Global and Stochastic Analysis
Vol. 13 No. 2 (2026)

DOI: 10.64837/GSA.13.2.4

Received: 20th December 2025 *Revised: 25th February 2026* *Accepted: 30th March 2026*

ON ECCENTRIC SOMBOR INDEX OF SOME CLASSES OF GRAPHS AND ITS CHEMICAL APPLICABILITY

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ABSTRACT: In this paper, we compute eccentric Sombor index for cycle graph, complete graph, complete bipartite graph, star graph, wheel graph, path graph and various thorn graphs, namely the thorn complete graph, thorn complete bipartite graph, thorn ring, thorn star, thorn rod and thorn path. Further, we investigate the chemical applicability of this index by comparing it with the physicochemical properties of hetero molecules, selected polycyclic aromatic hydrocarbons and octane isomers . Moreover, we extend our study for the chemical applicability of this index to regression analysis.

Key words: Eccentricity, hetero molecules, polycyclic aromatic hydrocarbons (PAHs), physicochemical properties, regression model, ecccentric Sombor index, thorn graphs.

2020 AMS Subject classification: 05C09, 05C10, 05C76, 05C92

1 Introduction

All the graphs discussed in this study are connected, simple, undirected and finite. A graph $G = (V, E)$ consisting the vertex set $V(G)$ and the edge set $E(G)$. In graph theory, the numerical value associated with the graph or molecular structure of chemical compound is called a topological index. A topological index, is also known as a molecular descriptor, is a graph invariant that provides valuable insight into the physical, chemical and structural properties of molecular graphs. In chemical graph theory, the molecular structure of chemical compound is modeled as a graph, where atoms correspond to vertices and bond correspond to edges. In recent years, topological indices have been progressively incorporated in the models of quantitative structure property relationships (QSPR) and quantitative structure activity property relationships (QSAR). A topological indices are mainly classified in to degree-based and distance-based categories. Among them, Wiener index [17] introduced by Wiener in 1947, is the earliest and most well-known distanced-based topological index and was used to calculate boiling point of Paraffins. In [7] Gutman and Trinajstic define Zagreb indices which are popular and have many applications in chemistry. Later eccentricity based first kind Zagreb index and second kind Zagreb index [5] are defined by Ghorbani and Hosseinzadeh. Gutman introduced Sombor index [8] and it is defined as,

$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2}$, this index has wide application in chemistry. Recently, in [13], Kulli introduced the eccentric version of the degree based Sombor index, called eccentric Sombor index (fourth Sombor index) of a graph G. For any graph G, eccentric Sombor index written as $S_e(G)$ and is defined as

$S_e(G) = \sum_{uv \in E(G)} \sqrt{\rho(u)^2 + \rho(v)^2}$, where $\rho(u)$ is the eccentricity of the vertex $u \in G$.

In [9] Gutman first studied the thorn graphs, which are of importance in polymer theory [3] discussed in the graph theoretical representation of some special class of chemical compound. Hetero molecules, PAHs and Octane isomers are organic compounds. Hetero molecules are used extensively in the chemical industry, pharmaceuticals and atmospheric chemistry. Whereas PAHs are used in industry but they are recognised as environmental pollutants . Further, octane isomers are used as a solvents and are also important in the petrochemical industry. moreover, all these organic compounds have many application. Many research works have been carried out on hetero molecules, PAHs and Octane isomers for this we refer [4, 12, 14, 16, 2].

In this study, we investigate the chemical applicability of eccentric Sombor index for hetero molecules, selected PAHs and octane isomers(C_8H_{18}) by correlating it with their physicochemical properties, which explores the chemical applicability of this index. Many studies molecules having hetero atoms, PAHs and Octane isomers establish the chemical applicability.

Before we proceed to discuss the main results the following definition which are useful in this paper. In a graph $G=(V,E)$ the degree of a vertex v denoted by $d(v)$ is defined as the number of edges incident with v. The shortest path between the vertices u and v is called the eccentricity of u in G and is denoted by $\rho(u)$ in this paper . The floor function $\lfloor x \rfloor$ gives the greatest integer less than or equal to x. The Ceil function $\lceil x \rceil$ gives the least integer greater than or equal to x. We refer [11] for undefined notations and terminologies.

2. Eccentric Sombor index for certain standard graphs.

In this section, we compute the eccentric Sombor index of certain standard graphs.

Theorem 2.1

(i) Let C_n be a cycle graph with $n \geq 3$. Then $S_e(C_n) = n\left\lfloor\frac{n}{2}\right\rfloor\sqrt{2}$.

(ii) Let K_n be a complete graph with $n \geq 2$. Then $S_e(K_n) = \frac{n(n-1)}{\sqrt{2}}$.

(iii) Let $G = K_{p,q}$ be a complete bipartite graph with $p > 1, q > 1$. Then $S_e(G) = 2\sqrt{2}pq$.

(iv) Let W_n be a wheel graph with $n \geq 5$. Then $S_e(W_n) = (n-1)\left[\sqrt{5} + 2\sqrt{2}\right]$.

(v) Let $G = K_{1,h-1}$ be a star graph with $h \geq 2$. Then $S_e(G) = (h-1)\sqrt{5}$.

Proof:

(i) Let $C_n, n \geq 3$ be a cycle graph with $|V(C_n)| = n, |E(C_n)| = n$.

For each vertex $v_\iota \in V(C_n), \rho(v_\iota) = \left\lfloor\frac{n}{2}\right\rfloor$, where $\iota = 1,2,\cdots,n$.

For each edge $e_\iota \in E(C_n)$, such that $e_1 = v_1v_2,\ e_2 = v_2v_3, \cdots, e_n = v_nv_1$.

Note that $v_{n+1} = v_1$

By the definition,

$$S_e(C_n) = \sum_{e_\iota,\iota=1}^{n} \sqrt{\rho(v_\iota)^2 + \rho(v_{\iota+1})^2}$$

$$= \sqrt{\left\lfloor\frac{n}{2}\right\rfloor^2 + \left\lfloor\frac{n}{2}\right\rfloor^2} + \sqrt{\left\lfloor\frac{n}{2}\right\rfloor^2 + \left\lfloor\frac{n}{2}\right\rfloor^2}, \cdots, n\ times$$

Hence, $S_e(C_n) = n\left\lfloor\frac{n}{2}\right\rfloor\sqrt{2}$.

(ii) Let K_n, $n \geq 2$ be a complete graph with $|V(k_n)| = n, |E(k_n)| = \frac{n(n-1)}{2}$.

For each vertex $v_\iota \in V(K_n), \rho(v_\iota) = 1$.

By the definition, $S_e(K_n) = \frac{n(n-1)}{2}\sqrt{1^2 + 1^2}$

Hence, $S_e(K_n) = \frac{n(n-1)}{\sqrt{2}}$.

(iii) In a bipartite graph $G = K_{p,q}$,

$|V(G)| = p + q, |E(G)| = pq$. For each vertex $v_\iota \in V(G), \rho(v_\iota) = 2$.

By the Definition, $S_e(G) = pq\sqrt{2^2 + 2^2}$

Hence, $S_e(K_{p,q}) = 2\sqrt{2}pq$.

(iv) Let wheel graph $W_n = K_1 + C_{n-1}$, where K_1 is the singleton graph and

C_{n-1} is the cycle graph. For W_n, $|V(W_n)| = n, |E(W_n)| = 2(n-1)$.
let $v_0 \in V(K_1)$, clearly $\rho(v_0) = 1$ and for each $v_\iota \in V(W_n)$, $\rho(v_\iota) = 2$ for $1 \leq \iota \leq (n-1)$. In W_n, there are $n-1$ spokes and end vertices eccentricity of each spoke is $(1,2)$. For remaining $n-1$ exterior edges, the end vertices eccentricity of each exterior edge is $(2,\ 2)$. By considering the eccentricity of these distinct vertex types, we discern a total of two distinct types of edge partitions in W_n

By the definition, $S_e(W_n) = (n-1)\sqrt{1^2 + 2^2} + (n-1)\sqrt{2^2 + 2^2}$

Hence, $S_e(W_n) = (n-1)[\sqrt{5} + 2\sqrt{2}]$.

(v) Consider a star graph $G = K_{1,h-1}$, with $|V(G)| = h, |E(G)| = h-1$. Let v_0 be the central vertex of $K_{1,h-1}$, for each $e_\iota \in G$ such that $e_\iota = v_0 v_\iota$, $\rho(v_0) = 1$, $\rho(v_\iota) = 2$ where $\iota = 1,2,\cdots,h-1$.

By the definition, $S_e(K_{1,h-1}) = \sum_{e_\iota,\iota=1}^{h-1} \sqrt{\rho(v_0)^2 + \rho(v_\iota)^2} \quad = (h-1)\sqrt{1^2 + 2^2}$

Hence, $S_e(K_{1,h-1}) = (h-1)\sqrt{5}$.

Theorem 2.2

(vi) For any path P_n,

$$S_e(P_n) = \begin{cases} 2\sum_{\mu=\frac{n-1}{2}}^{n-2} \sqrt{\mu^2 + (\mu+1)^2} & for\ n\ is\ odd, n \geq 3. \\ \frac{n}{\sqrt{2}} + 2\sum_{\mu=\frac{n}{2}}^{n-2} \sqrt{\mu^2 + (\mu+1)^2} & for\ n\ is\ even, n \geq 4. \end{cases}$$

Proof: Let P_n be a path with vertex set $V(P_n) = \{v_1, v_2, v_3, \cdots, v_n\}$ and edge set $E(P_n) = \{e_1, e_2, e_3, \cdots, e_{n-1}\}$ such that

$$e_1 = (v_1, v_2), e_2 = (v_2, v_3), \cdots, e_{n-1} = (v_{n-1}, v_n).$$

Case 1. Consider $n \geq 3$ is odd, the end vertices of the edges of each set $\{e_1, e_{n-1}\}, \{e_2, e_{n-2}\}, \{e_3, e_{n-3}\}, \cdots, \{e_{\frac{n-1}{2}}, e_{\frac{n+1}{2}}\}$ having the eccentricities

$$\rho(v_1) = \rho(v_n) = n-1$$
$$\rho(v_2) = \rho(v_{n-1}) = n-2,$$
$$\rho(v_3) = \rho(v_{n-2}) = n-3, \cdots,$$
$$\rho(v_{\frac{n+1}{2}}) = \frac{n-1}{2}$$

Since P_n is symmetric about the middle vertex $v_{\frac{n+1}{2}}$, we have,

$$S_e(P_n) = 2\sqrt{(n-1)^2 + (n-2)^2} + 2\sqrt{(n-2)^2 + (n-3)^2} + 2\sqrt{(n-3)^2 + (n-4)^2} + \cdots$$
$$+2\sqrt{\left(\frac{n+1}{2}\right)^2 + \left(\frac{n-1}{2}\right)^2}$$
$$= 2\sum_{\mu=\frac{n-1}{2}}^{n-2} \sqrt{\mu^2 + (\mu+1)^2}$$

Hence, $S_e(P_n) = 2\sum_{\mu=\frac{n-1}{2}}^{n-2} \sqrt{\mu^2 + (\mu+1)^2}$.

Case 2. Consider $n \geq 2$ is even, the end vertices of the edges of each set $\{e_1, e_{n-1}\}, \{e_2, e_{n-2}\}$, $\{e_3, e_{n-3}\}, \cdots, \{e_{\frac{n}{2}-1}, e_{\frac{n}{2}+1}\}$ having the eccentricities $\rho(v_1) = \rho(v_n) = n-1$,

$$\rho(v_2) = \rho(v_{n-1}) = n-2,$$

$\rho(v_3) = \rho(v_{n-2}) = n-3, \cdots, \rho(v_{\frac{n}{2}-1}) = \rho(v_{\frac{n}{2}+2}) = \frac{n}{2} + 1.$

Also, for edge $e_{\frac{n}{2}} = (v_{\frac{n}{2}}, v_{\frac{n}{2}+1})$ having $\rho(v_{\frac{n}{2}}) = \rho(v_{\frac{n}{2}+1}) = \frac{n}{2}$.

Since P_n is symmetric about the middle edge $e_{\frac{n}{2}}$, we have

$$S_e(P_n) = \sqrt{\left(\frac{n}{2}\right)^2 + \left(\frac{n}{2}\right)^2} + 2\sqrt{(n-1)^2 + (n-2)^2} + 2\sqrt{(n-2)^2 + (n-3)^2}$$

$$+2\sqrt{(n-3)^2 + (n-4)^2 +} \cdots + 2\sqrt{\left(\frac{n}{2}+1\right)^2 + \left(\frac{n}{2}\right)^2}$$

Hence, $S_e(P_n) = \sqrt{\left(\frac{n}{2}\right)^2 + (\frac{n}{2})^2} + 2\sum_{\mu=\frac{n}{2}}^{n-2} \sqrt{\mu^2 + (\mu+1)^2}$

Hence, $S_e(P_n) = \frac{n}{\sqrt{2}} + 2\sum_{\mu=\frac{n}{2}}^{n-2} \sqrt{\mu^2 + (\mu+1)^2}$.

3 Eccentric Sombor index for certain thorn graphs.

In this section we compute this index for certain special classes of thorn graphs, such as thorn complete graph, thorn complete bipartite graph, thorn cycle, thorn star, thorn rod, thorn path.

Thorn Graph. The thorn graph G^*[1, 3, 9, 12, 10] is obtained by attaching $u_j \geq 1$ novel pendant vertices to every vertex v_ι of the n-vertices parent graph G, where $\iota = 1,2,3,\cdots,n.$, $j = 1,2,3,\cdots,n$. The u_j novel pendant vertices attached to every vertex v_ι are called thorns of v_ι.

Thorn complete graph. Let $G = K_n$ be a complete graph with n vertices. Then the thorny complete graph $G^* = K_{n,u_j}$ is a graph [12] obtained from K_n by attaching u_j number of thorns to every vertex, $v_\iota \in K_n$. Let $v_\iota \in V(K_n)$, $e_\iota \in E(K_n)$,

such that $e_1 = v_1v_2$, $e_2 = v_2v_3, \cdots, e_n = v_nv_1$, where $\iota = 1,2,\cdots,n$. And also, $u_j \in V(G^*)$, $e_j \in E(G^*)$ but $u_j \notin V(G)$, $e_j \notin E(G)$, where $j = 1,2,\cdots,n$ as shown in the Figure 1.

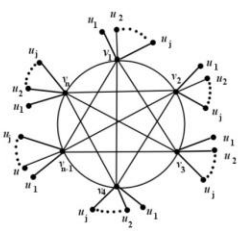

Figure 1: Thorn complete graph

Thorn complete bipartite graph. Let $G = K_{p,q}$ be a complete bipartite graph with $p > 1, q > 1$. Then the thorny complete bipartite graph $G^* = K_{p,q,u_j}$ is a graph [12] obtained from $K_{p,q}$ by attaching u_j number of thorns to every vertex, $v_\iota \in K_{p,q}$, where $\iota = 1,2,3,\cdots,p+q.$, $j = 1,2,3,\cdots,p+q$ as shown in the Figure 2.

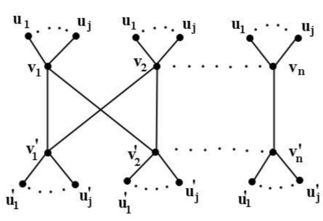

Figure 2: Thorn complete bipartite graph

Thorn Ring. Thorn ring $G^* = C_{n,r}$ obtained from the parent cycle $G = C_n$ by attaching $r-2$, $(r \geq 3)$ pendant vertices to each $G = C_n$ vertex. Let $v_\iota \in V(C_n)$, $e_\iota \in E(C_n)$, such that $e_1 = v_1v_2$, $e_2 = v_2v_3, , \cdots, e_n = v_nv_1$, where $\iota = 1,2,,\cdots,n$. And also, $u_j \in V(G^*)$, $e_j \in E(G^*)$ but $u_j \notin V(G)$, $e_j \notin E(G)$,

where $j = 1,2,\cdots,(r-2)n$ as shown in the Figure 3.

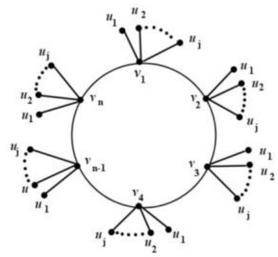

Figure 3: Thorn-ring

Thorn Star. Thorn star $G^* = K_{1,n-1,t}$ is obtained from the star $G = K_{1,n-1}$ by attaching $t-1$ $(t \geq 2)$ pendant vertices to each of $(n-1)$ star arms. Let $v_\iota \in V(G)$ for $\iota = 0,1,2,,\cdots,n-1$ and $e_\iota \in E(G)$, such that $e_1 = v_0v_1, e_2 = v_0v_2, \cdots, e_{n-1} = v_0v_{n-1}$. Also, $u_j \in G^*, e_j \in E(G^*)$ but $u_j \notin V(G)$, $e_j \notin E(G)$.
Where $j = 1,2,\cdots,(n-1)(t-1)$ as shown in the Figure 4.

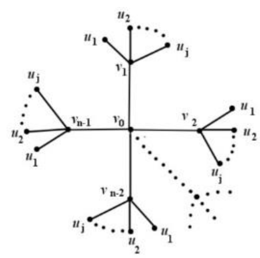

Figure 4: Thorn star

Thorn Rod. Thorn rod $G^* = P_{n,m}$ is obtained from the path $G = P_n$ by attaching $m-1$ pendant vertices to each extreme vertices of P_n. Let $v_\iota \in V(P_n)$, $e_\iota \in E(P_n)$ such that $e_1 = v_1v_2, e_2 = v_2v_3,,\cdots, e_{n-1} = v_{n-1}v_n$, for $\iota = 1,2,,\cdots,n$.
Also, $u_j \in V(G^*)$, $e_j \in E(G^*)$ but $u_j \notin V(P_n)$, $e_j \notin E(P_n)$,
for $j = 1,2,\cdots,2(m-1)$ as shown in the Figure 5.

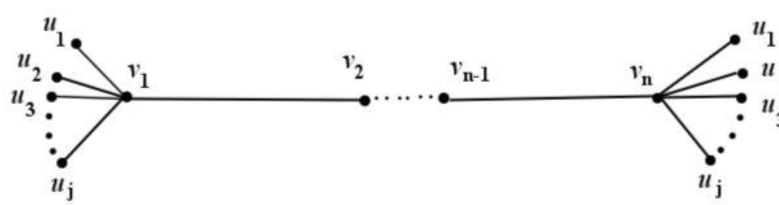

Figure 5: Thorn rod

Thorn Path. The thorn path $G^* = P_{n,h,l}$ is obtained from the path $G = P_n$ by attaching h pendant vertices to each of its non-extreme vertices and l pendant vertices to each of its extreme vertices.

Let $P_n (n \geq 3)$ be a path, its vertices labeled as $\{v_0, v_1, v_2, \ldots, v_{n-1}\}$ and $\{h_1, h_2, h_3, \cdots, h_i\}$ be a pendant vertices attached to each non-extreme vertices of P_n, where $i = 1,2,\cdots,h$. Also, let $\{l_1, l_2, l_3, \cdots, l_j\}$ be a pendant vertices attached to each extreme vertices of P_n, where $j = 1,2,\cdots,l$ as shown in the Figure 6.

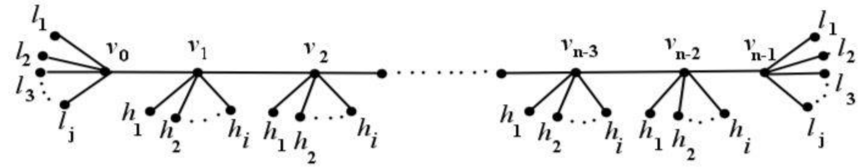

Figure 6: Thorn path

Theorem 3.1

Let $G^* = K_{n,u_j}$ be a thorn complete graph.

Then $S_e(K_{n,u_j}) = n(n-1)\sqrt{2} + nu_j\sqrt{13}$, for $n \geq 2$.

Proof:

Let $V(K_n) = \{v_1, v_2, v_3, \cdots, v_n\}$ and Let $V(u_j) = \{u_1, u_2, u_3, \cdots, u_n\}$, be the thorns attached to every vertex $v_\iota \in K_n$, to obtain the thorn graph G^*, where $\iota = 1,2,3, \cdots, n$. and $j = 1,2,3, \cdots, n$. We observed that $\forall \iota$, $\rho(v_\iota) = 2$ and $\forall j$, $\rho(u_j) = 3$. Based on the eccentricity of these distinct vertex types, we partition two distinct types of edges in G^*.

In first partition we considered the edges $e_\iota \in K_n$, such that $e_\iota = (v_\iota, v_{\iota+1})$. For each of these edges, end vertices eccentricity is (2,2) and in this partition $|E(K_n)| = \frac{n(n-1)}{2}$. In second partition we considered the edges $e_j \in G^*$, such that $e_j = (v_\iota, u_j)$, For each of these edges, end vertices eccentricity is (2,3) and the cardinality of the edges in this partition is nu_j.

By the definition,

$$S_e(K_{n,u_j}) = \frac{n(n-1)}{2}\sqrt{2^2 + 2^2} + nu_j\sqrt{2^2 + 3^2}$$

$$S_e(K_{n,u_j}) = n(n-1)\sqrt{2} + nu_j\sqrt{13}.$$

Theorem 3.2

Let $G^* = K_{p,q,u_j}$ be a thorn complete bipartite graph.

then $S_e(K_{p,q,u_j}) = 3\sqrt{2}pq + 5(p+q)u_j$.

Proof: Let $V(K_{p,q}) = \{v_1, v_2, v_3, \cdots, v_n\} \cup \{v_{1'}, v_{2'}, v_{3'}, \cdots, v_{n'}\}$. Let u_j and $u_{j'}$ be the number of thorns attached to v_ι and $v_{\iota'}$ respectively to obtain G^*, where $1 \leq \iota \leq p$, $1 \leq j \leq q$. Let $V(G^*) = V(K_{p,q}) \cup V' \cup V''$. Where $V' = \{x_\iota^k : 1 \leq k \leq u_j, 1 \leq \iota \leq p\}$ is the set of u_j thorns attached to v_ι, $1 \leq \iota \leq p$ and $V'' = \{y_j^k : 1 \leq k \leq u_{j'}, 1 \leq j \leq q\}$ is the set of $u_{j'}$ thorns attached to $v_{\iota'}$,$1 \leq \iota \leq q$. In G^*, we observed that $\forall$ $V_\iota, V_{\iota'}$, $\rho(v_\iota) = \rho(v_{\iota'}) = 3$ and $\forall u_j, u_{j'}$, $\rho(u_j) = \rho(u_{j'}) = 4$. By considering the eccentricity of these distinct vertex types, we discern a total of two distinct types of edge partitions of G^*. The first partition edges are $(v_\iota, v_{\iota'}) \in K_{p,q}$, for this partition each edge end vertices eccentricity is $(\rho(v_\iota), \rho(v_{\iota'})) = (3,3)$ and in this partition $|E(K_{p,q})| = pq$. In second partition we considered the edges $(v_\iota, u_j), (v_{\iota'}, u_{j'}) \in G^*$, for this, $(\rho(v_\iota), \rho(u_j)) = (\rho(v_{\iota'}), \rho(u_{j'})) = (3,4)$ and in this partition total number of edges are $(p+q)u_j$.

By the definition, $S_e(G^*) = pq\sqrt{3^2 + 3^2} + (p+q)u_j\sqrt{3^2 + 4^2}$

$$S_e(K_{p,q,u_j}) = 3\sqrt{2}pq + 5(p+q)u_j.$$

Theorem 3.3

For a thorn ring $G^* = C_{n,r}$,

$$S_e(C_{n,r}) = n\left(\left\lfloor\frac{n}{2}\right\rfloor + 1\right)\sqrt{2} + (r-2)n\sqrt{\left(\left\lfloor\frac{n}{2}\right\rfloor + 1\right)^2 + \left(\left\lfloor\frac{n}{2}\right\rfloor + 2\right)^2}.$$

Proof: Let C_n be a parent cycle and $G^* = C_{n,r}$ be a thorn ring with $|V(G^*)| = n(r-1), |E(G^*)| = n(r-1)$ and $(r-2)n$ thorns. For each vertex $v_\iota \in V(C_n)$, attach the pendant vertices u_j to obtain the graph G^*, where $\iota = 1,2,\cdots,n$ and $j = 1,2,,\cdots,(r-2)n$.

It is observed that, $\rho(v_\iota) = \left\lfloor\frac{n}{2}\right\rfloor + 1$, $\rho(u_j) = \left\lfloor\frac{n}{2}\right\rfloor + 2$. Based on the eccentricity of these distinct vertex types, we partitioned two types of edges, such as $e_\iota = (v_\iota, v_{\iota+1})$ and $e_j = (v_\iota, u_j)$. For these two types of edges, each edge end vertices eccentricity are $\left(\left\lfloor\frac{n}{2}\right\rfloor + 1\right), \left(\left\lfloor\frac{n}{2}\right\rfloor + 1\right)$ and $\left(\left\lfloor\frac{n}{2}\right\rfloor + 1\right), \left(\left\lfloor\frac{n}{2}\right\rfloor + 2\right)$ respectively. Also, $|E(e_\iota)| = n$, $|E(e_j)| = (r-2)n$

. By the definition,

$$S_e(G^*) = n\sqrt{\left(\left\lfloor\frac{n}{2}\right\rfloor + 1\right)^2 + \left(\left\lfloor\frac{n}{2}\right\rfloor + 1\right)^2} + (r-2)n\sqrt{\left(\left\lfloor\frac{n}{2}\right\rfloor + 1\right)^2 + \left(\left\lfloor\frac{n}{2}\right\rfloor + 2\right)^2}.$$

Hence, $S_e(C_{n,r}) = n\left(\left\lfloor\frac{n}{2}\right\rfloor + 1\right)\sqrt{2} + (r-2)n\sqrt{\left(\left\lfloor\frac{n}{2}\right\rfloor + 1\right)^2 + \left(\left\lfloor\frac{n}{2}\right\rfloor + 2\right)^2}.$

Theorem 3.4

For a thorn star $G^* = K_{1,n-1,t}$, $S_e(G^*) = (n-1)\sqrt{13} + 5(n-1)(t-1)$.

Proof: Consider, $G = K_{1,n-1}$ be a parent star with $n-1$ edges and let $G^* = K_{1,n-1,t}$ be thorn star with $|V(G^*)| = 1 + t(n-1), |E(G^*)| = (t-1)(n-1)$. Also in thorn star G^*, there are $(n-1)(t-1)$ thorns. For each $v_\iota \in G$, $\rho(v_\iota) = 3$, where $\iota = 1,2,\cdots,n-1$. and for central vertex $v_0 \in G$ having $\rho(v_0) = 2$. Also, for each edge $e_\iota \in G$ such that $e_\iota = v_0 v_\iota$. To obtain thorn star graph attach the pendant vertex, u_j to each $v_\iota \in G$ and for each edge $e_j \in G^*$ such that $e_j = v_\iota u_j$, where $j = 1,2,\cdots,(n-1)(t-1)$, having $\rho(u_j) = 4$. Based on the eccentricity of a vertex, we partition two type of edges such as, $e_\iota \in G$ and $e_j \in G^*$

By the definition,

$$S_e(G^*) = (n-1)\sqrt{2^2 + 3^2} + (n-1)(t-1)\sqrt{3^2 + 4^2}$$
$$Hence, S_e(K_{1,n-1,t}) = (n-1)\sqrt{13} + 5(n-1)(t-1).$$

Theorem 3.5

For a thorn rod $G^* = P_{n,m}$ $S_e(P_{n,m}) =$

$$\begin{cases} 2(m-1)\sqrt{n^2 + (n+1)^2} + 2\sum_{\mu=\frac{n+1}{2}}^{n-1}\sqrt{\mu^2 + (\mu+1)^2} & when\ n\ is\ odd, n \geq 3. \\ \frac{n+2}{\sqrt{2}} + 2(m-1)\sqrt{n^2 + (n+1)^2} + 2\sum_{\mu=\frac{n+2}{2}}^{n-1}\sqrt{\mu^2 + (\mu+1)^2} & when\ n\ is\ even, n \geq 4. \end{cases}$$

Proof: Let $V(P_n) = \{v_1, v_2, v_3, \cdots, v_n\}, E(P_n) = \{e_1, e_2, e_3, \cdots, e_{n-1}\}$ such that $e_1 = (v_1, v_2), e_2 = (v_2, v_3), \cdots, e_{n-1} = (v_{n-1}, v_n)$, where $\iota = 1,2,,\cdots,n$.

Let the thorn vertex set as, $V(u_j) = \{u_1, u_2, u_3, \cdots, u_n\}$ and edge set as $E(e_j) = \{(v_1, u_1), (v_1, u_2), (v_1, u_3),, \cdots, (v_1, u_j)\}$ $\cup$

$\{(v_n,u_1),(v_n,u_2),(v_n,u_3),,\cdots,(v_n,u_j)\}$,

where $j=1,2,\cdots,2(m-1)$. In each of the fallowing cases, we partition the edges based on the eccentricity of their end vertices.

Case 1. When $n\geq 3$ is odd. It is observed that the end vertices of the edges of each set $\{e_1,e_{n-1}\},\{e_2,e_{n-2}\}$, $\{e_3,e_{n-3}\},\cdots,\{e_{\frac{n-1}{2}},e_{\frac{n+1}{2}}\}$ having the eccentricity $\rho(v_1)=\rho(v_n)=n,\rho(v_2)=\rho(v_{n-1})=n-1,\rho(v_3)=\rho(v_{n-2})=n-2$ $,\cdots,\rho(v_{\frac{n-1}{2}})=\rho(v_{\frac{n+3}{2}})=\frac{n+3}{2}$ and the middle vertex, having $\rho(v_{\frac{n+1}{2}})=\frac{n+1}{2}$.

In thorn rod $P_{n,m}$, there are $2(m-1)$ thorns and each thorn u_j, having $\rho(u_j)=n+1$. Since $P_{n,m}$ is symmetric about $v_{\frac{n+1}{2}}$, we have

$$S_e(P_{n,m})=2(m-1)\sqrt{n^2+(n+1)^2}+2\sum_{\mu=\frac{n+1}{2}}^{n-1}\sqrt{\mu^2+(\mu+1)^2}.$$

Case 2. When $n\geq 4$ is even, the end vertices of the edges of each set, $\{e_1,e_{n-1}\},\{e_2,e_{n-2}\}$,

$\{e_3,e_{n-3}\},\cdots,\{e_{\frac{n}{2}-1},e_{\frac{n}{2}+1}\}$ having the eccentricity are $\rho(v_1)=\rho(v_n)=n,\rho(v_2)=\rho(v_{n-1})=n-1,\rho(v_3)=\rho(v_{n-2})=n-2,\cdots,\rho(v_{\frac{n}{2}})=\rho(v_{\frac{n}{2}+1})=\frac{n+2}{2}$. In thorn rod $P_{n,m}$, there are $2(m-1)$ thorns and each thorn u_j, having $\rho(u_j)=n+1$. Since $P_{n,m}$ is symmetric about $e_{\frac{n}{2}}$, we have

$$S_e(P_{n,m})=\sqrt{(\frac{n+2}{2})^2+(\frac{n+2}{2})^2}+2(m-1)\sqrt{n^2+(n+1)^2}$$
$$+2\sum_{\mu=\frac{n+2}{2}}^{n-1}\sqrt{\mu^2+(\mu+1)^2}$$

Hence, $S_e(P_{n,m})=\frac{n+2}{\sqrt{2}}+2(m-1)\sqrt{n^2+(n+1)^2}+2\sum_{\mu=\frac{n+2}{2}}^{n-1}\sqrt{\mu^2+(\mu+1)^2}$.

Theorem 3.6

For a thorn path $G^*=P_{n,h,l}$

$$S_e(P_{n,h,l})=\begin{cases}(h+2)\sqrt{(\frac{n+1}{2})^2+(\frac{n+3}{2})^2}+2(h+1)\sum_{\mu=\frac{n+3}{2}}^{n-1}\sqrt{\mu^2+(\mu+1)^2}\\ +2l\sqrt{n^2+(n+1)^2}\ \ for\ n\ is\ odd, n\geq 5.\\ \frac{n+2}{\sqrt{2}}+2l\sqrt{n^2+(n+1)^2}+2(h+1)\sum_{\mu=\frac{n+2}{2}}^{n-1}\sqrt{\mu^2+(\mu+1)^2} \quad for\ n\ is\ even, n\geq 4.\end{cases}$$

Proof: Let $V(P_n)=\{v_0,v_1,v_2,v_3,\cdots,v_{n-1}\},E(P_n)=\{e_1,e_2,e_3,\cdots,e_{n-1}\}$ such that $e_1=(v_0,v_1),e_2=(v_1,v_2),\cdots,e_{n-1}=(v_{n-1},v_{n-2})$

In each of the fallowing cases, we partition the edges based on the eccentricity of each edge end vertices.

Case 1. Consider odd n, $n\geq 5$.

In thorn path $P_{n,h,l}$, the non extreme vertices are $\{v_1,v_2,v_3,\cdots,v_{n-2}\}$. In this case,

$\rho(v_1) = \rho(v_{n-2}) = n-1$ and for each thorn h_ι , $\rho(h_\iota) = n$.

The thorns h_ι attached to v_1 , v_{n-2}, for $\iota = 1,2,\cdots,h$.

Similarly,

$\rho(v_2) = \rho(v_{n-3}) = n-2$ and for each thorn h_ι, $\rho(h_\iota) = n-1$.

The thorns h_ι attached to v_2, v_{n-3}, for $\iota = 1,2,\cdots,h$.

Also, $\rho(v_3) = \rho(v_{n-4}) = n-3$ and for each thorn h_ι, $\rho(h_\iota) = n-2$.

The thorns attached to v_3 , v_{n-4}, for $\iota = 1,2,\cdots,h$.

This process Continued till we reach the middle vertex $v_{\frac{n-1}{2}}$, for this vertex

$\rho\left(v_{\frac{n-1}{2}}\right) = \frac{n+1}{2}$ and thorns h_ι attached to $v_{\frac{n-1}{2}}$ have $\rho(h_\iota) = \frac{n+3}{2}$, where $\iota = 1,2,\cdots,h$.

Further, in $P_{n,h,l}$ there are l pendant vertices attached to each extreme vertex $v_0, v_{n-1} \in P_n$. Clearly, $\rho(v_0) = \rho(v_{n-1}) = n$ and for thorns l_j, $\rho(l_j) = n+1$, for $j = 1,2,\cdots,l$ attached to v_0, v_{n-1} . By considering the eccentricities of these distinct vertex types, we discern a total of three distinct types of partitions the edges of $P_{n,h,l}$, Since $P_{n,h,l}$ is symmetric about middle vertex $v_{\frac{n-1}{2}}$, we obtain

$$S_e(P_{n,h,l}) = (h+2)\sqrt{(\tfrac{n+1}{2})^2 + (\tfrac{n+3}{2})^2} + 2(h+1)\sum_{\mu=\frac{n+3}{2}}^{n-1} \sqrt{\mu^2 + (\mu+1)^2} + 2l\sqrt{n^2 + (n+1)^2}.$$

Case 2. Consider even n, $n \geq 4$.

From previous case we have, $\rho(v_1) = \rho(v_{n-2}) = n-1$ and for each $\rho(\iota) = n$, where $\iota = 1,2,\cdots,h$.

$\rho(v_2) = \rho(v_{n-3}) = n-2$ and for each $\rho(\iota) = n-1$, where $\iota = 1,2,\cdots,h$.

$\rho(v_3) = \rho(v_{n-4}) = n-3$ and for each $\rho(\iota) = n-2$, where $\iota = 1,2,\cdots,h$.

$,\cdots,$ $\rho(v_{\frac{n}{2}-1}) = \rho(v_{\frac{n}{2}+1}) = \frac{n+2}{2}$ and for each $\rho(\iota) = \frac{n+4}{2}$, where $\iota = 1,2,\cdots,h$.

Also, in thorn path $P_{n,h,l}$ there are l pendant vertices attached to each extreme vertex, having $\rho(v_0) = \rho(v_{n-1}) = n$, $\rho(l_j) = n+1$, where $j = 1,2,\cdots,l$. Since $P_{n,h,l}$ is symmetric about middle edge $e_{\frac{n}{2}}$, we have

$$S_e(P_{n,h,l}) = \frac{n+2}{\sqrt{2}} + 2l\sqrt{n^2 + (n+1)^2} + 2(h+1)\sum_{\mu=\frac{n+2}{2}}^{n-1} \sqrt{\mu^2 + (\mu+1)^2}.$$

4. Correlation analysis

In this section, we discuss the chemical applicability of the $S_e(G)$ index to validate its chemical significance. The study employs hetero molecules, selected polycyclic aromatic hydrocarbons(PAHs) and octane isomers. The chemical applicability is assessed through correlation analysis by correlating $S_e(G)$ index with relevant physico chemical properties of hetero molecules, PAHs and Octane isomers.

4.1. Correlation analysis between eccentric Sombor index of hetero molecules and their corresponding total π-electron energy(E_π)

In this section, the chemical applicability of $S_e(G)$ index is discussed by performing correlation analysis, considering total π-electron energy of hetero molecules ($E_\pi(HMO)$)[4] as the dependent variable (Y) and eccentric Sombor index of the hetero molecules as independent variable (X). Table 1 represents the computed $S_e(G)$ index value of selected hetero molecules and the experimental value of the ($E_\pi(HMO)$) and corresponding correlation graph is shown in Figure 7.

Hetero molecules Code	$S_e(G)$	E_π
$H1$	4.4721	2.23
$H2$	10.0395	5.66
$H3$	10.0395	5.76
$H4$	6.7082	6.96
$H5$	10.0395	6.82
$H6$	14.1421	5.23
$H7$	25.4558	6.69
$H8$	25.4558	9.06
$H9$	25.4558	9.1
$H10$	25.4558	9.07
$H11$	25.4558	9.65
$H12$	31.9705	8.19
$H13$	38.3847	12.21
$H14$	38.4852	12.22
$H15$	41.2915	12.21
$H16$	42.6946	11
$H17$	63.9972	14.23
$H18$	63.9972	14.23
$H19$	70.4004	16.15
$H20$	77.5174	16.12
$H21$	77.5174	13.46
$H22$	77.5174	13.59
$H23$	150.2567	20.1
$H24$	150.2567	21.02
$H25$	127.6728	20.56
$H26$	127.6728	21.62
$H27$	140.4790	24.23
$H28$	102.1083	19.39

Table 1: Computed value of the $S_e(G)$ of hetero molecules and their $E_\pi(HMO)$

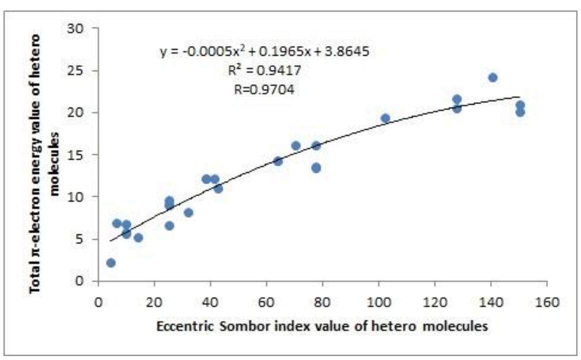

Figure 7: Correlation between $S_e(G)$ index value of hetero molecules and their $E_\pi(HMO)$

From the analysis, it is observed that there is a strong correlation between $S_e(G)$ index of hetero molecules and their $E_\pi(HMO)$

4.2. Correlation analysis between eccentric Sombor index of selected polycyclic aromatic hydrocarbons (PAHs) and their corresponding E_π

In this section, the chemical applicability of $S_e(G)$index is investigated through a correlation analysis, by considering total π-electron energy of selected PAHs($E_\pi(PAHs)$) [4, 14, 12] as the dependent variable (Y) and $S_e(G)$ index of the selected PAHs is taken independent variable (X). Table 2 presents the computed value of $S_e(G)$ index for some selected PAHs along with the corresponding $E_\pi(PAHs)$ and the associated correlation graph is shown in Figure 8 .

PAHs Molecules	$S_e(G)$	E_π
$Anthanthrene$	252.32	31.25
$Acenapthalene$	80.968	16.61
$Anthracene$	127.6727	19.31
$Azulene$	58.3404	13.36
$Benzene$	25.4558	8
$Benzo[a]anthracene$	201.29	25.1
$Benzo[a]pyrene$	225.3877	28.22
$Benzo[e]pyrene$	202.6422	28.33
$Benzo[g,h,i]perylene$	230.98	31.42
$Coronene$	259.3194	34.57
$Chrysene$	198.4584	25.19
$Dibenzo(a,c)anthracene$	262.1866	30.94
$Dibenzo[a,h]anthracene$	300.34	30.88
$Dibenzo(a,j)anthracene$	284.8658	30.88
$Dibenzo(a,h)pyrene$	308.7261	30.88
$Dibenzo(a,e)pyrene$	291.2052	33.92
$Fluoranthene$	132.6172	22.5
$Naphthalene$	63.9972	13.68
$Phenanthrene$	120.6017	19.44
$Pentacene$	317.2114	30.54
$Pyrene$	141.8149	22.5
$Perylene$	202.6422	28.24
$Picene$	300.3367	33.95
$Tetracene$	211.132	25.18
$Triphenylene$	174.3036	25.27

Table 2: Computed value of the $S_e(G)$ index of selected PAHs and their $E_\pi(PAHs)$

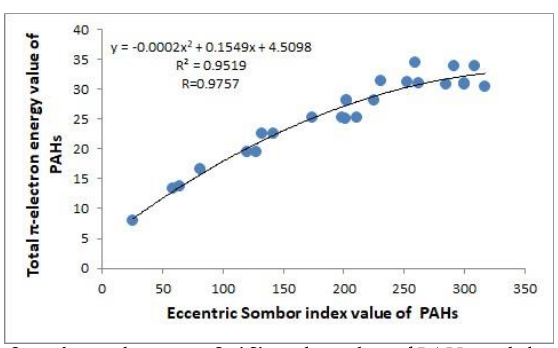

Figure 8: Correlation between $S_e(G)$ index value of PAHs and their $E_\pi(PAHs)$

From the analysis, it is observed that there is a strong correlation between $S_e(G)$ index of some selected PAHs molecules and their $E_\pi(PAHs)$

4.3. Correlation analysis between eccentric Sombor index of PAHs and their physicochemical properties.

In this section, the chemical applicability of the $S_e(G)$ is established correlation analysis, considering the physicochemical properties of 38 selected polycyclic aromatic hydrocarbons (PAHs). In the regression model, the physicochemical properties of PAHs namely melting point ($MP,\ {}^\circ\mathrm{C}$), complexity (C), polarizability ($PO, 10^{-24}cm^3$), Flash point ($FP,\ {}^\circ\mathrm{C}$), molecular weight ($MW,\ g/mol$), boiling point ($BP,\ {}^\circ\mathrm{C}$), molar refractivity (MR, cm^3), molar volume (MV, cm^3) are considered as dependent variable (Y), while the $S_e(G)$ of PAHs is taken as the independent variable(X). For each PAHs under consideration, the corresponding $S_e(G)$ value has been computed. The standard(experimental) values of the physicochemical properties, together with the calculated $S_e(G)$ values are provided in Table 3 and the associated correlation graph is shown in Figures 9-16 .

Name	$S_e(G)$	MP	C	PO	FP	MW	BP	MR	MV
Aceanthrylene	150.37	94	155	135.3	20.5	154.21	279	51.7	134.9
Acephenanthrylene	148.05	140	303	27.4	188.6	202.25	405.7	69.1	162.3
Anthracene	127.6728	217	154	24.5	146.6	178.23	337.4	61.9	157.7
Anthanthrene	252.32	261	411	40	247.2	276.3	497.1	100.8	200.4
Benzene	25.4558	5	15.5	10.4	−11.1	78.11	78.8	26.3	89.4
Benzo[a]anthracene	201.29	161	294	31.6	209.1	228.3	436.7	79.8	191.8
Benzo[a]pyrene	225.39	176	372	35.8	228.6	252.3	495	90.3	196.1
Benzo[b]fluoranthene	214.67	166	372	35.8	228.6	252.3	467.5	90.3	196.1
Benzo[k]fluoranthene	221.73	217	338	35.8	228.6	252.3	480	90.3	196.1
Benzo[e]pyrene	202.6422	177.5	336	35.8	228.6	252.3	467.5	90.3	196.1
Benzo[g,h,i]perylene	230.98	273	411	40	247.2	276.3	501	100.8	200.4
Biphenylene	96.451	115	339	19.8	187.2	152.19	469.9	50	129.9
Coronene	259.3194	440	376	44.1	265.2	300.4	525.6	111.4	204.7
Chrysene	198.4584	255	264	31.6	209.1	228.3	448	79.8	191.8
Corannulene	180.83	269	303	37.1	210.1	250.3	438	93.5	170.6
Dibenz[a,c]anthracene	262.1866	206	361	38.7	264.5	278.3	518	97.6	225.9
Dibenz[a,h]anthracene	300.34	266	361	38.7	264.5	278.3	524.7	97.6	225.9
Dibenz[a,i]anthracene	284.8658	196	363	38.7	264.5	278.3	524.7	97.6	225.9
Dibenzo[a,h]pyrene	308.7261	308	436	42.9	282	302.4	552.3	108.1	230.2
Dibenzo[a,i]pyrene	330.04	281.5	436	42.9	282	302.4	552.3	108.1	230.2
Dibenzo[a,l]pyrene	277.82	162.4	480	42.9	282	302.4	552.3	108.1	230.2
Fluoranthene	132.6172	110	243	28.7	168.4	202.25	375	72.5	162
Fluorene	102.11	115	165	21.3	133.1	166.22	293.6	53.8	148.3
Indeno[1,2,3-cd]pyrene	245.15	163.6	453	40	247.2	276.3	497.1	100.8	200.4
Indene	49.698	−2	124	15.1	58.9	116.16	181.6	38	111.8
Isochrysene	174.3	199	217	31.6	209.1	228.3	425	79.8	191.8
5-Methylchrysene	206.27	118	320	33.5	217.8	242.3	449.4	84.6	208.1
Naphthalene	63.9972	81	80.6	17.5	78.9	128.17	221.5	44.1	123.5
Naphthacene	211.3	350	236	31.6	209.1	228.3	436.7	79.8	53.5
Ovalene	201.94	257	696	38.7	264.5	398.5	524.7	97.6	225.9
Pentalene	37.251	–	174	38.7	97.2	102	308.9	34.2	96.1
Pentacene	317.2114	257	325	38.7	264.5	278.3	524.7	97.6	225.9
Phenanthrene	120.6017	100	174	24.6	146.6	178.23	337.4	61.9	157.7
perylene	202.6422	276	304	35.8	228.6	252.3	467.5	90.3	196.1
Picene	300.3367	367	361	38.7	264.5	278.3	519	97.6	225.9

Pyrene	141.8149	150	217	28.7	168.8	202.25	404	72.5	162
Rubicene	327.43	306	514	47	298.8	326.4	579	118.7	234.5
s-indacene	88.167	–	341	19.8	214.4	152.19	525.3	50	129.9

Table 3: Computed value of the $S_e(G)$ of PAHs and their physicochemical properties experimental values

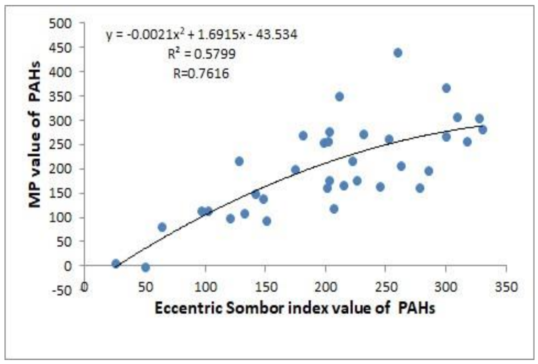

Figure 9: Correlation between $S_e(G)$ index of selected PAHs molecules and their MP

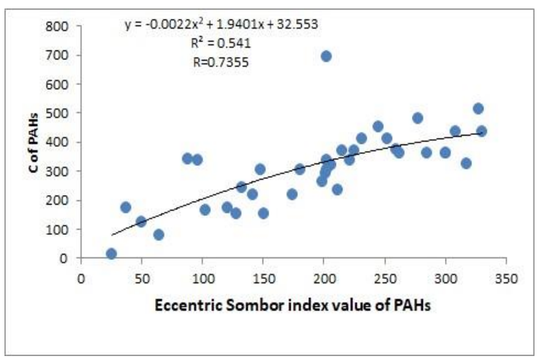

Figure 10: Correlation between $S_e(G)$ index of selected PAHs molecules and their Complexity

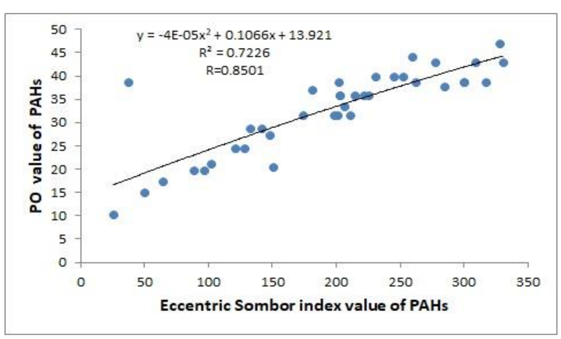

Figure 11: Correlation between $S_e(G)$ index of selected PAHs molecules and their PO

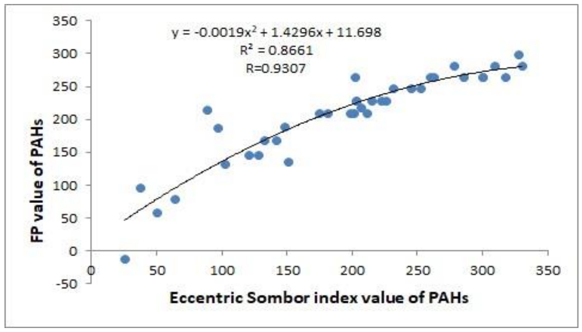

Figure 12: Correlation between $S_e(G)$ index of selected PAHs molecules and their FP

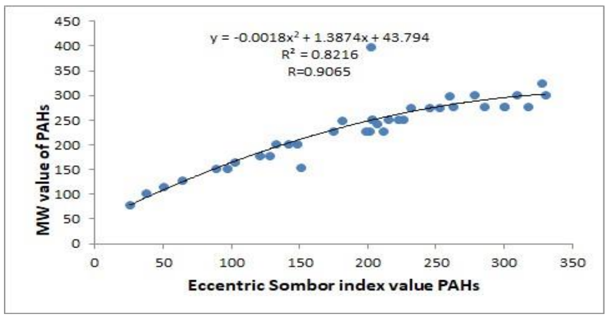

Figure 13: Correlation between $S_e(G)$ index of selected PAHs molecules and their MW

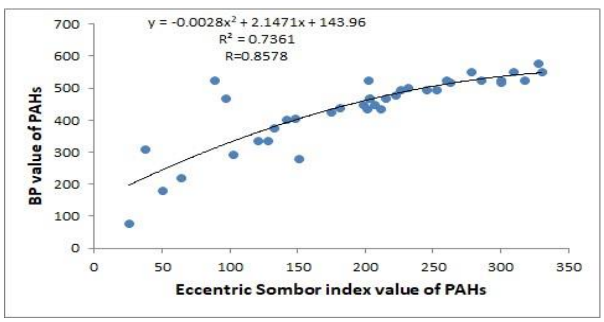

Figure 14: Correlation between $S_e(G)$ index of selected PAHs molecules and their BP

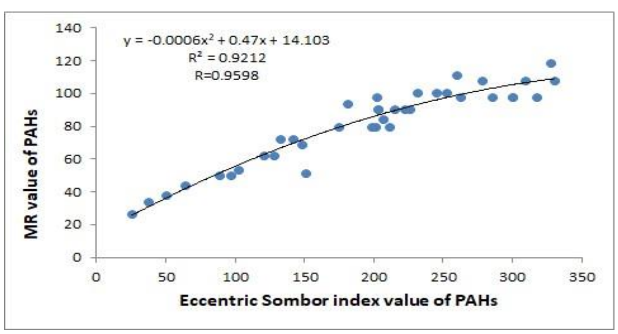

Figure 15: Correlation between $S_e(G)$ index of selected PAHs molecules and their MR

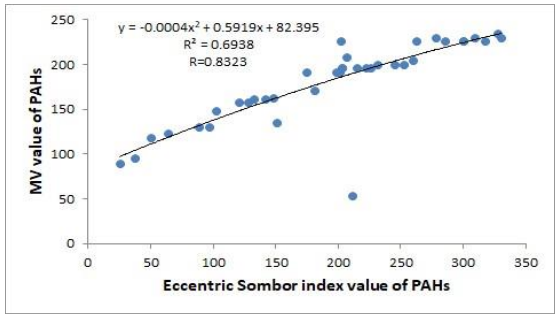

Figure 16: Correlation between $S_e(G)$ index of selected PAHs molecules and their MV

4.4. Correlation analysis between eccentric Sombor index of Octane isomers and their physicochemical properties.

In this section, the chemical applicability of the $S_e(G)$ is carried out between the $S_e(G)$ and the physico-chemcial properties of octane isomers. In this analysis, properties such as entropy (S), enthalpy of vaporization ($HVAP$), standard enthalpy of vaporization ($DHVAP$) and acentric factor (AF) were considered for each compound. For every octane isomer, the corresponding $S_e(G)$ value was computed. The standard(experimental) values of the physico-chemical properties, together with the calculated $S_e(G)$ values, are presented in Table 4 and the associated correlation graph is shown in Figures 17 - 20

Octane isomer	$S_e(G)$	S	HVAP	DHVAP	AF
n-octane	52.523	111.67	73.19	9.915	0.397898
2-methylheptane	46.237	109.84	70.30	9.484	0.377916
3-methylheptane	44.83	111.26	71.30	9.521	0.371002
4-methyl heptane	43.427	109.32	70.91	9.483	0.371504
3-ethyl hexane	38.452	109.43	71.70	9.476	0.362472
2, 2-dimethylhexane	44.83	103.42	67.70	8.915	0.339426
3, 3-dimethylhexane	38.452	108.02	70.20	9.272	0.348247
2,4-dimethyl hexane	38.452	106.98	68.50	9.029	0.344223
2,5-dimethyl hexane	46.237	105.72	68.60	9.051	0.35683
3,3-dimethyl hexane	37.049	104.74	68.50	8.973	0.322596
3,4-dimethyl hexane	37.049	106.59	70.20	9.316	0.340345
2-methyl 3-ethylpentane	30.8178	106.06	69.70	9.209	0.332433
3-methyl 3-ethyl pentane	29.422	101.48	69.30	9.081	0.306899
2,2,3-trimethyl pentane	30.817	101.31	67.30	8.826	0.300816
2,2,4-trimethyl pentane	32.211	104.09	64.87	8.402	0.30537
2,3,3-trimethyl pentane	37.049	102.06	68.10	8.897	0.293177
2,3,4-trimethyl pentane	30.817	102.39	68.37	9.014	0.317422
2,2,3,3-tetramethylbutane	24.462	93.06	66.20	8.410	0.255294

Table 4: Computed values of the $S_e(G)$ of octane isomers and their Physicochemical properties experimental values

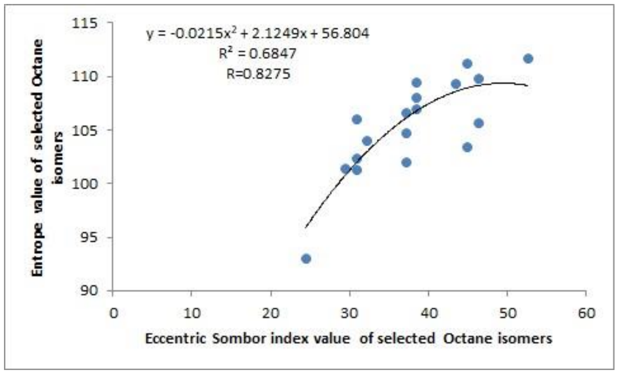

Figure 17: Correlation between $S_e(G)$ index of selected Octane isomers and their entropy

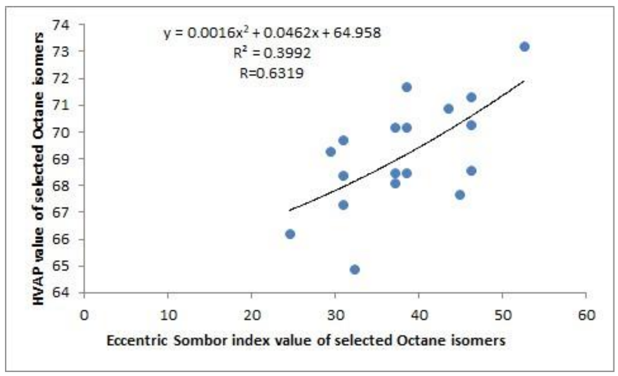

Figure 18: Correlation between $S_e(G)$ index of selected Octane isomers and their HVAP

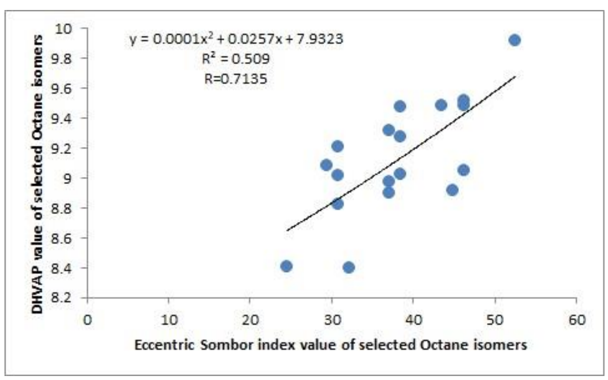

Figure 19: Correlation between $S_e(G)$ index of selected Octane isomers and their DHVAP

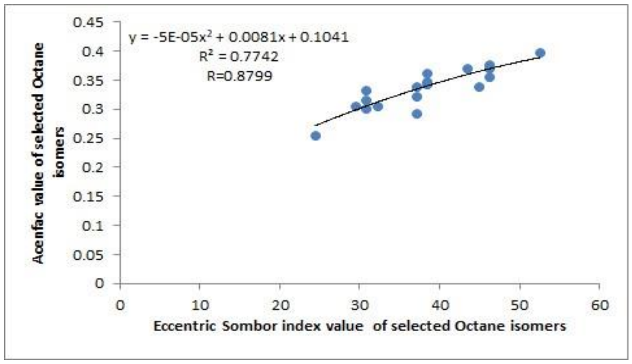

Figure 20: Correlation between $S_e(G)$ index of selected Octane isomers and their Acent fac

4.5. Regression analysis statistics.

In this section, regression model of Second ordered polynomial is presented and the Table 5, reported the statistical parameter values for studied properties

$$E_\pi(HMO) = -0.0005(S_e(G))^2 + 0.1965(S_e(G)) + 3.8645$$
$$E_\pi(PAHs) = -0.0002(S_e(G))^2 + 0.1549(S_e(G)) + 4.5098$$
$$MP = -0.00021(S_e(G))^2 + 1.6915(S_e(G)) - 43.534$$
$$C = -0.0022(S_e(G))^2 + 1.9401(S_e(G)) + 32.553$$
$$PO = -4\times10^{-5}(S_e(G))^2 + 0.1066(S_e(G)) + 13.921$$
$$FP = -0.0019(S_e(G))^2 + 1.4296(S_e(G)) + 11.698$$
$$MW = -0.0018(S_e(G))^2 + 1.3874(S_e(G)) + 43.794$$
$$BP = -0.0028(S_e(G))^2 + 2.1471(S_e(G)) + 143.96$$
$$MR = -0.0006(S_e(G))^2 + 0.47(S_e(G)) + 14.103$$
$$MV = -0.0004(S_e(G))^2 + 0.5919(S_e(G)) + 82.395$$
$$S = -0.0215(S_e(G))^2 + 2.1249(S_e(G)) + 56.804$$
$$HVAP = 0.0016(S_e(G))^2 + 0.0462(S_e(G)) + 64.948$$
$$DHVAP = 0.0001(S_e(G))^2 + 0.0257(S_e(G)) + 7.9323$$
$$AF = -5\times10^{-5}(S_e(G))^2 + 0.0081(S_e(G)) + 0.1041$$

Properties	R	F	SE	P-value	Sig.F
$E_\pi(HMO)$	0.9704	419.4162	1.4289	5.07818×10^{-06}	3.75668×10^{-16}
$E_\pi(PAHs)$	0.9757	147.9674	1.6341	0.00588732	3.18907×10^{-15}
MP	0.7616	22.7792	64.5859	0.4243	6.09256×10^{-07}
C	0.7355	20.6293	90.7766	0.6214	1.20538×10^{-06}
PO	0.8501	45.5789	4.8470	0.0003	1.79965×10^{-10}
FP	0.9307	113.1598	25.9114	0.5345	5.25631×10^{-16}
MW	0.9065	62.5738	32.7408	0.0602	2.76741×10^{-12}
BP	0.8579	48.8134	59.4173	0.0018	7.50131×10^{-11}
MR	0.9598	204.6083	6.8616	0.0071	4.87843×10^{-20}
MV	0.8323	39.6569	25.7542	8.47209×10^{-05}	1.01032×10^{-09}
S	0.8274	16.2889	2.7003	0.0029	0.00017
HVAP	0.6318	4.9828	1.6720	9.58476×10^{-06}	0.0219
DHVAP	0.7135	7.7756	0.2859	0.0003	0.00482
AF	0.8799	25.7094	0.0179	0.3447	1.42396×10^{-05}

Table 5: Statistical parameters value for studied properties

5. Conclusion

In this paper, we computed the eccentric Sombor index for several standard graphs such as cycle graph, complete graph, complete bipartite graph, star graph, wheel graph and path graph. Further, we extend this work to determine the eccentric Sombor index of thorn graphs, namely thorn complete graph, thorn complete bipartite graph, thorn ring, thorn star, thorn rod and thorn path graph. Moreover, we discussed the chemical applicability of eccentric Sombor index by performing correlation analysis between the eccentric Sombor index values of certain hetero molecules and their total π-electron energy. In addition, the eccentric Sombor index values of some selected PAHs are also correlated with their total π-electron energy. The correlation results indicate a very strong correlation between the eccentric Sombor index and the total π-electron energy. Furthermore, we investigate the Correlation analysis between eccentric Sombor index of certain PAHs and Octane isomers with their physicochemical properties. The comparitive study reveals that eccentric Sombor index has high chemical applicability, but HVAP have a weak correlation with eccentric Sombor index.We also compute the regression statistics for this correlation analysis, which further demonstrate the chemical applicability of this index. The authors would like to thank the referees for their valuable comments and suggestions, which helped improve the quality and clarity of this paper.

6. Acknowledgements

The authors would like to thank the referees for their valuable comments and suggestions, which helped improve the quality and clarity of this paper.

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