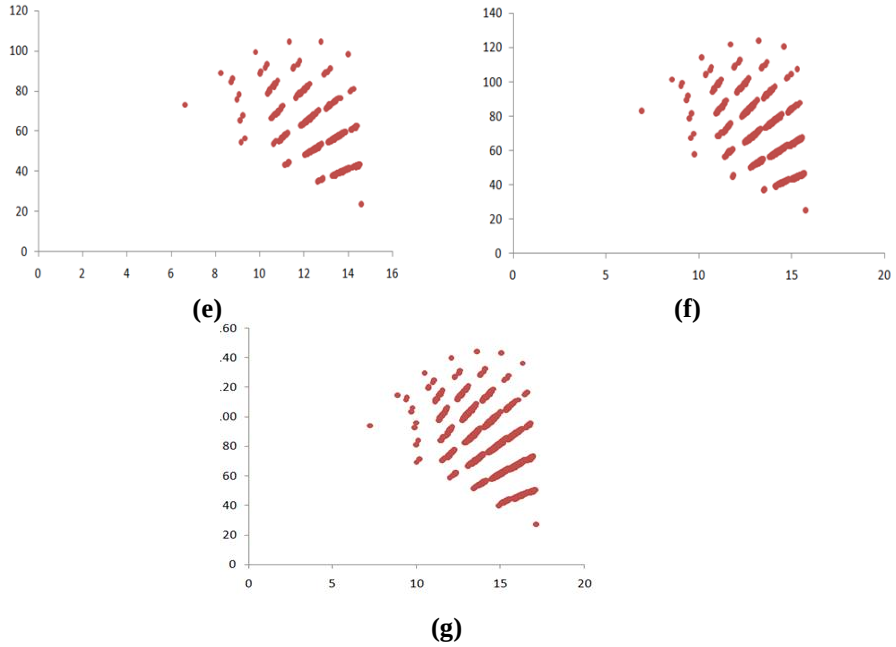


Figure 2. $\mathcal{ER}(G)$ vs $E(G)$ plotted for the set of trees.
(**a**) $\mathcal{ER}(G)$ vs $E(G)$ plotted for the set of trees with 8 vertices; (**b**) $\mathcal{ER}(G)$ vs energy $E(G)$ plotted for the set of trees with 9 vertices; **(c)**$\mathcal{ER}(G)$ vs energy $E(G)$ plotted for the set of trees with 10 vertices; **(d)**$\mathcal{ER}(G)$ vs energy $E(G)$ plotted for the set of trees with 11 vertices; (**e**)$\mathcal{ER}(G)$ vs that of energy $E(G)$ plotted for the set of trees with 12 vertices; **(f)**$\mathcal{ER}(G)$ vs that of energy $E(G)$ plotted for the set of trees with 13 vertices; **(g)**$\mathcal{ER}(G)$ vs energy $E(G)$ plotted for the set of trees with 14 vertices.

7. Conclusions

In this article, we have introduced the concept of reverse Sombor energy of a graph based on the reverse Sombor index of a graph. Further, we have observed some mathematical properties of the reverse Sombor matrix and the corresponding energy $\mathcal{ER}(G)$ and have established some bounds on $\mathcal{ER}(G)$. We have also discussed the chemical applicability of this parameter by comparing it with the π-electron energy of some polyaromatic hydrocarbons and with the graph energy of trees of order $n = 8,9,\cdots,14$ is presented. Based on the analysis, it has been found that there is a good correlation between $\mathcal{ER}(G)$ and π-electron energy, whereas the correlation between $\mathcal{ER}(G)$ and $E(G)$ on trees is found to be increasing with the order of the tree. These observations are purely experimental, and further theoretical investigation might shed some light on this behavior.

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Conflicts of Interest

The authors declare no conflict of interest.

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