Bol. Soc. Paran. Mat.
©SPM – E-ISSN-2175-1188
SPM: www.spm.uem.br/bspm

(3s.) **v. 2025 (43)** : 1–12.
ISSN-0037-8712
doi:10.5269/bspm.76033

On Cangul Stress Energy of Graphs

P. Somashekar, Howida Adel AlFran, P. Siva Kota Reddy*, M. Kirankumar and M. Pavithra

ABSTRACT: In this article, we introduce the Cangul stress matrix $CSM(G)$ for a connected graph G, which is associated with the Cangul stress index. We investigate the properties of this matrix, establish bounds on its eigenvalues, and define the Cangul stress energy $E_{CSM}(G)$ as the sum of the absolute values of the eigenvalues. Furthermore, we examine its potential relevance in chemistry by comparing $E_{CSM}(G)$ with the π-electron energy of benzene derivatives.

Key Words: Graph, stress of a vertex, energy, Cangul stress eigenvalues.

Contents

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 [8].

Gutman [6] 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. There are several matrices that can be associated with a graph, and their spectrums offer some useful insights about the graph (See for example [1,3,5,7,9-12,16,18-21,29,33]).

In 1953, Alfonso Shimbel [30] 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

* Corresponding author

Submitted March 08, 2025. Published May 23, 2025
2010 *Mathematics Subject Classification:* 05C50, 05C09, 05C92

concept has many applications including the study of biological and social networks. A number of authors have defined and examined numerous stress-related concepts in graphs and topological indices (See [2,14,15,17,22-28,31,32]). A graph G is k-stress regular [4] if $str(v) = k$ for all $v \in V(G)$. The stress-sum index $SS(G)$ [23] of a graph $G(V, E)$ is defined by

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

The second stress index $S_2(G)$ [24] of a graph $G(V, E)$ is defined by

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

The Cangul stress index $CS(G)$ [31] of a graph G is defined as

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

By the motivation of Cangul stress index, in this paper, we present the Cangul stress matrix for a graph G and define the Cangul stress energy $E_{CSM}(G)$ based on its eigenvalues. This novel approach broadens the concept of graph energy by integrating stress-related measures, providing a new perspective on graph invariants. We establish bounds for $E_{CSM}(G)$ in relation to other graph invariants and investigate the relationship between the Cangul stress energy of benzenoid hydrocarbons and their corresponding π-electron energy. This study aims to enhance our understanding of graph energy and its implications for molecular and structural analysis.

2. Cangul Stress Matrix and Energy

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

$$x_{ij} = \begin{cases} [str(v_i) + str(v_j)]str(v_i)\, str(v_j), & \text{if} \quad v_iv_j \in E(G); \\ 0, & \text{otherwise} . \end{cases}$$

The Cangul stress polynomial of a graph G is defined as

$$P_{CSM}(G) = |\lambda I - CSM(G)|,$$

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

All roots of the equation $P_{CSM}(G) = 0$ are real since the matrix $CSM(G)$ is both real and symmetric. Consequently, these roots can be arranged in descending order as $c_{s_1} \geq c_{s_2} \geq \cdots \geq c_{s_n}$, where c_{s_1} denotes the largest eigenvalue and c_{s_n} represents the smallest eigenvalue.

The Cangul stress energy $E_{CSM}(G)$ of a graph G is defined by

$$E_{CSM}(G) = \sum_{i=1}^{n} |c_{s_i}| .$$

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*

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

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 $M_1 = \max\limits_{1\leq i\leq n}\{c_i\}; M_2 = \max\limits_{1\leq i\leq n}\{d_i\}; m_1 = \min\limits_{1\leq i\leq n}\{c_i\}$ *and* $m_2 = \min\limits_{1\leq i\leq n}\{d_i\}$.

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 Cangul Stress Eigenvalues and Energy

Lemma 4.1 *Let $c_{s_1} \geq c_{s_2} \geq \ldots \geq c_{s_n}$ be the eigenvalues of the Cangul stress matrix $CSM(G)$. Then*

[(i)]

1. $\sum_{i=1}^{n} c_{s_i} = 0$
2. $\sum_{i=1}^{n} c_{s_i}^2 = 2\sum_{1\leq i<j\leq n}[(str(v_i) + str(v_j))(str(v_i)\, str(v_j))]^2 = 2\mathbb{C}$,

   where $\mathbb{C} = \sum_{1\leq i<j\leq n}[(str(v_i) + str(v_j))(str(v_i)\, str(v_j))]^2$.

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

$$\begin{aligned}
\sum_{i=1}^{n} c_{s_i}^2 &= \text{trace}[CSM(G)]^2 \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n}[(str(v_i) + str(v_j))(str(v_i)\, str(v_j))]^2 \\
&= 2\sum_{1\leq i<j\leq n}[(str(v_i) + str(v_j))(str(v_i)\, str(v_j))]^2 \\
&= 2\mathbb{C}.
\end{aligned}$$

□

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

$$P_{CSM}(K_{m,n}) = \lambda^{m+n-2}\left[\lambda^2 - \frac{mn}{8}\left(n^2m(n-1)^2(m-1) + nm^2(n-1)(m-1)^2\right)\right].$$

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

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

Hence,
$CSM(K_{m,n})=$

$$\begin{bmatrix} 0_m & \left[\frac{n(n-1)}{2} + \frac{m(m-1)}{2}\right]\left(\frac{(n(n-1))}{2}\frac{m(m-1)}{2}\right) J_{m\times n} \\ \left[\frac{n(n-1)}{2} + \frac{m(m-1)}{2}\right]\left(\frac{(n(n-1))}{2}\frac{m(m-1)}{2}\right) J_{n\times m} & 0_n \end{bmatrix}.$$

$$P_{CSM}(K_{m,n}) = |\lambda I - CSM(K_{m,n})|.$$

Thus we have,
$P_{CSM}(K_{m,n}) =$

$$\begin{vmatrix} \lambda I_m & -\left[\frac{n(n-1)}{2} + \frac{m(m-1)}{2}\right]\left(\frac{(n(n-1))}{2}\frac{m(m-1)}{2}\right) J_{m\times n} \\ -\left[\frac{n(n-1)}{2} + \frac{m(m-1)}{2}\right]\left(\frac{(n(n-1))}{2}\frac{m(m-1)}{2}\right) J_{n\times m} & \lambda I_n \end{vmatrix},$$

where I_r is the identity matrix of order $r\times r$, 0_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 4.2, we obtain the desired result.

□

Theorem 4.2 *The characteristic polynomial of fan graph F_n on $2n+1$ vertices and star graph S_n on $n+1$ vertices are λ^{2n+1} and λ^{n+1} respectively.*

Proof: In F_n graph, the stress of central vertex is $2n(n-1)$ and remaining $2n$ vertices have stress 0. Therefore $CSM(F_n) = [0]_{(2n+1)\times(2n+1)}$.

The characteristic polynomial of the above matrix is given by λ^{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 $CSM(S_n) = [0]_{(n+1)\times(n+1)}$. The characteristic polynomial of the above matrix is given by λ^{n+1}.
□

Theorem 4.3 *Let G be any graph with n-vertices. Then*

$$c_{s_1} \le \sqrt{\frac{(2\mathbb{C})(n-1)}{n}}.$$

Proof:
Setting $c_i = 1, d_i = c_{s_i}$, for $i = 2, 3, \ldots, n$ in Theorem 3.5, we have

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

From Lemma 4.1, we find that

$$\sum_{i=2}^{n} c_{s_i} = -c_{s_1} \text{ and } \sum_{i=2}^{n} c_{s_i}^2 = -c_{s_1}^2 + 2\mathbb{C}.$$

Employing the above in (4.1), we obtain

$$(-c_{s_1})^2 \leq (n-1)\left(2\mathbb{C} - c_{s_1}^2\right)$$
$$c_{s_1} \leq \sqrt{\frac{(2\mathbb{C})(n-1)}{n}}.$$

□

Theorem 4.4 *Let G be any graph with n-vertices. Then*

$$E_{CSM}(G) \leq \sqrt{(2\mathbb{C})n}.$$

Proof: Choosing $c_i = 1, d_i = |c_{s_i}|$, for $i = 2, 3, \ldots, n$ in Theorem 3.5, we get

$$\left(\sum_{i=1}^{n} |c_{s_i}|\right)^2 \leq n\sum_{i=1}^{n} c_{s_i}^2$$
$$\Longrightarrow (E_{CSM}(G))^2 \leq n(2\mathbb{C})$$
$$\Longrightarrow E_{CSM}(G) \leq \sqrt{n(2\mathbb{C})}.$$

□

Theorem 4.5 *If G is a graph with n vertices and $E_{CSM}(G)$ be the cangul stress energy of G, then*

$$\sqrt{2\mathbb{C}} \leq E_{CSM}(G).$$

Proof: By the definition of $E_{CSM}(G)$, we have

$$[E_{CSM}(G)]^2 = \left(\sum_{i=1}^{n} |c_{s_i}|\right)^2 \geq \sum_{i=1}^{n} |c_{s_i}|^2 = 2\mathbb{C}.$$
$$\Longrightarrow \quad \sqrt{2\mathbb{C}} \leq E_{CSM}(G).$$

□

Theorem 4.6 *Let G be any graph with n-vertices and Φ be the absolute value of the determinant of the cangul stress matrix $CSM(G)$. Then*

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

Proof: By the definition of cangul stress energy, we find that

$$(E_{CSM}(G))^2 = \left(\sum_{i=1}^{n} |c_{s_i}|\right)^2 = \sum_{i=1}^{n} |s_{\lambda_i}|^2 + 2\sum_{i<j} |c_{s_i}||c_{s_j}|$$
$$= (2\mathbb{C}) + \sum_{i \neq j} |c_{s_i}||c_{s_j}|.$$

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

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

Therefore,

$$\begin{aligned}&\sum_{i\neq j}|c_{s_i}|\,|c_{s_j}| \geq n(n-1)\Phi^{\frac{2}{n}}\\ \Longrightarrow\ & [E_{CSM}(G)]^2 \geq 2\mathbb{C} + n(n-1)\Phi^{2/n}\\ \Longrightarrow\ & E_{CSM}(G) \geq \sqrt{2\mathbb{C} + n(n-1)\Phi^{2/n}}.\end{aligned}$$

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

Lemma 4.3 *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 4.7 *Let G be a connected graph with n vertices. Then*

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

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

Proof: Let $c_i = |c_{s_i}|^2, i = 1, 2, \ldots, n$ and

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

By Lemma 4.3, we obtain

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

Upon simplification of the above equation, we find that

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

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

□

Theorem 4.8 *Let G be a graph of order n. Then*

$$E_{CSM}(G) \geq \sqrt{(2\mathbb{C})n - \frac{n^2}{4}\left(c_{s_1}-c_{s\min}\right)^2},$$

where $c_{s_1} = c_{s\max} = \max\limits_{1\leq i\leq n}\{|c_{s_i}|\}$ *and* $c_{s\min} = \min\limits_{1\leq i\leq n}\{|c_{s_i}|\}$.

Proof: Suppose $c_{s_1}, c_{s_2}, \ldots, c_{s_n}$ are the eigenvalues of $CSM(G)$. We choose $c_i = 1$ and $d_i = |c_{s_i}|$, which by Theorem 3.2 implies

$$\sum_{i=1}^{n} 1^2 \sum_{i=1}^{n} |c_{s_i}|^2 - \left(\sum_{i=1}^{n}|c_{s_i}|\right)^2 \leq \frac{n^2}{4}\left(c_{s_1}-c_{s\min}\right)^2$$

$$\text{i.e.,}\quad (2\mathbb{C})n - \left(E_{CSM}(G)\right)^2 \leq \frac{n^2}{4}\left(c_{s_1}-c_{s\min}\right)^2$$

$$\Longrightarrow\quad E_{CSM}(G) \geq \sqrt{(2\mathbb{C})n - \frac{n^2}{4}\left(c_{s_1}-c_{s\min}\right)^2}.$$

□

Theorem 4.9 *Suppose zero is not an eigenvalue of $CSM(G)$, then*

$$E_{CSM}(G) \geq \frac{2\sqrt{c_{s_1}c_{s\min}}\sqrt{(2\mathbb{C})n}}{c_{s_1}+c_{s\min}},$$

where $c_{s_1} = c_{s\max} = \max_{1\leq i\leq n}\{|c_{s_i}|\}$ *and* $c_{s\min} = \min_{1\leq i\leq n}\{|c_{s_i}|\}$.

Proof: Suppose $c_{s_1}, c_{s_2}, \ldots, c_{s_n}$ are the eigenvalues of $CSM(G)$.
Setting $c_i = |c_{s_i}|$ and $d_i = 1$ in Theorem 3.1, we have

$$\sum_{i=1}^{n}|c_{s_i}|^2 \sum_{i=1}^{n} 1^2 \leq \frac{1}{4}\left(\sqrt{\frac{c_{s_1}}{c_{s\min}}}+\sqrt{\frac{c_{s\min}}{c_{s_1}}}\right)^2\left(\sum_{i=1}^{n}|c_{s_i}|\right)^2$$

$$\text{i.e.,}\quad (2\mathbb{C})n \leq \frac{1}{4}\left(\frac{\left(c_{s_1}+c_{s\min}\right)^2}{c_{s_1}c_{s\min}}\right)\left(E_{CSM}(G)\right)^2$$

$$\Longrightarrow\quad E_{CSM}(G) \geq \frac{2\sqrt{c_{s_1}c_{s\min}}\sqrt{(2\mathbb{C})n}}{c_{s_1}+c_{s\min}}.$$

□

Theorem 4.10 *Let G be a graph of order n and $c_{s_1} \geq c_{s_2} \geq \ldots \geq c_{s_n}$ be the non zero eigenvalues of $CSM(G)$. Then*

$$E_{CSM}(G) \geq \frac{(2\mathbb{C}) + nc_{s_1}c_{s\min}}{c_{s_1}+c_{s\min}},$$

where $c_{s_1} = c_{s\max} = \max\limits_{1\leq i\leq n}\{|c_{s_i}|\}$ *and* $c_{s\min} = \min\limits_{1\leq i\leq n}\{|c_{s_i}|\}$.

Proof: Assigning $d_i = |c_{s_i}|, c_i = 1, R = |c_{s_1}|$ and $r = |c_{s\min}|$ in Theorem 3.4, we get

$$\sum_{i=1}^{n}|c_{s_i}|^2 + c_{s_1}c_{s\min}\sum_{i=1}^{n}1^2 \leq \left(c_{s_1}+c_{s\min}\right)\sum_{i=1}^{n}|c_{s_i}|$$

$$(2\mathbb{C}) + nc_{s_1}c_{s\min} \leq \left(c_{s_1}+c_{s\min}\right)E_{CSM}(G).$$

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

$$E_{CSM}(G) \geq \frac{(2\mathbb{C}) + nc_{s_1}c_{s\min}}{c_{s_1}+c_{s\min}}.$$

□

Theorem 4.11 *Let G be a graph of order n and $c_{s_1} \geq c_{s_2} \geq \ldots \geq c_{s_n}$ be the eigenvalues of $CSM(G)$. Then*

$$E_{CSM}(G) \geq \sqrt{(2\mathbb{C})n - \alpha(n)\left(c_{s_1} - c_{s\,\min}\right)^2},$$

where $c_{s_1} = c_{s\,\max} = \max\limits_{1\leq i\leq n}\{|c_{s_i}|\}$ and $c_{s\,\min} = \min\limits_{1\leq i\leq n}\{|c_{s_i}|\}$ 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 $c_i = |c_{s_i}| = d_i$, $A \leq |c_{s_i}| \leq B$ and $a \leq |c_{s_n}| \leq b$ in Theorem 3.3, we get

$$\left| n\sum_{i=1}^{n}|c_{s_i}|^2 - \left(\sum_{i=1}^{n}|c_{s_i}|\right)^2 \right| \leq \alpha(n)\left(c_{s_1} - c_{s\,\min}\right)^2$$
$$\left|(2\mathbb{C})n - (E_{CSM}(G))^2\right| \leq \alpha(n)\left(c_{s_1} - c_{s\,\min}\right)^2$$
$$E_{CSM}(G) \geq \sqrt{(2\mathbb{C})n - \alpha(n)\left(c_{s_1} - c_{s\,\min}\right)^2}.$$

□

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

In this section, we conduct a computational analysis of the cangul stress energy $E_{CSM}(G)$ and the π-electron energy of benzene derivatives. We investigate both power and logarithmic regression models to accommodate the nonlinear trends often present in real-world data. These adaptable methods allow researchers to identify the optimal fit for their specific datasets. Additionally, this section emphasizes the significance of Cangul stress energy in the formulation of power and logarithmic regression models aimed at assessing properties such as π-electron energy.

The regression models tested are as follows:

Power equation:

$$Y = AX^B$$

Logarithmic equation:

$$Y = A + B\log(X)$$

Here, Y is the dependent variable, A is the regression constant, and B is the regression coefficient for the independent variable X.

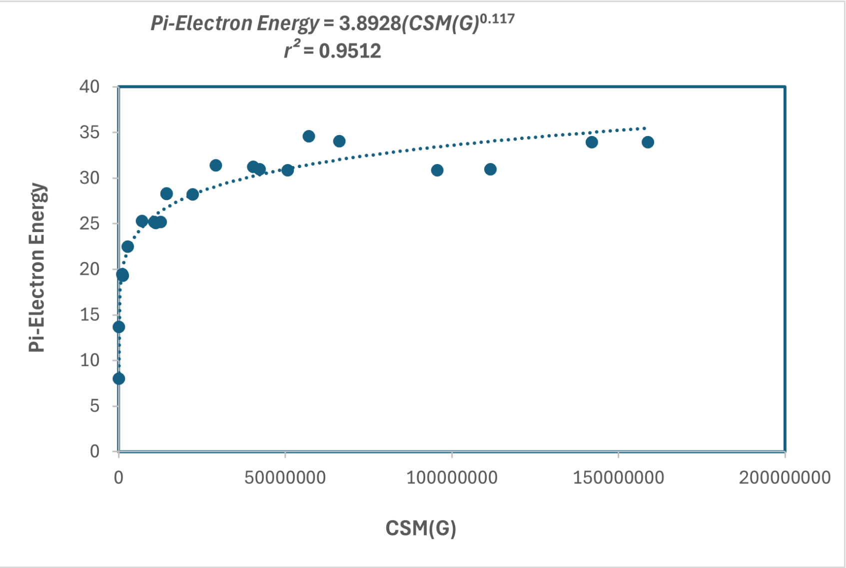
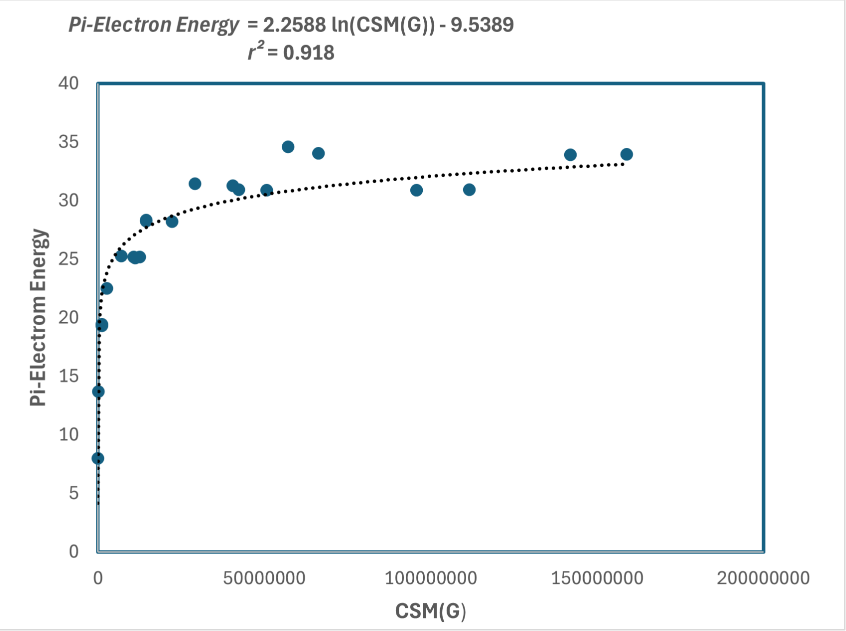


Table 1: Cangul Stress Energy and π-Electron Energy of Derivatives of Benzene

Derivatives of benzene	$E_{CSM}(G)$	π-electron energy
Benzene	432	8
Naphthalene	62305.07	13.683
Phenanthrene	1163588.90	19.448
Anthracene	1166559.36	19.314
Chrysene	12586044.99	25.192
Benzo[a]anthracene	11161172.27	25.10
Triphenylene	7000231.56	25.275
Tetracene	10687271.67	25.188
Benzo[a]pyrene	22238320.76	28.222
Benzo[e]pyrene	14395343.35	28.336
Perylene	14449828.65	28.245
Anthanthrene	40433942.11	31.253
Benzo[ghi]perylene	29168140.40	31.425
Dibenz[a,c]anthracene	42361213.334	30.492
Dibenz[a,h]anthracene	95641465.76	30.881
Dibenz[a,j]anthracene	50735054.62	30.88
Picene	111629104.23	30.943
Coronene	57042939.35	34.572
Dibenzo[a,h]pyrene	141956248.66	33.928
Dibenzo[a,i]pyrene	158846656.55	33.954
Dibenzo[a,l]pyrene	66257730.30	34.031
Pyrene	2683098.75	22.506

Table 2: The correlation coefficient r from power and logarithmic regression models between Cangul stress energy and π electron energy

Model	Correlation Coefficient r
Power	0.975
logarithmic	0.958



6. Conclusion

This study presents Cangul stress energy as a promising predictor of π-electron energy in chemical compounds. Understanding π-electron energy is essential for explaining the stability and reactivity of benzene derivatives. By employing regression models, we assess the predictive relationship between Cangul stress energy and π-electron energy.

Acknowledgments

The authors thank the anonymous reviewers for their careful reading of our manuscript and their many insightful comments and suggestions.

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), 50-59, (2024).
2. AlFran, H. A., Somashekar, P. and Siva Kota Reddy, P., *Modified Kashvi-Tosha Stress Index for Graphs*, Glob. Stoch. Anal., 12(1), 10-20, (2025).
3. Brouwer, A. E. and Haemers, W. H., *Spectra of Graphs-Monograph*, Springer, (2011).
4. Bhargava, K., Dattatreya, N. N. and Rajendra, R., *On stress of a vertex in a graph*, Palest. J. Math., 12(3), 15–25, (2023).
5. Cvetković, D. M., Doob, M. and Sachs, H., *Spectra of Graphs*, Academic Press, (1979).
6. Gutman, I., *The energy of a graph*, Ber. Math.-Stat. Sekt. Forschungszent. Graz, 103, 1-22, (1978).
7. 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, 435-442, (2007).
8. Harary, F., *Graph Theory*, Addison Wesley, Reading, Mass, (1972).
9. Hemavathi, P. S., Mangala Gowramma, H., Kirankumar, M., Pavithra, M. and Siva Kota Reddy, P., On Minimum Stress Energy of Graphs, *J. Appl. Math. Inform.*, 43(2), 543-557, (2025).
10. Kirankumar, M., Ruby Salestina, M., Harshavardhana, C. N., Kemparaju, R. and Siva Kota Reddy, P., *On Stress Product Eigenvalues and Energy of Graphs*, *Glob. Stoch. Anal.*, 12(1), 111-123, (2025).
11. Kirankumar, M., Harshavardhana, C. N., Ruby Salestina, M., Pavithra, M. and Siva Kota Reddy, P., On Sombor Stress Energy of Graphs, *J. Appl. Math. Inform.*, 43(2), 475-490, (2025).
12. Lokesha, V., Shanthakumari, Y. and Siva Kota Reddy, P., Skew-Zagreb Energy of Directed Graphs, *Proc. Jangjeon Math. Soc.*, 23(4), 557-568, (2020).
13. Mahesh, K. B., Rajendra, R. and Siva Kota Reddy, P., *Square Root Stress Sum Index for Graphs*, Proyecciones, 40(4), 927-937, (2021).
14. Mangala Gowramma, H., Siva Kota Reddy, P., Kim, T. and Rajendra, R., *Taekyun Kim Stress Power α-Index*, Bol. Soc. Parana. Mat. (3), 43, Article Id: 72273, 10 Pages, (2025).
15. Mangala Gowramma, H., Siva Kota Reddy, P., Kim, T. and Rajendra, R., *Taekyun Kim α-Index of Graphs*, Bol. Soc. Parana. Mat. (3), 43, Article Id: 72275, 10 Pages, (2025).
16. Nalina, C., Siva Kota Reddy, P., Kirankumar, M. and Pavithra, M., On Stress Sum Eigenvalues and Stress Sum Energy of Graphs, *Bol. Soc. Parana. Mat. (3)*, 43, Article Id: 75954, 15 Pages, (2025).
17. Poojary, R., Arathi Bhat, K., Arumugam, S. and Manjunatha Prasad, K., *The stress of a graph*, Commun. Comb. Optim., 8(1), 53-65, (2023).
18. Prakasha, K. N., Siva kota Reddy, P. and Cangul, I. N., *Partition Laplacian Energy of a Graph*, Adv. Stud. Contemp. Math., Kyungshang, 27(4), 477-494, (2017).
19. Prakasha, K. N., Siva Kota Reddy, P. and Cangul, I. N., *Minimum Covering Randic energy of a graph*, Kyungpook Math. J., 57(4), 701-709, (2017).
20. Prakasha, K. N., Siva Kota Reddy, P. and Cangul, I. N., *Sum-Connectivity Energy of Graphs*, Adv. Math. Sci. Appl., 28(1), 85-98, (2019).
21. Prakasha, K. N., Siva kota Reddy, P., Cangul, I. N. and Purushotham, S., *Atom-Bond-Connectivity Energy of Graphs*, TWMS J. App. Eng. Math., 14(4), 1689-1704, (2024).
22. Rai, P. S., Rajendra, R. and Siva Kota Reddy, P., *Vertex Stress Polynomial of a Graph*, Bol. Soc. Parana. Mat. (3), 43, Article Id: 68311, 6 Pages, (2025).
23. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N., *Stress-Sum index of graphs*, Sci. Magna, 15(1), 94-103, (2020).

24. Rajendra, R., Siva Kota Reddy, P. and Cangul, I. N., *Stress indices of graphs*, Adv. Stud. Contemp. Math. (Kyungshang), 31(2), 163-173, (2021).

25. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N., *Tosha Index for Graphs*, Proc. Jangjeon Math. Soc., 24(1), 141-147, (2021).

26. 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), 149-160, (2022).

27. 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), 483-493, (2023).

28. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N., *Stress-Difference Index for Graphs*, Bol. Soc. Parana. Mat. (3), 42, 1-10, (2024).

29. 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), 29-34, (2024).

30. Shimbel, A., *Structural Parameters of Communication Networks*, Bulletin of Mathematical Biophysics, 15, 501-507, (1953).

31. Somashekar, P., Siva Kota Reddy, P., Harshavardhana, C. N. and Pavithra, M., *Cangul Stress Index for Graphs*, J. Appl. Math. Inform., 42(6), 1379-1388, (2024).

32. Somashekar, P. and Siva Kota Reddy, P., *Kashvi-Tosha Stress Index for Graphs*, Dyn. Contin. Discrete Impuls. Syst., Ser. B, Appl. Algorithms, 32, 137-148, (2025).

33. Sureshkumar, S., Mangala Gowramma, H., Kirankumar, M., Pavithra, M. and Siva Kota Reddy, P., On Maximum Stress Energy of Graphs, *Glob. Stoch. Anal.*, 12(2), 56-69, (2025).

P. Somashekar,
Department of Mathematics
Maharani's Science College for Women (Autonomous)
Mysuru–570 005, India.
E-mail address: `somashekar2224@gmail.com`

and

Howida Adel AlFran,
Department of Mathematics
AL-Leith University College
Umm Al-Qura University, Kingdom of Saudi Arabia.
E-mail address: `hafran@uqu.edu.sa`

and

P. Siva Kota Reddy,
Department of Mathematics
JSS Science and Technology University
Mysuru–570 006, India.
E-mail address: `pskreddy@jssstuniv.in`

and

M. Kirankumar,
Department of Mathematics
Vidyavardhaka College of Engineering
Mysuru-570 002, India
Affiliated to Visvesvaraya Technological University, Belagavi-590 018, India.
E-mail address: `kiran.maths@vvce.ac.in`

and

M. Pavithra,
Department of Studies in Mathematics
Karnataka State Open University
Mysuru–570 006, India.
E-mail address: sampavi08@gmail.com