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Euler Sombor Energy of a Graph

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Abstract In this paper, we introduce and investigate the Euler Sombor matrix of a graph, defined with respect to the Euler Sombor index. For adjacent vertices u and v, the corresponding entry of this matrix is given by $\sqrt{d_u^2+d_v^2+d_ud_v}$, where d_u and d_v denote the degrees of vertices u and v, and is zero otherwise. The Euler Sombor energy of a graph is then defined as the sum of the absolute values of the eigenvalues of the Euler Sombor matrix. We compute the Euler Sombor energy for several standard classes of graphs, establish bounds for the spectral radius of the Euler Sombor matrix, and derive upper and lower bounds for the Euler Sombor energy. Furthermore, we investigate correlations of Euler Sombor energy, adjacency energy, and Sombor energy with the total π-electron energy of heteroatomic systems. Statistical analysis reveals strong correlations, with the Euler Sombor energy exhibiting the highest correlation coefficient ($R = 0.9825$) and coefficient of determination ($R^2 = 0.9654$) among the considered energies. These findings highlight the significance of the Euler Sombor energy in chemical graph theory and its potential applications in modeling molecular structures.

Keywords Euler-Sombor Index, Second Zagreb, Forgotten Index, Sombor Index.

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1. Introduction

Many topological indices in the literature were established primarily to study the structural relationships of chemical compounds. These indices are recognized as degree-based and distance-based topological indices. The degree-based topological indices are most commonly expressed as

$$T.I = \sum_{pq\in E(G)} f(d_p, d_q),$$

where $f(x,y)$ is an appropriately selected symmetric function. Several degree-based indices that have been extensively studied include the Randic index, forgotten topological index, first and second Zagreb indices, Sombor index, and others.

The widespread application of spectral graph theory (SGT) in the analysis of graph matrices via matrix theory and linear algebra has given rise to a lengthy and rich history. Because spectral properties and topological indices are tightly associated, they offer significant information about the stability and structure of chemical substances. Graph energy is defined as the sum of the absolute values of the eigenvalues of a graph G's adjacency matrix.A

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relationship between the graph energy and the molecular graph's total π-electron energy was discovered by Gutman [11] in 1978. Since then, researchers in pure and practical mathematics have become interested in spectral graph theory. It was discovered that their own understanding contains numerous, seemingly unrelated references to the idea of graph energy. Connecting one extreme characteristic to another, the eigenvalues are closely correlated with almost all of a graph's significant invariants. They are crucial for understanding graphs. In literature several graph matrices corresponding to the topological indices were defined and studies. The general form of the adjacency type matrix corresponding to the topological index is given by

$$M = \begin{cases} f(d_p, d_q) & \text{if } pq \in E(G) \\ 0 & \text{otherwise} \end{cases} \tag{1}$$

Some of the well studied matrices are listed below.

In this study, we assumed simple graphs, i.e., graphs without multiple edges and self loops. Let G be a such graph with vertex set $V(G) = \{v_1, v_2, v_3 ... v_n\}$ and edge set $E(G)$. If the vertices p and q are adjacent, then we write it as $p \sim q$ or $pq \in E(G)$. The degree of vertex p in G is denoted by d_p is the total number of edges connecting to p. For other graph theoretical notions, we refer [4].

Table 1. Topological indices and its corresponding matrices

Topological Index	**Mathematical expression**	**Corresponding Matrix** ($M = [a_{pq}]$)
First Zagreb Index [11]	$M_1 = \sum_{pq \in E(G)} (d_p + d_q)$	$a_{pq} = \begin{cases} d_p + d_q & \text{if } p \sim q \\ 0 & \text{otherwise} \end{cases}$ [18]
Second Zagreb Index [11]	$M_2 = \sum_{pq \in E(G)} d_p d_q$	$a_{pq} = \begin{cases} d_p d_q & \text{if } p \sim q \\ 0 & \text{otherwise} \end{cases}$ [18]
Randic Index [20, 25, 27]	$R(G) = \sum_{pq \in E(G)} \frac{1}{\sqrt{d_p \cdot d_q}}$	$a_{pq} = \begin{cases} \frac{1}{\sqrt{d_p \cdot d_q}} & \text{if } p \sim q \\ 0 & \text{otherwise} \end{cases}$ [5]
Sombor Index [12]	$SO(G) = \sum_{pq \in E(G)} \sqrt{d_p^2 + d_q^2}$	$a_{pq} = \begin{cases} \sqrt{d_p^2 + d_q^2} & \text{if } p \sim q \\ 0 & \text{otherwise} \end{cases}$ [9, 10]
Nirmala Index [16]	$N(G) = \sum_{pq \in E(G)} \sqrt{d_p + d_q}$	$a_{pq} = \begin{cases} \sqrt{d_p + d_q} & \text{if } p \sim q \\ 0 & \text{otherwise} \end{cases}$ [10]
Forgotten topological Index [8]	$F(G) = \sum_{pq \in E(G)} (d_p^2 + d_q^2)$	$a_{pq} = \begin{cases} d_p^3 & \text{if } p = q \\ 1 & \text{if } p \sim q \\ 0 & \text{otherwise} \end{cases}$ [15]

For other matrices and their energies we refer [17, 6, 19, 2]

In 2024 Gutman et.al [13] defined the new degree based topological index called Euler Sombor index as:

$$EU(G) = \sum_{pq \in E(G)} \sqrt{d_p^2 + d_q^2 + d_p d_q}. \tag{2}$$

The Euler Sombor index can be interpreted as an approximation of the perimeter of an ellipse, where the semi-major axis is taken as $d_p + d_q$ and the semi-minor axis as $\sqrt{d_p^2 + d_q^2}$ in a two-dimensional coordinate system. The details of this index we refer to [21, 22, 23, 24, 1, 26]. The broad applicability of the Euler Sombor index motivates the introduction of the Euler Sombor matrix and the corresponding Euler Sombor energy of a graph, which are defined in the following section.

2. Euler Sombor matrix and Energy of a Graph

The Euler Sombor matrix of a graph G with vertex set $V(G) = \{p_1, p_2, p_3, ..., p_n\}$ and edge set $E(G)$ is defined as $ES(G) = (e_{ij})_{n\times n}$, where

$$e_{ij} = \begin{cases} \sqrt{d_p^2 + d_q^2 + d_p d_q}, & \text{if} \quad pq \in E(G) \\ 0, & \text{otherwise} \end{cases} \tag{3}$$

where d_q indicates the degree of the vertex q. The Euler Sombor characteristic polynomial for a graph G is defined as:

$$P_{ES(G)}(\omega) = |\omega I - ES(G)|, \tag{4}$$

where I is an unit matrix of order $n \times n$. Since $ES(G)$ is a real symmetric matrix, all roots of $P_{ES(G)}(\omega) = 0$ are real. Thus, they can be arranged as $\omega_1 \geq \omega_2 \geq ... \geq \omega_n$.
The Euler Sombor energy of a graph G is given by

$$E_{ES}(G) = \sum_{i=1}^{n} |\omega_i|. \tag{5}$$

3. Euler Sombor energy of some standard graphs

Theorem 3.1. Let $A(G)$ be the adjacency matrix of an r-regular graph of order n. If λ_i is an eigenvalue of $A(G)$ then the eigenvalue of $ES(G)$ is $r\sqrt{3}\lambda_i$.

Proof
Let G be an r-regular of order n, then its $ES(G)$ is given by

$$e_{ij} = \begin{cases} r\sqrt{3}, & \text{if} \quad pq \in E(G) \\ 0, & \text{otherwise} \end{cases}. \tag{6}$$

It has been noted that $ES(G) = r\sqrt{3}A(G)$, if λ_i is an eigenvalue of $A(G)$ then the eigenvalue of $ES(G)$ is $r\sqrt{3}\lambda_i$. Hence the result follows. □

Corollary 3.1.1. Let K_n be a complete graph of order $n \geq 2$. Then $E_{ES}(K_n) = 2(n-1)^2\sqrt{3}$.

Corollary 3.1.2. Let C_n be a cycle graph of order $n \geq 3$. Then

$$E_{ES}(C_n) = \sum_{k=1}^{n} |2\sqrt{3}cos\left(\frac{2\pi k}{n}\right)|.$$

Lemma 1. For any positive integers m,n, the eigenvalues of $K_{m,n}$ are $\sqrt{mn}, -\sqrt{mn}$ and 0 with multiplicity $m+n-2$.

Theorem 3.2. Let $K_{m,n}$ be a complete bipartite graph of order $m+n$. Then

$$E_{ES}(K_{m,n}) = 2\sqrt{mn}\sqrt{m^2+n^2+mn}$$

Proof
Let $K_{m,n}$ be a complete bipartite graph of order $m+n$. The Euler Sombor matrix of $K_{m,n}$ is given by

$$ES(K_{m,n}) = \sqrt{m^2+n^2+mn}\,A(K_{m,n})$$

From Lemma 1 the eigenvalues of $A(K_{m,n})$ are $\sqrt{mn}, -\sqrt{mn}$ and 0 with multiplicity $m+n-2$. Thus, the adjacency spectrum of $K_{m,n}$, $specA(K_{m,n}) = \begin{pmatrix} -\sqrt{mn} & \sqrt{mn} & 0 \\ 1 & 1 & m+n-2 \end{pmatrix}$.

Hence the Euler Sombor Spectrum becomes,

$$spec\,ES(K_{m,n}) = \begin{pmatrix} -\sqrt{mn}\sqrt{m^2+n^2+mn} & \sqrt{mn}\sqrt{m^2+n^2+mn} & 0 \\ 1 & 1 & m+n-2 \end{pmatrix}.$$

Therefore the Euler Sombor energy of the $K_{m,n}$ is given by

$$E_{ES}(K_{m,n}) = 2\sqrt{mn}\sqrt{m^2+n^2+mn},$$

hence stated. □

Corollary 3.2.1. The Euler Sombor energy of a star graph $K_{1,n}$ of order $n+1$ is $2\sqrt{n^3+n^2+n}$.

Lemma 2. [7] If A and B are square matrices of order n then,

$$\sum_{1\leq i\leq j\leq n} \lambda_i(A+B) \leq \sum_{1\leq i\leq n} \lambda_i(A) + \sum_{1\leq i\leq n} \lambda_i(B) \tag{7}$$

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 3.3. For a path P_n of order $n \geq 4$, $E_{ES}(P_n) \leq 2\sqrt{3}\sum_{k=1}^{n} \left|cos\left(\frac{\pi k}{n+1}\right)\right| + 4(2\sqrt{3}-\sqrt{7})$.

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

$$\begin{aligned} ES(P_n) &= \begin{pmatrix} 0 & \sqrt{7} & 0 & 0 & \cdots & 0 \\ \sqrt{7} & 0 & 2\sqrt{3} & 0 & \cdots & 0 \\ 0 & 2\sqrt{3} & 0 & 2\sqrt{3} & \cdots & 0 \\ 0 & 0 & 2\sqrt{3} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \sqrt{7} \\ 0 & 0 & 0 & \cdots & \sqrt{7} & 0 \end{pmatrix} \\ &= 2\sqrt{3}\begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 1 \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix} + (\sqrt{7}-2\sqrt{3})\begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 1 \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix} \\ &= 2\sqrt{3}A(P_n) + (\sqrt{7}-2\sqrt{3})B \end{aligned}$$

where

$$B = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & 1 \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix}$$

has the spectrum, $spec(B) = \begin{pmatrix} -1 & 0 & 1 \\ 2 & (n-4) & 2 \end{pmatrix}$

so that $E(B) = 4$. Thus by the Lemma 2, we have

$$E_{ES}(P_n) \leq 2\sqrt{3}E(P_n) + E(B) = 2\sqrt{3}\sum_{k=1}^{n}\left|cos\left(\frac{\pi k}{n+1}\right)\right| + 4(2\sqrt{3} - \sqrt{7})$$

Hence stated. □

4. Some properties on the Euler Sombor matrix

Theorem 4.1. If C_0, C_1, C_2, C_3 are the first three coefficients of the Euler Sombor characteristic polynomial $P_{ES(G)}$ of G then

(i) $C_0 = 1$
(ii) $C_1 = 0$
(iii) $C_2 = -(M_2(G) + F(G))$
(iv) $C_3 = -(\sum_{\Delta} \prod_{pq\in E(G)} \sqrt{d_p^2 + d_q^2 + d_p d_q})$

where the summation runs over the triangles in G.

Proof
From equation 4,

$$C_0 = 1$$

$$C_1 = (-1)^1 \times Tr(EU(G)) = -1 \times 0 = 0.$$

$$\begin{aligned} C_2 &= \sum_{1\leq i<j\leq n} \begin{vmatrix} 0 & e_{ij} \\ e_{ji} & 0 \end{vmatrix} \\ &= -(\sum_{1\leq i<j\leq n} e_{ij}^2) \\ &= -\sum_{1\leq i<j\leq n} (d_p^2 + d_q^2 + d_p d_q) \\ &= -\left(\sum_{pq\in E(G)} (d_p^2 + d_q^2) + \sum_{pq\in E(G)} (d_p d_q)\right) \end{aligned}$$

$C_2 = -(M_2(G) + F(G))$ that links energy to Zagreb and forgotten indices.

$$\begin{aligned} C_3 &= (-1)^3 \sum_{1\leq i<j,k\leq n} \begin{vmatrix} 0 & e_{ij} & e_{ik} \\ e_{ij} & 0 & e_{jk} \\ e_{ki} & e_{kj} & 0 \end{vmatrix} \\ &= -2 \sum_{1\leq i<j,k\leq n} a_{ij}a_{jk}a_{ki} \\ C_3 &= -2(\sum_{\Delta} \prod_{pq\in E(G)} \sqrt{d_p^2 + d_q^2 + d_p d_q}) \end{aligned}$$

C_3 counts contributions from triangles (3-cycles) in the graph. □

Remark : $C_3 = 0$ if and only if G is a triangle free graph.

Theorem 4.2. Let $ES(G)$ be the Euler Sombor matrix and $\omega_1 \geq \omega_2 \geq \omega_3 \geq ... \geq \omega_n$ are its eigenvalues then

(i) $\sum_{i=1}^{n} \omega_i = 0$
(ii) $\sum_{i=1}^{n} \omega_i^2 = 2M^*$, where $M^* = M_2(G) + F(G)$

Proof
(i) Since, $ES(G)$ is a real symmetric matrix with Zero diagonals, So $Tr(ES(G)) = 0$ and hence $\sum_{i=1}^{n} \omega_i = 0$

$$(ii) \qquad \begin{aligned} \sum_{i=1}^{n} \omega_i^2 &= Tr(ES(G)^2) \\ &= \sum_{i=1}^{n} \sum_{j=1}^{n} e_{ij} e_{ji} \\ &= \sum_{i=1}^{n} e_{ii}^2 + 2 \sum_{i \neq j} e_{ij}^2 \\ &= 2 \sum_{pq \in E(G)} (d_p^2 + d_q^2 + d_p d_q) \\ &= 2(M_2(G) + F(G)) \\ &= 2M^*. \end{aligned} \tag{8}$$

It has been observed that the sum of second Zagreb and forgotten indices performs the same effect as the number of edges in normal graph energy. □

5. Bounds for the largest eigen value

Theorem 5.1. Let ω_1 be the largest Euler Sombor eigen value. Then $\omega_1 \geq \dfrac{2EU(G)}{n}$

Proof
From the Rayleigh-Ritz variational principal, if Y is any n-dimentional column unit vector then

$$\frac{Y^T ES(G) Y}{Y^T Y} \leq \omega_1. \tag{9}$$

Considering $Y = (1, 1, 1...1)^T$, we have

$$\begin{aligned} Y^T ES(G) Y &= \sum_{i=1}^{n} \sum_{j=1}^{n} e_{ij} \\ &= 2 \sum_{pq \in E(G)} e_{ij} \\ &= 2 \sum_{pq \in E(G)} \sqrt{(d_p^2 + d_q^2 + d_p d_q)} \\ &= 2EU(G) \end{aligned}$$

and $Y^T Y = n$. □

Lemma 3. [3] (The Cauchy -Schwartz inequality) Let $a=(a_1,a_2,...,a_n)$ and $b=(b_1,b_2,...,b_n)$ are n real vectors then

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right). \tag{10}$$

Equality holds if and only if a and b are proportional.

Theorem 5.2. Let $\omega_1 \geq \omega_2 \geq ... \geq \omega_n$ be the eigenvalues of the $ES(G)$ of the connected graph with n vertices then

$$\omega_1 \leq \frac{\sqrt{2(n-1)M^*}}{n}$$

Proof
Put $a_i = 1$ and $b_i = \omega_i$ for $i = 2,3,....,n$ in Lemma 3 we get:

$$(\sum_{i=2}^{n} \omega_i)^2 \leq (n-1)\sum_{i=2}^{n} \omega_i^2$$

on solving we get

$$\omega_1^2 \leq \frac{2(n-1)M^*}{n}$$

$$\omega_1 \leq \sqrt{\frac{2(n-1)M^*}{n}}$$

Hence the proof. □

6. Bounds for the Euler Sombor Energy

In this section, we present some bounds for the Euler Sombor energy by using following lemma's.

Lemma 4. [14] Suppose $(x_1,x_2,...,x_n)$ and $(y_1,y_2,...,y_n)$ are positive real, then

$$\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i^2 \leq \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}} + \sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2 \left(\sum_{i=1}^{n} x_i y_i\right)^2 \tag{11}$$

where $m_1 = min_{1\leq i\leq n}(x_i); m_2 = min_{1\leq i\leq n}(y_i); M_1 = max_{1\leq i\leq n}(x_i)$ and $M_2 = max_{1\leq i\leq n}(y_i);$.

Lemma 5. [14] Let $(a_1,a_2,...,a_n)$ and $(b_1,b_2,...,b_n)$ are non-negative real numbers, then

$$\sum_{i=1}^{n} b_i^2 + rR\sum_{i=1}^{n} a_i^2 \leq (r+R)\left(\sum_{i=1}^{n} a_i b_i\right) \tag{12}$$

where R and r are real constants, such that $ra_i \leq b_i \leq Ra_i$, for each i, $1 \leq i \leq n$.

Lemma 6. [14] Suppose $(a_1,a_2,...,a_n)$ and $(b_1,b_2,...,b_n)$ are non negative real numbers, then

$$\sum_{i=1}^{n} a_i^2 \sum_{i=1}^{n} b_i^2 - \left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \frac{n^2}{4}(M_1M_2 - m_1m_2)^2 \tag{13}$$

where m_i and M_i are defined as in the Lemma 4.

Lemma 7. [9] Let $(x_1,x_2,...,x_n)$ be the non-negative real numbers, then

$$n\left(\frac{1}{n}\sum_{i=1}^{n} x_i - \left(\prod_{i=1}^{n} x_i\right)^{\frac{1}{n}}\right) \leq n\sum_{i=1}^{n} x_i - \left(\sum_{i=1}^{n}\sqrt{x_i}\right)^2 \leq n(n-1)\left(\frac{1}{n}\sum_{i=1}^{n} x_i - \left(\prod_{i=1}^{n} x_i\right)^{\frac{1}{n}}\right) \tag{14}$$

6.1. Lower Bounds on the Euler Sombor Energy

Theorem 6.1. If zero is not an eigen value of $ES(G)$. Then

$$E_{ES}(G) \geq \frac{2\sqrt{\omega_1\omega_n}\sqrt{2M^*n}}{\omega_1+\omega_n} \tag{15}$$

Proof
Suppose $\omega_1, \omega_2, ..., \omega_n$ are the eigenvalues of $ES(G)$. If we set $x_i = |\omega_i|$ and $y_i = 1$ in Lemma 4, we get

$$\sum_{i=1}^{n} |\omega_i|^2 \sum_{i=1}^{n} 1^2 \leq \frac{1}{4}\left(\sqrt{\frac{\omega_n}{\omega_1}}+\sqrt{\frac{\omega_1}{\omega_n}}\right)^2 \left(\sum_{i=1}^{n} |\omega_i|\right)^2$$
$$2M^*n \leq \left(\frac{(\omega_1+\omega_n)^2}{\omega_1\omega_n}\right)(E_{ES}(G))^2$$
$$E_{ES}(G) \geq \frac{2\sqrt{\omega_1\omega_n}\sqrt{2M^*n}}{\omega_1+\omega_n}\ .$$

□

Theorem 6.2. Let $\omega_1, \omega_2, \ldots, \omega_n$ be the eigenvalues of $ES(G)$, arranged so that $|\omega_1| \geq |\omega_2| \geq \cdots \geq |\omega_n|$. Then

$$E_{ES}(G) \geq \frac{|\omega_1||\omega_n|n+2M^*}{|\omega_1|+|\omega_n|}. \tag{16}$$

Proof
Let $\omega_1, \omega_2, ..., \omega_n$ are the eigenvalues of $ES(G)$. We set $a_i = 1, b_i = |\omega_i|, r = |\omega_n|$ and $R = |\omega_1|$ in Lemma 5, we obtain

$$\sum_{i=1}^{n} |\omega_i|^2 + |\omega_1||\omega_n|n \leq (|\omega_1|+|\omega_n|)\sum_{i=1}^{n} |\omega_i|. \tag{17}$$

Since $E_{ES}(G) = \sum_{i=1}^{n} |\omega_i|$ and $\sum_{i=1}^{n} |\omega_i|^2 = 2M^*$. Therefore

$$2M^* + |\omega_1||\omega_n|n \leq (|\omega_1|+|\omega_n|)E_{ES}(G)$$

which yeilds the desired bound

$$E_{ES}(G) \geq \frac{|\omega_1||\omega_n|n+2M^*}{|\omega_1|+|\omega_n|}.$$

□

Theorem 6.3. Let $E_{ES}(G)$ be the Euler Sombor energy of a graph G of order n and size m then

$$\sqrt{2M^*n - \frac{n^2}{4}(\omega_1-\omega_n)^2} \leq E_{ES}(G). \tag{18}$$

Proof
Suppose $\omega_1, \omega_2, ..., \omega_n$ are the eigenvalues of $ES(G)$. Considering $a_i = |\omega_i|$ and $b_i = 1$ in Lemma 6, we get

$$\sum_{i=1}^{n} |\omega_i|^2 \sum_{i=1}^{n} 1 - \left(\sum_{i=1}^{n} \omega_i\right)^2 \leq \frac{n^2}{4}(\omega_1-\omega_n)^2$$

$$2M^*n - (E_{ES}(G))^2 \leq \frac{n^2}{4}(\omega_1-\omega_n)^2$$
$$\sqrt{2M^*n - \frac{n^2}{4}(\omega_1-\omega_n)^2} \leq E_{ES}(G).$$

□

6.2. Upper bounds on the Euler Sombor Energy

Theorem 6.4. If G is a graph on n vertices and $M_2(G), F(G)$ be its second Zagreb and forgotten indices then $E_{ES}(G) \leq \sqrt{2nM^*}$.

Proof
By setting $a_i = 1$ and $b_i = |\omega_i|$ in Lemma 3, we get

$$E_{ES}(G) = \sqrt{(\sum_{i=1}^{n} |\omega_i|)^2} \leq \sqrt{n \sum_{i=1}^{n} |\omega_i|^2} = \sqrt{2nM^*}$$

$$E_{ES}(G) \leq \sqrt{2nM^*}. \tag{19}$$

□

Theorem 6.5. Let G be a graph with n vertices with Euler Sombor index $EU(G)$ and sum of second Zagreb and Forgotten index $M^* = M_2(G) + F(G)$ respectively. Then

$$E_{ES}(G) \leq \frac{2EU(G)}{n} + \sqrt{(n-1)\left[2M^* - \left(\frac{2EU(G)}{n}\right)^2\right]}. \tag{20}$$

Proof
Applying Lemma 3 to $(|\omega_2| \geq |\omega_3| \geq ... \geq |\omega_n|)$ and (1.1.1...1), we arrive at

$$E_{ES}(G) \leq |\omega_1| + \sqrt{(n-1)[2M^* - |\omega_1|^2]} \tag{21}$$

Recall that $\omega_1 > 0$ and thus $|\omega_1| = \omega_1$

$$E_{ES}(G) \leq \omega_1 + \sqrt{(n-1)[2M^* - \omega_1^2]} \tag{22}$$

Let $f(x) = x + \sqrt{(n-1)[2M^* - x^2]}$, it is monotonically decreasing function in the interval (a, b) where $a = \sqrt{\frac{2M^*}{n}}$ and $b = \sqrt{2M^*}$. Therefore, the inequality 22 remains valid if on its right-hand side, ω is replaced by $\frac{2EU(G)}{n}$, from Theorem (5.1), we got the desired result. □

Theorem 6.6. Let G be a graph with n vertices, then

$$E_{ES}(G) \leq \sqrt{n\left\{Det(ES(G))^{\frac{2}{n}} + 2M^*\right\} - 2M^*} \tag{23}$$

Proof
Substituting $x_i = |\omega_i|^2$ in Lemma 7, we have

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

using the fact $\sum_{i=1}^{n} \omega_i^2 = 2M^*$, $\prod_{i=1}^{n} \omega_i$ = Det(ES(G)). The above inequality becomes

$$n\left(\frac{1}{n}2M^* - (\text{Det(ES(G))})^{\frac{2}{n}}\right) \leq n2M^* - (E_{ES}(G))^2$$

$$E_{ES}(G) \leq \sqrt{n\left\{Det(ES(G))^{\frac{2}{n}} + 2M^*\right\} - 2M^*}.$$

□

6.3. Numerical validation of the results

In this section, we consider path graphs (P_n) and cycle graphs (C_n) up to order $n = 20$ to numerically compare the Euler Sombor energy $E_{ES}(G)$ with its lower and upper bounds. These two graph families, representing linear and cyclic structures, enable a direct numerical comparison between $E_{ES}(G)$ and its bounds.

Table 2. Comparison of Euler Sombor energy $E_{ES}(G)$ with bounds (Lower bounds and Upper bounds).

Graph	E_{ES}	**Theorem 6.1**	**Theorem 6.2**	**Theorem 6.3**	**Theorem 6.4**	**Theorem 6.6**	**Theorem 6.7**
P2	3.4641	3.4641	3.4641	3.4641	3.4641	3.4641	3.4641
P3	7.4833		7.4833	7.2457	9.1652	9.1054	7.4833
P4	12.6491	12.0665	12.6491	12.6491	14.4222	14.3027	13.5647
P5	16.4270		13.6500	13.6473	19.4936	19.3251	17.4356
P6	21.4254	17.8768	19.7708	19.7142	24.4949	24.2895	23.4578
P7	25.3218		19.9446	19.8618	29.4618	29.2284	27.2764
P8	30.2168	22.8883	26.7189	26.6004	34.4093	34.1540	33.3065
P9	34.1941		26.4755	26.3313	39.3446	39.0719	37.0950
P10	39.0165	27.3844	33.6493	33.4977	44.2719	43.9850	43.1361
P11	43.0530		33.1353	32.9623	49.1935	48.8949	46.9068
P12	47.8215	31.4861	40.5786	40.4126	54.1110	53.8026	52.9558
P13	51.9031		39.8704	39.6869	59.0254	58.7086	56.7150
P14	56.6300	35.2716	47.5087	47.3384	63.9375	63.6134	62.7696
P15	60.7470		46.6530	46.4683	68.8477	68.5173	66.5245
P16	65.4411	38.7968	54.4394	54.2702	73.7564	73.4205	72.5796
P17	69.5867		53.4675	53.2862	78.6638	78.3231	76.3387
P18	74.2541	42.1037	61.3705	61.2050	83.5703	83.2252	82.3870
P19	78.4231		60.3044	60.1288	88.4760	88.1270	86.1537
P20	83.0684	45.2248	68.3017	68.1414	93.3809	93.0284	92.1926
C3	13.8564	13.8564	13.8564	13.7477	14.6969	13.8564	14.1826
C4	13.8564		13.8564	13.8564	19.5959	18.9282	16.9706
C5	22.4201	20.8042	21.4093	21.3720	24.4949	23.8988	23.6468
C6	27.7128	27.7128	27.7128	27.4955	29.3939	28.8371	28.8841
C7	31.1351	26.4644	28.6624	28.6456	34.2929	33.7610	33.3226
C8	33.4523		27.7128	27.7128	39.1918	38.6772	36.6606
C9	39.8979	31.3094	35.7897	35.7808	44.0908	43.5888	43.0579
C10	44.8403	41.6084	42.8187	42.7440	48.9898	48.4974	48.1492
C11	48.6822	35.5932	42.8524	42.8471	53.8888	53.4040	52.8179
C12	51.7128		41.5692	41.5692	58.7878	58.3091	56.2850
C13	57.4780	39.4650	49.8776	49.8742	63.6867	63.2132	62.5904
C14	62.2701	52.9289	57.3248	57.2912	68.5857	68.1164	67.6224
C15	66.2805	43.0197	56.8790	56.8766	73.4847	73.0190	72.3701
C16	69.6609		55.4256	55.4256	78.3837	77.9212	75.8949
C17	75.0875	46.3214	63.8644	63.8627	83.2827	82.8229	82.1543
C18	79.7959	62.6189	71.5794	71.5615	88.1816	87.7242	87.1549
C19	83.8975	49.4157	70.8385	70.8373	93.0806	92.6253	91.9416
C20	87.4859		69.2820	69.2820	97.9796	97.5262	95.5001

7. Chemical applicability of $E_{ES}(G)$

The Huckel molecular orbital (HMO) theory is a classical framework for analyzing the behavior of π-electron systems in conjugated hydrocarbons. Although originally formulated for all carbon systems, it can be extended to heteroatomic compounds by appropriately modifying the Coulomb (α) and resonance (β) integrals. In this study, we investigate the chemical applicability of the Euler Sombor energy, $E_{ES}(G)$, using a dataset of heteroatomic compounds [3]. To assess its predictive ability, we employed linear regression to compare $E_{ES}(G)$, adjacency energy $E(G)$ and Sombor energy $E_{SO}(G)$ with the total π-electron energy derived from HMO theory. The regression results summarized in Table 4 confirm strong linear correlations, with $E_{ES}(G)$ exhibiting the highest

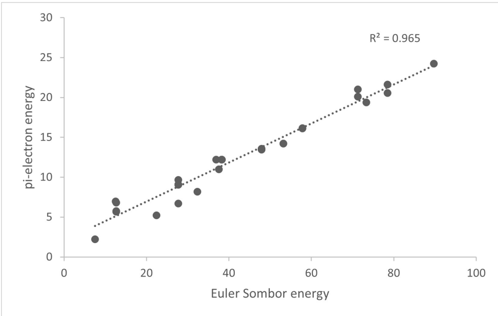
Table 3. Molecules containing hetero atoms with Euler Sombor energy $E_{ES}(G)$, Adjacency energy $E(G)$, Sombor energy $E_{SO}(G)$ and total π-electron energy

Molecules	$E_{ES}(G)$	E	$E_{SO}(G)$	**Total π-electron energy**
T_1	7.4833	2.83	6.3245	2.23
T_2	12.6491	4.4721	10.5830	5.66
T_3	12.6491	4.4721	10.5830	5.76
T_4	12.4900	3.4641	10.9544	6.96
T_5	12.6491	4.4721	6.3245	6.82
T_6	22.4201	6.4721	18.3059	5.23
T_7	27.7128	8.000	22.6274	6.69
T_8	27.7128	8.000	22.6274	9.06
T_9	27.7128	8.000	22.6274	9.1
T_{10}	27.7128	8.000	22.6274	9.07
T_{11}	27.7128	8.000	22.6274	9.65
T_{12}	32.3287	8.7206	26.7495	8.19
T_{13}	38.2077	9.954	31.8974	12.21
T_{14}	36.9240	9.4311	30.8519	12.22
T_{15}	38.2662	9.9248	32.0271	12.21
T_{16}	37.5954	10.424	30.9844	11
T_{17}	53.1912	13.683	43.6380	14.23
T_{18}	53.1912	13.683	43.6380	14.23
T_{19}	57.8761	14.495	47.7346	16.19
T_{20}	57.8441	14.427	47.7933	16.12
T_{21}	47.8953	12.171	39.3154	13.46
T_{22}	47.8953	12.171	39.3154	13.59
T_{23}	71.2908	18.878	58.5175	20.1
T_{24}	71.2908	18.878	58.5175	21.02
T_{25}	78.4958	19.314	64.5131	20.56
T_{26}	78.4972	19.314	64.5131	21.62
T_{27}	89.745	21.679	74.1517	24.23
T_{28}	73.3149	17.906	60.1785	19.39

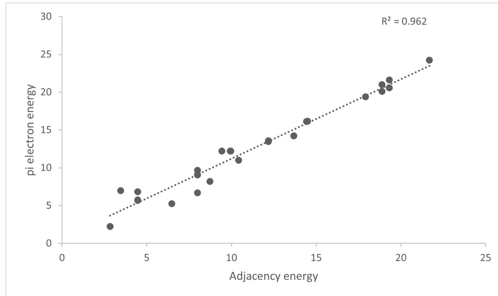
Table 4. Parameters of the linear model. Here R^2, R, SE, F and SF are the dettermination coefficient, correlation coefficient, standard error, F-test and significance factor respectively.

Energy()	R^2	R	SE	F	SF
$E_{ES}(G)$	0.9654	0.9825	1.0989	726.979	1.56×10^{-20}
$E_{SO}(G)$	0.9611	0.9803	3.8846	643.515	7.211×10^{-20}
$E(G)$	0.9629	0.9812	1.0623	675.681	3.91×10^{-20}

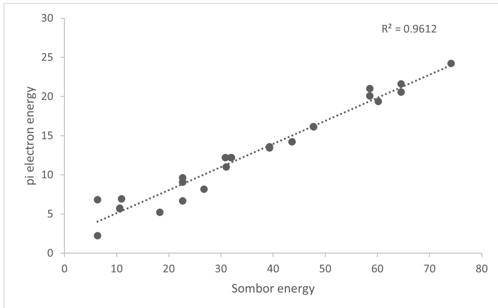
correlation with total π-electron energy ($R = 0.9825$, $R^2 = 0.9654$). This is also illustrated in Figure 1, which highlights the predictive strength of Euler Sombor energy. The following molecules containing hetero atoms are used to obtain the correlation of Euler Sombor energy with total π-electron energy [9].



(a) Correlation graph of $E_{ES}(G)$ with the total π electron energy



(b) Correlation graph of $E(G)$ with the total π electron energy



(c) Correlation graph of $SE(G)$ with the total π electron energy

Figure 1. Correlation graphs of different graph energies with the total π-electron energy: (a) Euler Sombor energy $E_{ES}(G)$, (b) adjacency energy $E(G)$, and (c) Sombor energy $SE(G)$.

8. Conclusion

In this work, we introduced the Euler Sombor matrix and the corresponding Euler Sombor energy of a graph. We computed the Euler Sombor energy for several standard graph classes and established bounds for both the spectral radius and the Euler Sombor energy. Our statistical analysis showed that Euler Sombor energy E_{ES} exhibits stronger correlations with the total π-electron energy of heteroatomic systems compared to adjacency energy $E(G)$ and Sombor energy $E_{SO}(G)$. These results demonstrate that Euler Sombor energy $E_{ES}(G)$ provides an effective spectral parameter in chemical graph theory and may serve as a useful tool for modeling molecular structures and studying graph invariants in mathematical chemistry.

As a continuation of this research, several possible directions for future work can be considered. Additional studies on Euler Sombor energy for directed graphs may provide deeper insights. The problem becomes more challenging when weights are assigned to the edges of the graph. Determining the graphs that maximize and minimize the Euler Sombor energy also remains an open problem. Furthermore, the Euler Sombor energy for various graph operations, such as corona products, tensor graph products, and lexicographic graph products, is still unexplored.

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