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ON ADJACENCY SQUARE ROOT STRESS SUM EIGENVALUES AND ENERGY OF GRAPHS

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Abstract. The stress of a vertex is a node centrality index, which has been introduced by Shimbel (1953). The stress of a vertex in a graph is the number of geodesics (shortest paths) passing through it. In this paper, we introduce a new topological index for graphs called squares stress sum index using stresses of vertices. We establish some inequalities, prove some results and compute squares stress sum index for some standard graphs. Further, a QSPR analysis is carried for squares stress sum index of molecular graphs and physical properties of lower alkanes and linear regression models are presented for some physical properties.

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1. Introduction

In this paper, we consider finite, unweighted, simple, and undirected graphs. A graph is represented as $G = (V, E)$, where V is the set of vertices and E is the set of edges. The degree of a vertex $v \in V$ is denoted by $d(v)$. The distance between two vertices u and v, represented as $d(u, v)$, refers to the length of the shortest path (geodesic) between them, measured by the number of edges. A geodesic path P is said to traverse a vertex v if v is an internal vertex of P, that is v is located on P but is not one of its endpoints.

Graph energy, introduced by Ivan Gutman [7] in 1978, is a graph invariant connected to the total π-electron energy in molecular graphs. It is calculated as the sum of the absolute values of the eigenvalues of the graph's adjacency matrix. This concept plays a significant role in chemical graph theory, particularly in analyzing molecular stability and properties influenced by the structure of chemical compounds.Subsequently, several matrices were introduced to represent various structural features of graphs, such as distance, adjacency, and vertex degrees. Notable examples include the distance matrix, Seidel matrix, Laplacian matrix, Seidel Laplacian matrix, signless Laplacian matrix, Seidel signless Laplacian matrix, and the degree sum matrix. These matrices are essential tools for analyzing different graph invariants and topological indices. Numerous matrices can be related to a graph, and their spectrums provide certain helpful information about the

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graph [2, 4, 6, 7, 9–12, 17, 22, 25, 26].

In 1953, Alfonso Shimbel [23] 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 [1,3,5,13–16,18–21,24]. A graph G is k-stress regular [5] if $str(v) = k$ for all $v \in V(G)$.

The square root stress sum index [20] of a simple graph $G = (V, E)$ is given by

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

The stress-sum index $SS(G)$ [?] of a simple graph $G = (V, E)$ is given by

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

Motivated by advancements in topological indices and their associated matrices, as well as eigenvalue bounds, We introduce the square root stress sum matrix of a graph G and define its corresponding energy, called the square root stress sum energy and denoted by $E_{SRS}(G)$. This extends the concept of graph energy by incorporating stress-based measures. Furthermore, we establish bounds for $E_{SRS}(G)$ and explore its relationship with the π-electron energy of molecular graphs, particularly those with heteroatoms.

2. Square Root Stress Sum Matrix and Energy

The square root stress sum matrix of a graph G with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ is defined as $A_{SRS}(G) = ((SRS)_{ij})$, where

$$(SRS)(i,j) = \begin{cases} \sqrt{\text{str}(v_i) + \text{str}(v_j)} & \text{if } v_i v_j \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

The square root stress sum polynomial of a graph G is defined as

$$P_{A_{SRS}}(G) = |s_r I - A_{SRS}(G)|,$$

where I is the $n \times n$ identity matrix.

All the roots of the equation $P_{A_{SRS}(G)}(s_r) = 0$ are real, since the matrix $A_{SRS}(G)$ is real and symmetric. These roots can therefore be ordered as

$$s_{r_1} \geq s_{r_2} \geq \cdots \geq s_{r_n},$$

with s_{r_1} being the largest and s_{r_n} the smallest eigenvalue.

The square root stress sum energy of a graph G is given by

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

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*

$$\sum_{i=1}^{n} c_i^2 \sum_{i=1}^{n} d_i^2 \leq \frac{1}{4}\left(\sqrt{\frac{M_1M_2}{m_1m_2}}+\sqrt{\frac{m_1m_2}{M_1M_2}}\right)^2\left(\sum_{i=1}^{n} c_i d_i\right)^2,$$

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*

$$\sum_{i=1}^{n} c_i^2 \sum_{i=1}^{n} d_i^2 - \left(\sum_{i=1}^{n} c_i d_i\right)^2 \leq \frac{n^2}{4}\left(M_1M_2 - m_1m_2\right)^2,$$

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 non-negative 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 Square Root Stress Eigenvalues and Energy

Lemma 4.1. *Let $G = (V, E)$ be a graph and $P_{A_{SRS}}(G) = s_r^n + c_1 s_r^{n-1} + c_2 s_r^{n-2} + \cdots + c_n$ be the characteristic polynomial of$A_{SRS}(G)$. Then*

(i) $\mathrm{c}_1 = 0$

(ii) $\mathrm{c}_2 = -SS(G)$

(iii) $\mathrm{c}_3 = -2\sum_{\Delta} \prod_{uv \in E(\Delta)} \sqrt{str(u) + str(v)},$

where the summation is taken over all cycles $\triangle$ of length 3 in G.

Proof. Since each coefficient $c_i, i = 1, 2, \cdots, n, (-1)^i \mathrm{c_i}$ corresponds to the sum of all the principal minors of $A_{SRS}(G)$ with i rows and i columns, we have the following:
(i) $c_1 = 0$ as all the principal diagonal elements of $A_{SRS}(G)$ are zero.

$$(ii)\ c_2 = \sum_{1 \le i < j \le n} \begin{vmatrix} 0 & b_{ij} \\ b_{ji} & 0 \end{vmatrix} = -\sum_{1 \le i < j \le n} b_{ij}^2 = -\sum_{1 \le i < j \le n} (str\,(v_i) + str\,(v_j)) = -SS(G).$$

(iii) From the definition of $P_{A_{SRS}}(G)$, we have

$$(-1)^3 C_3 = \text{sum of all } 3 \times 3 \text{ principal minors of } A_{SRS}(G)$$

$$\begin{aligned}
\implies C_3 &= (-1)^3 \sum_{1 \le i < j < k \le n} \begin{vmatrix} b_{ii} & b_{ij} & b_{ik} \\ b_{ji} & b_{jj} & b_{jk} \\ b_{ki} & b_{kj} & b_{kk} \end{vmatrix} \\
&= -\sum_{1 \le i < j < k \le n} \left[b_{ii}\left(b_{jj}b_{kk} - b_{kj}b_{jk}\right) - b_{ij}\left(b_{ji}b_{kk} - b_{ki}b_{jk}\right) + b_{ik}\left(b_{ji}b_{kj} - b_{ki}b_{jj}\right) \right] \\
&= -\sum_{1 \le i < j < k \le n} b_{ii}a_{jj}b_{kk} + \sum_{1 \le i < j < k \le n} \left(b_{ii}b_{jk}^2 + b_{jj}b_{ik}^2 + b_{kk}b_{ij}^2\right) \\
&\quad - \sum_{1 \le i < j < k \le n} b_{ij}b_{jk}b_{ki} - \sum_{1 \le i < j < k \le n} b_{ik}b_{kj}b_{ji} \\
&= -2\sum_{\Delta} \prod_{uv \in E(\Delta)} \sqrt{str(u) + str(v)}.
\end{aligned}$$

□

Lemma 4.2. *Let $A_{SRS}(G)$ be the square root stress sum matrix with $s_{r_1} \ge s_{r_2} \ge \ldots \ge s_{r_n}$representing its square root stress sum adjacency eigenvalues. Then*

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

(ii) $\sum_{i=1}^{n} s_{r_i}^2 = 2SS(G)$.

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

ii) We have

$$\begin{aligned}\sum_{i=1}^{n} s_{r_i}^2 &= \text{Trace}\left(A_{SRS}(G)^2\right)\\ &= \sum_{i=1}^{n}\sum_{j=1}^{n} A_{SRS}(G)(i,j)A_{SRS}(G)(j,i)\\ &= 2\sum_{uv\in E(G)} A_{SRS}(G)(u,v)A_{SRS}(G)(v,u)\\ &= 2\sum_{uv\in E(G)} \sqrt{str(u)+str(v)}\sqrt{str(v)+str(u)}\\ &= 2\sum_{uv\in E(G)} [str(u)+str(v)]\\ &= 2SS(G).\end{aligned}$$

□

Lemma 4.3. *If a, b, c, and d are real numbers, then the determinant of the form*

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

is given by:

$$= (\lambda+a)^{m-1}(\lambda+b)^{n-1}\left[(\lambda-(m-1)a)(\lambda-(n-1)b) - mncd\right].$$

Theorem 4.4. *If $K_{m,n}$ is a complete biparite graph, then*

$$P_{A_{SRS}}(K_{m,n}) = s_r^{m+n-2}\left[s_r^2 - mn\left(\frac{n(n-1)+m(m-1)}{2}\right)\right].$$

Proof. The graph $K_{m,n}$ of order $m+n$ has two types of verices namely, m vertices are of stress $\frac{n(n-1)}{2}$ and n of stress $\frac{m(m-1)}{2}$. Hence,

$$A_{SRS}(K_{m,n}) = \begin{bmatrix} 0_{m\times m} & \sqrt{\frac{n(n-1)}{2}+\frac{m(m-1)}{2}}J_{m\times n} \\ \sqrt{\frac{n(n-1)}{2}+\frac{m(m-1)}{2}}J_{n\times m} & 0_{n\times n}\end{bmatrix}.$$

$$\begin{aligned}P_{A_{SRS}}(K_{m,n}) &= |s_r I - A_{SRS}(K_{m,n})|\\ &= \begin{vmatrix} s_r I_m & -\sqrt{\frac{n(n-1)}{2}+\frac{m(m-1)}{2}}J_{m\times n} \\ -\sqrt{\frac{n(n-1)}{2}+\frac{m(m-1)}{2}}J_{n\times m} & s_r I_n\end{vmatrix},\end{aligned}$$

where I_r is the identity matrix of order $r\times r$, $0_{m\times m}$ is the zero matrix of order $m\times m$, and $J_{m\times n}$ is the $m\times n$ matrix with all entries equal to 1. Thus, by applying Lemma 4.3, we obtain the desired result.

□

Theorem 4.5. *If $K_{1\times n-1}$ is a star graph, then*

$$P_{A_{SRS}}(K_{1\times n-1}) = s_r^{n-2}\left[s_r^2 - (n-1)\left(\frac{(n-1)(n-2)}{2}\right)\right].$$

Proof. The star graph $K_{1\times n-1}$ has two types of vertices: Internal vertex has stress $\frac{(n-1)(n-2)}{2}$ and remaining vertex have stress 0. Hence,

$$A_{SRS}\left(K_{1\times n-1}\right)=\begin{bmatrix} (0)_{1\times 1} & \sqrt{\frac{(n-1)(n-2)}{2}}J_{1\times(n-1)} \\ \sqrt{\frac{(n-1)(n-2)}{2}}J_{(n-1)\times 1} & (0)_{(n-1)\times(n-1)} \end{bmatrix}.$$

$$\begin{aligned} P_{A_{SRS}}(K_{1\times n-1}) &= |s_r I - A_{SRS}(K_{1\times n-1})| \\ &= \begin{vmatrix} s_r I_1 & -\sqrt{\frac{(n-1)(n-2)}{2}}J_{1\times(n-1)} \\ -\sqrt{\frac{(n-1)(n-2)}{2}}J_{(n-1)\times 1} & s_r I_{(n-1)} \end{vmatrix}, \end{aligned}$$

where I_r is the identity matrix of order $r\times r$, $0_{m\times m}$ is the zero matrix of order $m\times m$, and $J_{m\times n}$ is the $m\times n$ matrix with all entries equal to 1. Thus, by applying Lemma 4.3, we obtain the desired result. □

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

$$s_{r_1}\le\sqrt{\frac{2\,SS(G)(n-1)}{n}}.$$

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

$$\left(\sum_{i=2}^{n} s_{r_i}\right)^2 \le (n-1)\sum_{i=2}^{n} s_{r_i}^2 \tag{4.1}$$

From Lemma 4.2, we find that

$$\sum_{i=2}^{n} s_{r_i} = -s_{r_1} \text{ and } \sum_{i=2}^{n} s_{r_i}^2 = -s_{r_1}^2 + 2SS(G).$$

Employing the above in (4.1) we obtain

$$\begin{aligned} (-s_{r_1})^2 &\le (n-1)\left(2SS(G)-s_{r_1}^2\right) \\ \implies s_{r_1} &\le \sqrt{\frac{2SS(G)(n-1)}{n}}. \end{aligned}$$

□

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

$$E_{SRS}(G)\le\sqrt{2\,SS(G)\,n}.$$

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

$$\begin{aligned} \left(\sum_{i=1}^{n} |s_{r_i}|\right)^2 &\le n\sum_{i=1}^{n} s_{r_i}^2 \\ (E_{SRS}(G))^2 &\le n(2\,SS(G)) \\ \implies E_{SRS}(G) &\le \sqrt{2n\,SS(G)}. \end{aligned}$$

□

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

$$\sqrt{2SS(G)} \leq E_{SRS}(G).$$

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

$$[E_{SRS}(G)]^2 = \left(\sum_{i=1}^{n} |s_{r_i}|\right)^2 \geq \sum_{i=1}^{n} |s_{r_i}|^2 = 2\,SS(G)$$

which gives

$$\sqrt{2SS(G)} \leq E_{SRS}(G).$$

□

Theorem 4.9. *Let G be any graph with n vertices, and let Φ be the absolute value of the determinant of the Square root stress sum matrix $A_{SRS}(G)$. Then*

$$\sqrt{2SS(G) + n(n-1)\Phi^{2/n}} \leq E_{SRS}(G).$$

Proof. By the definition of square root stress sum energy,we find that

$$\begin{aligned}(E_{SRS}(G))^2 &= \left(\sum_{i=1}^{n} |s_{r_i}|\right)^2 \\ &= \sum_{i=1}^{n} |s_{\gamma_i}|^2 + 2\sum_{i<j} |s_{r_i}||s_{r_j}| \\ &= 2SS(G) + \sum_{i\neq j} |s_{r_i}||s_{r_j}|.\end{aligned}$$

Since for non-negative numbers the arithmetic mean is not smaller than the geometric mean,

$$\begin{aligned}\frac{1}{n(n-1)}\sum_{i\neq j} |s_{r_i}|||s_{r_j}| &\geq \left(\prod_{i\neq j} |s_{r_i}||s_{r_j}|\right)^{\frac{1}{n(n-1)}} \\ &= \left(\prod_{i=1}^{n} |s_{r_i}|^{2(n-1)}\right)^{\frac{1}{n(n-1)}} \\ &= \prod_{i=1}^{n} |s_{r_i}|^{2/n} \\ &= \Phi^{2/n}.\end{aligned}$$

Therefore,

$$\sum_{i\neq j} |s_{r_i}|\,|s_{r_j}| \geq n(n-1)\Phi^{\frac{2}{n}}$$

$$\implies [E_{SRS}(G)]^2 \geq 2SS(G) + n(n-1)\Phi^{2/n}$$
$$\implies E_{SRS}(G) \geq \sqrt{2SS(G) + n(n-1)\Phi^{2/n}}.$$

Equality in AM-GM inequality is attained if and only if all $s_{r_i}; i = 1, 2, \ldots, n$ 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*

$$\sqrt{2SS(G) + n(n-1)\Phi^{2/n}} \leq E_{SRS}(G) \leq \sqrt{2SS(G)(n-1) + n\Phi^{2/n}}.$$

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

$$V = n\left[\frac{1}{n}\sum_{i=1}^{n}|s_{r_i}|^2 - \left(\prod_{i=1}^{n}|s_{r_i}|^2\right)^{1/n}\right]$$
$$= n\left[\frac{2SS(G)}{n} - \left(\prod_{i=1}^{n}|s_{r_i}|\right)^{2/n}\right]$$
$$= n\left[\frac{2SS(G)}{n} - \Phi^{2/n}\right]$$
$$= 2SS(G) - n\Phi^{2/n}.$$

By Lemma 4.10, we obtain

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

that is

$$2SS(G) - n\Phi^{2/n} \leq 2nSS(G) - (E_{SRS}(G))^2 \leq (n-1)\left(2SS(G) - n\Phi^{2/n}\right)$$

on simplifying of above equation, we find that

$$\sqrt{2SS(G) + n(n-1)\Phi^{2/n}} \leq E_{SRS}(G) \leq \sqrt{2SS(G)(n-1) + n\Phi^{2/n}}.$$

□

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

$$E_{SRS}(G) \geq \sqrt{2SS(G)n - \frac{n^2}{4}\left(s_{r_1} - s_{r\min}\right)^2},$$

where $s_{r_1} = s_{r\max} = \max_{1\leq i\leq n}|s_{r_i}|$ and $s_{r\min} = \min_{1\leq i\leq n}|s_{r_i}|$.

Proof. Suppose $s_{r_1}, s_{r_2}, \ldots, s_{r_n}$ are the eigenvalues of$A_{SRS}(G)$ We assume that $c_i = 1$ and $d_i = |s_{r_i}|$, which by Theorem 3.2 implies

$$\sum_{i=1}^{n} 1^2 \sum_{i=1}^{n} |s_{r_i}|^2 - \left(\sum_{i=1}^{n} |s_{r_i}|\right)^2 \leq \frac{n^2}{4} \left(s_{r_1} - s_{r\,\min}\right)^2$$

$$2SS(G)n - (E_{SRS}(G))^2 \leq \frac{n^2}{4} \left(s_{r_1} - s_{r\,\min}\right)^2$$

$$\implies E_{SRS}(G) \geq \sqrt{2SS(G)n - \frac{n^2}{4} \left(s_{r_1} - s_{r\,\min}\right)^2}.$$

□

Theorem 4.13. *Suppose zero is not an eigenvalue of $A_{SRS}(G)$, then*

$$E_{SRS}(G) \geq \frac{2\sqrt{s_{r_1} s_{r\,\min}}\sqrt{2SS(G)n}}{s_{r_1} + s_{r\,\min}},$$

where $s_{r_1} = s_{r\,\max} = \max_{1 \leq i \leq n} |s_{r_i}|$ and $s_{r\,\min} = \min_{1 \leq i \leq n} |s_{r_i}|$.

Proof. Suppose $s_{r_1}, s_{r_2}, \ldots, s_{r_n}$ are the eigenvalues of$A_{SRS}(G)$ We assume that $c_i = |s_{r_i}|$ and $d_i = 1$, which by Theorem 3.1, we have

$$\sum_{i=1}^{n} |s_{r_i}|^2 \sum_{i=1}^{n} 1^2 \leq \frac{1}{4} \left(\sqrt{\frac{s_{r_1}}{s_{r\,\min}}} + \sqrt{\frac{s_{r\,\min}}{s_{r_1}}}\right)^2 \left(\sum_{i=1}^{n} |s_{r_i}|\right)^2$$

$$2SS(G)n \leq \frac{1}{4} \left(\frac{\left(s_{r_1} + s_{r\,\min}\right)^2}{s_{r_1} s_{r\,\min}}\right) (E_{SRS}(G))^2$$

$$\implies E_{SRS}(G) \geq \frac{2\sqrt{s_{r_1} s_{r\,\min}}\sqrt{2SS(G)n}}{s_{r_1} + s_{r\,\min}}.$$

□

Theorem 4.14. *Let G be a graph of order n. Let $s_{r_1} \geq s_{r_2} \geq \ldots \geq s_{r_n}$ be the eigenvalues of$A_{SRS}(G)$ Then*

$$E_{SRS}(G) \geq \frac{2SS(G) + n s_{r_1} s_{r\,\min}}{s_{r_1} + s_{r\,\min}},$$

where $s_{r_1} = s_{r\,\max} = \max_{1 \leq i \leq n} |s_{r_i}|$ and $s_{r\,\min} = \min_{1 \leq i \leq n} |s_{r_i}|$.

Proof. Assigning $d_i = |s_{r_i}|, c_i = 1, R = |s_{r_1}|$ and $r = |s_{r\,\min}|$.
Then by Theorem 3.4, we get

$$\sum_{i=1}^{n} |s_{r_i}|^2 + s_{r_1} s_{r\,\min} \sum_{i=1}^{n} 1^2 \leq \left(s_{r_1} + s_{r\,\min}\right) \sum_{i=1}^{n} |s_{r_i}|$$

$$\implies 2SS(G) + n s_{r_1} s_{r\,\min} \leq \left(s_{r_1} + s_{r\,\min}\right) E_{SRS}(G).$$

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

$$E_{SRS}(G) \geq \frac{2SS(G) + n s_{r_1} s_{r\,\min}}{s_{r_1} + s_{r\,\min}}.$$

□

Theorem 4.15. *Let G be a graph of order n. Let $s_{r_1} \geq s_{r_2} \geq \ldots \geq s_{r_n}$ be the eigenvalues of $A_{SRS}(G)$ Then*

$$E_{SRS}(G) \geq \sqrt{2SS(G)n - \alpha(n)\left(s_{r_1} - s_{r\min}\right)^2},$$

where $s_{r_1} = s_{r\max} = \max_{1\leq i\leq n} |s_{r_i}|$ and $s_{r\min} = \min_{1\leq i\leq n} |s_{r_i}|$ 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 $c_i = |s_{r_i}| = d_i, A \leq |s_{r_i}| \leq B$ and $a \leq |s_{r_n}| \leq b$, then by Theorem 3.3 we get

$$\left| n\sum_{i=1}^{n} |s_{r_i}|^2 - \left(\sum_{i=1}^{n} |s_{r_i}|\right)^2 \right| \leq \alpha(n)\left(s_{r_1} - s_{r\min}\right)^2$$

$$\text{i.e., } \left| 2SS(G)n - \left(E_{SRS}(G)\right)^2 \right| \leq \alpha(n)\left(s_{r_1} - s_{r\min}\right)^2$$

$$\Longrightarrow E_{SRS}(G) \geq \sqrt{2SS(G)n - \alpha(n)\left(s_{r_1} - s_{r\min}\right)^2}.$$

□

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

In this section, we perform a computational analysis of the square root stress sum energy $E_{SRS}(G)$ and π-electron energy of heteroatoms. This study explores linear, 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 square root stress sum energy in developing linear, quadratic, and cubic regression models for properties such as π-electron energy.

The regression models tested are as follows:
Linear equation:

$$Y = A + B_1X_1$$

Quadratic equation:

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

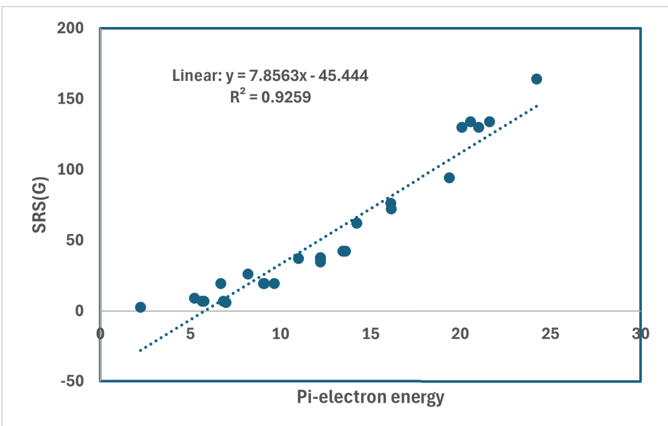
Cubic equation:

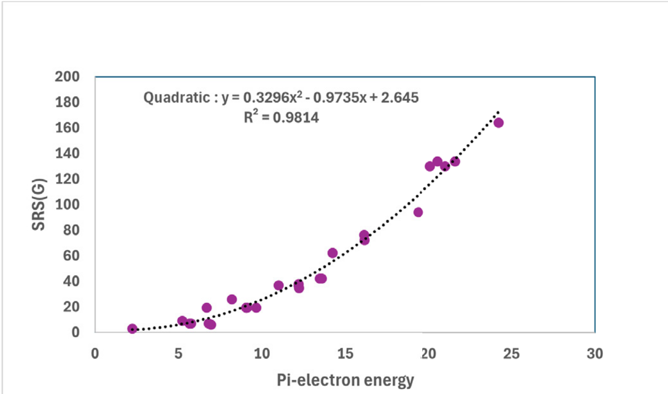
$$Y = A + B_1X_3 + B_2X_3^2 + B_3X_3^3$$

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 square root stress sum energy.

Molecule	Total π-electron energy	$E_{SRS}(G)$
Veny chloride like system	2.23	2.828
Acrolein like systems	5.76	6.928
1,1-Dichloro-ethylene like systems	6.96	5.91
Glyoxal like and 1,2-Dichloro-ethylene like systems	6.82	6.928
Butadiene perturbed at C2	5.66	6.928
Pyrrole like systems	5.23	9.152
Pyridine like systems	6.69	19.595
Pyridazine like systems	9.06	19.595
Pyrimidine like systems	9.10	19.595
Pyrazine like systems	9.07	19.595
S-Triazene like systems	9.65	19.595
Aniline like systems	8.19	26.093
O-Phenylene-diamine like systems	12.21	36.497
m-Phenylene-diamine like systems	12.22	34.691
p-Phenylene-diamine like systems	12.21	37.864
Benzaldehyde like systems	11.00	37.027
Quinoline like systems	14.23	62.13
Iso-quinoline like systems	14.23	62.13
1-Naphthalein like systems	16.15	72.132
2-Naphthalein like systems	16.12	76.183
Acridine like systems	20.56	133.766
Phenazine like systems	21.62	133.766
Iso-indole like systems	13.46	42.307
Indole like systems	13.59	42.307
Azobenzene like systems	21.02	122.995
Benzylidine-aniline-like systems	20.10	122.995
9,10-Anthraquinoline structures	24.23	164.02
Cabazole like structures	19.39	94.246





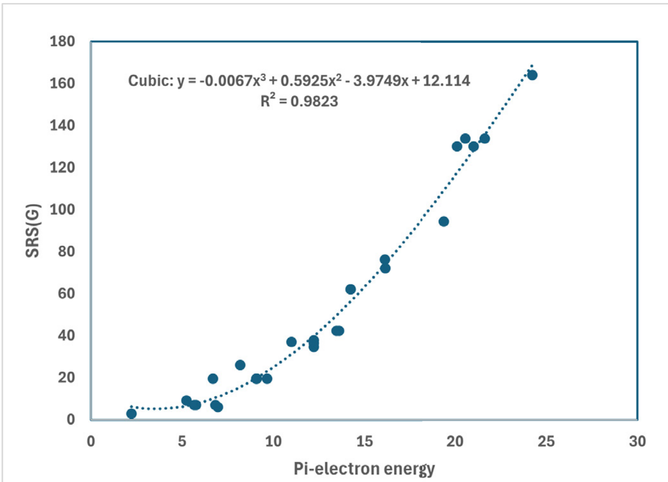


TABLE 2. The correlation coefficient r from linear, quadratic, and cubic regression model between square root stress sum energy and π electron energy

Model	Correlation Coefficient r
Linear	0.962
Quadratic	0.991
Cubic	0.991

TABLE 3. Comparison of statistical parameters among the regression models

Model	R^2	F-value	SE	Significant
Linear	0.9259	325.068	13.139	0.000
Quadratic	0.9814	661.326	6.70	0.000
Cubic	0.9823	443.416	6.69	0.000

6. Conclusion

The square root stress sum 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 square root stress sum energy and π-electron energy. We have observed the following:

(1) The square root stress sum energy has been shown to be a strong predictive measure for π-electron energy through regression models
(2) The statistical parameters computed from the regression models indicate a minimal SE, a significant p-value ($p \leq 0.05$), and an R^2 value close to 1, demonstrating a strong correlation between square root stress sum energy and π-electron energy
(3) The square root stress sum energy is an effective predictive tool for π-electron energy in chemical systems.Regression models applied to π-electron energy show strong correlations, with statistical measures such as SE, p-value, and R^2 supporting its predictive capacity. This study establishes the square root stress sum energy as a promising approach for predicting π-electron energy in molecules containing heteroatoms.

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