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A study on the temperature Sombor energy and entropy of a graph

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ABSTRACT: The temperature Sombor index is one of the variations of the recently introduced Sombor index, a degree based topological index, found to have nice mathematical properties and very useful applications. In our current study, we introduce the temperature Sombor matrix $\mathcal{T}(G)$, an associated matrix of the temperature Sombor index of a graph G and present certain bounds on its eigenvalues. Additionally, we define the temperature Sombor energy $\mathcal{ET}(G)$ of G and determine some bounds on it. We also discuss the chemical applicability of this parameter by comparing it with the π-electron energy of certain chemical compounds. Additionally, we perform the regression analysis of the temperature Sombor energy with the graph energy of trees with fixed orders $n = 8, 9, \cdots, 18$. Further, we compute the temperature Sombor entropy of the silicon carbide compound and analyze it in conjunction with its temperature Sombor index.

Key Words: Graph energy, Sombor index, temperature Sombor index, temperature forgotten index, temperature Sombor energy, entropy, temperature Sombor entropy.

Contents

1. Introduction

One of the significant ideas employed in chemical graph theory is that of the chemical indices that depend on the structure of the associated graph, commonly known as topological indices. Topological indices are numerical values that a graph inherits and can be correlated with the physical properties, biological activities and chemical reactivity of individual chemical molecules. Many characteristics of the chemical structures, including toughness, entropy, rigidity, boiling point, strain energy, enthalpy of formation and enthalpy of vaporization are known to be closely related to their underlying graphical

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structures. These topological indices are therefore generally considered descriptors of chemical structures. Generally, a vertex-degree-based (VDB) topological index can be expressed in the form

$$TI(G) = \sum_{vw \in E(G)} f(\mathbf{d}(v), \mathbf{d}(w))$$

where $\mathbf{d}(v)$ represents the number of vertices adjacent with the vertex v, called the degree of v in the graph G. Zagreb index [11], Randić index [25], Sombor index [32] and harmonic index [24] are some of the commonly known vertex-degree-based topological indices. Sombor index [22], a recently introduced vertex-degree-based topological index, has drawn a lot of interest in the literature. It is being thoroughly investigated because of its broad range of applicability [31,32,19,35,12,42,16,41]. Since then, numerous studies on various versions of the Sombor index have been proposed and investigated [8,43,14,5,27].

In 1988, Fajtolowicz defines a new parameter called the temperature of a vertex [36]. Motivated by the definition of Sombor index and Fajtolowicz's research, Kulli introduces a new Sombor index variant called the temperature Sombor index of G [44], denoted as $\mathcal{TSO}(G)$ and studies some of its mathematical properties. It is being extensively studied in the field of graph theory because of its interesting characteristics. For related work, we cite [13,37,38,45].

On the other hand, spectral graph theory involves linear algebra in general and matrix theory in particular, to explore and interpret the topological and physico-chemical properties of a graph and related chemical structures. With its rapid development, spectral graph theory has gained a lot of attention even from mathematicians and researchers whose interests are quite different from this domain. Study of graph energies is one of the main concepts that comes under spectral graph theory.

As defined by Gutman [10], the sum of the absolute values of eigenvalues of the adjacency matrix $\mathcal{A}(G)$ of a graph G is the energy $\mathcal{E}(G)$ of G. Notably, eigenvalues connect with all extreme properties and are strongly related to nearly all critical graph invariants, offering a key to the fundamental understanding of graphs and therefore, graph energy has generated interest in both pure and applied mathematics. Over the years, a lot of work has been made on the energy of graphs and chemical structures. Many kind of graph energies and matrices are introduced and studied [20,22,18,30,28].

In addition to graph energy, the concept of graph entropy plays a vital role in the analysis of the structural properties of molecular structures. Shannon introduces the concept of entropy in 1948 [3], defining it as "a measure of the unpredictability of information content or the uncertainty of a system" within a probability distribution. This foundational work has increased the importance of entropy across various fields, including graph and chemical network analysis, particularly in measuring structural information. In 1955, Rashevsky contributes significantly to the field by introducing the idea of graph entropy, which focuses on classifying vertex orbits. The concept of an edge-weighted graph characterized by entropy is first introduced by Chen *et* al. [46] in 2014. Recently, the application of graph entropy has expanded to multiple disciplines, including chemistry, biology, ecology, sociology, discrete mathematics and statistics. Its primary purpose is to analyze entropies in relational structures. In mathematical chemistry, graph entropy is used to effectively characterize the structure of graphical representations. It can also be employed to evaluate chemical databases or groups of molecules based on their structural diversity. A higher entropy value indicates greater structural diversity, which may result in a more varied range of chemical substances. For related work, we cite [17,26,33,39].

Semiconductors are both cost-effective and environmentally friendly, serving a vital role in the electronics sector. They are essential for the functionality of nearly all electronic devices, highlighting their significance in contemporary technology. Silicon carbide (SiC) is composed of lightweight components and is recognized for its low coefficient of thermal expansion. This material is characterized by robust covalent bonds, excellent thermal conductivity and remarkable hardness. Until 1929, it was considered the hardest substance on Earth. Its appearance varies, displaying colors such as green or black, depending on the presence of impurities such as aluminum (Al), iron (Fe) or oxygen (O). Silicon carbide is extensively used in various furnace components, including heating elements, core tubes and refractory bricks, because of its exceptional heat resistance. Furthermore, it serves as a foundational material for advances in electronics, transportation technologies and applications in quantum physics.

Motivated by the definition of the temperature Sombor index of G, in this article, we define the temperature Sombor energy $\mathcal{ET}(G)$ of a graph G by introducing its temperature Sombor matrix and determining its eigenvalues. Besides that, we establish some bounds on $\mathcal{ET}(G)$ in terms of other graph invariants. Additionally, we study the correlation of the temperature Sombor energy of some molecules having hetero atoms, alkanes and cubic compounds with their respective π-electron energies, compute regression analysis of temperature Sombor energy with the graph energies of trees with fixed orders $n = 8, 9, \cdots, 18$. Further, we derive the formulae for the temperature Sombor index and temperature Sombor entropy related to the Silicon Carbide ($SiC_4 - I[a, b]$) semiconductor compound [29] and perform regression analysis of the temperature Sombor index with temperature Sombor entropy of $SiC_4 - I[a, b]$ as well.

2. Preliminaries

Throughout this article, we consider only graphs that are simple, finite, undirected and connected. Given a graph $G = (V, E)$ with $V(G)$ being the vertex set and $E(G)$ being the edge set, two vertices $v, w \in V(G)$ are said to be adjacent if they share a common edge. Vertices with degree zero and one are respectively called isolated and pendant vertices.

The adjacency matrix of a graph G with $V(G) = \{u_1, u_2, \cdots, u_n\}$ is defined as $\mathcal{A}(G) = (a_{ij})_{n\times n}$ where

$$a_{ij} = \begin{cases} 1 & \text{if } u_iu_j \in E(G) \\ 0 & \text{if } u_iu_j \notin E(G) \\ 0 & \text{otherwise.} \end{cases}$$

The Sombor index [32] of a graph G is defined as

$$\mathcal{SO}(G) = \sum_{vw\in E(G)} \sqrt{\mathbf{d}(v)^2 + \mathbf{d}(w)^2}.$$

Correspondingly, the Sombor matrix [22] of G, having its vertex set $V(G) = \{u_1, u_2, \cdots, u_n\}$, is defined as $\mathcal{A}_{\mathcal{SO}}(G) = ((a_{\mathcal{SO}})_{ij})$ where

$$(a_{\mathcal{SO}})_{ij} = \begin{cases} \sqrt{\mathbf{d}(u_i)^2 + \mathbf{d}(u_j)^2} & \text{if } u_iu_j \in E(G) \\ 0 & \text{if } u_iu_j \notin E(G) \\ 0 & \text{otherwise.} \end{cases}$$

Further, the sum of the absolute values of the eigenvalues of $\mathcal{A}_{\mathcal{SO}}(G)$ is defined as the Sombor energy of G.

The temperature Sombor index [44] of a graph G is defined as

$$\mathcal{TSO}(G) = \sum_{vw\in E(G)} \sqrt{\mathcal{T}(v)^2 + \mathcal{T}(w)^2}$$

where $\mathcal{T}(v) = \dfrac{\mathbf{d}(v)}{n - \mathbf{d}(v)}$ is called the temperature of a vertex v in G [36].

The forgotten index $\mathcal{F}(G)$ [1] of G is defined as

$$\mathcal{F}(G) = \sum_{vw\in E(G)} \left(\mathbf{d}(v)^2 + \mathbf{d}(w)^2\right).$$

Further, its corresponding temperature version, named as the temperature forgotten index [44], is defined as

$$\mathcal{FT}(G) = \sum_{vw\in E(G)} \left(\mathcal{T}(v)^2 + \mathcal{T}(w)^2\right).$$

3. Temperature Sombor matrix and temperature Sombor energy of a graph

Definition 3.1 *For a graph G with $V(G) = \{u_1, u_2, \cdots, u_n\}$, the temperature Sombor matrix of G, denoted by $\mathcal{T}(G)$, is defined as $\mathcal{T}(G) = (t_{ij})_{n\times n}$ where*

$$t_{ij} = \begin{cases} \sqrt{\mathcal{T}(u_i)^2 + \mathcal{T}(u_j)^2} & \text{if } u_iu_j \in E(G) \\ -1 & \text{if } u_iu_j \notin E(G) \\ 0 & \text{otherwise,} \end{cases}$$

where $\mathcal{T}(u_i)$ denotes the temperature of $u_i \in V(G)$.

Further, given the identity matrix $I_{n\times n}$, the temperature Sombor polynomial $\mathcal{P}_G(\beta)$ of G is defined as

$$\mathcal{P}_G(\beta) = |\beta I - \mathcal{T}(G)|.$$

$\mathcal{T}(G)$ is a real symmetric matrix so that all its n eigenvalues, being real, can be ordered as $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_n$. Accordingly, the temperature Sombor energy $\mathcal{ET}(G)$ of G is defined as

$$\mathcal{ET}(G) = \sum_{i=1}^{n} |\beta_i|.$$

Remark 3.1 *By the definition of the temperature Sombor matrix $\mathcal{T}(G)$, it is observed that $tr(\mathcal{T}(G)) = 0$. Therefore, the eigenvalues of $\mathcal{T}(G)$ must satisfy the relation that $\sum_{i=1}^{n} \beta_i = 0$ from which it follows that $\sum_{i=2}^{n} \beta_i = -\beta_1$.*

Lemma 3.1 *[4]*

$$\left(\sum_{j=1}^{n} \mathcal{X}_j \mathcal{Y}_j\right)^2 \leq \sum_{j=1}^{n} \mathcal{X}_j^2 \sum_{j=1}^{n} \mathcal{Y}_j^2$$

where $\mathcal{X}_1, \mathcal{X}_2, \cdots, \mathcal{X}_n$ and $\mathcal{Y}_1, \mathcal{Y}_2, \cdots, \mathcal{Y}_n$ are two sequences of real numbers. Further, equality holds if and only if there exists a real number α with $\mathcal{X}_j = \alpha \mathcal{Y}_j$, for each $j = 1, 2, \cdots, n$.

Remark 3.2 *For a graph G with order n and size m, if $\mathcal{P}(G)(\beta) = C_0\beta^n + C_1\beta^{n-1} + C_2\beta^{n-2} + C_3\beta^{n-3} \cdots + C_n$ is the temperature Sombor polynomial of G, then*

(i) $C_0 = 1$,

(ii) $C_1 = 0$,

(iii) $C_2 = -\left(\mathcal{FT}(G) + \dfrac{n^2 - n - 2m}{2}\right)$.

Theorem 3.1 *Let $\mathcal{T}(G)$ be the temparature Sombor matrix of G with eigenvalues $\beta_1 \geq \beta_2 \geq \cdots \geq \beta_n$. Then, the following results hold good.*

(i) $\sum \beta_i = 0$,

(ii) $\sum_{i=1}^{n} \beta_i^2 = 2\mathcal{FT}(G) + n(n-1) - 2m$.

Proof:

(i) Since $tr(\mathcal{T}(G)) = 0$, the eigenvalues of $\mathcal{T}(G)$ satisfy the relation $\sum_{i=1}^{n} \beta_i = 0$.

(ii) We have

$$\begin{aligned}\sum_{i=1}^{n} \beta_i^2 &= tr\left(\mathcal{T}(G)^2\right) \\ &= \sum_{i=1}^{n}\sum_{j=1}^{n} t_{ij}t_{ji} \\ &= \sum_{i=1}^{n} t_{ii}^2 + \sum_{i\neq j} t_{ij}t_{ji}\end{aligned}$$

Now, since $t_{ii} = 0$ for each $i = 1, 2, 3, \cdots, n$ in $\mathcal{T}(G)$,

$$\begin{aligned}\sum_{i=1}^{n} \beta_i^2 &= 2\sum_{i<j} t_{ij}^2 \\ &= 2\sum_{vw\in E(G)} \left(\mathcal{T}(v)^2 + \mathcal{T}(w)^2\right) + 2\sum_{vw\notin E(G)} (-1)^2 \text{ so that} \\ \sum_{i=1}^{n} \beta_i^2 &= 2\mathcal{FT}(G) + n(n-1) - 2m.\end{aligned}$$

□

4. Bounds for the temperature Sombor energy

The following classical inequalities are used to establish some bounds on the temperature Sombor energy $\mathcal{ET}(G)$ of graph G.

Lemma 4.1 *[15] [Diaz-Metcalf Inequality] Let $a_1, a_2, \cdots, a_n$ and $b_1, b_2, \cdots, b_n$ be two sequences, with $a_i, b_i \in \mathbb{R}^+$, $r, R \in \mathbb{R}$, such that $ra_i \leq b_i \leq Ra_i$, for each $i = 1, 2, \cdots, n$. Then,*

$$\sum_{i=1}^{n} b_i^2 + rR\sum_{i=1}^{n} a_i^2 \leq (r+R)\sum_{i=1}^{n} a_ib_i.$$

In the above expression, equality holds if and only if $b_i = Ra_i$ or $b_i = ra_i$, for $1 \leq i \leq n$.

Lemma 4.2 *[6] Let $a_1, a_2, a_3, \cdots, a_n$ be a sequence of non-negative real numbers. Then,*

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

Lemma 4.3 *[4] [Radon's Inequality] Let $a_1, a_2, \cdots, a_n$ and $b_1, b_2, \cdots, b_n$ be two sequences with $a_i, b_i \in \mathbb{R}^+$. Then, for any $r \geq 0$,*

$$\sum_{i=1}^{n}\left(\frac{b_i^{r+1}}{a_i^r}\right) \geq \frac{\left(\sum_{i=1}^{n} b_i\right)^{r+1}}{\left(\sum_{i=1}^{n} a_i\right)^{r}}$$

with equality if and only if $r = 0$ or $\frac{b_1}{a_1} = \frac{b_2}{a_2} = \cdots = \frac{b_n}{a_n}$.

Lemma 4.4 *[28] [Holder's Inequality] Let $a_1, a_2, a_3, \cdots, a_n$ and $b_1, b_2, b_3, \cdots, b_n$ be two sequences, with $a_i, b_i \in \mathbb{R}^+$ and p and q be strictly greater than 1 such that $\frac{1}{p} + \frac{1}{q} = 1$. Then,*

$$\sum_{i=1}^{n} a_i b_i \leq \left(\sum_{i=1}^{n} a_i^p\right)^{\frac{1}{p}} \left(\sum_{i=1}^{n} b_i^q\right)^{\frac{1}{q}}$$

with equality if and only if

$$\frac{a_1^p}{b_1^q} = \frac{a_2^p}{b_2^q} = \frac{a_3^p}{b_3^q} = \cdots = \frac{a_n^p}{b_n^q}.$$

Lemma 4.5 *[22] Let $a_1, a_2, a_3, \cdots, a_n$ be a sequence of non-negative real numbers such that $a_1 \leq a_2 \leq \cdots \leq a_n$. Then,*

$$\sum_{i=1}^{n} a_i + n(n-1)\left(\prod_{i=1}^{n} a_i\right)^{\dfrac{1}{n}} \leq n\left(\sum_{i=1}^{n} \sqrt{a_i}\right)^2 \leq (n-1)\sum_{i=1}^{n} a_i + n\left(\prod_{i=1}^{n} a_i\right)^{\dfrac{1}{n}}.$$

Lemma 4.6 *[6] If $a_1, a_2, a_3, \cdots, a_n$ and $b_1, b_2, b_3, \cdots, b_n$ are two sequences of non-negative real numbers, then*

$$\left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right) - \left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \frac{n^2}{4}\left(AB - ab\right)^2$$

where $A = \max\limits_{1\leq i\leq n} a_i, B = \max\limits_{1\leq i\leq n} b_i, a = \min\limits_{1\leq i\leq n} a_i$ and $b = \min\limits_{1\leq i\leq n} b_i$.

Lemma 4.7 *[7][Abel's inequality] Let $\eta_1, \eta_2, \cdots, \eta_n$ and $\mathcal{X}_1, \mathcal{X}_2, \cdots, \mathcal{X}_n$ be two sequences, with $\eta_i, \mathcal{X}_i \in \mathbb{R}$, such that $\mathcal{X}_n \geq \mathcal{X}_{n+1} \geq 0$ for all n. Then,*

$$|\eta_1\mathcal{X}_1 + \eta_2\mathcal{X}_2 + \cdots + \eta_n\mathcal{X}_n| \leq A\mathcal{X}_1 \quad \textit{where}$$

$$A = max\left\{|\eta_1|, |\eta_1| + |\eta_2|, \cdots, |\eta_1| + |\eta_2| + \cdots + |\eta_n|\right\}.$$

Lemma 4.8 *[28][Polya-Szego inequality] Let $a_1, a_2, \cdots, a_n$ and $b_1, b_2, \cdots, b_n$ be two sequences, with $a_i, b_i \in \mathbb{R}^+$, such that $a \leq a_i \leq A$ and $b \leq b_i \leq B$ for each $i = 1, 2, 3, \cdots, n$. Then,*

$$\sum_{i=1}^{n} b_i^2 \sum_{i=1}^{n} a_i^2 \leq \frac{1}{4}\left(\sqrt{\frac{AB}{ab}} + \sqrt{\frac{ab}{AB}}\right)^2 \left(\sum_{i=1}^{n} a_i b_i\right)^2$$

4.1. Lower bounds for the temperature Sombor energy

Theorem 4.1 *For any graph G of order n and size m, let $\mathcal{P}$ be the absolute value of $det(\mathcal{T}(G))$. Then,*

$$\mathcal{ET}(G) \geq \sqrt{2\mathcal{FT}(G) + n(n-1)(\mathcal{P}^{\frac{2}{n}} + 1) - 2m}.$$

Proof: From the definition of temperature Sombor energy and Theorem 3.1, we have

$$\begin{aligned}
\mathcal{ET}(G) &= \left(\sum_{i=1}^{n} |\beta_i|\right) \\
\implies (\mathcal{ET}(G))^2 &= \left(\sum_{i=1}^{n} |\beta_i|\right)^2 \\
&= 2\mathcal{FT}(G) + n^2 - n - 2m + \sum_{i\neq j} |\beta_i||\beta_j|. \qquad (4.1)
\end{aligned}$$

Since, for non-negative numbers, the arithmetic mean $A.M. \geq G.M.$, its geometric mean, we have

$$\begin{aligned}\sum_{i\neq j}|\beta_i||\beta_j| &\geq n(n-1)\left(\prod_{i\neq j}|\beta_i||\beta_j|\right)^{\frac{1}{n(n-1)}}\\ &= \left(\prod_{i=1}^{n}|\beta_i|^{2(n-1)}\right)^{\frac{1}{n(n-1)}}\\ &= \prod_{i=1}^{n}|\beta_i|^{\frac{2}{n}} = \mathcal{P}^{\frac{2}{n}}\\ \text{so that}\quad \sum_{i\neq j}|\beta_i||\beta_j| &\geq n(n-1)\mathcal{P}^{\frac{2}{n}}. \end{aligned} \tag{4.2}$$

Thus, we get

$$\begin{aligned}(\mathcal{ET}(G))^2 &\geq 2\mathcal{FT}(G) - n^2 - n - 2m + n(n-1)\mathcal{P}^{\frac{2}{n}}\\ &\geq 2\mathcal{FT}(G) - 2m + n(n-1)(\mathcal{P}^{\frac{2}{n}}+1)\\ \text{or}\quad \mathcal{ET}(G) &\geq \sqrt{2\mathcal{FT}(G) - 2m + n(n-1)(\mathcal{P}^{\frac{2}{n}}+1)}.\end{aligned}$$

. □

Theorem 4.2 *Let G be any graph of order n and size m. Then,*

$$\frac{2\mathcal{FT}(G) + n(|\beta_1||\beta_n| + n - 1) - 2m}{|\beta_1| + |\beta_n|} \leq \mathcal{ET}(G).$$

Further, equality holds if and only if for each $1 \leq i \leq n$, either $|\beta_i| = |\beta_1|$ or $|\beta_i| = |\beta_n|$.

Proof: Choosing $b_i = |\beta_i|$, $a_i = 1$, $r = |\beta_n|$ and $R = |\beta_1|$ in Lemma 4.1, we get

$$\begin{aligned}&\sum_{i=1}^{n}|\beta_i|^2 + |\beta_n||\beta_1|\sum_{i=1}^{n}1 \leq (|\beta_1| + |\beta_n|)\,\mathcal{ET}(G)\\ \Longrightarrow\quad &\sum_{i=1}^{n}|\beta_i|^2 + |\beta_n||\beta_1|n \leq (|\beta_1| + |\beta_n|)\,\mathcal{ET}(G)\\ \Longrightarrow\quad &\frac{2\mathcal{FT}(G) + n(|\beta_1||\beta_n| + n - 1) - 2m}{|\beta_1| + |\beta_n|} \leq \mathcal{ET}(G).\end{aligned}$$

□

Theorem 4.3 *Let G be any non-trivial graph. Then, $\mathcal{ET}(G) \geq \sqrt[4]{\dfrac{tr(\mathcal{T}(G)^2)^5}{tr(\mathcal{T}(G)^6)}}$.*

Proof: Taking $a_i = |\beta_i|^{\frac{4}{5}}$, $b_i = |\beta_i|^{\frac{6}{5}}$, $p = \frac{5}{4}$ and $q = 5$ in Lemma 4.4, we get

$$\sum_{i=1}^{n} |\beta_i|^{\frac{4}{5}} |\beta_i|^{\frac{6}{5}} \leq \left(\sum_{i=1}^{n} |\beta_i|\right)^{\frac{4}{5}} \left(\sum_{i=1}^{n} |\beta_i|^6\right)^{\frac{1}{5}}$$

$$\implies \sum_{i=1}^{n} |\beta_i|^2 \leq \left(\sum_{i=1}^{n} |\beta_i|\right)^{\frac{4}{5}} \left(\sum_{i=1}^{n} |\beta_i|^6\right)^{\frac{1}{5}}$$

$$\implies \left(\sum_{i=1}^{n} |\beta_i|\right) \geq \left(\frac{\left(\sum_{i=1}^{n} |\beta_i|^2\right)^5}{\sum_{i=1}^{n} |\beta_i|^6}\right)^{\frac{1}{4}}.$$

The result then follows from the definition of $\mathcal{ET}(G)$ and the property of $tr(\mathcal{T}(G))$. □

Theorem 4.4 *Let G be any graph of order n and size m. Then,*

$$\mathcal{ET}(G) \geq \frac{2\mathcal{FT}(G) + n(n-1) - 2m}{|\beta_1|}$$

where $|\beta_1| \geq |\beta_2| \cdots \geq |\beta_n|$ are the absolute values of eigenvalues of $\mathcal{T}(G)$. Further, equality holds when $|\beta_1| = |\beta_2| = \cdots = |\beta_n|$ or $|\beta_1| = |\beta_r|, 2 \leq r \leq n$ and $|\beta_s| = 0$ where, $s \neq r$, $2 \leq s \leq n$.

Proof: Taking $\eta_i = \mathcal{X}_i = |\beta_i|$ for all $1 \leq i \leq n$ in Lemma 4.7 and observing that

$$A = max\{|\beta_1|, |\beta_1| + |\beta_2|, \cdots, |\beta_1| + |\beta_2| + |\beta_3| + \cdots + |\beta_n|\} = \mathcal{ET}(G),$$

we get

$$\left||\beta_1|^2 + |\beta_2|^2 + \cdots + |\beta_n|^2\right| \leq \mathcal{ET}(G)\,|\beta_1|$$

$$\implies \frac{tr\left(\mathcal{T}(G)^2\right)}{|\beta_1|} \leq \mathcal{ET}(G).$$

Thus, by Theorem 3.1, we get

$$\mathcal{ET}(G) \geq \frac{2\mathcal{FT}(G) + n(n-1) - 2m}{|\beta_1|}.$$

Further,

$$\frac{tr\left(\mathcal{T}(G)^2\right)}{|\beta_1|} = \mathcal{ET}(G)$$

$$\iff |\beta_1|\left(|\beta_1| + |\beta_2| + |\beta_3| + \cdots + |\beta_n|\right) = \sum_{i=1}^{n} |\beta_i|^2$$

$$\iff |\beta_1|\left(|\beta_2| + |\beta_3| + \cdots + |\beta_n|\right) = \sum_{i=2}^{n} |\beta_i|^2$$

This is possible if and only if
$|\beta_1| = |\beta_2| = \cdots = |\beta_n|$ or $|\beta_1| = |\beta_r|, 2 \leq r \leq n$ and $|\beta_s| = 0$ where $s \neq r$ and $2 \leq s \leq n$. □

Theorem 4.5 *For a graph G of order n and size m,*

$$2n\mathcal{FT}(G) \leq \frac{1}{4}\left(\sqrt{\frac{\beta_1}{\beta_n}}+\sqrt{\frac{\beta_n}{\beta_1}}\right)\mathcal{ET}(G)^2 - n^2(n-1) + 2mn.$$

Proof: Substituting $a_i = |\beta_i|$ and $b_i = 1$ in Lemma 4.8, we get

$$\sum_{i=1}^{n} 1 \sum_{i=1}^{n} |\beta_i|^2 \leq \frac{1}{4}\left(\sqrt{\frac{AB}{ab}}+\sqrt{\frac{ab}{AB}}\right)^2 \left(\sum_{i=1}^{n}|\beta_i|\right)^2.$$

Clearly, $\beta_n \leq \beta_i \leq \beta_1$. Choosing $A = \beta_1, a = \beta_n, B = b = 1$ and using Theorem 3.1, we obtain

$$2n\mathcal{FT}(G) \leq \frac{1}{4}\left(\sqrt{\frac{\beta_1}{\beta_n}}+\sqrt{\frac{\beta_n}{\beta_1}}\right)\mathcal{ET}(G)^2 - n^2(n-1) + 2mn.$$

□

Theorem 4.6 *For a graph G of order n and size m,*

$$\sqrt{2n\mathcal{FT}(G) + n^2(n-1) - 2mn - \frac{n^2}{4}(\beta_1-\beta_n)^2} \leq \mathcal{ET}(G).$$

Proof: Setting $a_i = |\beta_i|, b_i = 1, A = \beta_1, B = 1, a = \beta_n$ and $b = 1$ in Lemma 4.6, we obtain

$$\left(\sum_{i=1}^{n}|\beta_i|^2\right)\left(\sum_{i=1}^{n}1\right) - \left(\sum_{i=1}^{n}|\beta_i|\right)^2 \leq \frac{n^2}{4}(\beta_1-\beta_n)^2.$$

Using Theorem 3.1, we get

$$2n\mathcal{FT}(G) + n^2(n-1) - 2mn - \mathcal{ET}(G)^2 \leq \frac{n^2}{4}(\beta_1-\beta_n)^2.$$

Regrouping and simplifying the above expression gives the required result. □

Theorem 4.7 *For a graph G of order n and size m,*

$$\sqrt{(2\mathcal{FT}(G) + n(n-1) - 2m)} \leq \mathcal{ET}(G).$$

Proof: We have

$$\begin{aligned}
\mathcal{ET}(G) &= \sum_{i=1}^{n}|\beta_i| \\
\implies (\mathcal{ET}(G))^2 &= \left(\sum_{i=1}^{n}|\beta_i|\right)^2 \geq \sum_{i=1}^{n}|\beta_i|^2 \\
\implies (\mathcal{ET}(G))^2 &\geq \sum_{i=1}^{n}|\beta_i|^2,
\end{aligned}$$

Using Theorem 3.1 in this equation, followed by simplification, gives the required result. □

4.2. Upper bounds for the temperature Sombor energy

Theorem 4.8 *If G be a graph of order n and size m, then*

$$\mathcal{ET}(G) \leq \sqrt{n(2\mathcal{FT}(G) + n^2 - n - 2m)}.$$

.

Proof: Taking $\mathcal{Y}_j = 1$ and $\mathcal{X}_j = |\beta_i|$ in Lemma 3.1, we get

$$[\mathcal{ET}(G)]^2 \leq n \sum_{i=1}^{n} |\beta_i|^2 = n(2\mathcal{FT}(G) + n^2 - n - 2m)$$
$$\implies \mathcal{ET}(G) \leq \sqrt{n(2\mathcal{FT}(G) + n(n-1) - 2m)}.$$

□

Theorem 4.9 *If G is a graph of order n and size m, then*

$$\mathcal{ET}(G) \leq \sqrt{(n-1)(2\mathcal{FT}(G) + n^2 - n - 2m) + n\,[det(\mathcal{T}(G))^2]^{\frac{1}{n}}}$$

where, $det(\mathcal{T}(G))$ is the determinant of the temperature Sombor matrix $\mathcal{T}(G)$.

Proof: Choosing $a_i = \beta_i^2$ in Lemma 4.2, we get

$$n\left(\frac{1}{n}\sum_{i=1}^{n}\beta_i^2 - \left(\prod_{i=1}^{n}\beta_i^2\right)^{\frac{1}{n}}\right) \leq n\sum_{i=2}^{n}\beta_i^2 - \left(\sum_{i=1}^{n}|\beta_i|\right)^2.$$

Using Theorem 3.1, we have

$$n\left(\frac{1}{n}(2\mathcal{FT}(G) + n^2 - n - 2m) - \left[det(T(G))^2\right]^{\frac{1}{n}}\right) \leq n(2\mathcal{FT}(G) + n^2 - n - 2m) - (\mathcal{ET}(G))^2$$
$$\implies (\mathcal{ET}(G))^2 - n\left[det(T(G))^2\right]^{\frac{1}{n}} \leq (n-1)(2\mathcal{FT}(G) + n^2 - n - 2m)$$
$$\implies \mathcal{ET}(G) \leq \sqrt{(n-1)(2\mathcal{FT}(G) + n^2 - n - 2m) + n\,[det(T(G))^2]^{\frac{1}{n}}}.$$

□

Theorem 4.10 *Let G be a simple connected graph of order n. Then,*

$$\mathcal{ET}(G) \leq tr(\mathcal{T}(G)^4)tr(\mathcal{T}(G)^{-2}).$$

.

Proof: Taking $r = 1$, $b_i = |\beta_i|$ and $a_i = |\beta_i|^4$ in Lemma 4.3, we get

$$\sum_{i=1}^{n}\frac{|\beta_i|^2}{|\beta_i|^4} \geq \frac{\left(\sum_{i=1}^{n}|\beta_i|\right)^2}{\left(\sum_{i=1}^{n}|\beta_i|^4\right)}$$
$$\implies \sum_{i=1}^{n}\frac{1}{\beta_i^2} \geq \frac{\mathcal{ET}(G)^2}{\sum_{i=1}^{n}\beta_i^4}.$$

Simplifying the above expression gives the required result. □

Theorem 4.11 *Let G be a graph of order $n \geq 2$, size m and $|\beta_n|$ be the absolute value of the eigenvalue β_n. Then,*

$$\mathcal{ET}(G) \leq |\beta_n| + \sqrt{(n-1)(2\mathcal{FT}(G) + n^2 - n - 2m - \beta_n^2)}.$$

Proof: Taking $a_i = \beta_i^2$ for each $i = 1, 2, 3, \cdots, n-1$ in Lemma 4.2, we get

$$\begin{aligned}(n-1)\left(\frac{1}{n-1}\sum_{i=1}^{n-1}\beta_i^2 - \left(\prod_{i=1}^{n-1}\beta_i^2\right)^{\frac{1}{n-1}}\right) &\leq (n-1)\sum_{i=1}^{n-1}\beta_i^2 - \left(\sum_{i=1}^{n-1}\sqrt{\beta_i^2}\right)^2 \\ &\leq (n-2)(n-1)\left(\frac{1}{n-1}\sum_{i=1}^{n-1}\beta_i^2 - \left(\prod_{i=1}^{n-1}\beta_i^2\right)^{\frac{1}{n-1}}\right). \end{aligned} \tag{4.3}$$

Suppose

$$\mathcal{S} = (n-1)\left(\frac{1}{n-1}\sum_{i=1}^{n-1}\beta_i^2 - \left(\prod_{i=1}^{n-1}\beta_i^2\right)^{\frac{1}{n-1}}\right).$$

Then, Equation 4.3 becomes

$$\mathcal{S} \leq (n-1)(2\mathcal{FT}(G) + n^2 - n - 2m - \beta_n^2) - (\mathcal{ET}(G) - |\beta_n|)^2 \leq (n-2)\mathcal{S}.$$

From this equation, it is clear that

$$\begin{aligned}&(\mathcal{ET}(G) - |\beta_n|)^2 \leq (n-1)(2\mathcal{FT}(G) + n^2 - n - 2m - \beta_n^2) - \mathcal{S} \\ \text{and}\quad &(\mathcal{ET}(G) - |\beta_n|)^2 \geq (n-1)(2\mathcal{FT}(G) + n^2 - n - 2m - \beta_n^2) - (n-2)\mathcal{S}.\end{aligned} \tag{4.4}$$

But we have

$$\begin{aligned}\mathcal{S} &= (n-1)\left(\frac{1}{n-1}\sum_{i=1}^{n-1}\beta_i^2 - \left(\prod_{i=1}^{n-1}\beta_i^2\right)^{\frac{1}{n-1}}\right) \\ &= \sum_{i=1}^{n-1}\beta_i^2 - (n-1)\left(\prod_{i=1}^{n-1}\beta_i^2\right)^{\frac{1}{n-1}} \\ &= (2\mathcal{FT}(G) + n^2 - n - 2m - \beta_n^2) - (n-1)\left(\frac{\mathcal{P}}{|\beta_n|}\right)^{\frac{2}{n-1}}\end{aligned}$$

$$\mathcal{S} = (2\mathcal{FT}(G) + n^2 - n - 2m - \beta_n^2) - (n-1)\left(\frac{\mathcal{P}}{|\beta_n|}\right)^{\frac{2}{n-1}} \tag{4.5}$$

where $\mathcal{P}$ is the absolute value of the determinant of the temperature Sombor matrix $\mathcal{T}(G)$.

Also, we know that $A.M. \geq G.M.$ Therefore,

$$\frac{1}{n-1}\sum_{i=1}^{n-1}\beta_i^2 \geq \left(\prod_{i=1}^{n-1}\beta_i^2\right)^{\dfrac{1}{n-1}}$$
$$\implies \frac{(2\mathcal{FT}(G)+n^2-n-2m-\beta_n^2)}{n-1} \geq \left(\frac{\mathcal{P}}{|\beta_n|}\right)^{\dfrac{2}{n-1}}$$
$$\implies \left(\frac{2\mathcal{FT}(G)+n^2-n-2m-\beta_n^2}{n-1}\right)^{n-1} \geq \left(\frac{\mathcal{P}}{|\beta_n|}\right)^{2}. \tag{4.6}$$

Bearing in mind the upper bound, using Equations 4.5 and 4.6 in Equation 4.4, we get

$$(\mathcal{ET}(G)-|\beta_n|)^2 \leq (n-1)(2\mathcal{FT}(G)+n^2-n-2m-\beta_n^2).$$

On further simplification, we get the required result. □

Theorem 4.12 *Let G be any non-trivial graph of order n and size m. Then,*

$$\mathcal{ET}(G) \geq \sqrt{\frac{tr(\mathcal{T}(G)^2)^3}{tr(\mathcal{T}(G)^4)}}.$$

Proof: Taking $a_i = |\beta_i|^{\frac{2}{3}}$, $b_i = |\beta_i|^{\frac{4}{3}}$, $p = \dfrac{3}{2}$ and $q = 3$ in Lemma 4.4, we get

$$\sum_{i=1}^{n}|\beta_i|^2 = \sum_{i=1}^{n}|\beta_i|^{\frac{2}{3}}|\beta_i|^{\frac{4}{3}} \leq \left(\sum_{i=1}^{n}|\beta_i|\right)^{\dfrac{2}{3}}\left(\sum_{i=1}^{n}|\beta_i|^4\right)^{\dfrac{1}{3}}$$
$$\implies \mathcal{ET}(G) \geq \left(\frac{\sum_{i=1}^{n}|\beta_i|^2}{\left(\sum_{i=1}^{n}|\beta_i|^4\right)^{\dfrac{1}{3}}}\right)^{\dfrac{3}{2}} = \sqrt{\frac{tr(\mathcal{T}(G)^2)^3}{tr(\mathcal{T}(G)^4)}}.$$

□

Theorem 4.13 *Let G be a graph of order $n \geq 2$ and size m. Then,*

$$\sqrt{\frac{2\mathcal{FT}(G)+n(n-1)[\Phi^{\frac{2}{n}}+1]-2m}{n}} \leq \mathcal{ET}(G) \leq \sqrt{\frac{2(n-1)\mathcal{FT}(G)+n[\Phi^{\frac{2}{n}}+(n-1)^2]-2m(n-1)}{n}}.$$

where Φ is the absolute value of $det(\mathcal{T}(G))$.

Proof: Taking $a_i = \beta_i^2$ in Lemma 4.5, we get

$$\sum_{i=1}^{n}\beta_i^2 + n(n-1)\left(\prod_{i=1}^{n}\beta_i^2\right)^{\dfrac{1}{n}} \leq n\left(\sum_{i=1}^{n}\sqrt{\beta_i^2}\right)^2 \leq (n-1)\sum_{i=1}^{n}\beta_i^2 + n\left(\prod_{i=1}^{n}\beta_i^2\right)^{\dfrac{1}{n}}$$

Using Theorem 3.1 and the properties of eigenvalues, we obtain

$$2\mathcal{FT}(G)+n(n-1)-2m+n(n-1)[\Phi^2]^{\frac{1}{n}} \leq n\mathcal{ET}(G)^2 \leq (n-1)\left(2\mathcal{FT}(G)+n(n-1)-2m\right)+n[\Phi^2]^{\frac{1}{n}}$$

$$\implies \frac{2\mathcal{FT}(G)+n(n-1)[\Phi^{\frac{2}{n}}+1]-2m}{n} \leq \mathcal{ET}(G)^2 \leq \frac{2(n-1)\mathcal{FT}(G)+n[\Phi^{\frac{2}{n}}+(n-1)^2]-2m(n-1)}{n}.$$

□

5. Chemical applicability of $\mathcal{ET}(G)$

In this section, we have discussed the chemical applicability of temperature Sombor energy by performing a correlation analysis between $\mathcal{ET}(G)$ and the π-electron energy of molecules having hetero atoms, alkanes and cubic compounds.

5.1. Statistical computation

Polynomial regression analysis involves analysing the relationship between the independent variable X and the dependent variable Y by modelling it as an n^{th} degree polynomial in X, thus fitting a non-linear relationship between the value of X and the corresponding condition Y. Even though this type of regression fits a non-linear model to the data, it is linear as a statistical estimation problem, as the regression function $E(Y|X)$ is linear in the unknown parameters that are estimated from the data. Therefore, polynomial regression is considered to be a special case of multiple linear regression.
The main aim of regression analysis is to model the expected value of a dependent variable Y in terms of the value of an independent variable X. The model

$$Y\,(Property) = a + bX$$

is used in simple linear regression where the conditional expectation of Y rises by b units for every unit increase in the value of X. Further, we employ the polynomial regression model in situations where linear relationships may not hold true and represent the expected value of Y as a n^{th} degree polynomial in this model in the form

$$Y\,(Property) = a_0 + a_1X + a_2X^2 + a_3X^3 + \cdots + a_nX^n.$$

Here, we use polynomial regression model where we model the expected value of Y as a sixth degree polynomial of the form

$$Y\,(Property) = a_0 + a_1X + a_2X^2 + a_3X^3 + a_4X^4 + a_5X^5 + a_6X^6.$$

where X stands for computed temperature Sombor energy $\mathcal{ET}(G)$ and Y stands for the π-electron energy property of that compound.
In QSPR studies, the correlation coefficient (r) is a real number ranges from -1 to $+1$ that shows the strength and direction of a link between two variables X and Y. It is important to note that the absolute value of correlation coefficient above 0.7 is considered strong, while the absolute value of correlation coefficient above 0.5 is moderate. Similarly, the F-value helps to determine whether the relationship between the independent and dependent variables is statistically significant. In any test, value of F is greater than or equal to 2.5 indicates that all estimated values are significant.

5.2. Correlation analysis of π-electron energy with $\mathcal{ET}(G)$

The main focus of the Hückel molecular orbital (HOM) theory is on conjugated, all-carbon compounds. The range of those compounds can be discussed by comparing the energy values for hetero atoms. This is achieved by modifying the resonance integral (β) and Coulomb (α) values for hetero atoms as seen in [21,2,23,9,22]. Here, we have performed the regression analysis by comparing $\mathcal{ET}(G)$ with the total π-electron energy values of molecules containing hetero atoms, cubic compounds and alkanes which are found in [34,40,6,22] and have found the corresponding values of r, r^2 and F value as given below.

Compound	**Molecules containing hetero compounds**
Y	π-electron energy
Polynomial	$-5.449 \times 10^{-7}X^6 + 7.245 \times 10^{-5}X^5 - 0.003859X^4 + 0.1052X^3$ $-1.542X^2 + 12.07X - 32.1$
r^2	0.9649
r	0.9822
Number of compounds	28
F	102.7052

Compound	**Cubic compounds**
Y	π-electron energy
Polynomial	$-0.004607X^6 + 0.7035X^5 - 44.41X^4 + 1485X^3$ $-2.776 \times 10^4X^2 + 2.753 \times 10^5X - 1.132 \times 10^6$
r^2	0.8250
r	0.9083
Number of compounds	21
F	14.0732

5.3. Regression analysis of graph energy with temperature Sombor energy of trees

In this section, we perform a regression analysis relating temperature Sombor energy with the graph energy of all trees with fixed orders $n = 8, 9, \cdots, 18$. Using the MATLAB Software, we compute the graph energy and temperature Sombor energy and present the 6^{th} degree polynomial regression models between these two parameters in Table 4 and their graphical representation in Fig. 4 and 5.

6. Temperature Sombor Entropy

The concept of an edge-weighted graph, characterized by entropy, is first introduced by Chen *et* al. in 2014 [46]. An edge-weighted graph is expressed by the equation $G = (V(G), E(G), \Phi(vw))$, where $\Phi(vw)$

Compound	**Alkanes**
Y	π-electron energy
Polynomial	$-5.202 \times 10^{-5}X^6 + 0.003988X^5 - 0.1268X^4 + 2.148119X^3$ $-20.52X^2 + 105.2X - 222.2$
r^2	0.6246
r	0.7903
Number of compounds	68
F	16.9161

Table 1: Molecules containing hetero atoms with π-electron energy and the temperature Sombor energy

Sl. No.	**Molecule**	**π-electron energy**	$\mathcal{ET}(G)$
1	H1	2.23	6.92
2	H2	5.66	7.18
3	H3	5.76	7.18
4	H4	6.96	12.65
5	H5	6.82	7.18
6	H6	5.23	8.80
7	H7	6.69	10.83
8	H8	9.06	10.83
9	H9	9.10	10.83
10	H10	9.07	10.83
11	H11	9.65	10.83
12	H12	8.19	13.80
13	H13	12.21	16.75
14	H14	12.22	16.69
15	H15	12.21	16.19
16	H16	11	16.08
17	H17	14.23	21.50
18	H18	14.23	21.50
19	H19	16.15	24.10
20	H20	16.12	24.10
21	H21	13.46	21.50
22	H22	13.59	21.50
23	H23	20.10	31.96
24	H24	21.02	31.96
25	H25	20.56	31.96
26	H26	21.62	31.96
27	H27	24.23	36.77
28	H28	19.39	29.54

Table 2: Cubic compounds of order 10 with π-electron energy and the temperature Sombor energy

Sl. No.	**Molecule**	**π-electron energy**	$\mathcal{ET}(G)$
1	G1	15.1231	22.653
2	G2	14.8596	23.046
3	G3	14.8212	22.261
4	G4	13.5143	21.038
5	G5	14.2925	21.988
6	G6	14.9443	22.395
7	G7	15.0777	23.367
8	G8	15.1231	24.653
9	G9	15.3164	23.847
10	G10	14.4721	21.183
11	G11	14.702	21.948
12	G12	16	24.061
13	G13	14.378	22.305
14	G14	15.0895	23.055
15	G15	14.7943	22.642
16	G16	14	22.849
17	G17	16	26.061
18	G18	13.5569	21.523
19	G19	15.5791	23.4
20	G20	14	21.67
21	G21	12	20.819

Table 3: Alkanes with π-electron energy and the temperature Sombor energy

Sl. No.	**Alkanes**	**π-electron energy**	$\mathcal{ET}(G)$
1	Butane	2.828	7.1817
2	2-methylpropane	2.828	12.646
3	Pentane	4.472	8.6636
4	2-methylbutane	5.226	10.466
5	2, 2 dimethylpropane	4	19.31
6	Hexane	6.988	10.671
7	2-methylpentane	6.064	11.512
8	3-methyalpentane	6.9	11.849
9	2, 2-methylbutane	5.818	14.317
10	2, 3-dimethylbutane	6.004	12.617
11	Heptanes	8.054	12.975
12	2-methylhexane	7.728	13.263
13	3-methylhexane	7.88	13.588
14	3-ethylpentane	6.9	13.859
15	2, 2-dimethylpentane	6.72	14.517
16	2, 3-dimethylpentane	7.664	14.426
17	2, 4-dimethylpentane	6.156	14.163
18	3, 3-dimethylpentane	6.5969	15.043
19	Octane	9.516	15.74
20	2-methylheptane	8.764	15.618
21	3-methylheptane	9.408	15.654
22	4-methylheptane	8.828	16.151
23	3-ethylhexane	7.88	16.016
24	2, 2-dimethylhexane	8.312	16.026
25	2, 3-dimethylhexane	8.646	16.013
26	2, 4-dimethylhexane	8.564	16.109
27	2, 5-dimethylhexane	8.472	15.63
28	3, 3-dimethylhexane	8.523	16.527
29	3, 4-dimethylhexane	9.332	16.266

Sl. No.	**Alkanes**	**π-electron energy**	$\mathcal{ET}(G)$
30	3-ethyl-2-methylpentane	7.664	16.543
31	3-ethyl-3-methylpentane	7.596	16.814
32	2, 2, 3-trimethylpentane	7.3	17.168
33	2, 2, 4-trimethylpentane	7.384	16.909
34	2, 3, 3-trimethylpentane	8.054	17.286
35	2, 3, 4-trimethylpentane	8.424	17.056
36	2, 2, 3, 3-tetramethylbutane	7.212	17.784
37	Nonane	10.628	18.089
38	2-methyloctane	10.252	18.427
39	3-methyloctane	10.472	18.326
40	4-methyloctane	10.384	18.397
41	3-ethylheptane	10.564	18.178
42	4-ethylheptane	10.492	18.35
43	2, 2-dimethylheptane	9.336	18.302
44	2, 3-dimethylheptane	10.176	18.182
45	2, 4-dimethylheptane	9.508	18.811
46	2, 5-dimethylheptane	10.152	18.087
47	2, 6-dimethylheptane	10.096	18.248
48	3, 3-dimethylheptane	9.464	18.41
49	3, 4-dimethylheptane	10.312	18.682
50	3, 5-dimethylheptane	10.29	18.204
51	4, 4-dimethylheptane	9.43	19.027
52	3-ethyl-2-methylhexane	10.198	18.702
53	4-ethyl-2-methylhexane	10.176	18.508
54	3-ethyl-3-methylhexane	10.262	18.841
55	2, 2, 4-trimethylhexane	9.13	18.779
56	2, 2, 5-trimethylhexane	9.06	18.212
57	2, 3, 3-trimethylhexane	9.3	18.776
58	2, 3, 4-trimethylhexane	10.096	18.94
59	2, 3, 5-trimethylhexane	9.336	18.58

Sl. No.	Alkanes	π-electron energy	$\mathcal{ET}(G)$
60	3, 3, 4-trimethylhexane	10.036	19.058
61	3, 3-diethylpentane	10.472	18.806
62	2, 2-dimethyl-3-ethylpentane	9.3	19.224
63	2, 3-dimethyl-3-ethylpentane	10.062	19.341
64	2, 4-dimethyl-3-ethylpentane	8.884	19.249
65	2, 2, 3, 3-tetramethylpentane	8.98	19.761
66	2, 2, 3, 4-tetramethylpentane	9.02	19.72
67	2, 2, 4, 4-tetramethylpentane	7.936	19.451
68	2, 3, 3, 4-tetramethylpentane	9.152	19.797

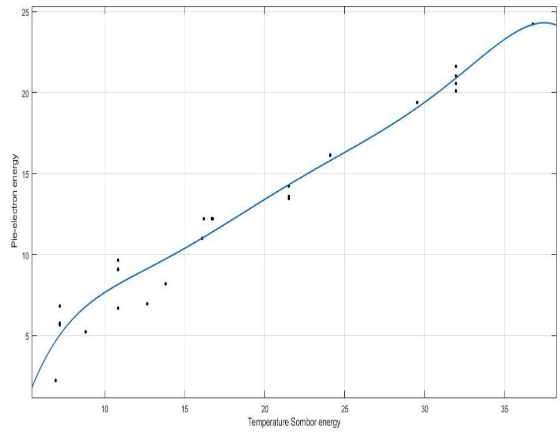


Figure 1: Correlation graph for molecules containing hetero atoms

indicates the weight of the edge (vw). The entropy of an edge-weighted graph is defined as

$$ENT_{TI}(G) = -\sum_{vw\in E(G)} \frac{\Phi(vw)}{\sum\limits_{vw\in E(G)} \Phi(vw)} log \left(\frac{\Phi(vw)}{\sum\limits_{vw\in E(G)} \Phi(vw)} \right).$$

On replacing $\sum\limits_{vw\in E(G)} \Phi(vw)$ with $TI(G)$, we get the required edge-weighted entropy of G, w. r. t. the topological index $TI(G)$ as

$$ENT_{TI}(G) = log\left(TI(G)\right) - \frac{1}{TI(G)} \sum_{vw\in E(G)} \Phi(vw) log\left(\Phi(vw)\right).$$

In this article, we introduce a new edge-weighted entropy of G, called the temperature Sombor entropy

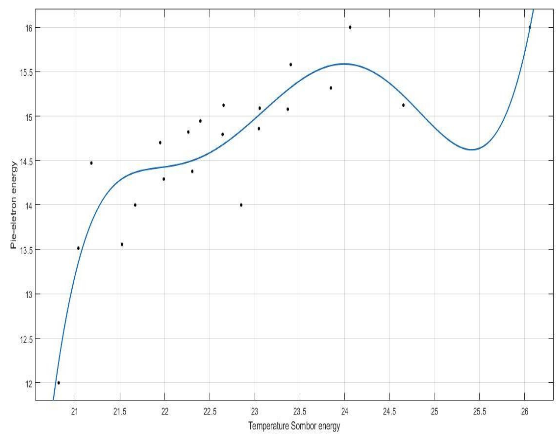


Figure 2: Correlation graph for cubic compounds

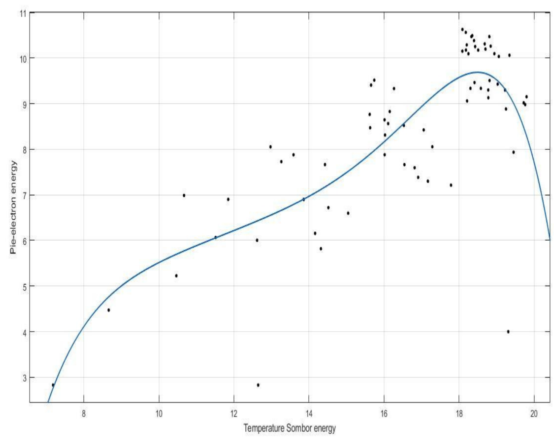


Figure 3: Correlation graph for alkanes

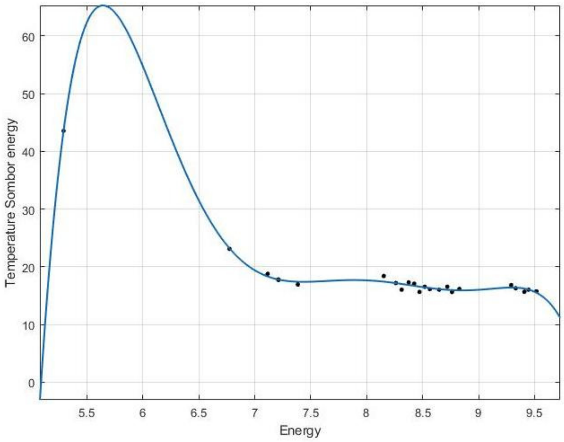
$(ENT_{\mathcal{TSO}}(G))$, defined as

$$ENT_{\mathcal{TSO}}(G) = log\left(\mathcal{TSO}(G)\right) - \frac{1}{\mathcal{TSO}(G)} \sum_{vw \in E(G)} \left[\sqrt{T(v)^2 + T(w)^2} \cdot log\left(\sqrt{T(v)^2 + T(w)^2}\right) \right].$$

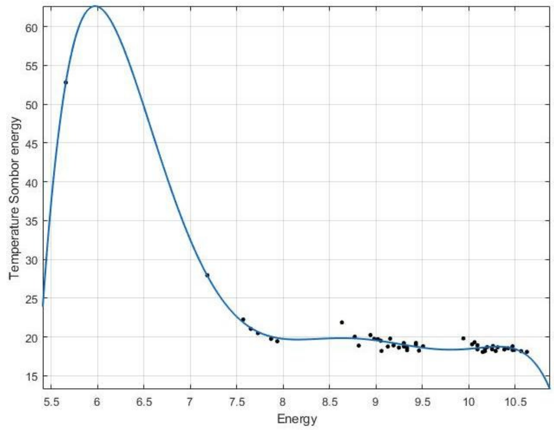
where $\Phi(vw) = \sqrt{T(v)^2 + T(w)^2}$ and $E(G)$ is the edge set of graph G.

6.1. Results and Discussion

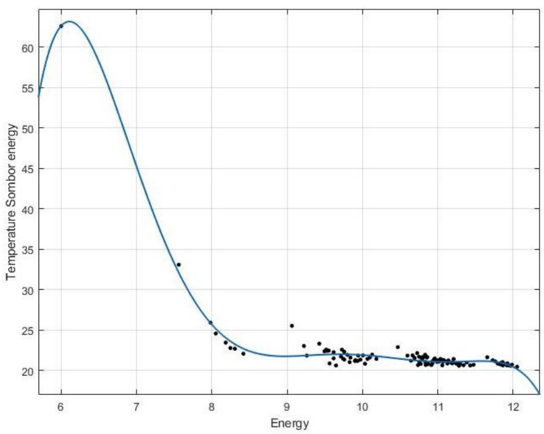
It is commonly known that the unit cell is the primary building block of all chemical substances. A molecular structure is composed of several unit cells arranged in a specific way. The compound that we have taken into consideration for our discussion is silicon carbide ($SiC_4 - I[a, b]$), commonly known as Carborundum, is a compound made of silicon and carbon atom. It is an emerging semiconductor material for various applications in semiconductor devices. While a is the total number of rows in this arrangement b denotes the number of unit cells in each row. The two-dimensional molecular structure of $SiC_4 - I[a, b]$ are illustrated in Figure 6.



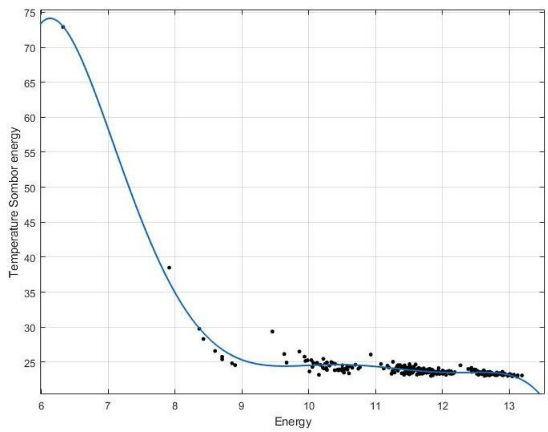
Trees of order 8



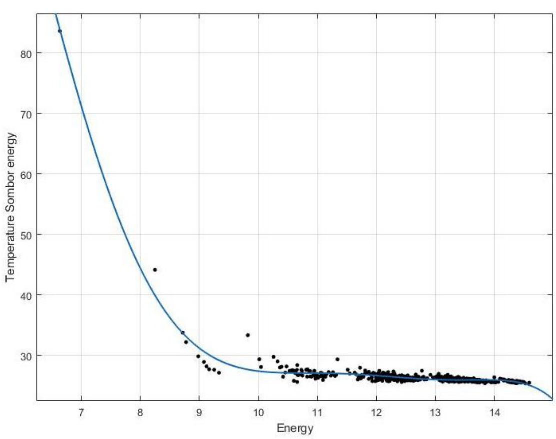
Trees of order 9



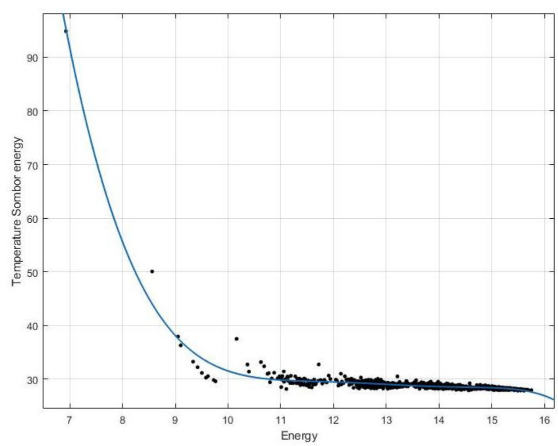
Trees of order 10



Trees of order 11

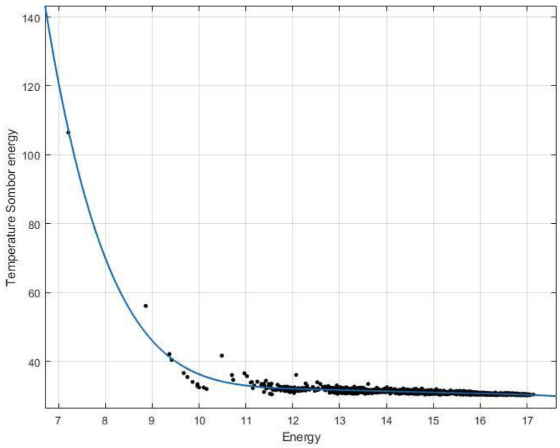


Trees of order 12

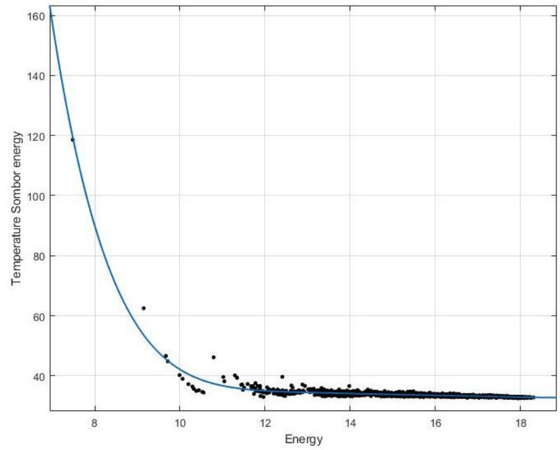


Trees of order 13

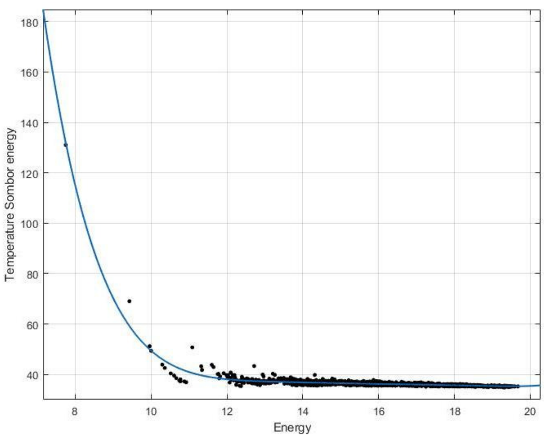
Figure 4: Graphical representation of energy vs. temperature Sombor energy of trees of order between 8 and 13



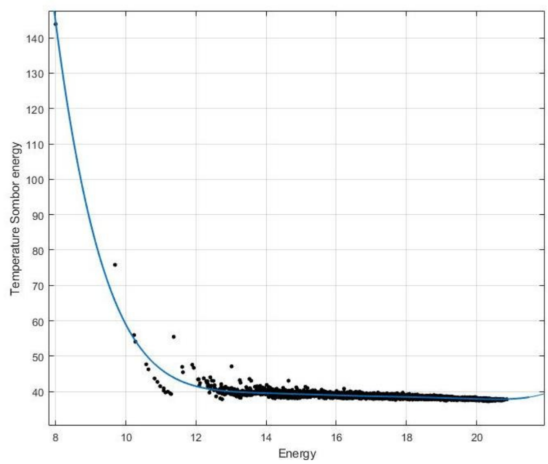
Trees of order 14



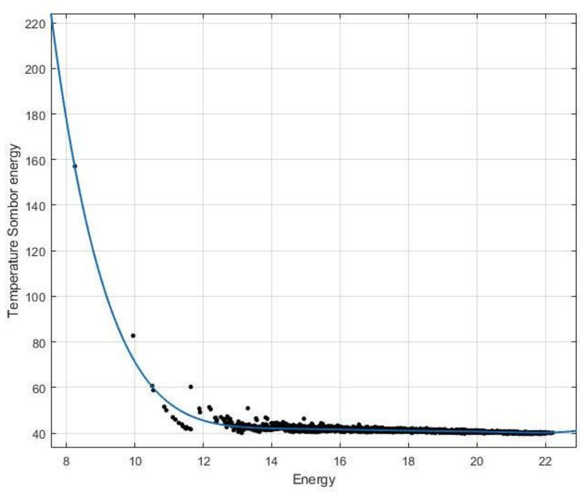
Trees of order 15



Trees of order 16



Trees of order 17



Trees of order 18

Figure 5: Graphical representation of energy vs. temperature Sombor energy of trees of order between 14 and 18

Table 4: The 6^{th} degree polynomial regression models for temperature Sombor energy of graph for all trees of order $n = 8, 9, \cdots, 18$

Order	**Number of trees**	**Polynomial**	r^2	r
8	23	$-0.9918X^6 - 2.555X^5 + 3.049X^4 + 4.598X^3$ $-2.178X^2 - 2.684X + 17.15$	0.9936	0.9968
9	47	$-0.2604X^6 + 13.4X^5 - 285X^4 + 3207X^3$ $-2.01 \times 10^4X^2 + 6.646 \times 10^4X - 9.043 \times 10^4$	0.9885	0.9942
10	106	$-0.05009X^6 + 2.853X^5 - 67.02X^4 + 829.7X^3$ $-5700X^2 + 2.055 \times 10^4X - 3.027 \times 10^4$	0.9788	0.9893
11	235	$-0.03714X^6 - 0.2882X^5 - 0.333X^4 + 0.6685X^3$ $+0.6717X^2 - 0.947X + 23.75$	0.9713	0.9852
12	551	$-0.01017X^6 - 0.1061X^5 - 0.1778X^4 + 0.2709X^3$ $+0.4962X^2 - 0.6394X + 26.12$	0.9601	0.9798
13	1301	$-0.00204X^6 - 0.03833X^5 - 0.1101X^4 + 0.01441X^3$ $+0.2472X^2 - 0.3794X + 28.59$	0.9501	0.9747
14	3159	$0.001125X^6 - 0.001162X^5 - 0.01826X^4 - 0.01234X^3$ $+0.04287X^2 - 0.3696X + 31.05$	0.9375	0.9682
15	7741	$0.000426X^6 - 0.03921X^5 + 1.499X^4 - 30.44X^3$ $+346.6X^2 - 2098X + 5315$	0.9226	0.9605
16	19320	$0.0003736X^6 - 0.03581X^5 + 1.424X^4 - 30.08X^3$ $+356X^2 - 2239X + 5888$	0.90	0.9487
17	48629	$0.00128X^6 0.01001X^5 + 0.01694X^4 - 0.03194X^3$ $-0.07153X^2 - 0.3013X + 38.36$	0.8684	0.9319
18	123867	$0.0002101X^6 - 0.02232X^5 + 0.9828X^4 - 22.96X^3$ $+300X^2 - 2081X + 6026$	0.8256	0.9086

In Figure 6, carbon atoms are represented by the color yellow, while silicon atoms are represented by the color blue.

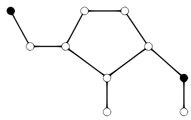
Based on their degree, the vertices in $SiC_4 - I[a, b]$ can be categorized into three groups. Table 5 uses the letters V_1, V_2 and V_3 to represent first, second and third degree vertices respectively.

In the same way, the edges in $SiC_4 - I[a, b]$ can be separated into five different edge sections, which are shown in Table 6.

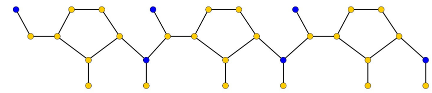
Theorem 6.1 *For silicon carbide compound $G = SiC_4 - I[a, b]$, the temperature Sombor index ($\mathcal{TSO}(G)$) and the temperature Sombor entropy ($ENT_{\mathcal{TSO}}(G)$) are given below.*

1.

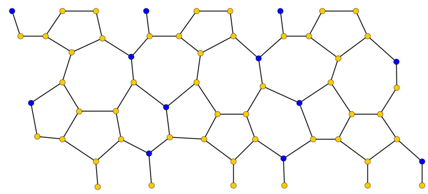
$$\begin{aligned}\mathcal{TSO}(G) = 2\left(\frac{\sqrt{500(ab)^2 - 120(ab) + 8}}{(10ab-2)(10ab-1)}\right) + (3a-b)\left(\frac{\sqrt{1000(ab)^2 - 240(ab) + 18}}{(10ab-3)(10ab-1)}\right)\\ + (a+2b-2)\left(\frac{2\sqrt{2}}{(10ab-2)}\right) + (15ab - 10a - 8b + 5)\left(\frac{3\sqrt{2}}{(10ab-3)}\right)\\ + (2a+4b-2)\left(\frac{\sqrt{1300(ab)^2 - 600(ab) + 72}}{(10ab-3)(10ab-2)}\right).\end{aligned}$$



(a) Unit structure of $SiC_4 - I[a,b]$



(b) Structure of $SiC_4 - I[3,1]$



(c) Structure of $SiC_4 - I[a,b]$

Figure 6: Two-dimensional molecular structure of $SiC_4 - I[a,b]$

Table 5: Vertex partition of $SiC_4 - I[a,b]$

$\mathbf{d}(v)$	**Cardinality**
V_1	$3a$
V_2	$2a + 4b - 2$
V_3	$10ab - 5a - 4b + 2$
$\|V(G)\|$	$10ab$

2.

$$\begin{aligned}
ENT_{\mathcal{TSO}}(G) = log\left(\mathcal{TSO}(G)\right) - \frac{1}{\mathcal{TSO}(G)}\Bigg[2\left(\frac{\sqrt{500(ab)^2 - 120(ab) + 8}}{(10ab-2)(10ab-1)}\right) \cdot log\left(\frac{\sqrt{500(ab)^2 - 120(ab) + 8}}{(10ab-2)(10ab-1)}\right) \\
+ (3a - b)\left(\frac{\sqrt{1000(ab)^2 - 240(ab) + 18}}{(10ab-3)(10ab-1)}\right) \cdot log\left(\frac{\sqrt{1000(ab)^2 - 240(ab) + 18}}{(10ab-3)(10ab-1)}\right) \\
+ (a + 2b - 2)\left(\frac{2\sqrt{2}}{(10ab-2)}\right) \cdot log\left(\frac{2\sqrt{2}}{(10ab-2)}\right) \\
+ (15ab - 10a - 8b + 5)\left(\frac{3\sqrt{2}}{(10ab-3)}\right) \cdot log\left(\frac{3\sqrt{2}}{(10ab-3)}\right) \\
+ (2a + 4b - 2)\left(\frac{\sqrt{1300(ab)^2 - 600(ab) + 72}}{(10ab-3)(10ab-2)}\right) \cdot log\left(\frac{\sqrt{1300(ab)^2 - 600(ab) + 72}}{(10ab-3)(10ab-2)}\right)\Bigg].
\end{aligned}$$

Proof:

Table 6: Edge partition of $SiC_4 - I[a,b]$

$(\mathbf{d}(u), \mathbf{d}(v))$	**Cardinality**
$(2,1)$	2
$(3,1)$	$3a-2$
$(2,2)$	$a+2b-2$
$(3,2)$	$2a+4b-2$
$(3,3)$	$15ab-10a-8b+5$
$\lvert E(G)\rvert$	$12ab-a$

1. From the definition of temperature Sombor index and using Table 5 and Table 6, we have

$$\begin{aligned}\mathcal{TSO}(G) = 2\cdot\sqrt{\frac{4}{(10ab-2)^2}+\frac{1}{10ab-1)^2}} + (3a-b)\cdot\sqrt{\frac{9}{(10ab-3)^2}+\frac{1}{(10ab-1)^2}}\\ +(a+2b-2)\cdot\sqrt{\frac{4}{(10ab-2)^2}+\frac{4}{(10ab-2)^2}}+(15ab-10a-8b+5)\cdot\sqrt{\frac{9}{(10ab-3)^2}+\frac{9}{(10ab-3)^2}}\\ +(2a+4b-2)\cdot\sqrt{\frac{9}{(10ab-3)^2}+\frac{4}{(10ab-4)^2}}\end{aligned}$$

On further simplification, we get the required result.

2. From the definition and Table 6, we have

$$\begin{aligned}ENT_{\mathcal{TSO}}(G) &= log\,(\mathcal{TSO}(G))\\ &-\frac{1}{\mathcal{TSO}(G)}\sum_{vw\in E(G)}\Bigg[2\cdot\sqrt{\frac{4}{(10ab-2)^2}+\frac{1}{(10ab-1)^2}}\cdot log\left(\sqrt{\frac{4}{(10ab-2)^2}+\frac{1}{(10ab-1)^2}}\right)\\ &+(3a-b)\cdot\sqrt{\frac{9}{(10ab-3)^2}+\frac{1}{(10ab-1)^2}}\cdot log\left(\sqrt{\frac{9}{(10ab-3)^2}+\frac{1}{(10ab-1)^2}}\right)\\ &+(a+2b-2)\cdot\sqrt{\frac{4}{(10ab-2)^2}+\frac{4}{(10ab-2)^2}}\cdot log\left(\sqrt{\frac{4}{(10ab-2)^2}+\frac{4}{(10ab-2)^2}}\right)\\ &+(15ab-10a-8b+5)\cdot\sqrt{\frac{9}{(10ab-3)^2}+\frac{9}{(10ab-3)^2}}\cdot log\left(\sqrt{\frac{9}{(10ab-3)^2}+\frac{9}{(10ab-3)^2}}\right)\\ &+(2a+4b-2)\cdot\sqrt{\frac{9}{(10ab-3)^2}+\frac{4}{(10ab-4)^2}}\cdot log\left(\sqrt{\frac{9}{(10ab-3)^2}+\frac{4}{(10ab-4)^2}}\right)\Bigg]\end{aligned}$$

On further simplification, we get the required result. □

6.2. Regression analysis of $\mathcal{TSO}(G)$ with $ENT_{\mathcal{TSO}}(G)$

In this section, we have established a regression analysis relating $\mathcal{TSO}(G)$ with $ENT_{\mathcal{TSO}}(G)$ of $SiC_4 - I[a,b]$ and have presented the regression model of degree 6 between these two parameters in Table 8.

7. Conclusion

In this study, we have introduced new variants called the temperature Sombor matrix $\mathcal{T}(G)$ and the temperature Sombor energy $\mathcal{ET}(G)$, which are based on the Sombor index and the temperature Sombor index of a graph G. Here, we have discussed some mathematical properties of $\mathcal{T}(G)$ and some

Table 7: Temperature Sombor index ($\mathcal{TSO}(G)$) and its entropy ($ENT_{\mathcal{TSO}}(G)$) of $SiC_4 - I[a, b]$

(a, b)	$\mathcal{TSO}(G)$	$ENT_{\mathcal{TSO}}(G)$	(a, b)	$\mathcal{TSO}(G)$	$ENT_{\mathcal{TSO}}(G)$
(1, 1)	4.54027	2.26965	(21, 21)	6.19457	8.77685
(2, 2)	5.04694	3.87846	(22, 22)	6.20203	8.87081
(3, 3)	5.38422	4.76213	(23, 23)	6.20886	8.96055
(4, 4)	5.58772	5.37359	(24, 24)	6.21514	9.04645
(5, 5)	5.72204	5.84143	(25, 25)	6.22093	9.1288
(6, 6)	5.81701	6.22041	(26, 26)	6.22628	9.2079
(7, 7)	5.8876	6.53893	(27, 27)	6.23125	9.28398
(8, 8)	5.94211	6.81364	(28, 28)	6.23587	9.35728
(9, 9)	5.98545	7.05515	(29, 29)	6.24019	9.42799
(10, 10)	6.02073	7.27062	(30, 30)	6.24422	9.49628
(11, 11)	6.05	7.46513	(31, 31)	6.24799	9.56232
(12, 12)	6.07468	7.64239	(32, 32)	6.25154	9.62624
(13, 13)	6.09576	7.80521	(33, 33)	6.25488	9.68919
(14, 14)	6.11398	7.95577	(34, 34)	6.25802	9.74827
(15, 15)	6.12989	8.09579	(35, 35)	6.26099	9.80661
(16, 16)	6.14389	8.22664	(36, 36)	6.26379	9.86329
(17, 17)	6.15632	8.34946	(37, 37)	6.26645	9.9184
(18, 18)	6.16741	8.46517	(38, 38)	6.26897	9.97204
(19, 19)	6.17738	8.57455	(39, 39)	6.27136	10.0243
(20, 20)	6.18639	8.67825	(40, 40)	6.27364	10.0752

bounds on $\mathcal{ET}(G)$ as well. Followed by this, we have also discussed chemical applicability of the invariant $\mathcal{ET}(G)$ by comparing it with the π-electron energy of some molecules containing hetero compounds, cubic compounds and alkanes. From this study, it has been found that there is a good correlation between $\mathcal{ET}(G)$ and the π-electron energy of above mentioned compounds, which is found to be $r = 0.9822$, 0.9083 and 0.7903 respectively. Additionally, we conducted a regression analysis on trees of a fixed order, ranging from 8 to 18, to explore the relationship between graph energy and temperature Sombor energy. The results revealed that the correlation coefficient values tend to decrease with an increase in the order of the trees, with a minimum observed value of $r = 0.9086$. Furthermore, we performed a regression analysis of Silicon carbide ($SiC_4 - I[a, b]$), a semiconductor, assessing its temperature Sombor index and temperature Sombor entropy values. From this analysis, we found that there is a strong correlation between $\mathcal{TSO}(G)$ and the $ENT_{\mathcal{TSO}}(G)$ with $r = 0.9999$. The results of the correlation analysis are highly significant, as they satisfy the criteria that the absolute value of the correlation coefficient r is at least 0.7 and F-value is at least 2.5. These observations are purely experimental and further theoretical investigations might throw more light on this behavior.

Table 8: Regression analysis table for $SiC_4 - I[a, b]$ semiconductor compound

Compound	$SiC_4 - I[a, b]$
Y	Temperature Sombor entropy
X	Temperature Sombor index
Polynomial	$12.25X^6 - 400.9X^5 + 5456X^4 - 3.952 \times 10^4 X^3$ $+1.607 \times 10^5 X^2 - 3.479 \times 10^5 X + 3.13 \times 10^5$
r^2	0.9999
r	0.9999
F	23737.7018

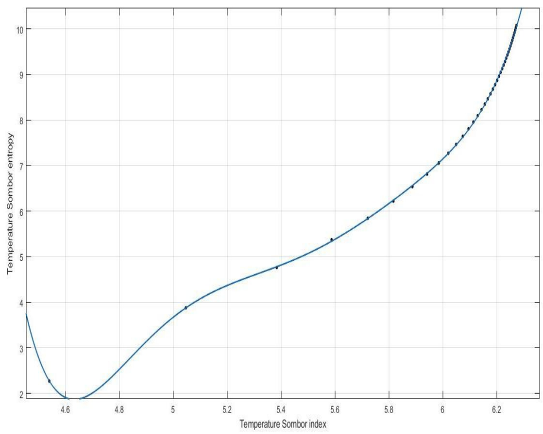


Figure 7: Correlation graph for $SiC_4 - I[a, b]$

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