



On a New Variant Sombor Matrix and Energy of Total Transformation Graphs of Regular Graphs

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ABSTRACT: In this paper, we study the spectral properties of a new variant of Sombor matrix $\mathcal{NSo}(G)$ for simple graph G . The $\mathcal{NSo}(G)$ is defined as, for $i \neq j$ its (i, j) -entry is equal to $\sqrt{d_i^2 + d_j^2}$ and 0 otherwise, where d_i represents the degree of i^{th} vertex. Explicit expressions for the spectrum, the spectral radius η_1 and the Sombor energy $E_{\mathcal{NSo}}(G)$ are obtained for total transformation graphs G^{xyz} of regular graphs using the relation $E_{\mathcal{NSo}}(G) = 2\eta_1$. Also as an application, a set of 26 hetero atoms with total π -electron energy is analyzed, and a regression analysis is performed using $E_{\mathcal{NSo}}(G)$ for the hetero atoms. The linear regression model yields a correlation coefficient of $r = 0.982$.

Keywords: Sombor matrix, Sombor energy, spectrum, total transformation graphs.

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1. Introduction

Let $G = (V, E)$ be a simple graph, where $V(G)$ denotes the vertex set with $|V(G)| = n$ and $E(G)$ denotes the edge set with $|E(G)| = m$. For a vertex $v_i \in V(G)$, the degree of v_i , denoted by d_i , is the number of edges incident with v_i . The maximum and minimum degrees among all vertices of G are denoted by Δ and δ , respectively, while the maximum and minimum degrees among all edges are denoted by Δ' and δ' . A graph G is called a complete graph if every pair of distinct vertices is adjacent. In this case, each vertex has degree $n - 1$, and the graph is denoted by K_n . A graph G is said to be bipartite if its vertex set can be divided into two disjoint subsets M and N , with $|M| = p$ and $|N| = q$, such that every edge joins a vertex of M to a vertex of N . If every vertex in M is adjacent to every vertex in N , then G is called a complete bipartite graph and is denoted by $K_{p,q}$. The complete bipartite graph $K_{1,n-1}$ is known as a star graph and is denoted by S_n . Moreover, when $p = q$, the graph $K_{p,p}$ is referred to as an equi-bipartite graph. A graph G is called s -regular, if every vertex of G has the same degree s . The complement of a graph G , denoted by \bar{G} , is the graph defined on the same vertex set as G in which two distinct vertices are adjacent if and only if they are not adjacent in G . The Petersen graph is a well-known cubic (3-regular) graph consisting of 10 vertices and 15 edges.

Spectral graph theory provides powerful tools for studying structural properties of graphs using matrices and their eigenvalues. Among various graph matrices, the adjacency matrix has been extensively studied, with the associated graph energy, introduced by I. Gutman [3], playing a significant role in chemical graph theory and related fields. In recent years, numerous alternative matrices and their energies have been explored to capture different structural and topological features of graphs.

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Notable examples include the extended adjacency matrix [17], the edge-weighted matrix [11], the Randić matrix [4], and the arithmetic-geometric matrix [7]. The Sombor matrix, derived from the Sombor index, has also been investigated for its spectral properties and energy [18,13]. Other variants, such as the degree sum matrix [8], degree square sum matrix [1], common neighbourhood matrix [15], eccentricity sum matrix [10], combined degree sum matrix [2], and degree sum exponent distance matrix [12], have gained attention due to their applications in chemical graph theory, QSPR analysis, and network analysis.

Motivated by these studies, a new variant of the Sombor matrix, denoted by $\mathcal{NSo}(G)$, has been introduced in [14]. For a simple graph G with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and vertex degrees d_i , the (i, j) -entry of $\mathcal{NSo}(G)$ is defined as

$$\mathcal{NSo}(G)_{ij} = \begin{cases} \sqrt{d_i^2 + d_j^2}, & i \neq j, \\ 0, & i = j. \end{cases}$$

The characteristic polynomial for $\mathcal{NSo}(G)$ is defined as $\psi(G, \eta) = |\eta I - \mathcal{NSo}(G)| = \eta^n + \vartheta_1 \eta^{n-1} + \dots + \vartheta_n$, here I represents the identity matrix of order n . Since $\mathcal{NSo}(G)$ is a real symmetric matrix, the roots of $\psi(G, \eta) = 0$ are real and it can be written in descending order as $\eta_1 \geq \eta_2 \geq \dots \geq \eta_n$. The spectral radius η_1 is defined as the absolute value of the largest eigenvalue, and the Sombor energy $E_{\mathcal{NSo}}(G)$ is the sum of the absolute values of all eigenvalues. For certain classes of graphs, it has been shown that $E_{\mathcal{NSo}}(G) = 2\eta_1$.

The paper is structured as follows. In Section 2, we recall necessary preliminaries and definitions related to $\mathcal{NSo}(G)$ and total transformation graphs. Section 3 presents preliminary results and lemmas essential for our computations. Section 4 lists auxiliary results for standard graphs, while Section 5 contains the spectral analysis and QSPR applications.

Example: Let G be a simple graph as shown in the Figure 1.

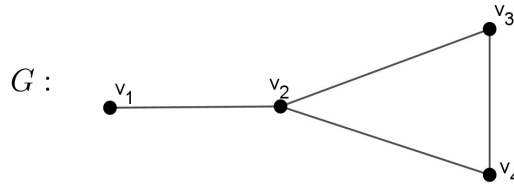


Figure 1: Simple graph G .

The degree of each vertex of G is $d_1 = 1$, $d_2 = 3$, $d_3 = 2$, $d_4 = 2$. A new variant of Sombor matrix $\mathcal{NSo}(G)$ of G is

$$\mathcal{NSo}(G) = \begin{bmatrix} 0 & \sqrt{10} & \sqrt{5} & \sqrt{5} \\ \sqrt{10} & 0 & \sqrt{13} & \sqrt{13} \\ \sqrt{5} & \sqrt{13} & 0 & 2\sqrt{2} \\ \sqrt{5} & \sqrt{13} & 2\sqrt{2} & 0 \end{bmatrix}$$

The eigenvalues are $\eta_1 = 8.9153$, $\eta_2 = -4.04155$, $\eta_3 = -2.82843$, $\eta_4 = -2.04532$.

The Sombor energy $E_{\mathcal{NSo}}(G)$ is 17.8306.

In 2001, Wu and Meng [16] gave new transformation G^{xyz} for G generalizing the concept of the total Graph. The total transformation graph is defined as follows.

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

- $u, v \in V$, u and v are adjacent in G if $x = +$ and are nonadjacent in G if $x = -$.

- $u, v \in E$, u and v are adjacent in G if $y = +$ and are nonadjacent in G if $y = -$.
- $u \in V$ and $v \in E$, u and v are incident in G if $z = +$ and are nonincident in G if $z = -$.

The eight graphical transformations for a given graph G , are G^{+++} , G^{-++} , G^{+-+} , G^{++-} and their complements G^{---} , G^{+--} , G^{-+-} , G^{--+} . Many other transformation graphs is discussed in [5].

2. Preliminary Results

Proposition 2.1 [9] For a s -regular graph G , let $u, v \in V$ and $e = uv \in E$. Then the degrees of corresponding vertices in G^{xyz} are:

- $d_{G^{+++}}(v) = 2s$ and $d_{G^{+++}}(e) = 2s$
- $d_{G^{++-}}(v) = m$ and $d_{G^{++-}}(e) = 2s + n - 4$
- $d_{G^{+-+}}(v) = 2s$ and $d_{G^{+-+}}(e) = m - 2s + 3$
- $d_{G^{-++}}(v) = n - 1$ and $d_{G^{-++}}(e) = 2s$
- $d_{G^{---}}(v) = n + m - 2s - 1$ and $d_{G^{---}}(e) = n + m - 2s - 1$
- $d_{G^{-+-}}(v) = n - 1$ and $d_{G^{-+-}}(e) = m - 2s + 3$
- $d_{G^{+--}}(v) = n + m - 2s - 1$ and $d_{G^{+--}}(e) = 2s + n - 4$
- $d_{G^{--+}}(v) = m$ and $d_{G^{--+}}(e) = n + m - 2s - 1$

Lemma 2.1 [9] If a and b are scalars then,

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

where I is the identity matrix and J is the matrix with all the entries as 1.

Lemma 2.2 [9] If a, b, c and d are real numbers then the characteristic polynomial of the determinant $\begin{vmatrix} (\lambda + a)I_n - aJ_n & -cJ_{n \times m} \\ -dJ_{m \times n} & (\lambda + b)I_m - bJ_m \end{vmatrix}_{n+m \times n+m}$ is given by $(\lambda + a)^{n-1}(\lambda + b)^{m-1} \{[\lambda - (n - 1)a][\lambda - (m - 1)b] - nmcd\}$. Also if $\lambda_1, \lambda_2, \dots, \lambda_{n+m}$ are eigenvalues of the same determinant then the eigenvalues are given by

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

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. Auxiliary Results

- The $E_{\mathcal{NSo}}(K_n)$ is $2\sqrt{2}(n-1)^2$
- The $E_{\mathcal{NSo}}(G)$ of s -regular graph is $2\sqrt{2}s(n-1)$
- The $E_{\mathcal{NSo}}(C_n)$ is $4\sqrt{2}(n-1)$
- The $E_{\mathcal{NSo}}(K_{n,n})$ is $2\sqrt{2}n(2n-1)$

4. Main Results

In this section, we have obtained Sombor energy for total transformation graphs. By the definition of total transformation graphs of an s -graph G with n vertices and $m = \frac{ns}{2}$ edges, G^{xyz} have $n+m$ vertices. Let the vertices be labelled as $v_i, i = 1, 2, \dots, n$ and the edges as $e_j, j = 1, 2, \dots, m$.

Theorem 4.1 For any s -regular graph G , we have

$$E_{\mathcal{NSo}}(G^{+++}) = 2\sqrt{2}s(ns + 2n - 2)$$

Proof: As G is a s -regular graph, by the definition of G^{+++} and Lemma 2.1, we have characteristic polynomial of Sombor matrix as $|\eta I - \mathcal{NSo}(G^{+++})| = 0$.

Now,

$$|\eta I - \mathcal{NSo}(G^{+++})| = \begin{vmatrix} \eta & -2\sqrt{2}s & -2\sqrt{2}s & \cdots & -2\sqrt{2}s & -2\sqrt{2}s \\ -2\sqrt{2}s & \eta & -2\sqrt{2}s & \cdots & -2\sqrt{2}s & -2\sqrt{2}s \\ -2\sqrt{2}s & -2\sqrt{2}s & \eta & \cdots & -2\sqrt{2}s & -2\sqrt{2}s \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -2\sqrt{2}s & -2\sqrt{2}s & -2\sqrt{2}s & \cdots & \eta & -2\sqrt{2}s \\ -2\sqrt{2}s & -2\sqrt{2}s & -2\sqrt{2}s & \cdots & -2\sqrt{2}s & \eta \end{vmatrix}_{(n+m) \times (n+m)}$$

By using Lemma 2.1,

$$|\eta I - \mathcal{NSo}(G^{+++})| = (\eta + 2\sqrt{2}s)^{n+m-1}[\eta - (n+m-1)2\sqrt{2}s] = 0$$

$$\text{spectra}(\mathcal{NSo}(G^{+++})) = \left(\begin{array}{cc} -2\sqrt{2}s & 2\sqrt{2}s(n+m-1) \\ (n+m-1) & 1 \end{array} \right)$$

Hence

$$E_{\mathcal{NSo}}(G^{+++}) = 4\sqrt{2}s(n+m-1) = 2\sqrt{2}s(ns + 2n - 2)$$

□

Theorem 4.2 For any s -regular graph G , we have

$$E_{\mathcal{NSo}}(G^{---}) = \frac{1}{\sqrt{2}}(ns + 2n - 2)(2n + ns - 4s - 2)$$

Proof: As G is a s -regular graph, by the definition of G^{----} and Lemma 2.1, we have characteristic polynomial of Sombor matrix as $|\eta I - \mathcal{NSo}(G^{----})| = 0$.

Now,

$$|\eta I - \mathcal{NSo}(G^{----})| = |\eta I - \sqrt{2}(n+m-2s-1)(J-I)|_{(n+m) \times (n+m)}$$

By using Lemma 2.1,

$$|\eta I - \mathcal{NSo}(G^{----})| = (\eta + \sqrt{2}(n+m-2s-1))^{n+m-1} [\eta - (n+m-1)\sqrt{2}(n+m-2s-1)] = 0$$

$$\text{spectra}(\mathcal{NSo}(G^{----})) = \begin{pmatrix} -\sqrt{2}(n+m-2s-1) & (n+m-1)\sqrt{2}(n+m-2s-1) \\ (n+m-1) & 1 \end{pmatrix}$$

Hence

$$E_{\mathcal{NSo}(G^{----})} = 2\sqrt{2}(n+m-1)(n+m-2s-1) = \frac{1}{\sqrt{2}}(ns+2n-2)(2n+ns-4s-2)$$

□

Theorem 4.3 For any s -regular graph G , we have

$$\begin{aligned} E_{\mathcal{NSo}(G^{++-})} &= \sqrt{2}m(n-1) + \sqrt{2}(m-1)(2s+n-4) \\ &+ \sqrt{[\sqrt{2}m(n-1) - \sqrt{2}(m-1)(2s+n-4)]^2 + 4nm[m^2 + (2s+n-4)^2]} \end{aligned}$$

Proof: As G is a s -regular graph, by the definition of G^{++-} and Lemma 2.2, we have characteristic polynomial of Sombor matrix as $|\eta I - \mathcal{NSo}(G^{++-})| = 0$.

Now, $|\eta I - \mathcal{NSo}(G^{++-})| =$

$$\begin{vmatrix} \eta & -\sqrt{2}m & \cdots & -\sqrt{2}m & -\sqrt{m^2 + (2s+n-4)^2} & \cdots & \cdots & -\sqrt{m^2 + (2s+n-4)^2} \\ -\sqrt{2}m & \eta & \cdots & -\sqrt{2}m & -\sqrt{m^2 + (2s+n-4)^2} & \cdots & \cdots & -\sqrt{m^2 + (2s+n-4)^2} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\sqrt{2}m & -\sqrt{2}m & \cdots & \eta & -\sqrt{m^2 + (2s+n-4)^2} & \cdots & \cdots & \sqrt{m^2 + (2s+n-4)^2} \\ -\sqrt{m^2 + (2s+n-4)^2} & \cdots & \cdots & -\sqrt{m^2 + (2s+n-4)^2} & \eta & -\sqrt{2}(2s+n-4) & \cdots & -\sqrt{2}(2s+n-4) \\ -\sqrt{m^2 + (2s+n-4)^2} & \cdots & \cdots & -\sqrt{m^2 + (2s+n-4)^2} & -\sqrt{2}(2s+n-4) & \eta & \cdots & -\sqrt{2}(2s+n-4) \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ -\sqrt{m^2 + (2s+n-4)^2} & \cdots & \cdots & -\sqrt{m^2 + (2s+n-4)^2} & -\sqrt{2}(2s+n-4) & -\sqrt{2}(2s+n-4) & \cdots & \eta \end{vmatrix}$$

i.e.,

$$|\eta I - \mathcal{NSo}(G^{++-})| = \begin{vmatrix} (\eta I - \sqrt{2}m(J-I))_{n \times n} & (-\sqrt{m^2 + (2s+n-4)^2})_{J_n \times m} \\ (-\sqrt{m^2 + (2s+n-4)^2})_{J_m \times n} & (\eta I - \sqrt{2}(2s+n-4)(J-I))_{m \times m} \end{vmatrix}$$

Expanding using the Lemma 2.2 we get

$$\begin{aligned} |\eta I - \mathcal{NSo}(G^{++-})| &= (\eta + \sqrt{2}m)^{n-1} (\eta + \sqrt{2}(2s+n-4))^{m-1} [\eta - (n-1)\sqrt{2}m] \\ &[\eta - (m-1)\sqrt{2}(2s+n-4)] - nm[m^2 + (2s+n-4)^2] = 0 \end{aligned}$$

$$\begin{aligned} |\eta I - \mathcal{NSo}(G^{++-})| &= (\eta + \sqrt{2}m)^{n-1} (\eta + \sqrt{2}(2s+n-4))^{m-1} [\eta^2 - \eta[(n-1)\sqrt{2}m \\ &+ (m-1)\sqrt{2}(2s+n-4)] + 2m(n-1)(m-1)(2s+n-4) \\ &- nm[m^2 + (2s+n-4)^2] = 0 \end{aligned}$$

$\text{spectra}(\mathcal{NSo}(G^{++-}))$

$$= \begin{cases} -\sqrt{2}m & (n-1)\text{times} \\ -\sqrt{2}(2s+n-4) & (m-1)\text{times} \\ \frac{[\sqrt{2}m(n-1) + \sqrt{2}(m-1)(2s+n-4)] \pm \sqrt{[\sqrt{2}m(n-1) - \sqrt{2}(m-1)(2s+n-4)]^2 + 4nm[m^2 + (2s+n-4)^2]}}{2} \end{cases}$$

In this,

$$\begin{aligned}\eta_1 &= [\sqrt{2}m(n-1) + \sqrt{2}(m-1)(2s+n-4)] \\ &+ \sqrt{[\sqrt{2}m(n-1) - \sqrt{2}(m-1)(2s+n-4)]^2 + 4nm[m^2 + (2s+n-4)^2]}/2\end{aligned}$$

is the largest and only one positive eigenvalue.

Hence

$$\begin{aligned}E_{\mathcal{NSo}}(G^{+-}) &= 2\eta_1 = \sqrt{2}m(n-1) + \sqrt{2}(m-1)(2s+n-4) \\ &+ \sqrt{[\sqrt{2}m(n-1) - \sqrt{2}(m-1)(2s+n-4)]^2 + 4nm[m^2 + (2s+n-4)^2]}\end{aligned}$$

□

Theorem 4.4 For any s -regular graph G , we have

$$\begin{aligned}E_{\mathcal{NSo}}(G^{-+}) &= \sqrt{2}(n-1)^2 + \sqrt{2}(m-1)(m-2s+3) \\ &+ [[\sqrt{2}(n-1)^2 - \sqrt{2}(m-1)(m-2s+3)]^2 \\ &+ 4nm[(n-1)^2 + (m-2s+3)^2]]^{1/2}\end{aligned}$$

Proof: As G is a s -regular graph, by the definition of G^{-+} and Lemma 2.2, we have characteristic polynomial of Sombor matrix as $|\eta I - \mathcal{NSo}(G^{-+})| = 0$.

i.e., $|\eta I - \mathcal{NSo}(G^{-+})| =$

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

Expanding using the Lemma 2.2, we get

$$\begin{aligned}|\eta I - \mathcal{NSo}(G^{-+})| &= (\eta + \sqrt{2}(n-1))^{n-1}(\eta + \sqrt{2}(m-2s+3))^{m-1}[\eta - \sqrt{2}(n-1)^2] \\ &[\eta - (m-1)\sqrt{2}(m-2s+3)] - nm[(n-1)^2 + (m-2s+3)^2] = 0\end{aligned}$$

$$\begin{aligned}|\eta I - \mathcal{NSo}(G^{-+})| &= (\eta + \sqrt{2}(n-1))^{n-1}(\eta + \sqrt{2}(m-2s+3))^{m-1}[\eta^2 - \eta[\sqrt{2}(n-1)^2 \\ &+ (m-1)\sqrt{2}(m-2s+3)] + 2(n-1)^2(m-1)(m-2s+3) \\ &- nm[(n-1)^2 + (m-2s+3)^2] = 0\end{aligned}$$

$spectra(\mathcal{NSo}(G^{-+}))$

$$= \begin{cases} -\sqrt{2}(n-1) & (n-1)\text{times} \\ -\sqrt{2}(m-2s+3) & (m-1)\text{times} \\ \frac{[\sqrt{2}(n-1)^2 + \sqrt{2}(m-1)(m-2s+3)] \pm \sqrt{[\sqrt{2}(n-1)^2 - \sqrt{2}(m-1)(m-2s+3)]^2 + 4nm[(n-1)^2 + (m-2s+3)^2]}}{2} \end{cases}$$

In this,

$$\begin{aligned}\eta_1 &= [\sqrt{2}(n-1)^2 + \sqrt{2}(m-1)(m-2s+3)] \\ &+ \sqrt{[\sqrt{2}(n-1)^2 - \sqrt{2}(m-1)(m-2s+3)]^2 + 4nm[(n-1)^2 + (m-2s+3)^2]}/2\end{aligned}$$

is the largest and only one positive eigenvalue.

Hence

$$\begin{aligned}E_{\mathcal{NSo}}(G^{-+}) &= 2\eta_1 = \sqrt{2}(n-1)^2 + \sqrt{2}(m-1)(m-2s+3) \\ &+ [[\sqrt{2}(n-1)^2 - \sqrt{2}(m-1)(m-2s+3)]^2 \\ &+ 4nm[(n-1)^2 + (m-2s+3)^2]]^{1/2}\end{aligned}$$

□

Theorem 4.5 For any s -regular graph G , we have

$$\begin{aligned} E_{\mathcal{NSo}}(G^{+--}) &= \sqrt{2}m(n-1) + \sqrt{2}(m-1)(n+m-2s-1) \\ &+ [[\sqrt{2}m(n-1) - \sqrt{2}(m-1)(n+m-2s-1)]^2 \\ &+ 4nm[m^2 + (n+m-2s-1)^2]]^{1/2} \end{aligned}$$

Proof: As G is a s -regular graph, by the definition of G^{+--} and Lemma 2.2, we have characteristic polynomial of Sombor matrix as $|\eta I - \mathcal{NSo}(G^{+--})| = 0$.

i.e., $|\eta I - \mathcal{NSo}(G^{+--})| =$

$$\begin{vmatrix} (\eta I - \sqrt{2}m(J-I))_{n \times n} & (-\sqrt{m^2 + (n+m-2s-1)^2})_{n \times m} \\ (-\sqrt{m^2 + (n+m-2s-1)^2})_{m \times n} & (\eta I - \sqrt{2}(n+m-2s-1)(J-I))_{m \times m} \end{vmatrix}$$

Expanding using the Lemma 2.2, we get

$$\begin{aligned} |\eta I - \mathcal{NSo}(G^{+--})| &= (\eta + \sqrt{2}m)^{n-1}(\eta + \sqrt{2}(n+m-2s-1))^{m-1}[\eta - (n-1)\sqrt{2}m] \\ &[\eta - (m-1)\sqrt{2}(n+m-2s-1)] - nm[m^2 + (n+m-2s-1)^2] = 0 \end{aligned}$$

$\text{spectra}(\mathcal{NSo}(G^{+--}))$

$$= \begin{cases} -\sqrt{2}m & (n-1)\text{times} \\ -\sqrt{2}(n+m-2s-1) & (m-1)\text{times} \\ \frac{[\sqrt{2}m(n-1) + \sqrt{2}(m-1)(n+m-2s-1)] \pm \sqrt{[\sqrt{2}m(n-1) - \sqrt{2}(m-1)(n+m-2s-1)]^2 + 4nm[m^2 + (n+m-2s-1)^2]}}{2} \end{cases}$$

In this,

$$\begin{aligned} \eta_1 &= [\sqrt{2}m(n-1) + \sqrt{2}(m-1)(n+m-2s-1) \\ &+ \sqrt{[\sqrt{2}m(n-1) - \sqrt{2}(m-1)(n+m-2s-1)]^2 + 4nm[m^2 + (n+m-2s-1)^2]}/2 \end{aligned}$$

is the largest and only one positive eigenvalue.

Hence

$$\begin{aligned} E_{\mathcal{NSo}}(G^{+--}) &= 2\eta_1 = \sqrt{2}m(n-1) + \sqrt{2}(m-1)(n+m-2s-1) \\ &+ [[\sqrt{2}m(n-1) - \sqrt{2}(m-1)(n+m-2s-1)]^2 \\ &+ 4nm[m^2 + (n+m-2s-1)^2]]^{1/2} \end{aligned}$$

□

Theorem 4.6 For any s -regular graph G , we have

$$\begin{aligned} E_{\mathcal{NSo}}(G^{-++}) &= \sqrt{2}(n-1)^2 + 2\sqrt{2}s(m-1) \\ &+ \sqrt{[\sqrt{2}(n-1)^2 - 2\sqrt{2}s(m-1)]^2 + 4nm[(n-1)^2 + 4s^2]} \end{aligned}$$

Proof: As G is a s -regular graph, by the definition of G^{-++} and Lemma 2.2, we have characteristic polynomial of Sombor matrix as $|\eta I - \mathcal{NSo}(G^{-++})| = 0$. i.e.,

$$|\eta I - \mathcal{NSo}(G^{-++})| = \begin{vmatrix} (\eta I - \sqrt{2}(n-1)(J-I))_{n \times n} & (-\sqrt{(n-1)^2 + (2s)^2})_{n \times m} \\ (-\sqrt{(n-1)^2 + (2s)^2})_{m \times n} & (\eta I - 2\sqrt{2}s(J-I))_{m \times m} \end{vmatrix}$$

Expanding using the Lemma 2.2, we get

$$\begin{aligned} |\eta I - \mathcal{NSo}(G^{-++})| &= (\eta + \sqrt{2}(n-1))^{n-1}(\eta + 2\sqrt{2}s)^{m-1}[\eta - \sqrt{2}(n-1)^2] \\ &[\eta - (m-1)2\sqrt{2}s] - nm[(n-1)^2 + 4s^2] = 0 \end{aligned}$$

$spectra(\mathcal{NSo}(G^{-++}))$

$$= \begin{cases} -\sqrt{2}(n-1) & (n-1)\text{times} \\ -2\sqrt{2}s & (m-1)\text{times} \\ \frac{[\sqrt{2}(n-1)^2 + 2\sqrt{2}s(m-1)] \pm \sqrt{[\sqrt{2}(n-1)^2 - 2\sqrt{2}s(m-1)]^2 + 4nm[(n-1)^2 + 4s^2]}}{2} \end{cases}$$

In this,

$$\eta_1 = \frac{[\sqrt{2}(n-1)^2 + 2\sqrt{2}s(m-1)] + \sqrt{[\sqrt{2}(n-1)^2 - 2\sqrt{2}s(m-1)]^2 + 4nm[(n-1)^2 + 4s^2]}}{2}$$

is the largest and only one positive eigenvalue.

Hence

$$E_{\mathcal{NSo}(G^{-++})} = 2\eta_1 = \frac{[\sqrt{2}(n-1)^2 + 2\sqrt{2}s(m-1)] + \sqrt{[\sqrt{2}(n-1)^2 - 2\sqrt{2}s(m-1)]^2 + 4nm[(n-1)^2 + 4s^2]}}{2}$$

□

Theorem 4.7 For any s -regular graph G , we have

$$E_{\mathcal{NSo}(G^{+-+})} = \frac{2\sqrt{2}s(n-1) + \sqrt{2}(m-2s+3)(m-1) + [[2\sqrt{2}s(n-1) - \sqrt{2}(m-2s+3)(m-1)]^2 + 4nm[4s^2 + (m-2s+3)^2]]^{1/2}}{2}$$

Proof: As G is a s -regular graph, by the definition of G^{+-+} and Lemma 2.2, we have characteristic polynomial of Sombor matrix as $|\eta I - \mathcal{NSo}(G^{+-+})| = 0$.

i.e., $|\eta I - \mathcal{NSo}(G^{+-+})| =$

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

Expanding using the Lemma 2.2, we get

$$|\eta I - \mathcal{NSo}(G^{+-+})| = (\eta + 2\sqrt{2}s)^{n-1}(\eta + \sqrt{2}(m-2s+3))^{m-1}[\eta - (n-1)2\sqrt{2}s] [\eta - (m-1)\sqrt{2}(m-2s+3)] - nm[4s^2 + (m-2s+3)^2] = 0$$

$spectra(\mathcal{NSo}(G^{+-+}))$

$$= \begin{cases} -2\sqrt{2}s & (n-1)\text{times} \\ -\sqrt{2}(m-2s+3) & (m-1)\text{times} \\ \frac{[2\sqrt{2}s(n-1) + \sqrt{2}(m-2s+3)(m-1)] \pm \sqrt{[2\sqrt{2}s(n-1) - \sqrt{2}(m-2s+3)(m-1)]^2 + 4nm[4s^2 + (m-2s+3)^2]}}{2} \end{cases}$$

In this,

$$\eta_1 = \frac{[2\sqrt{2}s(n-1) + \sqrt{2}(m-2s+3)(m-1)] + \sqrt{[2\sqrt{2}s(n-1) - \sqrt{2}(m-2s+3)(m-1)]^2 + 4nm[4s^2 + (m-2s+3)^2]}}{2}$$

is the largest and only one positive eigenvalue.

Hence,

$$\begin{aligned} E_{\mathcal{N}So}(G^{+-+}) &= 2\eta_1 = 2\sqrt{2}s(n-1) + \sqrt{2}(m-2s+3)(m-1) \\ &+ [[2\sqrt{2}s(n-1) - \sqrt{2}(m-2s+3)(m-1)]^2 \\ &+ 4nm[4s^2 + (m-2s+3)^2]]^{1/2} \end{aligned}$$

□

Theorem 4.8 For any s -regular graph G , we have

$$\begin{aligned} E_{\mathcal{N}So}(G^{-+-}) &= \sqrt{2}(n+m-2s-1)(n-1) + \sqrt{2}(m-1)(2s+n-4) \\ &+ [[\sqrt{2}(n+m-2s-1)(n-1) - \sqrt{2}(m-1)(2s+n-4)]^2 \\ &+ 4nm[(n+m-2s-1)^2 + (2s+n-4)^2]]^{1/2} \end{aligned}$$

Proof: As G is a s -regular graph, by the definition of G^{-+-} and Lemma 2.2, we have characteristic polynomial of Sombor matrix as $|\eta I - \mathcal{N}So(G^{-+-})| = 0$.

i.e., $|\eta I - \mathcal{N}So(G^{-+-})| =$

$$\begin{vmatrix} (\eta I - \sqrt{2}(n+m-2s-1)(J-I))_{n \times n} & (-\sqrt{(n+m-2s-1)^2 + (2s+n-4)^2})_{n \times m} J_{n \times m} \\ (-\sqrt{(n+m-2s-1)^2 + (2s+n-4)^2})_{m \times n} J_{m \times n} & (\eta I - \sqrt{2}(2s+n-4)(J-I))_{m \times m} \end{vmatrix}$$

Expanding using the Lemma 2.2, we get

$$\begin{aligned} |\eta I - \mathcal{N}So(G^{-+-})| &= (\eta + \sqrt{2}(n+m-2s-1))^{n-1} (\eta + \sqrt{2}(2s+n-4))^{m-1} [\eta \\ &- (n-1)\sqrt{2}(n+m-2s+1)] [\eta - (m-1)\sqrt{2}(2s+n-4)] \\ &- nm[(n+m-2s-1)^2 + (2s+n-4)^2] = 0 \end{aligned}$$

$spectra(\mathcal{N}So(G^{-+-}))$

$$= \begin{cases} -\sqrt{2}(n+m-2s-1) & (n-1) \text{ times} \\ -\sqrt{2}(2s+n-4) & (m-1) \text{ times} \\ \frac{[\sqrt{2}(n+m-2s-1)(n-1) + \sqrt{2}(m-1)(2s+n-4)] \pm \\ [[\sqrt{2}(n+m-2s-1)(n-1) - \sqrt{2}(m-1)(2s+n-4)]^2 \\ + 4nm[(n+m-2s-1)^2 + (2s+n-4)^2]]^{1/2}}{2} \end{cases}$$

In this,

$$\begin{aligned} \eta_1 &= [\sqrt{2}(n+m-2s-1)(n-1) + \sqrt{2}(m-1)(2s+n-4) \\ &+ [[\sqrt{2}(n+m-2s-1)(n-1) - \sqrt{2}(m-1)(2s+n-4)]^2 \\ &+ 4nm[(n+m-2s-1)^2 + (2s+n-4)^2]]^{1/2}]/2 \end{aligned}$$

is the largest and only one positive eigenvalue.

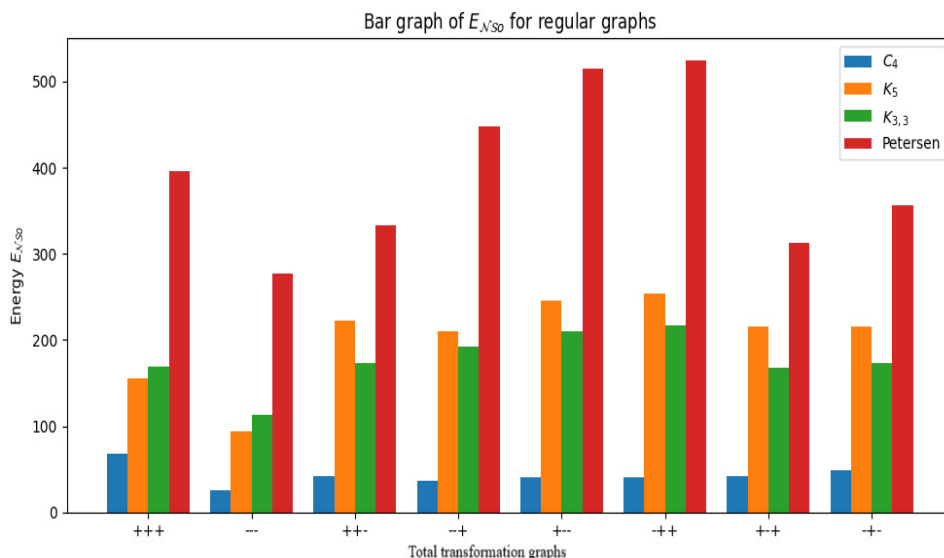
Hence

$$\begin{aligned} E_{\mathcal{N}So}(G^{-+-}) &= 2\eta_1 = \sqrt{2}(n+m-2s-1)(n-1) + \sqrt{2}(m-1)(2s+n-4) \\ &+ [[\sqrt{2}(n+m-2s-1)(n-1) - \sqrt{2}(m-1)(2s+n-4)]^2 \\ &+ 4nm[(n+m-2s-1)^2 + (2s+n-4)^2]]^{1/2} \end{aligned}$$

□

Table 1: $E_{\mathcal{NS}_o}(G)$ of total transformation graph derived from C_4 , K_5 , $K_{3,3}$ and the Peterson graph

Graphs	C_4	K_5	$K_{3,3}$	Peterson Graph
$E_{\mathcal{NS}_o}(G^{+++})$	67.882	155.563	169.706	395.979
$E_{\mathcal{NS}_o}(G^{---})$	25.456	93.338	113.137	277.185
$E_{\mathcal{NS}_o}(G^{++-})$	42.426	222.281	173.241	333.093
$E_{\mathcal{NS}_o}(G^{--+})$	36.770	210.019	192.969	447.409
$E_{\mathcal{NS}_o}(G^{+-})$	40.012	245.840	209.657	515.240
$E_{\mathcal{NS}_o}(G^{-++})$	41.231	253.435	216.333	523.847
$E_{\mathcal{NS}_o}(G^{+--})$	42.426	215.424	168.293	312.996
$E_{\mathcal{NS}_o}(G^{-+-})$	48.497	215.424	173.241	356.383

Figure 2: Bar graph of $E_{\mathcal{NS}_o}(G)$ of total transformation graph derived from C_4 , K_5 , $K_{3,3}$ and the Peterson graph

5. Applications of a New Variant Sombor Energy $E_{\mathcal{NS}_o}(G)$

In this section, a data set of total π -electron energy values of 26 hetero atoms are considered and respective $E_{\mathcal{NS}_o}(G)$ is calculated for each atom by drawing its molecular graph structure. The following total π -electron energy [2] and the $E_{\mathcal{NS}_o}(G)$ for 26 hetero items are listed in Table 2. Further the correlation coefficient r between the total π -electron energy and $E_{\mathcal{NS}_o}(G)$ is analysed which comes out to be $r = 0.982$, and the graph for linear regression model is depicted in Figure 3. The $E_{\mathcal{NS}_o}(G)$ for the 26 hetero atoms shows an improved correlation coefficient r compared to the actual Sombor energy for these hetero atoms, which is 0.976 [6].

Table 2: Molecules containing hetero atoms with total π -electron energy [2] and $E_{NS_o}(G)$

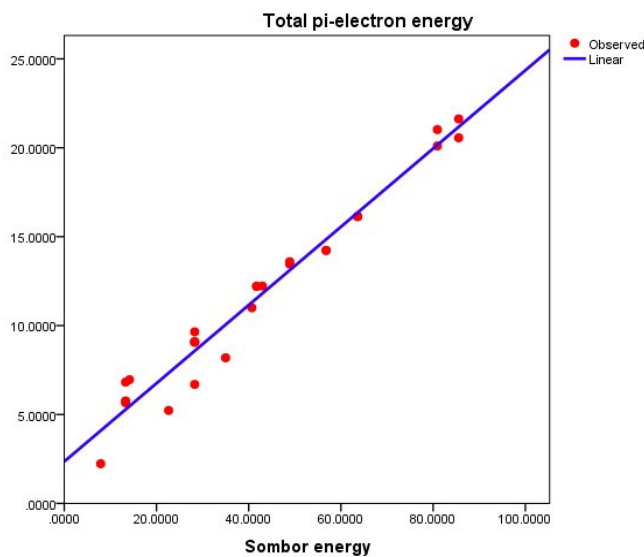
Molecule	Code	Total π -electron energy	$E_{NS_o}(G)$
Venyl chloride like systems	S_1	2.23	7.8949
Butadiene perturbed at C2	S_2	5.66	13.2980
Acrolein like systems	S_3	5.76	13.2980
1, 1-dichloro-ethylene like systems	S_4	6.96	14.1421
Glyoxal like and 1, 2-dichloro-ethylene like systems	S_5	6.82	13.2980
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
Benzylidene-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

The linear regression model is given by

$$\text{total } \pi\text{-electron energy} = a(E_{NS_o}(G)) + b$$

The linear regression model of total π -electron energy with $E_{NS_o}(G)$ is

$$\begin{aligned} \text{total } \pi\text{-electron energy} &= 0.220(\pm 0.009)(E_{NS_o}(G)) + 2.355(\pm 0.420) \\ r &= 0.982, \quad F = 640.581, \quad SF = 1.031 \end{aligned}$$

Figure 3: Linear regression model of total π -electron energy with $E_{NS_o}(G)$

6. Conclusion

In this paper, a new variant Sombor matrix $\mathcal{NSo}(G)$ is defined as, if $i \neq j$ its (i, j) -entry is equal to $\sqrt{d_i^2 + d_j^2}$ and 0 in the either case. $E_{\mathcal{NSo}}(G)$ is obtained for total transformation graphs G^{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 $E_{\mathcal{NSo}}(G)$ for the hetero atoms. The linear regression model yields a correlation coefficient of $r = 0.982$. Further the $E_{\mathcal{NSo}}(G)$ for the 26 hetero atoms shows an improved correlation coefficient r compared to the actual Sombor energy for these hetero atoms, which is 0.976.

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