Global and Stochastic Analysis
Vol. 12 No. 1 (January, 2025)

Received: 06th August 2024 **Revised: 17th September 2024** **Accepted: 29th September 2024**

ON STRESS PRODUCT EIGENVALUES AND ENERGY OF GRAPHS

M. KIRANKUMAR, M. RUBY SALESTINA, C. N. HARSHAVARDHANA, R. KEMPARAJU, AND P. SIVA KOTA REDDY*

Abstract. In this paper, we introduce the stress product matrix $SPM(G)$ for a connected graph G, which is related to the second stress index. We explore the properties of this matrix, establish bounds on its eigenvalues, and define the stress product energy $E_{SP}(G)$ as the sum of the absolute eigenvalues. Additionally, we discuss its potential chemical relevance by comparing $E_{SP}(G)$ with the π-electron energy of polyaromatic hydrocarbons.

1. Introduction

In this article, we will be focusing on finite, unweighted, simple, and undirected graphs. Let $G = (V, E)$ denote a graph. The degree of a vertex v in G is denoted by $d(v)$. The distance between two vertices u and v in G, denoted $d(u, v)$, is the number of edges in the shortest path (or geodesic) connecting them. A geodesic path P is said to pass through a vertex v if v is an internal vertex of P, meaning v lies on P but is not an endpoint of P. For standard terminology and notion in graph theory, we follow the text-book of Harary [7].

Gutman [5] defined the energy of a graph G as the sum of the absolute values of its eigenvalues, denoted by $\mathcal{E}(G)$. Eigenvalues are crucial in understanding graphs because they relate closely to almost every major graph invariant and extreme property. Consequently, graph energy, a specific type of matrix norm, has attracted attention from both pure and applied mathematicians. Spectral graph theory focuses on matrices associated with graphs, including their eigenvalues and energies, and is vital for analyzing graph matrices through matrix theory and linear algebra. Graph energy provides valuable insights into various structural and dynamic properties of graphs. It is a measure that captures the collective influence of a graph's eigenvalues, linking to diverse applications from chemical graph theory to network analysis. Different graph energies associated with topological indices have been introduced and extensively studied in the literature, highlighting their significance in understanding complex systems. Numerous matrices can be related to a graph, and their spectrums provide certain helpful information about

2000 *Mathematics Subject Classification.* 05C50, 05C09, 05C92.

Key words and phrases. Graph, Stress of a vertex, Energy, Stress Product Eigenvalues, Stress Product Energy.

*Corresponding author.

the graph [1, 2, 4, 6, 9–11, 18].

In 1953, Alfonso Shimbel [20] introduced the notion of vertex stress for graphs as a centrality measure. Stress of a vertex v in a graph G is the number of shortest paths (geodesics) passing through v. This concept has many applications including the study of biological and social networks. Many stress related concepts in graphs and topological indices have been defined and studied by several authors [12–17, 19]. A graph G is k-stress regular [3] if $str(v) = k$ for all $v \in V(G)$. The stress-sum index $SS(G)$ [12] of a graph $G(V, E)$ is defined by

$$SS(G) = \sum_{uv \in E(G)} [str(u) + str(v)].$$

The second stress index $S_2(G)$ [13] of a graph $G(V, E)$ is defined by

$$S_2(G) = \sum_{uv \in E(G)} str(u)str(v).$$

In this paper, we introduce the stress product matrix of a graph G and define the stress product energy $E_{SP}(G)$ based on its eigenvalues. This new approach extends the concept of graph energy to incorporate stress-related measures, offering a fresh perspective on graph invariants. We also establish bounds for $E_{SP}(G)$ in relation to other graph invariants and explore the correlation between the stress product energy of molecules with heteroatoms and their respective π-electron energy. This work aims to deepen our understanding of graph energy and its implications for molecular and structural analysis.

2. Stress Product Matrix and Energy

The stress product matrix of a graph G with $V(G) = \{v_1, v_2, \cdots, v_n\}$ is defined as $SPM(G) = (x_{ij})$, where

$$x_{ij} = \begin{cases} str(v_i)\, str(v_j), & \text{if} \quad i \neq j; \\ 0, & \text{otherwise}. \end{cases}$$

The stress product polynomial of a graph G is defined as

$$P_{SPM(G)}(s_\lambda) = |s_p I - SPM(G)|,$$

where I is an $n \times n$ unit matrix.

All the roots of the equation $P_{SPM(G)}(s_\lambda) = 0$ are real because the matrix $SPM(G)$ is real and symmetric. Therefore, these roots can be ordered as $s_{p_1} \geq s_{p_2} \geq \cdots \geq s_{p_n}$, with s_{p_1} being the largest and s_{p_n} being the smallest eigenvalue. The stress product energy $E_{SP}(G)$ of a graph G is defined by

$$E_{SP}(G) = \sum_{i=1}^{n} |s_{p_i}|.$$

3. Preliminary results

In this section, we will document the necessary results to support our main findings in section 4.

Theorem 3.1. *Let c_i and d_i, for $1 \leq i \leq n$, be non-negative real numbers. Then*

$$\sum_{i=1}^{n} c_i^2 \sum_{i=1}^{n} d_i^2 \leq \frac{1}{4} \left(\sqrt{\frac{M_1 M_2}{m_1 m_2}} + \sqrt{\frac{m_1 m_2}{M_1 M_2}} \right)^2 \left(\sum_{i=1}^{n} c_i d_i \right)^2 ,$$

where $M_1 = \max_{1 \leq i \leq n} \{c_i\}; M_2 = \max_{1 \leq i \leq n} \{d_i\}; m_1 = \min_{1 \leq i \leq n} \{c_i\}$ and $m_2 = \min_{1 \leq i \leq n} \{d_i\}$.

Theorem 3.2. *Let c_i and d_i, for $1 \leq i \leq n$ be positive real numbers. Then*

$$\sum_{i=1}^{n} c_i^2 \sum_{i=1}^{n} d_i^2 - \left(\sum_{i=1}^{n} c_i d_i \right)^2 \leq \frac{n^2}{4} \left(M_1 M_2 - m_1 m_2 \right)^2 ,$$

where $M_1 = \max_{1 \leq i \leq n} \{c_i\}; M_2 = \max_{1 \leq i \leq n} \{d_i\}; m_1 = \min_{1 \leq i \leq n} \{c_i\}$ and $m_2 = \min_{1 \leq i \leq n} \{d_i\}$.

Theorem 3.3. *(BPR Inequality) Let c_i and $d_i, for 1 \leq i \leq n$ be non-negative real numbers. Then*

$$\left| n \sum_{i=1}^{n} c_i d_i - \sum_{i=1}^{n} c_i \sum_{i=1}^{n} d_i \right| \leq \alpha(n)(A-a)(B-b),$$

where a, b, A and B are real constants, that for each $i, 1 \leq i \leq n, a \leq c_i \leq A$ and $b \leq d_i \leq B$. Further, $\alpha(n) = n \left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n} \left\lceil \frac{n}{2} \right\rceil \right)$.

Theorem 3.4. *(Diaz–Metcalf Inequality) If c_i and $d_i, 1 \leq i \leq n$, are nonnegative real numbers. Then*

$$\sum_{i=1}^{n} d_i^2 + rR \sum_{i=1}^{n} c_i^2 \leq (r+R) \left(\sum_{i=1}^{n} c_i d_i \right),$$

where r and R are real constants, so that for each $i, 1 \leq i \leq n$, holds $rc_i \leq d_i \leq Rc_i$.

Theorem 3.5. *(The Cauchy-Schwarz inequality) If $c = (c_1, c_2, \ldots, c_n)$ and $d = (d_1, d_2, \ldots, d_n)$ are real n-vectors, then*

$$\left(\sum_{i=1}^{n} c_i d_i \right)^2 \leq \left(\sum_{i=1}^{n} c_i^2 \right) \left(\sum_{i=1}^{n} d_i^2 \right).$$

4. Bounds for the Stress Product Eigenvalues and Energy

Lemma 4.1. *Let $s_{p_1} \geq s_{p_2} \geq \ldots \geq s_{p_n}$ be the eigenvalues of the stress product matrix $SPM(G)$. Then*

(i) $\sum_{i=1}^{n} s_{p_i} = 0$

(ii) $\sum_{i=1}^{n} s_{p_i}^2 = 2 \sum_{1 \leq i \leq j \leq n} (str(v_i)\, str(v_j))^2 = 2\mathbb{S}$

where $\mathbb{S} = \sum_{1 \leq i < j \leq n} (str(v_i) str(v_j))^2$.

Proof. i) The first equality is a direct consequence of $SPM(G)_{ii} = 0$ for all $1, 2, \ldots, n$.
ii) We have

$$\begin{aligned}
\sum_{i=1}^{n} s_{\beta_i}^2 &= \text{trace}[SPM(G)]^2 \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} (str(v_i) str(v_j))^2 \\
&= 2 \sum_{1 \leq i < j \leq n} (str(v_i) str(v_j))^2 \\
&= 2\mathbb{S}.
\end{aligned}$$

□

Lemma 4.2. *If a, b, c and d are real numbers, then the determinant of the form* $\begin{vmatrix} (\lambda + a) I_{n\times n} - aJ_{n\times n} & -cJ_{n\times m} \\ -dJ_{m\times n} & (\lambda + b) I_{m\times m} - bJ_{m\times m} \end{vmatrix}$
$= (\lambda + a)^{n-1} (\lambda + b)^{m-1} [(\lambda - (n-1)a)(\lambda - (m-1)b) - mncd]$.

Theorem 4.3. *If $K_{m,n}$ is a complete bipartite graph, then the characteristic polynomial is given by*

$$\left(s_p + \frac{m^2(m-1)^2}{4}\right)^{n-1} \left(s_p + \frac{n^2(n-1)^2}{4}\right)^{m-1} \times \left[\left(s_p - \frac{m^2(m-1)^2(n-1)}{4}\right)\left(s_p - \frac{n^2(n-1)^2(m-1)}{4}\right) - \frac{n^3(n-1)^2}{4}\frac{m^3(m-1)^2}{4}\right].$$

Proof. In a complete bipartite graph $K_{m,n}$, the vertex set $V(K_{m,n})$ can be partitioned into two disjoint sets $A = \{u_1, u_2, ..., u_m\}$ and $B = \{v_1, v_2, ..., v_n\}$. The stress of any vertex v in $K_{m,n}$ is given by

$$Str(v) = \begin{cases} \frac{n(n-1)}{2} & if\ v \in A \\ \frac{m(m-1)}{2} & if\ v \in B \end{cases}$$

Using the above and the definition of stress product matrix, we find that $SPM(K_{m,n}) =$
$$\begin{bmatrix} \frac{m^2(m-1)^2}{4}(-I_{n\times n} + J_{n\times n}) & \frac{n(n-1)}{2}\frac{m(m-1)}{2}J_{n\times m} \\ \frac{n(n-1)}{2}\frac{m(m-1)}{2}J_{m\times n} & \frac{n^2(n-1)^2}{4}(-I_{m\times m} + J_{m\times m}) \end{bmatrix},$$

where I_n is the identity matrix and $J_{n\times m}$ is the matrix with all entries as 1. The characteristic polynomial of the above matrix is given by the following determinant:

$$\begin{vmatrix} \left(s_p+\frac{m^2(m-1)^2}{4}\right)I_{n\times n}-\frac{m^2(m-1)^2}{4}J_{n\times n} & -\frac{n(n-1)}{2}\frac{m(m-1)}{2}J_{n\times m} \\ -\frac{n(n-1)}{2}\frac{m(m-1)}{2}J_{m\times n} & \left(s_p+\frac{n^2(n-1)^2}{4}I_{m\times m}\right)-\frac{n^2(n-1)^2}{4}J_{m\times m} \end{vmatrix}$$

Using the Lemma 4.2 in the above, we have the characteristic polynomial $=$

$$\left(s_p+\frac{m^2(m-1)^2}{4}\right)^{n-1}\left(s_p+\frac{n^2(n-1)^2}{4}\right)^{m-1} \times\left[\left(s_p-\frac{m^2(m-1)^2(n-1)}{4}\right)\left(s_p-\frac{n^2(n-1)^2(m-1)}{4}\right)-\frac{n^3(n-1)^2}{4}\frac{m^3(m-1)^2}{4}\right].$$

□

Theorem 4.4. *If C_n is cycle graph, then the characteristic polynomial is given by*

$$\begin{cases} \left(s_p-\frac{(n-1)^3(n-3)^2}{8^2}\right)\left(s_p+\frac{(n-1)^2(n-3)^2}{8^2}\right)^{n-1} & if\ n\ is\ odd \\ \left(s_p-\frac{n^2(n-1)(n-2)^2}{8^2}\right)\left(s_p+\frac{n^2(n-2)^2}{8^2}\right)^{n-1} & if\ n\ is\ even \end{cases}$$

Proof. The stress of any vertex v in C_n is given by

$$Str(v)=\begin{cases} \frac{(n-1)(n-3)}{8}, & if\ n\ is\ odd \\ \frac{n(n-2)}{8}, & if\ n\ is\ even \end{cases}$$

Using the above and the definition of stress product matrix for n being odd, we find that

$$SPM\left(C_n\right)=\begin{bmatrix} 0 & \frac{(n-1)^2(n-3)^2}{8^2} & \frac{(n-1)^2(n-3)^2}{8^2} & \cdots & \frac{(n-1)^2(n-3)^2}{8^2} \\ \frac{(n-1)^2(n-3)^2}{8^2} & 0 & \frac{(n-1)^2(n-3)^2}{8^2} & \cdots & \frac{(n-1)^2(n-3)^2}{8^2} \\ \vdots & \vdots & \ddots & \vdots & \\ \frac{(n-1)^2(n-3)^2}{8^2} & \frac{(n-1)^2(n-3)^2}{8^2} & \frac{(n-1)^2(n-3)^2}{8^2} & \cdots & 0 \end{bmatrix}.$$

Using the Lemma 4.2 in the above, the characteristic polynomial of the above matrix is given by

$$\left(s_p-\frac{(n-1)^3(n-3)^2}{8^2}\right)\left(s_p+\frac{(n-1)^2(n-3)^2}{8^2}\right)^{n-1}.$$

Likewise for the case of n being even can be obtained. □

Theorem 4.5. *The characteristic polynomial of fan graph F_n on $2n+1$ vertices and star graph S_n on $n+1$ vertices are s_p^{2n+1} and s_p^{n+1} respectively.*

Proof. In F_n graph, the stress of central vertex is $2n\left(n-1\right)$ and remaining $2n$ vertices have stress 0. Therefore $SPM\left(F_n\right)=[0]_{(2n+1)\times(2n+1)}$
The characteristic polynomial of the above matrix is given by s_p^{2n+1}.

In S_n graph, the stress of common vertex is $\frac{n(n-1)}{2}$ and remaining n vertices have stress 0. Therefore $SPM\left(S_n\right)=[0]_{(n+1)\times(n+1)}$. The characteristic polynomial of the above matrix is given by s_p^{n+1}. □

Theorem 4.6. *Let G be any graph with n-vertices. Then*

$$s_{p_1} \leq \sqrt{\frac{(2\mathbb{S})(n-1)}{n}}.$$

Proof. Setting $c_i = 1, d_i = s_{p_i}$, for $i = 2, 3, \ldots, n$ in Theorem 3.5, we have

$$\left(\sum_{i=2}^{n} s_{p_i}\right)^2 \leq (n-1)\sum_{i=2}^{n} s_{p_i}^2. \tag{4.1}$$

From Lemma 4.1, we find that

$$\sum_{i=2}^{n} s_{p_i} = -s_{p_1} \text{ and } \sum_{i=2}^{n} s_{p_i}^2 = -s_{p_1}^2 + 2\mathbb{S}.$$

Employing the above in (4.1), we obtain

$$(-s_{p_1})^2 \leq (n-1)\left(2\mathbb{S} - s_{p_1}^2\right)$$
$$s_{p_1} \leq \sqrt{\frac{(2\mathbb{S})(n-1)}{n}}.$$

□

Theorem 4.7. *Let G be any graph with n vertices. Then*

$$E_{SP}(G) \leq \sqrt{(2\mathbb{S})n}.$$

Proof. Choosing $c_i = 1, d_i = |s_{p_i}|$, for $i = 2, 3, \ldots, n$ in Theorem 3.5, we get

$$\left(\sum_{i=1}^{n} |s_{p_i}|\right)^2 \leq n\sum_{i=1}^{n} s_{p_i}^2$$
$$\Longrightarrow (E_{SP}(G))^2 \leq n(2\mathbb{S})$$
$$\Longrightarrow E_{SP}(G) \leq \sqrt{n(2\mathbb{S})}.$$

□

Theorem 4.8. *If G is a graph with n vertices and $E_{SP}(G)$ be the stress product energy of G, then*

$$\sqrt{2\mathbb{S}} \leq E_{SP}(G).$$

Proof. By the definition of $E_{SP}(G)$, we have

$$[E_{SP}(G)]^2 = \left(\sum_{i=1}^{n} |s_{p_i}|\right)^2 \geq \sum_{i=1}^{n} |s_{p_i}|^2 = 2\mathbb{S}.$$
$$\Longrightarrow \sqrt{2\mathbb{S}} \leq E_{SP}(G).$$

□

Theorem 4.9. *Let G be any graph with n-vertices and Φ be the absolute value of the determinant of the stress product matrix $SPM(G)$. Then*

$$\sqrt{(2\mathbb{S})+n(n-1)\Phi^{2/n}} \leq E_{SP}(G).$$

Proof. By the definition of stress product energy, we find that

$$(E_{SP}(G))^2 = \left(\sum_{i=1}^{n} |s_{p_i}|\right)^2 = \sum_{i=1}^{n} |s_{\lambda_i}|^2 + 2\sum_{i<j} |s_{p_i}||s_{p_j}|$$
$$= (2\mathbb{S}) + \sum_{i\neq j} |s_{p_i}||s_{p_j}|.$$

Since for non-negative numbers, the Arithmetic mean is greater than Geometric mean, we have

$$\frac{1}{n(n-1)} \sum_{i\neq j} |s_{p_i}||s_{p_j}| \geq \left(\prod_{i\neq j} |s_{p_i}||s_{p_j}|\right)^{\frac{1}{n(n-1)}}$$
$$= \left(\prod_{i=1}^{n} |s_{p_i}|^{2(n-1)}\right)^{\frac{1}{n(n-1)}}$$
$$= \prod_{i=1}^{n} |s_{p_i}|^{2/n}$$
$$= \Phi^{2/n}.$$

Therefore,

$$\sum_{i\neq j} |s_{p_i}|\left|s_{p_j}\right| \geq n(n-1)\Phi^{\frac{2}{n}}$$
$$\Longrightarrow [E_{SP}(G)]^2 \geq 2\mathbb{S} + n(n-1)\Phi^{2/n}$$
$$\Longrightarrow E_{SP}(G) \geq \sqrt{2\mathbb{S}+n(n-1)\Phi^{2/n}}.$$

Equality in AM-GM inequality is attained if and only if all $s_{p_i}; i = 1, 2, \ldots, n$ are equal. □

Lemma 4.10. *Let $c_1, c_2, \ldots, c_n$ be non-negative numbers. Then*

$$n\left[\frac{1}{n}\sum_{i=1}^{n} c_i - \left(\prod_{i=1}^{n} c_i\right)^{1/n}\right] \leq n\sum_{i=1}^{n} c_i - \left(\sum_{i=1}^{n} \sqrt{c_i}\right)^2 \leq n(n-1)\left[\frac{1}{n}\sum_{i=1}^{n} c_i - \left(\prod_{i=1}^{n} c_i\right)^{1/n}\right].$$

Theorem 4.11. *Let G be a connected graph with n vertices. Then*

$$\sqrt{(2\mathbb{S})+n(n-1)\Phi^{2/n}} \leq$$
$$E_{SP}(G) \leq \sqrt{(2\mathbb{S})(n-1)+n\Phi^{2/n}}.$$

Proof. Let $c_i = |s_{p_i}|^2, i = 1, 2, \ldots, n$ and

$$\begin{aligned} V &= n\left[\frac{1}{n}\sum_{i=1}^{n}|s_{p_i}|^2 - \left(\prod_{i=1}^{n}|s_{p_i}|^2\right)^{1/n}\right] \\ &= n\left[\frac{(2\mathbb{S})}{n} - \left(\prod_{i=1}^{n}|s_{p_i}|\right)^{2/n}\right] \\ &= n\left[\frac{(2\mathbb{S})}{n} - \Phi^{2/n}\right] \\ &= (2\mathbb{S}) - n\Phi^{2/n}. \end{aligned}$$

By Lemma 4.10, we obtain

$$V \leq n\sum_{i=1}^{n}|s_{p_i}|^2 - \left(\sum_{i=1}^{n}|s_{p_i}|\right)^2 \leq (n-1)V.$$

Upon simplification of the above equation, we find that

$$\sqrt{(2\mathbb{S}) + n(n-1)\Phi^{2/n}} \leq$$

$$E_{SP}(G) \leq \sqrt{(2\mathbb{S})(n-1) + n\Phi^{2/n}}.$$

□

Theorem 4.12. *Let G be a graph of order n. Then*

$$E_{SP}(G) \geq \sqrt{(2\mathbb{S})n - \frac{n^2}{4}\left(s_{p_1} - s_{p\min}\right)^2},$$

where $s_{p_1} = s_{p\max} = \max_{1\leq i\leq n}\{|s_{p_i}|\}$ and $s_{p\min} = \min_{1\leq i\leq n}\{|s_{p_i}|\}$.

Proof. Suppose $s_{p_1}, s_{p_2}, \ldots, s_{p_n}$ are the eigenvalues of $SPM(G)$. We choose $c_i = 1$ and $d_i = |s_{p_i}|$, which by Theorem 3.2 implies

$$\begin{aligned} \sum_{i=1}^{n}1^2\sum_{i=1}^{n}|s_{p_i}|^2 - \left(\sum_{i=1}^{n}|s_{p_i}|\right)^2 &\leq \frac{n^2}{4}\left(s_{p_1} - s_{p\min}\right)^2 \\ \text{i.e., } (2\mathbb{S})n - \left(E_{SP}(G)\right)^2 &\leq \frac{n^2}{4}\left(s_{p_1} - s_{p\min}\right)^2 \\ \implies E_{SP}(G) &\geq \sqrt{(2\mathbb{S})n - \frac{n^2}{4}\left(s_{p_1} - s_{p\min}\right)^2}. \end{aligned}$$

□

Theorem 4.13. *Suppose zero is not an eigenvalue of $SPM(G)$, then*

$$E_{SP}(G) \geq \frac{2\sqrt{s_{p_1}s_{p\min}}\sqrt{(2\mathbb{S})n}}{s_{p_1} + s_{p\min}},$$

where $s_{p_1} = s_{p\max} = \max_{1\leq i\leq n}\{|s_{p_i}|\}$ and $s_{p\min} = \min_{1\leq i\leq n}\{|s_{p_i}|\}$.

Proof. Suppose $s_{p_1}, s_{p_2}, \ldots, s_{p_n}$ are the eigenvalues of $SPM(G)$.
Setting $c_i = |s_{p_i}|$ and $d_i = 1$ in Theorem 3.1, we have

$$\sum_{i=1}^{n} |s_{p_i}|^2 \sum_{i=1}^{n} 1^2 \leq \frac{1}{4}\left(\sqrt{\frac{s_{p_1}}{s_{p\min}}} + \sqrt{\frac{s_{p\min}}{s_{p_1}}}\right)^2 \left(\sum_{i=1}^{n} |s_{p_i}|\right)^2$$

$$\text{i.e., } (2\mathbb{S})n \leq \frac{1}{4}\left(\frac{(s_{p_1} + s_{p\min})^2}{s_{p_1} s_{p\min}}\right) (E_{SP}(G))^2$$

$$\Longrightarrow E_{SP}(G) \geq \frac{2\sqrt{s_{p_1} s_{p\min}}\sqrt{(2\mathbb{S})n}}{s_{p_1} + s_{p\min}}.$$

□

Theorem 4.14. *Let G be a graph of order n and $s_{p_1} \geq s_{p_2} \geq \ldots \geq s_{p_n}$ be the non zero eigenvalues of $SPM(G)$. Then*

$$E_{SP}(G) \geq \frac{(2\mathbb{S}) + n s_{p_1} s_{p\min}}{s_{p_1} + s_{p\min}},$$

where $s_{p_1} = s_{p\max} = \max_{1\leq i\leq n}\{|s_{p_i}|\}$ and $s_{p\min} = \min_{1\leq i\leq n}\{|s_{p_i}|\}$.

Proof. Assigning $d_i = |s_{p_i}|, c_i = 1, R = |s_{p_1}|$ and $r = |s_{p\min}|$ in Theorem 3.4, we get

$$\sum_{i=1}^{n} |s_{p_i}|^2 + s_{p_1} s_{p\min} \sum_{i=1}^{n} 1^2 \leq (s_{p_1} + s_{p\min}) \sum_{i=1}^{n} |s_{p_i}|$$

$$(2\mathbb{S}) + n s_{p_1} s_{p\min} \leq (s_{p_1} + s_{p\min}) E_{SP}(G)$$

After simplifying and using the definition of $E_{SP}(G)$, we obtain

$$E_{SP}(G) \geq \frac{(2\mathbb{S}) + n s_{p_1} s_{p\min}}{s_{p_1} + s_{p\min}}.$$

□

Theorem 4.15. *Let G be a graph of order n and $s_{p_1} \geq s_{p_2} \geq \ldots \geq s_{p_n}$ be the eigenvalues of $SPM(G)$. Then*

$$E_{SP}(G) \geq \sqrt{(2\mathbb{S})n - \alpha(n)\,(s_{p_1} - s_{p\min})^2},$$

where $s_{p_1} = s_{p\max} = \max_{1\leq i\leq n}\{|s_{p_i}|\}$ and $s_{p\min} = \min_{1\leq i\leq n}\{|s_{p_i}|\}$ and $\alpha(n) = n\left\lceil\frac{n}{2}\right\rceil\left(1 - \frac{1}{n}\left\lceil\frac{n}{2}\right\rceil\right)$.

Proof. Setting $c_i = |s_{p_i}| = d_i, A \leq |s_{p_i}| \leq B$ and $a \leq |s_{p_n}| \leq b$ in Theorem 3.3, we get

$$\left| n\sum_{i=1}^{n} |s_{p_i}|^2 - \left(\sum_{i=1}^{n} |s_{p_i}|\right)^2 \right| \leq \alpha(n)\left(s_{p_1} - s_{p\,\min}\right)^2$$

$$\left|(2\mathbb{S})n - (E_{SP}(G))^2\right| \leq \alpha(n)\left(s_{p_1} - s_{p\,\min}\right)^2$$

$$E_{SP}(G) \geq \sqrt{(2\mathbb{S})n - \alpha(n)\left(s_{p_1} - s_{p\,\min}\right)^2}.$$

□

5. Chemical Applicability of $E_{SP}(G)$

In this section, we perform a computational analysis of the stress product energy $E_{SP}(G)$ and π-electron energy of heteroatoms. This study explores quadratic and cubic regression models. Since real-world data can exhibit nonlinear patterns, flexible approaches are necessary to capture such variations. These models enable researchers to determine the best fit for their specific data. This section highlights the chemical relevance of stress product energy in developing quadratic and cubic regression models for properties such as π-electron energy.
The regression models tested are as follows:
Quadratic equation:

$$Y = A + B_1X_1 + B_2X_1^2$$

Cubic equation:

$$Y = A + B_1X_2 + B_2X_2^2 + B_3X_2^3$$

Here, Y is the dependent variable, A being the regression constant, and B_i (where $i = 1, 2, 3$) are the regression coefficients and X_i (where $i = 1, 2, 3$) are the independent variables.

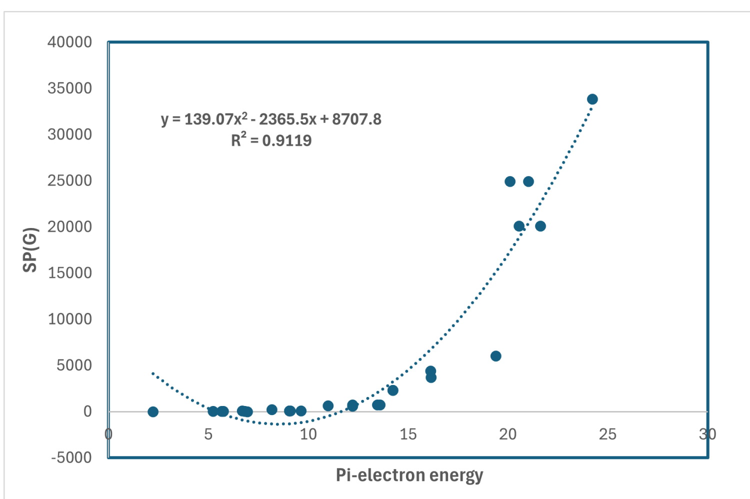
TABLE 1. Molecules containing hetero atoms with total π-electron energy and the stress product energy.

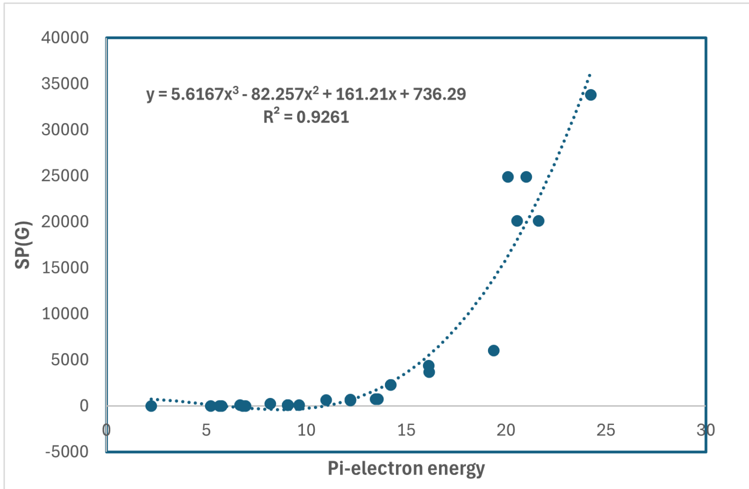
Molecule	Total π-electron energy	$E_{SP}(G)$
Veny chloride like system	2.23	0
Acrolein like systems	5.76	8
1,1-Dichloro-ethylene like systems	6.96	0
Glyoxal like and 1,2-Dichloro-ethylene like systems	6.82	8
Butadiene perturbed at C2	5.66	8
Pyrrole like systems	5.23	8
Pyridine like systems	6.69	90
Pyridazine like systems	9.06	90
Pyrimidine like systems	9.10	90
Pyrazine like systems	9.07	90
S-Triazene like systems	9.65	90

Molecule	Total π-electron energy	$E_{SP}(G)$
Aniline like systems	8.19	224.24
O-Phenylene-diamine like systems	12.21	629.21
m-Phenylene-diamine like systems	12.22	585.7
p-Phenylene-diamine like systems	12.21	704.4
Benzaldehyde like systems	11.00	626.142
Quinoline like systems	14.23	2292.83
Iso-quinoline like systems	14.23	2292.83
1-Naphthalein like systems	16.15	3699.47
2-Naphthalein like systems	16.12	4396.37
Acridine like systems	20.56	20093.626
Phenazine like systems	21.62	20093.626
Iso-indole like systems	13.46	734.3
Indole like systems	13.59	734.3
Azobenzene like systems	21.02	24910.36
Benzylidine-aniline-like systems	20.10	24910.36
9,10-Anthraquinoline structures	24.23	33819.071
Cabazole like structures	19.39	6016.893

TABLE 2. The correlation coefficient r from quadratic and cubic regression model between stress product energy and π electron energy

Model	Correlation Coefficient r
Quadratic	0.954
Cubic	0.962





Conclusion. The stress product energy is proposed with potential predictive capability for π-electron energy in chemical compounds.π-electron energy plays a crucial role in the stability and reactivity of molecules, particularly in molecules containing heteroatoms. In this study, we apply regression models to assess the predictive relationship between stress product energy and π-electron energy.

Acknowledgement. We would also like to thank our reviewers for their valuable comments.

References

1. AlFran, H. A., Rajendra, R., Siva Kota Reddy, P., Kemparaju, R. and Altoum, Sami H.: Spectral Analysis of Arithmetic Function Signed Graphs, *Glob. Stoch. Anal.*, **11**(3) (2024), 50–59.
2. Brouwer, A. E. and Haemers, W. H.: *Spectra of Graphs-Monograph*, Springer, 2011.
3. Bhargava, K., Dattatreya, N. N. and Rajendra, R.: On stress of a vertex in a graph, *Palest. J. Math.*, **12**(3) (2023), 15—25.
4. Cvetković, D. M., Doob, M. and Sachs, H.: *Spectra of Graphs*, Academic Press, 1979.
5. Gutman, I.: The energy of a graph, *Ber. Math.-Stat. Sekt. Forschungszent. Graz*, **103** (1978), 1–22.
6. Gutman, I., Firoozabadi, S. Z., de la Peña, J. A. and Rada, J.: On the energy of regular graphs, *MATCH Commun. Math. Comput. Chem.*, **57** (2007), 435–442
7. Harary, F.: *Graph Theory*, Addison Wesley, Reading, Mass, 1972.
8. Mahesh, K. B., Rajendra, R. and Siva Kota Reddy, P.: Square Root Stress Sum Index for Graphs, *Proyecciones*, **40**(4) (2021), 927–937.
9. Prakasha, K. N., Siva kota Reddy, P. and Cangul, I. N.: Partition Laplacian Energy of a Graph, *Adv. Stud. Contemp. Math., Kyungshang*, **27**(4) (2017), 477–494.
10. Prakasha, K. N., Siva kota Reddy, P. and Cangul, I. N.: Minimum Covering Randic energy of a graph, *Kyungpook Math. J.*, **57**(4) (2017), 701–709.
11. Prakasha, K. N., Siva kota Reddy, P. and Cangul, I. N.: Sum-Connectivity Energy of Graphs, *Adv. Math. Sci. Appl.*, **28**(1) (2019), 85–98.
12. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N.: Stress-Sum index of graphs, *Sci. Magna*, **15**(1) (2020), 94–103.
13. Rajendra, R., Siva Kota Reddy, P. and Cangul, I. N.: Stress indices of graphs, *Adv. Stud. Contemp. Math. (Kyungshang)*, **31**(2) (2021), 163–173.

14. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N.: Tosha Index for Graphs, *Proc. Jangjeon Math. Soc.*, **24**(1) (2021), 141–147.
15. Rajendra, R., Siva Kota Reddy, P., Mahesh, K.B. and Harshavardhana, C. N.: Richness of a Vertex in a Graph, *South East Asian J. Math. Math. Sci.*, **18**(2) (2022), 149–160.
16. Rajendra, R., Siva Kota Reddy, P., Harshavardhana, C. N., and Alloush, Khaled A. A.: Squares Stress Sum Index for Graphs, *Proc. Jangjeon Math. Soc.*, **26**(4) (2023), 483–493.
17. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N.: Stress-Difference Index for Graphs, *Bol. Soc. Parana. Mat. (3)*, **42** (2024), 1–10.
18. Rajendra, R., Siva Kota Reddy, P. and Kemparaju, R.: Eigenvalues and Energy of Arithmetic Function Graph of a Finite Group, *Proc. Jangjeon Math. Soc.*, **27**(1) (2024), 29–34.
19. Poojary, R., Arathi Bhat, K., Arumugam, S. and Manjunatha Prasad, K.: The stress of a graph, *Commun. Comb. Optim.*, **8**(1) (2023), 53–65.
20. Shimbel, A.: Structural Parameters of Communication Networks, *Bulletin of Mathematical Biophysics*, **15** (1953), 501–507.

M. Kirankumar: Department of Mathematics, Vidyavardhaka College of Engineering, Mysuru-570 002, INDIA
Email address: kiran.maths@vvce.ac.in

M. Ruby Salestina: Department of Mathematics, Yuvaraja's College, University of Mysore, Mysuru-570 005, INDIA
Email address: ruby.salestina@gmail.com

C. N. Harshavardhana: Department of Mathematics, Government Science College (Autonomous), Hassan-573 201, INDIA
Email address: cnhmaths@gmail.com

R. Kemparaju: Department of Mathematics, Government First Grade College, T. Narasipura-571 124, INDIA
Email address: kemps007@gmail.com

P. Siva Kota Reddy: Department of Mathematics, JSS Science and Technology University, Mysuru-570 006, India
Email address: pskreddy@jssstuniv.in; pskreddy@sjce.ac.in