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On a new variant Sombor matrix and energy of total transformation graphs of regular graphs

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Abstract

In this study, we introduce a new variant of the Sombor matrix, denoted by $\mathcal{NS}o(\zeta)$, associated with a simple graph $\zeta(\mathcal{V}, \mathcal{E})$, where the (i, j)-entry for $i \neq j$ is equal to $\sqrt{(\varsigma_i^2 + \varsigma_j^2)}$ and 0 in the either case, where ς_i represents the degree of i^{th} vertex. The Sombor energy $E_{\mathcal{NS}o}(\zeta)$ represents the sum of the absolute values of the eigenvalues of the Sombor matrix. The spectrum and $E_{\mathcal{NS}o}(\zeta)$ is obtained for total transformation graphs ζ^{xyz} of regular graphs. Also as an application, a set of 26 hetero atoms with total π-electron energy is analyzed, and a regression analysis is performed using $E_{\mathcal{NS}o}(\zeta)$ for the hetero atoms. The linear regression model yields a correlation coefficient of $r = 0.982$.

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1. Introduction

Let $\zeta(\mathcal{V}, \mathcal{E})$ be a simple graph, with $|\mathcal{V}| = \rho$ and $|\mathcal{E}| = \varrho$. The degree of a vertex $v_i \in \mathcal{V}$ is the count of edges connected to v_i denoted by ς_i. The maximum(minimum) vertex and edge degree of a graph is denoted by $\Delta(\delta)$ and $\Delta'(\delta')$ respectively. A graph ζ is said to be complete if $\Delta = \delta = \rho - 1$ denoted by K_ρ. If a vertex set of a graph ζ is partitioned into two sets say $|\mathcal{M}| = \upsilon$ and $|\mathcal{N}| = \nu$ (partite sets) such that every edge meet both $\mathcal{M}$ and $\mathcal{N}$ then the graph is bipartite graph. If every vertex of $\mathcal{M}$ is adjacent to every vertex of $\mathcal{N}$ then the graph is complete bipartite graph denoted as $K_{\upsilon,\nu}$. The graph $K_{1,\rho-1}$ is called as star graph denoted by $\mathcal{S}_\rho$ and the graph $K_{\nu,\nu}$ is called equi-bipartite graph. The complement of a graph ζ denoted by $\overline{\zeta}$ is a graph defined on same vertex set as of ζ such that if two vertices are adjacent in $\overline{\zeta}$, then they are not adjacent in ζ. For more terminologies refer the following [4].

A square matrix $\mathcal{A}(\zeta)$ of order ρ is an adjacency matrix of ζ whose (i, j)-entry is 1 if the vertex v_i is adjacent to v_j, and is 0 otherwise. The energy $E(\zeta)$ of a graph ζ is the sum of the absolute values of eigenvalues of $\mathcal{A}(\zeta)$. This quantity is introduced in [7]. Suppose $\kappa_1 \geq \kappa_2 \geq \ldots \geq \kappa_\rho$ are the eigenvalues of the adjacency matrix $\mathcal{A}(\zeta)$ then the energy of the graph ζ is given by

$$E = E(\zeta) = \sum_{i=1}^{\rho} |\kappa_i| \tag{1}$$

Ramane, Revankar and Patil, [9] proposed the degree sum matrix of graph ζ, denoted as $DS(\zeta)$, further obtained bounds on degree sum energy. Also Basavanagoud and Chitra, [1] proposed degree square sum matrix and obtained bounds on degree square sum energy. Motivated by this a new variant of Sombor matrix $\mathcal{NS}o(\zeta)$ is defined as if $i \neq j$ its (i, j)-entry is equal to $\sqrt{\varsigma_i^2 + \varsigma_j^2}$ and 0 in the either case. Here ς_i represents the degree of v_i, for every $i = 1,2,\ldots,\rho$.

The characteristic polynomial for $\mathcal{NS}o(\zeta)$ is defined as $\psi(\zeta,\eta) = det(\eta I - \mathcal{NS}o(\zeta)) = |\eta I - \mathcal{NS}o(\zeta)| = \eta^\rho + r_1\eta^{\rho-1} + \ldots + r_\rho = 0$, here I

represents the identity matrix of order ρ. Since $\mathcal{NS}o(\zeta)$ is a real symmetric matrix, the roots of $\psi(\zeta,\eta)=0$ are real and it can written in descending order as $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_\rho$, with respective multiplicities $\tau_1, \tau_2, \ldots, \tau_\rho$ then the spectrum can be written as,

$$Spectra(\mathcal{NS}o(\zeta)) = \begin{pmatrix} \eta_1 & \eta_2 & \cdots & \eta_\rho \\ \tau_1 & \tau_2 & \cdots & \tau_\rho \end{pmatrix}$$

where η_1 is the spectral radius. Sombor energy of ζ is given as,

$$E_{\mathcal{NS}o}(\zeta) = \sum_{i=1}^{\rho} |\eta_i| \tag{2}$$

For recent research on graph energy, see references [1], [5], [6], [8], [9], [13].

In 2001, Wu and Meng [14] introduced a novel transformation, denoted by ζ^{xyz}, which extends the idea of the total graph. This transformation, known as the total transformation graph, is defined as follows.

Definition 1.1: For graph $\zeta(\mathcal{V},\mathcal{E})$ on $\rho \geq 3$ vertices and x, y, z be three variables taking values $+$ or $-$. Total transformation graph ζ^{xyz} for ζ, is a graph having $\mathcal{V}(\zeta) \cup \mathcal{E}(\zeta)$ as a vertex set and for $u, v \in \mathcal{V}(\zeta) \cup \mathcal{E}(\zeta)$, u and v are adjacent in ζ^{xyz} if and only if

- $u, v \in \mathcal{V}(\zeta)$, u and v are adjacent in ζ if $x=+$ and are nonadjacent in ζ if $x=-$.
- $u, v \in \mathcal{E}(\zeta)$, u and v are adjacent in ζ if $y=+$ and are nonadjacent in ζ if $y=-$.
- $u \in \mathcal{V}(\zeta)$ and $v \in \mathcal{E}(\zeta)$, u and v are incident in ζ if $z=+$ and are nonincident in ζ if $z=-$.

The eight graphical transformations for a given graph ζ, are ζ^{+++}, ζ^{-++}, ζ^{+-+}, ζ^{++-} and their complements ζ^{---}, ζ^{+--}, ζ^{-+-}, ζ^{--+}. Many other transformation graphs are discussed in [11], and generalized transformation graphs are put forwarded in [12].

2. Preliminary results

Proposition 2.1: [3] For a s-regular graph $\zeta(\mathcal{V},\mathcal{E})$, let $u, v \in \mathcal{V}(\zeta)$ and $e = uv \in \mathcal{E}$. Then the degrees of corresponding vertices in ζ^{xyz} are:

- $\varsigma_{\zeta^{+++}}(v) = 2s$ and $\varsigma_{\zeta^{+++}}(e) = 2s$
- $\varsigma_{\zeta^{++-}}(v) = \varrho$ and $\varsigma_{\zeta^{++-}}(e) = 2s + \rho - 4$
- $\varsigma_{\zeta^{+-+}}(v) = 2s$ and $\varsigma_{\zeta^{+-+}}(e) = \rho - 2s + 3$
- $\varsigma_{\zeta^{-++}}(v) = \rho - 1$ and $\varsigma_{\zeta^{-++}}(e) = 2s$
- $\varsigma_{\zeta^{---}}(v) = \rho + \rho - 2s - 1$ and $\varsigma_{\zeta^{---}}(e) = \rho + \rho - 2s - 1$
- $\varsigma_{\zeta^{--+}}(v) = \rho - 1$ and $\varsigma_{\zeta^{--+}}(e) = \varrho - 2s + 3$
- $\varsigma_{\zeta^{-+-}}(v) = \rho + \varrho - 2s - 1$ and $\varsigma_{\zeta^{-+-}}(e) = 2s + \rho - 4$
- $\varsigma_{\zeta^{+--}}(v) = \varrho$ and $\varsigma_{\zeta^{+--}}(e) = \rho + \varrho - 2s - 1$

Lemma 2.2: [3] If a and b are scalars then,

$$|aI + b(J-I)|_{\rho\times\rho} = \begin{vmatrix} a & b & \cdots & b \\ b & a & \cdots & b \\ \vdots & \vdots & \ddots & \vdots \\ b & b & \cdots & a \end{vmatrix} = (a-b)^{\rho-1}[a+(\rho-1)b],$$

where I denotes the identity matrix and J represents the matrix with all entries equal to 1.

Lemma 2.3: [10] *If a, b, c and d are real numbers then the characteristic polynomial of the determinant is given by*

$$\begin{vmatrix} (\lambda+a)I_n - aJ_n & -cJ_{n\times m} \\ -dJ_{m\times n} & (\lambda+b)I_m - bJ_m \end{vmatrix}_{n+m\times n+m}$$

is given by $(\lambda+a)^{n-1}(\lambda+b)^{m-1}\{[\lambda-(n-1)a][\lambda-(m-1)b]-nmcd\}$. *Also if $\lambda_1, \lambda_2, \ldots, \lambda_{n+m}$ are eigenvalues of the same determinant then the eigenvalues are given by*

$$Spectra = \begin{cases} -a & (n-1)times \\ -b & (m-1)times \\ [a(n-1)+b(m-1) \ \pm & \sqrt{[a(n-1)-b(m-1)]^2+4mcd}/2 \end{cases}$$

Further,

Case (i): If $(n-1)(m-1)ab \leq nmcd$,

$$\lambda_1 = \sum_{i=2}^{n+m} |\lambda_i| = [a(n-1)+b(m-1) + \sqrt{[a(n-1)-b(m-1)]^2+4nmcd}]/2$$

Case (ii): If $(n-1)(m-1)ab > nmcd$,

$$\lambda_1 + \lambda_2 = \sum_{i=3}^{n+m} |\lambda_i| = a(n-1)+b(m-1)$$

Where,

$$\lambda_1 = \sum_{i=2}^{n+m} |\lambda_i| = [a(n-1)+b(m-1) + \sqrt{[a(n-1)-b(m-1)]^2+4nmcd}]/2$$

and

$$\lambda_2 = \sum_{i=2}^{n+m} |\lambda_i| = [a(n-1)+b(m-1) - \sqrt{[a(n-1)-b(m-1)]^2+4nmcd}]/2$$

3. Main Results

In this section we present the computation of Sombor energy for total transformation graphs. Given a graph ζ with ρ vertices and $\varrho = \frac{\rho s}{2}$ edges, the total transformation graph ζ^{xyz} consists of $\rho + \varrho$ vertices. We denote the vertices by v_i, where $i = 1,2,\ldots,\rho$ and the edges by e_j, where $j = 1,2,\ldots,\varrho$.

Theorem 3.1: *For any s-regular graph $\zeta(\rho,\varrho)$, we have*

$$E_{\mathcal{NS}o}(\zeta^{+++}) = \sqrt{2}s(\rho s + 2\rho - 2)$$

Proof: As $\zeta(\rho,\varrho)$ is an s-regular graph, according to the definition of ζ^{+++} and Lemma 2.2, the characteristic polynomial associated with the Sombor matrix satisfies $|\eta I - \mathcal{NS}o(\zeta^{+++})| = 0$.

Now,

$$|\eta I - \mathcal{NS}o(\zeta^{+++})| = \begin{vmatrix} \eta & -\sqrt{2}s & -\sqrt{2}s & \cdots & -\sqrt{2}s & -\sqrt{2}s \\ -\sqrt{2}s & \eta & -\sqrt{2}s & \cdots & -\sqrt{2}s & -\sqrt{2}s \\ -\sqrt{2}s & -\sqrt{2}s & \eta & \cdots & -\sqrt{2}s & -\sqrt{2}s \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -\sqrt{2}s & -\sqrt{2}s & -\sqrt{2}s & \cdots & \eta & -\sqrt{2}s \\ -\sqrt{2}s & -\sqrt{2}s & -\sqrt{2}s & \cdots & -\sqrt{2}s & \eta \end{vmatrix}_{(\rho+\varrho)\times(\rho+\varrho)}$$

By using Lemma 2.2,

$$|\eta I - \mathcal{NS}o(\zeta^{+++})| = (\eta + \sqrt{2}s)^{\rho+\varrho-1}[\eta - (\rho+\varrho-1)\sqrt{2}s] = 0$$

$$spectra(\mathcal{NS}o(\zeta^{+++})) = \begin{pmatrix} -\sqrt{2}s & \sqrt{2}s(\rho+\varrho-1) \\ (\rho+\varrho-1) & 1 \end{pmatrix}$$

Hence

$$E_{\mathcal{NS}o}(\zeta^{+++}) = 2\sqrt{2}s(\rho+\varrho-1) = \sqrt{2}s(\rho s + 2\rho - 2)$$

Theorem 3.2: *For any s-regular graph $\zeta(\rho,\varrho)$, we have*

$$E_{\mathcal{NS}o}(\zeta^{---}) = \frac{1}{\sqrt{2}}(\rho s + 2\rho - 2)(2\rho + \rho s - 4s - 2)$$

Proof: As $\zeta(\rho,\varrho)$ is an s-regular graph, according to the definition of ζ^{---} and Lemma 2.2, the characteristic polynomial associated with the Sombor matrix satisfies $|\eta I - \mathcal{NS}o(\zeta^{---})| = 0$.

Now,

$$|\eta I - \mathcal{NS}o(\zeta^{---})| = |\eta I - \sqrt{2}(\rho+\varrho-2s-1)(J-I)|_{(\rho+\varrho)\times(\rho+\varrho)}$$

By using Lemma 2.2,

$$|\eta I - \mathcal{NS}o(\zeta^{---})| = (\eta + \sqrt{2}(\rho+\varrho-2s-1))^{\rho+\rho-1}$$
$$[\eta - (\rho+\varrho-1)\sqrt{2}(\rho+\varrho-2s-1)] = 0$$

$$spectra(\mathcal{NS}o(\zeta^{---})) = \begin{pmatrix} -\sqrt{2}(\rho+\varrho-2s-1) & (\rho+\varrho-1)\sqrt{2}(\rho+\varrho-2s-1) \\ (\rho+\varrho-1) & 1 \end{pmatrix}$$

Hence

$$E_{\mathcal{NS}o}(\zeta^{---}) = 2\sqrt{2}(\rho+\varrho-1)(\rho+\varrho-2s-1)$$
$$= \frac{1}{\sqrt{2}}(\rho s+2\rho-2)(2\rho+\rho s-4s-2)$$

Theorem 3.3: *For any s-regular graph $\zeta(\rho,\varrho)$, we have*

$$E_{\mathcal{NS}o}(\zeta^{++-}) = \sqrt{2}\varrho(\rho-1)+\sqrt{2}(\varrho-1)(2s+\rho-4)$$
$$+\sqrt{[\sqrt{2}\varrho(\rho-1)-\sqrt{2}(\varrho-1)(2s+\rho-4)]^2+4\rho\varrho[\varrho^2+(2s+\rho-4)^2]}$$

Proof: As $\zeta(\rho,\varrho)$ is an s-regular graph, according to the definition of ζ^{++-} and Lemma 2.3, the characteristic polynomial associated with the Sombor matrix satisfies $|\eta I-\mathcal{NS}o(\zeta^{++-})|=0$.

Now, $|\eta I-\mathcal{NS}o(\zeta^{++-})| =$

$$\begin{vmatrix}
\eta & -\sqrt{2}\varrho & \cdots & -\sqrt{2}\varrho & -\sqrt{\varrho^2+(2s+\rho-4)^2} & \cdots & \cdots & -\sqrt{\varrho^2+(2s+\rho-4)^2}\\
-\sqrt{2}\varrho & \eta & \cdots & -\sqrt{2}\varrho & -\sqrt{\varrho^2+(2s+\rho-4)^2} & \cdots & \cdots & -\sqrt{\varrho^2+(2s+\rho-4)^2}\\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots\\
-\sqrt{2}\varrho & -\sqrt{2}\varrho & \cdots & \eta & -\sqrt{\varrho^2+(2s+\rho-4)^2} & \cdots & \cdots & \sqrt{\varrho^2+(2s+\rho-4)^2}\\
-\sqrt{\varrho^2+(2s+\rho-4)^2} & \cdots & \cdots & -\sqrt{\varrho^2+(2s+\rho-4)^2} & \eta & & \cdots & -\sqrt{2}(2s+\rho-4)\\
-\sqrt{\varrho^2+(2s+\rho-4)^2} & \cdots & \cdots & -\sqrt{\varrho^2+(2s+\rho-4)^2} & -\sqrt{2}(2s+\rho-4) & & \cdots & -\sqrt{2}(2s+\rho-4)\\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots\\
-\sqrt{\varrho^2+(2s+\rho-4)^2} & \cdots & \cdots & -\sqrt{\varrho^2+(2s+\rho-4)^2} & -\sqrt{2}(2s+\rho-4) & & \cdots & \eta
\end{vmatrix}_{(\rho+\varrho)\times(\rho+\varrho)}$$

i.e.,

$$|\eta I-\mathcal{NS}o(\zeta^{++-})| =$$
$$\begin{vmatrix}
(\eta I-\sqrt{2}\varrho(J-I))_{\rho\times\rho} & (-\sqrt{\varrho^2+(2s+\rho-4)^2})J_{\rho\times\varrho}\\
(-\sqrt{\varrho^2+(2s+\rho-4)^2})J_{\varrho\times\rho} & (\eta I-\sqrt{2}(2s+\rho-4)(J-I))_{\varrho\times\varrho}
\end{vmatrix}$$

Expanding using the Lemma 2.3 we get

$$|\eta I-\mathcal{NS}o(\zeta^{++-})| = (\eta+\sqrt{2}\varrho)^{\rho-1}(\eta+\sqrt{2}(2s+\rho-4))^{\varrho-1}[\eta-(\rho-1)$$
$$\sqrt{2}\varrho]\,[\eta-(\varrho-1)\sqrt{2}(2s+\rho-4)]-\rho\varrho[\varrho^2+(2s+\rho-4)^2]$$

$$|\eta I-\mathcal{NS}o(\zeta^{++-})| = (\eta+\sqrt{2}\varrho)^{\rho-1}(\eta+\sqrt{2}(2s+\rho-4))^{\rho-1}[\eta^2$$
$$-\eta[(\rho-1)\sqrt{2}\varrho+ (\varrho-1)\sqrt{2}(2s+\rho-4)]$$
$$+2\varrho(\rho-1)(\varrho-1)(2s+\rho-4)$$
$$-\rho\varrho[\varrho^2+(2s+\rho-4)^2]$$

$$spectra(\mathcal{NS}o(\zeta^{++-})) =$$
$$\begin{cases}
-\sqrt{2}\varrho & (\rho-1)times\\
-\sqrt{2}(2s+\rho-4) & (\rho-1)times\\
[\sqrt{2}\varrho(\rho-1)+\sqrt{2}\rho(\varrho-1)(2s+\rho-4)\pm & \\
\sqrt{[\sqrt{2}\varrho(\rho-1)-\sqrt{2}\rho(\varrho-1)(2s+\rho-4)]^2+4\rho\varrho[\varrho^2+(2s+\rho-4)^2]}]/2 &
\end{cases}$$

In this,

$$\eta_1 = [\sqrt{2}\varrho(\rho-1)+\sqrt{2}(\varrho-1)(2s+\rho-4) + \sqrt{[\sqrt{2}\varrho(\rho-1)-\sqrt{2}(\varrho-1)(2s+\rho-4)]^2+4\rho\varrho[\varrho^2+(2s+\rho-4)^2]}]/2$$

is the largest and only one positive eigenvalue.

Hence

$$E_{\mathcal{NS}o}(\zeta^{++-}) = 2\eta_1 = \sqrt{2}\varrho(\rho-1)+\sqrt{2}(\varrho-1)(2s+\rho-4) + \sqrt{[\sqrt{2}\varrho(\rho-1)-\sqrt{2}(\varrho-1)(2s+\rho-4)]^2+4\rho\varrho[\varrho^2+(2s+\rho-4)^2]}$$

Theorem 3.4: *For any s-regular graph $\zeta(\rho,\varrho)$, we have*

$$E_{\mathcal{NS}o}(\zeta^{--+}) = \sqrt{2}(\rho-1)^2+2\rho\varrho(\rho-1)(\varrho-2s+3) + \sqrt{[\sqrt{2}(\rho-1)^2-\sqrt{2}(\varrho-1)(\varrho-2s+3)]^2+4\rho\varrho[(\rho-1)^2+(\varrho-2s+3)^2]}$$

Proof: As $\zeta(\rho,\varrho)$ is an s-regular graph, according to the definition of ζ^{--+} and Lemma 2.3, the characteristic polynomial associated with the Sombor matrix satisfies $|\eta I-\mathcal{NS}o(\zeta^{--+})|=0$. i.e.,

$$|\eta I-\mathcal{NS}o(\zeta^{--+})| = \begin{vmatrix} (\eta I-\sqrt{2}(\rho-1)(J-I))_{\rho\times\rho} & (-\sqrt{(\rho-1)^2+(\varrho-2s+3)^2})J_{\rho\times\varrho} \\ (-\sqrt{(\rho-1)^2+(\varrho-2s+3)^2})J_{\varrho\times\rho} & (\eta I-\sqrt{2}(\varrho-2s+3)(J-I))_{\varrho\times\varrho} \end{vmatrix}$$

Expanding using the Lemma 2.3 we get

$$|\eta I-\mathcal{NS}o(\zeta^{--+})| = (\eta+\sqrt{2}(\rho-1))^{\rho-1}(\eta+\sqrt{2}(\varrho-2s+3))^{\varrho-1}[\eta-\sqrt{2}(\rho-1)^2][\eta - (\varrho-1)\sqrt{2}(\varrho-2s+3)]-\rho\varrho[(\rho-1)^2+(\varrho-2s+3)^2]$$

$$|\eta I-\mathcal{NS}o(\zeta^{--+})| = (\eta+\sqrt{2}(\rho-1))^{\rho-1}(\eta+\sqrt{2}(\varrho-2s+3))^{\varrho-1}[\eta^2-\eta[\sqrt{2}(\rho-1)^2 + (\varrho-1)\sqrt{2}(\varrho-2s+3)]+2(\rho-1)^2(\varrho-1)(\varrho-2s+3) - \rho\varrho[(\rho-1)^2+(\varrho-2s+3)^2]$$

$$spectra(\mathcal{NS}o(\zeta^{--+})) = \begin{cases} -\sqrt{2}(\rho-1) & (\rho-1)times \\ -\sqrt{2}(\rho-2s+3) & (\varrho-1)times \\ [\sqrt{2}(\rho-1)^2+\sqrt{2}(\varrho-2s+3) \pm \\ \sqrt{[\sqrt{2}(\rho-1)^2-\sqrt{2}(\varrho-1)(\varrho-2s+3)]^2+4\rho\varrho[(\rho-1)^2+(\varrho-2s+3)^2]}]/2 & \end{cases}$$

In this,

$$\eta_1 = [\sqrt{2}(\rho-1)^2 + 2\rho\varrho(\rho-1)(\varrho-2s+3)$$
$$+\sqrt{[\sqrt{2}(\rho-1)^2 - \sqrt{2}(\varrho-1)(\varrho-2s+3)]^2 + 4\rho\varrho[(\rho-1)^2 + (\varrho-2s+3)^2]}]/2$$

is the largest and only one positive eigenvalue.

Hence

$$E_{\mathcal{NS}o}(\zeta^{--+}) = 2\eta_1 = \sqrt{2}(\rho-1)^2 + 2\rho\varrho(\rho-1)(\varrho-2s+3)$$
$$+\sqrt{[\sqrt{2}(\rho-1)^2 - \sqrt{2}(\varrho-1)(\rho-2s+3)]^2 + 4\rho\varrho[(\rho-1)^2 + (\varrho-2s+3)^2]}$$

Theorem 3.5: *For any s-regular graph $\zeta(\rho,\varrho)$, we have*

$$E_{\mathcal{NS}o}(\zeta^{+--}) = \sqrt{2}\varrho(\rho-1) + \sqrt{2}(\varrho-1)(\rho+\varrho-2s-1)$$
$$+\sqrt{[\sqrt{2}\varrho(\rho-1) - \sqrt{2}(\varrho-1)(\rho+\varrho-2s-1)]^2 + 4\rho\varrho[\varrho^2 + (\rho+\varrho-2s-1)^2]}$$

Proof: As $\zeta(\rho,\varrho)$ is an s-regular graph, according to the definition of ζ^{+--} and Lemma 2.3, the characteristic polynomial associated with the Sombor matrix satisfies $|\eta I - \mathcal{NS}o(\zeta^{+--})| = 0$. i.e.,

$$|\eta I - \mathcal{NS}o(\zeta^{+--})| =$$
$$\begin{vmatrix} (\eta I - \sqrt{2}\varrho(J-I))_{\rho\times\rho} & (-\sqrt{\varrho^2 + (\rho+\varrho-2s-1)^2})J_{\rho\times\varrho} \\ (-\sqrt{\varrho^2 + (\rho+\varrho-2s-1)^2})J_{\varrho\times\rho} & (\eta I - \sqrt{2}(\varrho+\rho-2s-1)(J-I))_{\varrho\times\varrho} \end{vmatrix}$$

Expanding using the Lemma 2.3 we get

$$|\eta I - \mathcal{NS}o(\zeta^{+--})| = (\eta+\sqrt{2}\varrho)^{\varrho-1}(\eta+\sqrt{2}(\varrho+\rho-2s-1))^{\rho-1}[\eta-(\rho-1)\sqrt{2}\varrho][\eta$$
$$-(\rho-1)\sqrt{2}(\varrho+\rho-2s-1)] - \rho\varrho[\rho^2 + (\rho+\varrho-2s-1)^2]$$

$$spectra\big(\mathcal{NS}o(\zeta^{+--})\big) =$$
$$\begin{cases} -\sqrt{2}\varrho & (\rho-1)times \\ -\sqrt{2}(\rho+\varrho-2s-1) & (\varrho-1)times \\ [\sqrt{2}\varrho(\rho-1) + \sqrt{2}(\varrho-1)(\rho+\varrho-2s-1) \pm & \\ \sqrt{[\sqrt{2}\varrho(\rho-1) - \sqrt{2}(\varrho-1)(\rho+\varrho-2s-1)]^2 + 4\rho\varrho[\varrho^2 + (\rho+\varrho-2s-1)^2]}]/2 & \end{cases}$$

In this,

$$\eta_1 = [\sqrt{2}\varrho(\rho-1) + \sqrt{2}(\varrho-1)(\rho+\varrho-2s-1)$$
$$+\sqrt{[\sqrt{2}\varrho(\rho-1) - \sqrt{2}(\varrho-1)(\rho+\varrho-2s-1)]^2 + 4\rho\varrho[\varrho^2 + (\rho+\varrho-2s-1)^2]}]/2$$

is the largest and only one positive eigenvalue.

Hence

$$E_{\mathcal{NS}o}(\zeta^{+--}) = 2\eta_1 = \sqrt{2}\varrho(\rho-1) + \sqrt{2}(\varrho-1)(\rho+\varrho-2s-1)$$
$$+\sqrt{[\sqrt{2}\varrho(\rho-1) - \sqrt{2}(\varrho-1)(\rho+\varrho-2s-1)]^2 + 4\rho\varrho[\varrho^2 + (\rho+\varrho-2s-1)^2]}$$

Theorem 3.6: *For any s-regular graph $\zeta(\rho,\rho)$, we have*

$$E_{\mathcal{NS}o}(\zeta^{-++}) = \sqrt{2}(\rho-1)^2 + 2\sqrt{2}s(\varrho-1) + \sqrt{[\sqrt{2}(\rho-1)^2 - 2\sqrt{2}s(\varrho-1)]^2 + 4\rho\varrho[(\rho-1)^2+4s^2]}$$

Proof: As $\zeta(\rho,\varrho)$ is an s-regular graph, according to the definition of ζ^{-++} and Lemma 2.3, the characteristic polynomial associated with the Sombor matrix satisfies $|\eta I - \mathcal{NS}o(\zeta^{-++})| = 0$. i.e.,

$$|\eta I - \mathcal{NS}o(\zeta^{-++})| = \begin{vmatrix} (\eta I - \sqrt{2}(\rho-1)(J-I))_{\rho\times\rho} & (-\sqrt{(\rho-1)^2+(2s)^2})J_{\rho\times\varrho} \\ (-\sqrt{(\rho-1)^2+(2s)^2})J_{\varrho\times\rho} & (\eta I - 2\sqrt{2}s(J-I))_{\varrho\times\varrho} \end{vmatrix}$$

Expanding using the Lemma 2.3 we get

$$|\eta I - \mathcal{NS}o(\zeta^{-++})| = (\eta+\sqrt{2}(\rho-1))^{\rho-1}(\eta+2\sqrt{2}s)^{\varrho-1}[\eta-\sqrt{2}(\rho-1)^2][\eta - (\varrho-1)2\sqrt{2}s] - \rho\varrho[(\rho-1)^2+4s^2]$$

$$spectra(\mathcal{NS}o(\zeta^{-++}))= \begin{cases} -\sqrt{2}(\rho-1) & (\rho-1)times \\ -2\sqrt{2}s & (\varrho-1)times \\ [\sqrt{2}(\rho-1)^2 + 2\sqrt{2}s(\varrho-1) \pm \\ \sqrt{[\sqrt{2}(\rho-1)^2 - 2\sqrt{2}s(\varrho-1)]^2 + 4\rho\varrho[(\rho-1)^2+4s^2]}]/2 \end{cases}$$

In this,

$$\eta_1 = [\sqrt{2}(\rho-1)^2 + 2\sqrt{2}s(\varrho-1) + \sqrt{[\sqrt{2}(\rho-1)^2 - 2\sqrt{2}s(\varrho-1)]^2 + 4\rho\varrho[(\rho-1)^2+4s^2]}]/2$$

is the largest and only one positive eigenvalue.

Hence

$$E_{\mathcal{NS}o}(\zeta^{-++}) = 2\eta_1 = \sqrt{2}(\rho-1)^2 + 2\sqrt{2}s(\varrho-1) + \sqrt{[\sqrt{2}(\rho-1)^2 - 2\sqrt{2}s(\varrho-1)]^2 + 4\rho\varrho[(\rho-1)^2+4s^2]}$$

Theorem 3.7: *For any s-regular graph $\zeta(\rho,\rho)$, we have*

$$E_{\mathcal{NS}o}(\zeta^{+-+}) = 2\sqrt{2}s(\rho-1) + \sqrt{2}(\varrho-2s+3)(\varrho-1) + \sqrt{[2\sqrt{2}s(\rho-1) - \sqrt{2}(\varrho-2s+3)(\varrho-1)]^2 + 4\rho\varrho[4s^2+(\varrho-2s+3)^2]}$$

Proof: As $\zeta(\rho,\rho)$ is an s-regular graph, according to the definition of ζ^{+-+} and Lemma 2.3, the characteristic polynomial associated with the Sombor matrix satisfies $|\eta I - \mathcal{NS}o(\zeta^{+-+})| = 0$. i.e.,

$|\eta I - \mathcal{NS}o(\zeta^{+-+})| =$

$$\begin{vmatrix} (\eta I - 2\sqrt{2}s(J-I))_{\rho\times\rho} & (-\sqrt{(2s)^2+(\varrho-2s+3)^2})J_{\rho\times\varrho} \\ (-\sqrt{(2s)^2+(\varrho-2s+3)^2})J_{\rho\times\rho} & (\eta I - \sqrt{2}(\varrho-2s+3)(J-I))_{\varrho\times\varrho} \end{vmatrix}$$

Expanding using the Lemma 2.3 we get

$|\eta I - \mathcal{NS}o(\zeta^{+-+})| =$

$$(\eta+2\sqrt{2}s)^{\rho-1}(\eta+\sqrt{2}(\varrho-2s+3))^{\varrho-1}[\eta-(\rho-1)2\sqrt{2}s][\eta - (\varrho-1)\sqrt{2}(\varrho-2s+3)] - \rho\varrho[4s^2+(\varrho-2s+3)^2]$$

$spectra(\mathcal{NS}o(\zeta^{+-+})) =$

$$\begin{cases} -2\sqrt{2}s & (\rho-1)times \\ -\sqrt{2}(\varrho-2s+3) & (\varrho-1)times \\ [2\sqrt{2}s(\rho-1)+\sqrt{2}(\varrho-2s+3)(\varrho-1) \pm \\ \sqrt{[2\sqrt{2}s(\rho-1)+\sqrt{2}(\varrho-2s+3)(\varrho-1)]^2+4\rho\rho[4s^2+(\rho-2s+3)^2]}]/2 \end{cases}$$

In this,

$$\eta_1 = [2\sqrt{2}s(\rho-1)+\sqrt{2}(\varrho-2s+3)(\varrho-1) + \sqrt{[2\sqrt{2}s(\rho-1)-\sqrt{2}(\varrho-2s+3)(\varrho-1)]^2+4\rho\varrho[4s^2+(\varrho-2s+3)^2]}]/2$$

is the largest and only one positive eigenvalue.

Hence,

$$E_{\mathcal{NS}o}(\zeta^{+-+}) = 2\eta_1 = 2\sqrt{2}s(\rho-1)+\sqrt{2}(\varrho-2s+3)(\varrho-1) + \sqrt{[2\sqrt{2}s(\rho-1)-\sqrt{2}(\varrho-2s+3)(\varrho-1)]^2+4\rho\varrho[4s^2+(\varrho-2s+3)^2]}$$

Theorem 3.8: *For any s-regular graph $\zeta(\rho,\rho)$, we have*

$$\begin{aligned} E_{\mathcal{NS}o}(\zeta^{-+-}) = {} & \sqrt{2}(\rho+\varrho-2s+1)(\rho-1)+\sqrt{2}(\varrho-1)(\varrho-2s+3) \\ & + [[\sqrt{2}(\rho+\varrho-2s+1)(\rho-1)-\sqrt{2}(\varrho-1)(\varrho-2s+3)]^2 \\ & + 4\rho\varrho[(\rho-1)^2+(\varrho-2s+3)^2]]^{1/2} \end{aligned}$$

Proof. As $\zeta(\rho,\varrho)$ is an s-regular graph, according to the definition of ζ^{-+-} and Lemma 2.3, the characteristic polynomial associated with the Sombor matrix satisfies $|\eta I - \mathcal{NS}o(\zeta^{-+-})| = 0$. i.e.,

$|\eta I - \mathcal{NS}o(\zeta^{-+-})|$

$$= \begin{vmatrix} (\eta I - \sqrt{2}(\rho+\varrho-2s+1)(J-I))_{\rho\times\rho} & (-\sqrt{(\rho-1)^2+(\varrho-2s+3)^2})J_{\rho\times\varrho} \\ (-\sqrt{(\rho-1)^2+(\varrho-2s+3)^2})J_{\varrho\times\rho} & (\eta I - \sqrt{2}(\varrho-2s+3)(J-I))_{\varrho\times\varrho} \end{vmatrix}$$

Expanding using the Lemma 2.3 we get

$$|\eta I - \mathcal{NS}o(\zeta^{-+-})| = (\eta + \sqrt{2}(\rho + \varrho - 2s + 1))^{\rho-1}(\eta + \sqrt{2}(\varrho - 2s + 3))^{\varrho-1}$$
$$[\eta - (\rho - 1)\sqrt{2}(\rho + \varrho - 2s + 1)][\eta - (\varrho - 1)\sqrt{2}(\varrho - 2s + 3)]$$
$$- \rho\varrho[(\rho - 1)^2 + (\varrho - 2s + 3)^2]$$

$$spectra(\mathcal{NS}o(\zeta^{-+-})) =$$
$$\begin{cases} -\sqrt{2}(\rho + \varrho - 2s + 1) & (\rho - 1) times \\ -\sqrt{2}(\varrho - 2s + 3) & (\varrho - 1) times \\ [\sqrt{2}(\rho + \varrho - 2s + 1)(\rho - 1) + \sqrt{2}(\varrho - 1)(\varrho - 2s + 3) \pm & \\ [[\sqrt{2}(\rho + \varrho - 2s + 1)(\rho - 1) - \sqrt{2}(\varrho - 1)(\varrho - 2s + 3)]^2 & \\ +4\rho\rho[(\rho - 1)^2 + (\rho - 2s + 3)^2]]^{1/2}]/2 & \end{cases}$$

In this,

$$\eta_1 = [\sqrt{2}(\rho + \varrho - 2s + 1)(\rho - 1) + \sqrt{2}(\varrho - 1)(\rho - 2s + 3)$$
$$+ [[\sqrt{2}(\rho + \varrho - 2s + 1)(\rho - 1) - \sqrt{2}(\varrho - 1)(\varrho - 2s + 3)]^2$$
$$+ 4\rho\varrho[(\rho - 1)^2 + (\varrho - 2s + 3)^2]]^{1/2}]/2$$

Table 1

Molecules composed of hetero atoms and their total π-electron energy [2] and $E_{\mathcal{NS}o}(\zeta)$

Molecule	Code	Total π-electron energy	$E_{\mathcal{NS}o}(\zeta)$
Venyl chloride like systems	S_1	2.23	7.8949
Butadiene perturbed at C2	S_2	5.66	13.2980
Acrolein like systems	S_3	5.76	13.2980
1, 1-dichloro-ethylene like systems	S_4	6.96	14.1421
Glyoxal like and 1, 2-dichloro-ethylene like systems	S_5	6.82	13.2980
Pyrrole like systems	S_6	5.23	22.6274
Pyridine like systems	S_7	6.69	28.2842
Pyridazine like systems	S_8	9.06	28.2842
Pyrimidine like systems	S_9	9.10	28.2842
Pyrazine like systems	S_{10}	9.07	28.2842
S-Triazene like systems	S_{11}	9.65	28.2842
Aniline like systems	S_{12}	8.19	34.9870
O-phenylene-diamine like systems	S_{13}	12.21	41.7170
m-phenylene-diamine like systems	S_{14}	12.22	42.9786
p-phenylene-diamine like systems	S_{15}	12.21	41.7170
Benzaldehyde like systems	S_{16}	11.00	40.6817
Quinoline like systems	S_{17}	14.23	56.7858
Iso-quinoline like systems	S_{18}	14.23	56.7858
1-Naphthalein like systems	S_{19}	16.15	63.6301
2-Naphthalein like systems	S_{20}	16.12	63.6301
Iso-indole like systems	S_{21}	13.46	48.8959
Indole like systems	S_{22}	13.59	48.8959
Benzylidine-aniline like systems	S_{23}	20.10	80.9168
Azobenzene like systems	S_{24}	21.02	80.9168
Acridine like systems	S_{25}	20.56	85.5335
Phenazine like systems	S_{26}	21.62	85.5335

is the largest and only one positive eigenvalue.

Hence

$$E_{\mathcal{N}So}(\zeta^{-+-}) = 2\eta_1 = \sqrt{2}(\rho+\varrho-2s+1)(\rho-1)+\sqrt{2}(\varrho-1)(\varrho-2s+3) + [[\sqrt{2}(\rho+\varrho-2s+1)(\rho-1)-\sqrt{2}(\varrho-1)(\varrho-2s+3)]^2 + 4\rho\varrho[(\rho-1)^2+(\varrho-2s+3)^2]]^{1/2}$$

4. Applications of a new variant Sombor energy $E_{\mathcal{N}So}(\zeta)$

This section focuses on a dataset of total π-electron energies corresponding to 26 different heteroatoms, and the respective $E_{\mathcal{N}So}(\zeta)$ is calculated for each atom by constructing its molecular graph structure. The following total π-electron energy [2] and the $E_{\mathcal{N}So}(\zeta)$ for 26 hetero items are listed in Table 1. Further the correlation coefficient r between the total π-electron energy and $E_{\mathcal{N}So}(\zeta)$ is analysed which comes out to be $r = 0.982$, and the graph for linear regression model is depicted in Figure 1.

The linear regression model is given by

$$\text{total } \pi\text{-electron energy } = a(E_{\mathcal{N}So}(\zeta)) + b$$

The linear regression model of total π-electron energy with $E_{\mathcal{N}So}(\zeta)$ is

$$\text{total } \pi\text{-electron energy} = 0.220(\pm 0.009)(E_{\mathcal{N}So}(\zeta)) + 2.355(\pm 0.420)$$

$$n = 26, r = 0.982, F = 640.581, SF = 1.031$$

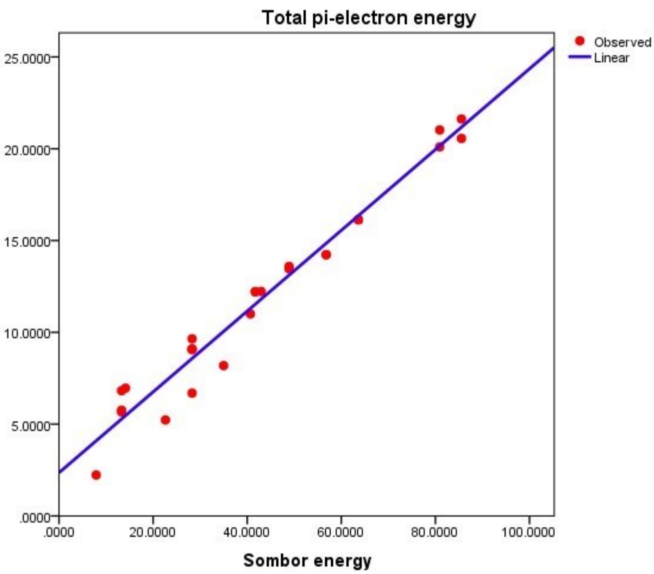

Figure 1
Linear regression model of total π-electron energy with $E_{\mathcal{N}So}(\zeta)$

5. Conclusion

In this paper, a novel variant of the Sombor matrix, denoted by $\mathcal{NS}o(\zeta)$, is defined such that for $i \neq j$, its (i,j)-entry is equal to $\sqrt{\varsigma_i^2 + \varsigma_j^2}$ and 0 in the either case. $E_{\mathcal{NS}o}(\zeta)$ is obtained for total transformation graphs ζ^{xyz} of regular graphs. Also as an application, a collection of 26 hetero atoms, along with their total π-electron energy, is examined, and a regression analysis is conducted using $E_{\mathcal{NS}o}(\zeta)$ for these hetero atoms. The linear regression model yields a correlation coefficient of $r = 0.982$.

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