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Research Paper

AN ELLIPTIC-ECCENTRIC SOMBOR INDEX OF A GRAPH AND ITS CHEMICAL APPLICABILITIES

Neelakantappa Harish[1], Channabasappa Nandeesh Kumar[2] and Basavaraju Chaluvaraju[1,*]

[1]Department of Mathematics, Bangalore University, Jnana Bharathi Campus, Bangalore, India, harish.jaga16@gmail.com

[2]Department of Mathematics, R. V. College of Engineering, R. V. Vidyaniketan, Bangalore, India, nandeeshkumarc@rvce.edu.in

[1] Department of Mathematics, Bangalore University, Jnana Bharathi Campus, Bangalore, India, bchaluvaraju@gmail.com

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ABSTRACT

An elliptic Sombor index of a graph was introduced by Gutman et al., [14]. Based on their work, in this paper we initiated the distance based graphical indices called an elliptic-eccentric Sombor index of graphs. Here, we compute the exact values of a certain class of graphs. Also, some bounds and characterizations in terms order, size, degrees, radius, diameter and other graphical indices are obtained. Further, we obtained the comparative analysis of molecular graph of Heptane isomers.

1. INTRODUCTION

1.1. **Fundamental graph notions:** In this paper, we assumed all graphs are finite and simple connected graph. A graph $G = (V(G), E(G))$, is a simple connected graph, that is, no loops and no multiedges. As usual, we denotes the order and size of the graphs are $n = |V(G)|$ and $m = |E(G)|$ of a graph G. The number of vertices are adjacent u is the degree

$*$ Address correspondence to B. Chaluvaraju; Department of Mathematics, Bangalore University, Jnana Bharathi Campus, Bangalore -560 056, India, E-mail: bchaluvaraju@gmail.com.

of u and is represented by $d_G(u)$. In the same way, the minimum and maximum degree of u are represented by $\delta(G) = \delta$ and $\Delta(G) = \Delta$, respectively. A graph G is a r-regular graph with $\delta = r = \Delta$ for all $u \in V(G)$. The distance $d(u, v)$ between any two vertices u and v in a graph G is the length of (number of edges in) the shortest path connecting them. The eccentricity of a vertex u in a graph G is the length of the longest distance between any two pair of vertices, that is $\varepsilon_G(u)$. The value of maximum eccentricity among the vertices called diameter, $diam(G)$ of G. The value of minimum eccentricity among all the vertices called radius $rad(G)$ of G. Hence, $rad(G) \leq \varepsilon_G(u) \leq diam(G)$ for every $u \in V(G)$. For more graph theoretic terminology not given here, the reader is referred to [9, 19].

1.2. **Elements of Chemical graphs:** Graphical indices are indeed topological indices / molecular descriptors that provide quantitative information about the molecular structure of chemical compounds. These descriptor indices are derived from the graph theoretic principles applied to molecular graphs, where atoms are represented as vertices and bonds as edges. These indices are useful in various areas of chemistry, bio-chemistry and drug design because they encode structural information that correlates with molecular properties such as reactivity, biological activity, and physico-chemical properties such as QSPR / QSAR / QSTR studies. For more information on chemical graph we refer to [4, 5].

1.3. **Degree based graphical indices:** Here, we can take some of the degree based graphical indices are as shown in Table 1. In 2024, Gutman et al., [14] was introduced the vertex

Graphical indices	Mathematical Representation
First Zagreb index, [15]	$M_1(G) = \sum_{uv \in E(G)} d_G(u) + d_G(v)$
Second Zagreb index, [15]	$M_2(G) = \sum_{uv \in E(G)} d_G(u).d_G(v)$
Forgotten index, [12]	$F(G) = \sum_{uv \in E(G)} d_G^2(u) + d_G^2(v)$
Sombor index, [16]	$SO(G) = \sum_{u,v \in E(G)} \sqrt{d_G^2(u) + d_G^2(v)}.$

Table 1. Degree based graphical indices and its mathematical representation.

degree-based elliptic Sombor index of a graph G and is defined as

$$ESO(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))\sqrt{d_G^2(u) + d_G^2(v)}.$$

For more details on the elliptic Sombor index, we refer to [10, 17, 23, 24, 30, 31, 34] and mathematical properties and their application of other graphical indices, we refer to [20, 21, 25, 29].

1.4. **Eccentricity based graphical indices.** In 1997, Sharma et al., [32] introduced the eccentric-based graphical indices. Here, we used some of the eccentricity based families of graphical indices are as shown in Table 2. For more information on many eccentricity-based graphical indices are in [1, 2, 3, 7, 11, 13, 18, 27, 37, 38].

Graphical indices	Mathematical Representation
first Zagreb eccentricity index, [36]	${}^{\varepsilon}M_1(G) = \sum_{uv\in E(G)} \varepsilon_G(u) + \varepsilon_G(v)$
second Zagreb eccentricity index, [36]	${}^{\varepsilon}M_2(G) = \sum_{uv\in E(G)} \varepsilon_G(u)\,\varepsilon_G(v)$
eccentricity Forgotten index, [28]	${}^{\varepsilon}F(G) = \sum_{uv\in E(G)} \varepsilon_G^2(u) + \varepsilon_G^2(v)$
eccentricity Harmonic index, [33]	${}^{\varepsilon}H(G) = \sum_{uv\in E(G)} \frac{2}{\varepsilon_G(u) + \varepsilon_G(v)}$

Table 2. Eccentricity based graphical indices and its mathematical representation.

In 2021 [22], Kulli initiated the eccentric Sombor index (fourth Sombor index) of a graph G and is defined as

$$(1.1)\qquad {}^{\varepsilon}SO(G) = \sum_{uv\in E(G)} \sqrt{\varepsilon_G^2(u) + \varepsilon_G^2(v)}.$$

In this paper, we introduced the new eccentricity based graphical index called as an Elliptic-Eccentric Sombor index of a graph G, and is defined as

$$(1.2)\qquad {}^{\varepsilon}ES(G) = \sum_{uv\in E(G)} (\varepsilon_G(u) + \varepsilon_G(v))\sqrt{\varepsilon_G^2(u) + \varepsilon_G^2(v)}.$$

Obviously, the equation (1.1) and equation (1.2) can be expressed as

$$ {}^{\varepsilon}SO(G) = \sum_{uv\in E(G)} \sqrt{\varepsilon_G^2(u) + \varepsilon_G^2(v)}$$

$$ {}^{\varepsilon}SO(G) = \sum_{uv\in E(G)} \sqrt{(n - d_G(u))^2 + (n - d_G(v))^2}$$

$$(1.3)\qquad {}^{\varepsilon}SO(G) = \sum_{uv\in E(G)} \sqrt{2n^2 + d_G^2(u) + d_G^2(v) - 2n(d_G(u) + d_G(v))}.$$

and

$$(1.4)\qquad {}^{\varepsilon}ES(G) = \sum_{uv\in E(G)} (2n-(d_G(u)+d_G(v)))\sqrt{2n^2 + d_G^2(u) + d_G^2(v) - 2n(d_G(u) + d_G(v))}.$$

2. Some specific classes of graphs

Proposition 2.1. *Let K_n be a complete graph with $n \geq 2$. Then*

$$ {}^{\varepsilon}ES(K_n) = \sqrt{2}n(n-1).$$

Proof. Let K_n be a complete graph with $n \geq 2$. If the eccentricity of each vertices in K_n are $\varepsilon_G(u) = 1$, then

$$\begin{aligned} {}^{\varepsilon}ES(K_n) &= \sum_{uv\in E(G)} (\varepsilon_{K_n}(u) + \varepsilon_{K_n}(v))\sqrt{\varepsilon_{K_n}^2(u) + \varepsilon_{K_n}^2(v)}. \\ &= \frac{n(n-1)}{2}[(1+1)\sqrt{1+1}]. \\ &= \sqrt{2}n(n-1). \end{aligned}$$

□

Proposition 2.2. *Let C_n be a cycle with $n \geq 3$. Then*

$$^{\varepsilon}ES(C_n) = \begin{cases} \dfrac{n^3}{\sqrt{2}}, & \text{if } n \text{ is even} \\ \dfrac{n(n-1)^2}{\sqrt{2}}, & \text{if } n \text{ is odd.} \end{cases}$$

Proof. Let C_n be a cycle graph with $n \geq 3$. We have

Case 1. If n is even, then the eccentricity of each vertex $\varepsilon_{C_n}(u) = \frac{n}{2}$, we have

$$\begin{aligned} ^{\varepsilon}ES(C_n) &= \sum_{uv \in E(C_n)} (\varepsilon_{C_n}(u) + \varepsilon_{C_n}(v)) \sqrt{\varepsilon^2_{C_n}(u) + \varepsilon^2_{C_n}(v)} \\ &= n\left[\left(\frac{n}{2} + \frac{n}{2}\right)\sqrt{\frac{n^2}{4} + \frac{n^2}{4}}\right]. \\ &= \frac{n^3}{\sqrt{2}}. \end{aligned}$$

Case 2. If n is odd, then the eccentricity of each vertex $\varepsilon_{C_n}(v) = \frac{n-1}{2}$. Therefore

$$\begin{aligned} ^{\varepsilon}ES(C_n) &= \sum_{uv \in E(C_n)} (\varepsilon_{C_n}(u) + \varepsilon_{C_n}(v)) \sqrt{\varepsilon^2_{C_n}(u) + \varepsilon^2_{C_n}(v)} \\ &= n\left[\left(\frac{n-1}{2} + \frac{n-1}{2}\right)\sqrt{\left(\frac{n-1}{2}\right)^2 + \left(\frac{n-1}{2}\right)^2}\right]. \\ &= \frac{n(n-1)^2}{\sqrt{2}}. \end{aligned}$$

□

Proposition 2.3. *Let W_n be a wheel graph with $n \geq 5$. Then*

$$^{\varepsilon}ES(W_n) = (n-1)[3\sqrt{5} + 8\sqrt{2}].$$

Proof. Let $W_n = K_1 + C_{n-1}$ be a wheel graph with $n \geq 5$. If the eccentricity of center vertex in W_n is $\varepsilon_{W_n}(v_1) = 1$ and $\varepsilon_{W_n}(v_i)$, for $i = 2, 3, 4, \ldots$, we have

$$\begin{aligned} ^{\varepsilon}ES(W_n) &= \sum_{uv \in E(W_n)} (\varepsilon_{W_n}(u) + \varepsilon_{W_n}(v)) \sqrt{\varepsilon^2_{W_n}(u) + \varepsilon^2_{W_n}(v)} \\ &= (n-1)\left[(1+2)\sqrt{1^2 + 2^2} + (2+2)\sqrt{2^2 + 2^2}\right]. \\ &= (n-1)[3\sqrt{5} + 8\sqrt{2}]. \end{aligned}$$

□

Proposition 2.4. *Let $K_{t,s}$ be a complete bipartite graph. Then*

$$^{\varepsilon}ES(K_{t,s}) = \begin{cases} 8\sqrt{2}\, t\, s, & \text{if } t,\ s > 1 \\ 3\sqrt{5}(s-1), & \text{if } t=1 \text{ and } s > 1. \end{cases}$$

Proof. Let $K_{t,s}$ be a complete bipartite graph. We have

Case 1. If the eccentricity of u_0 and u_1 is 2 and the eccentricity of u_i's is 2.

$$\begin{aligned} ^{\varepsilon}ES(K_{t,s}) &= \sum_{uv \in E(K_{t,s})} (\varepsilon_{K_{t,s}}(u) + \varepsilon_{K_{t,s}}(v)) \sqrt{\varepsilon^2_{K_{t,s}}(u) + \varepsilon^2_{K_{t,s}}(v)} \\ &= ts[(2+2)\sqrt{2^2 + 2^2} + (2+2)\sqrt{2^2 + 2^2}]. \\ &= 8\sqrt{2}\, t\, s. \end{aligned}$$

Case 2. Let $K_{1,s}$ be a star graph with $s \geq 2$. If the eccentricity of $u_0 = 1$ and $u_i = 2$ for

$i = 1, 2, 3, \ldots$, we have

$$^{\varepsilon}ES(K_{1,s}) = \sum_{uv \in E(K_{1,s})} (\varepsilon_{K_{1,s}}(u) + \varepsilon_{K_{1,s}}(v)) \sqrt{\varepsilon^2_{K_{1,s}}(u) + \varepsilon^2_{K_{1,s}}(v)}.$$
$$= (s-1)[(1+2)\sqrt{1^2+2^2}].$$
$$= 3\sqrt{5}(s-1). \qquad \square$$

Proposition 2.5. *Let $DS_{t,t}$ be a double star graph with $n = 2(t+1)$ vertices and $t \geq 2$. Then*

$$^{\varepsilon}ES(DS_{t,t}) = 10t\sqrt{13} + 8\sqrt{2},$$

where $DS_{t,t}$ is a double star, which is obtained by joining the apex vertices of two copies of star $S_{1,t}$ by an edge.

Proof. Let $DS_{t,t}$ be a double star graph with $n = 2(t+1)$ vertices and $t \geq 2$. If u and v are adjacent to every other u_i's, for $i = 1, 2, 3, \ldots$, in $DS_{t,t}$, then eccentricity of u and v is 2 and the eccentricity of u_i's is 3.

$$^{\varepsilon}ES(DS_{t,t}) = \sum_{uv \in E(DS_{t,t})} (\varepsilon_{DS_{t,t}}(u) + \varepsilon_{DS_{t,t}}(v)) \sqrt{\varepsilon^2_{DS_{t,t}}(u) + \varepsilon^2_{DS_{t,t}}(v)}$$
$$= t\ [(2+3)\sqrt{2^2+3^2}] + (2+2)\sqrt{2^2+2^2}.$$
$$= 10t\sqrt{13} + 8\sqrt{2}. \qquad \square$$

Proposition 2.6. *Let F_n be a fan graph with $n \geq 5$. Then*

$$^{\varepsilon}ES(F_n) = 3(n-1)\sqrt{5} + 8(n-2)\sqrt{2},$$

where $F_n = K_1 + P_{n-1}$ is the fan graph defined the graph is obtained by joining all the vertices of path P_n to a new vertex named center.

Proof. Let F_n be a fan graph with $n \geq 5$. If u_0 is adjacent to every other u_i's and u_i is adjacent to every other u_{i+1} vertices for $i = 1, 2, 3, \ldots$, in F_n, then the eccentricity of $u_0 = 1$ and the eccentricity of $u_i = 2$.

$$^{\varepsilon}ES(F_n) = \sum_{uv \in E(F_n)} (\varepsilon_{F_n}(u) + \varepsilon_{F_n}(v)) \sqrt{\varepsilon^2_{F_n}(u) + \varepsilon^2_{F_n}(v)}$$
$$= (n-1)[(1+2)\sqrt{1^2+2^2} + 2(n-2)(2+2)\sqrt{2^2+2^2}].$$
$$= 3(n-1)\sqrt{5} + 8(n-2)\sqrt{2}. \qquad \square$$

Proposition 2.7. *Let FS_n be a friendship graph with $n \geq 5$. Then*

$$^{\varepsilon}ES(FS_n) = (n-3)[6\sqrt{5} + 8\sqrt{2}],$$

where FS_n is the friendship graph defined a graph in which every two distinct vertices have exactly one common adjacent vertex.

Proof. Let FS_n be a friendship graph with $n \geq 2$. If u_0 is adjacent to every other vertex u_i's and u_i is adjacent to every other vertex u_{i+1} for $i = 1, 2, 3, \ldots$ in FS_n, then the eccentricity of $u_0 = 1$ and the eccentricity of $u_i = 2$.

$$^{\varepsilon}ES(FS_n) = \sum_{uv \in E(FS_n)} (\varepsilon_{FS_n}(u) + \varepsilon_{FS_n}(v))\sqrt{\varepsilon^2_{FS_n}(u) + \varepsilon^2_{FS_n}(v)}$$
$$= (n-3)[(1+2)\sqrt{1^2+2^2} + (2+2)\sqrt{2^2+2^2}].$$
$$= (n-3)[3\sqrt{5} + 8\sqrt{2}].$$ □

3. BOUNDS INTERMS OF ORDER, SIZE, MINIMUM / MAXIMUM DEGREE, RADIUS AND DIAMETER

To prove next couple of results, we make use of the following Lemma.

Lemma 3.1. [6],[8] *For any connected graph G with $n \geq 2$,*

(i) $rad(G) \leq \varepsilon_G(u) \leq diam(G)$.
(ii) $(n - \Delta) \leq \varepsilon_G(u) \leq (n - \delta)$.

Theorem 3.2. *For any connected graph G,*

$$2\sqrt{2}\, m\, rad^2(G) \leq \ ^{\varepsilon}ES(G) \leq 2\sqrt{2}\, m\, diam^2(G).$$

Proof. For any connected graph G,

$$rad(G) \leq \varepsilon_G(u) \leq diam(G).$$
$$2rad^2(G) \leq \{\varepsilon^2_G(u) + \varepsilon^2_G(v)\} \leq 2diam^2(G).$$
$$\sqrt{2}rad(G) \leq \sqrt{\varepsilon^2_G(u) + \varepsilon^2_G(v)} \leq \sqrt{2}diam(G). \tag{3.1}$$
$$rad(G) \leq \varepsilon_G(u) \leq diam(G).$$
$$2rad(G) \leq \varepsilon_G(u) + \varepsilon_G(v) \leq 2diam(G). \tag{3.2}$$

Multipliying equations (3.1) and (3.2), we have

$$2\sqrt{2}rad^2(G) \leq \big(\varepsilon_G(u) + \varepsilon_G(v)\big)\sqrt{\varepsilon^2_G(u) + \varepsilon^2_G(v)} \leq 2\sqrt{2}diam^2(G).$$

The above inequality satisfies for each edge $uv \in E(G)$ and apply summation to all over the inequalities, we have

$$\sum_{uv \in E(G)} 2\sqrt{2}\, rad^2(G) \leq \sum_{uv \in E(G)} \big(\varepsilon_G(u) + \varepsilon_G(v)\big)\sqrt{\varepsilon^2_G(u) + \varepsilon^2_G(v)}$$
$$\leq \sum_{uv \in E(G)} 2\sqrt{2}\, diam^2(G).$$

Therefore, $$2\sqrt{2}\, m\, rad^2(G) \leq \ ^{\varepsilon}ES(G) \leq 2\sqrt{2}\, m\, diam^2(G).$$ □

Theorem 3.3. *For any connected graph G,*

$$2\sqrt{2}m(n-\Delta)^2 \leq \ ^{\varepsilon}ES(G) \leq 2\sqrt{2}m(n-\delta)^2.$$

Further, the inequality holds if and only if G is regular.

Proof. For any connected graph G,

$$(n - \Delta) \leq \varepsilon_G(u) \leq (n - \delta).$$

$$2(n-\Delta)^2 \leq \{\varepsilon_G^2(u)+\varepsilon_G^2(v)\} \leq 2(n-\delta)^2.$$

$$\sqrt{2}(n-\Delta) \leq \sqrt{\varepsilon_G^2(u)+\varepsilon_G^2(v)} \leq \sqrt{2}(n-\delta). \tag{3.3}$$

$$(n-\Delta) \leq \varepsilon_G(u) \leq (n-\delta).$$

$$2(n-\Delta) \leq \varepsilon_G(u)+\varepsilon_G(v) \leq 2(n-\delta). \tag{3.4}$$

Multipliying equations (3.3) and (3.4), we have

$$2\sqrt{2}(n-\Delta)^2 \leq \big(\varepsilon_G(u)+\varepsilon_G(v)\big)\sqrt{\varepsilon_G^2(u)+\varepsilon_G^2(v)} \leq 2\sqrt{2}(n-\delta)^2.$$

The above inequality satisfies for each edge $uv \in E(G)$ and apply summation to all over inequalities, we have

$$\sum_{uv\in E(G)} 2\sqrt{2}\,(n-\Delta)^2 \leq \sum_{uv\in E(G)} \big(\varepsilon_G(u)+\varepsilon_G(v)\big)\sqrt{\varepsilon_G^2(u)+\varepsilon_G^2(v)}$$

$$\leq \sum_{uv\in E(G)} 2\sqrt{2}\,(n-\delta)^2.$$

Therefore, $2\sqrt{2}m(n-\Delta)^2 \leq {}^{\varepsilon}ES(G) \leq 2\sqrt{2}m(n-\delta)^2.$

Further, the inequality holds if and only if G is regular. □

4. BOUNDS INTERMS OF OTHER ECCENTRIC BASED GRAPHICAL INDICES

Theorem 4.1. *Let G be a connected graph. Then*

$$^{\varepsilon}ES(G) \leq {}^{\varepsilon}M_1(G)\,{}^{\varepsilon}SO(G).$$

Proof. Let G be a connected graph. Then

$$^{\varepsilon}ES(G) = \sum_{uv\in E(G)} \big(\varepsilon_G(u)+\varepsilon_G(v)\big)\sqrt{\varepsilon_G^2(u)+\varepsilon_G^2(v)}.$$

$$\leq \sum_{uv\in E(G)} \big(\varepsilon_G(u)+\varepsilon_G(v)\big) \sum_{uv\in E(G)} \sqrt{\varepsilon_G^2(u)+\varepsilon_G^2(v)}.$$

Therefore, $^{\varepsilon}ES(G) \leq {}^{\varepsilon}M_1(G)\,{}^{\varepsilon}SO(G).$ □

Theorem 4.2. *Let G be a connected graph. Then*

$$2rad(G)\,{}^{\varepsilon}SO(G) \leq {}^{\varepsilon}ES(G) \leq 2diam(G)\,{}^{\varepsilon}SO(G).$$

Proof. Let G be a connected graph. Then

$$^{\varepsilon}ES(G) = \sum_{uv\in E(G)} \big(\varepsilon_G(u)+\varepsilon_G(v)\big)\sqrt{\varepsilon_G^2(u)+\varepsilon_G^2(v)}.$$

$$\leq 2diam(G) \sum_{uv\in E(G)} \sqrt{\varepsilon_G^2(u)+\varepsilon_G^2(v)}.$$

$$\leq 2\; diam(G)\,{}^{\varepsilon}SO(G).$$

Similarly, we prove the lower bound.

$$^{\varepsilon}ES(G) \geq 2rad(G)\,{}^{\varepsilon}SO(G).$$

Hence, the proof complete. □

Theorem 4.3. *Let G be a connected graph. Then*

$$\sqrt{2}\, rad(G)\, {}^{\varepsilon}M_1(G) \leq {}^{\varepsilon}ES(G) \leq \sqrt{2}\, diam(G)\, {}^{\varepsilon}M_1(G).$$

Proof. Let G be a connected graph. Then

$$\begin{aligned} \varepsilon ES(G) &= \sum_{uv\in E(G)} \big(\varepsilon_G(u)+\varepsilon_G(v)\big)\sqrt{\varepsilon_G^2(u)+\varepsilon_G^2(v)}. \\ &\leq \sqrt{diam^2(G)+diam^2(G)} \sum_{uv\in E(G)} \big(\varepsilon_G(u)+\varepsilon_G(v)\big). \\ &\leq \sqrt{2}\, diam(G)\, {}^{\varepsilon}M_1(G). \end{aligned}$$

Similarly, we prove the lower bound.

$${}^{\varepsilon}ES(G) \geq \sqrt{2}\, rad(G)\, {}^{\varepsilon}M_1(G).$$

Thus, the desired result follows. □

Corollary 4.1. *Let G be a connected graph. Then*

(i) $2(n-\Delta)\, {}^{\varepsilon}SO(G) \leq {}^{\varepsilon}ES(G) \leq 2(n-\delta)\, {}^{\varepsilon}SO(G)$

(ii) $\sqrt{2}(n-\Delta)\, {}^{\varepsilon}M_1(G) \leq {}^{\varepsilon}ES(G) \leq \sqrt{2}(n-\delta)\, {}^{\varepsilon}M_1(G)$.

Further, the inequality holds if and only if G is regular.

Proof. By Theorem 4.2, Theorem 4.3 and Lemma 3.1 (i) and (ii) we obtain the desired results. □

Theorem 4.4. *Let G be a connected graph. Then*

$${}^{\varepsilon}M_2^2(G)\frac{2\sqrt{2}}{diam^2(G)} \leq {}^{\varepsilon}ES(G) \leq {}^{\varepsilon}M_2^2(G)\frac{2\sqrt{2}}{rad^2(G)}.$$

Proof. Let G be a connected graph. Then

$$\begin{aligned} {}^{\varepsilon}ES(G) &= \sum_{uv\in E(G)} \big(\varepsilon_G(u)+\varepsilon_G(v)\big)\sqrt{\varepsilon_G^2(u)+\varepsilon_G^2(v)}. \\ &\geq \sum_{uv\in E(G)} \big(\varepsilon_G(u).\varepsilon_G(v)\big)^2\Big[\frac{1}{\varepsilon_G(u)}+\frac{1}{\varepsilon_G(v)}\Big]\sqrt{\frac{1}{\varepsilon_G^2(u)}+\frac{1}{\varepsilon_G^2(v)}} \\ &\geq \frac{2\sqrt{2}}{diam^2(G)}\, {}^{\varepsilon}M_2^2(G). \end{aligned}$$

Similarly, we prove the upper bound

$${}^{\varepsilon}ES(G) \leq \frac{2\sqrt{2}}{rad^2(G)}\, {}^{\varepsilon}M_2^2(G).$$

Therefore,

$${}^{\varepsilon}M_2^2(G)\frac{2\sqrt{2}}{diam^2(G)} \leq {}^{\varepsilon}ES(G) \leq {}^{\varepsilon}M_2^2(G)\frac{2\sqrt{2}}{rad^2(G)}.$$

Hence, the proof complete. □

Theorem 4.5. *Let G be a connected graph. Then*

$$\frac{2}{diam(G)}\, {}^{\varepsilon}M_2(G)\, {}^{\varepsilon}SO(G) \leq {}^{\varepsilon}ES(G) \leq \frac{2}{rad(G)}\, {}^{\varepsilon}M_2(G)\, {}^{\varepsilon}SO(G).$$

Proof. By Theorem4.4, we obtain the desired result. □

Corollary 4.2. *Let G be a connected graph. Then*

(i) ${}^{\varepsilon}M_2^2(G)\dfrac{2\sqrt{2}}{(n-\delta)^2} \leq \varepsilon ES(G) \leq {}^{\varepsilon}M_2^2(G)\dfrac{2\sqrt{2}}{(n-\Delta)^2}$.

(ii) $\dfrac{2}{(n-\delta)}\, {}^{\varepsilon}M_2(G)\, {}^{\varepsilon}SO(G) \leq {}^{\varepsilon}ES(G) \leq \dfrac{2}{(n-\Delta)}\, {}^{\varepsilon}M_2(G)\, {}^{\varepsilon}SO(G)$.

Further, the inequality holds if and only if G is regular.

Proof. By Theorem 4.4, Theorem 4.5 and Lemma 3.1 (ii), we obtain the desired results. □

Theorem 4.6. *Let G be a connected graph. Then*

$$^{\varepsilon}ES(G) \leq \frac{diam(G) + rad(G)}{diam(G)\; rad(G)}\, {}^{\varepsilon}M_2(G)\, {}^{\varepsilon}SO(G).$$

Proof. Let G be a connected graph. Then

$$\begin{aligned} {}^{\varepsilon}ES(G) &= \sum_{uv\in E(G)} \big(\varepsilon_G(u) + \varepsilon_G(v)\big)\sqrt{\varepsilon_G^2(u) + \varepsilon_G^2(v)}. \\ &= \sum_{uv\in E(G)} \big(\varepsilon_G(u).\varepsilon_G(v)\big)\left[\frac{\varepsilon_G(u) + \varepsilon_G(v)}{\varepsilon_G(u).\varepsilon_G(v)}\right]\sqrt{\varepsilon_G^2(u) + \varepsilon_G^2(v)} \\ &\leq \frac{diam(G) + rad(G)}{diam(G) rad(G)}\, {}^{\varepsilon}M_2(G)\, {}^{\varepsilon}SO(G). \end{aligned}$$

Hence, the result. □

Lemma 4.7. *(Chebyschev's inequality) Let a_i and b_i are real numbers. Then*

$$n\sum_{i=1}^{n} a_i b_i \geq \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i,$$

with equality holds if and only if $a_1 = a_2 = ... = a_n$ or $b_1 = b_2 = ... = b_n$.

Lemma 4.8. *Root mean square inequalities are Arithmatic Mean and Quadratic Mean (AM-QM). For positive real number $a_1, a_2, ..., a_n$, we have*

$$\frac{\sum_{i=1}^{n} a_i}{n} \leq \sqrt{\frac{\sum_{i=1}^{n} a_i^2}{n}}.$$

Theorem 4.9. *Let G be a connected graph. Then*

$$^{\varepsilon}ES(G) \geq \frac{1}{n}\, {}^{\varepsilon}M_1(G)\, {}^{\varepsilon}SO(G).$$

Proof. Let $a_i = \varepsilon_G(u_i) + \varepsilon_G(v_i)$ and $b_i = \sqrt{\varepsilon_G^2(u_i) + \varepsilon_G^2(v_i)}$ for $i = 1, 2, 3, ...,$ we have

$$^{\varepsilon}ES(G) = \sum_{uv\in E(G)} \big(\varepsilon_G(u_i) + \varepsilon_G(v_i)\big)\sqrt{\varepsilon_G^2(u_i) + \varepsilon_G^2(v_i)}.$$

By Lemma 4.7, we have

$$n\sum_{i=1}^{n} \big(\varepsilon_G(u_i) + \varepsilon_G(v_i)\big)\sqrt{\varepsilon_G^2(u_i) + \varepsilon_G^2(v_i)}$$

$$\geq \sum_{i=1}^{n} \varepsilon_G(u_i) + \varepsilon_G(v_i) \sum_{i=1}^{n} \sqrt{\varepsilon_G^2(u_i) + \varepsilon_G^2(v_i)}.$$

$$\geq \frac{1}{n}\, {}^{\varepsilon}M_1(G)\, {}^{\varepsilon}SO(G).$$

Hence, the proof. □

Theorem 4.10. *Let G be a connected graph. Then*

$$^{\varepsilon}ES(G) \leq \sqrt{n}\, ^{\varepsilon}ES(G).$$

Proof. Let $a_i = \big(\varepsilon_G(u_i) + \varepsilon_G(v_i)\big)\sqrt{\varepsilon_G^2(u_i) + \varepsilon_G^2(v_i)}$, for $i = 1, 2, 3, \cdots$. By Lemma 4.8, we have

$$\frac{\sum_{i=1}^{n} \big(\varepsilon_G(u_i) + \varepsilon_G(v_i)\big)\sqrt{\varepsilon_G^2(u_i) + \varepsilon_G^2(v_i)}}{n} \leq \sqrt{\frac{\Big(\sum_{i=1}^{n} \big(\varepsilon_G(u_i) + \varepsilon_G(v_i)\big)\sqrt{\varepsilon_G^2(u_i) + \varepsilon_G^2(v_i)}\Big)^2}{n}}.$$

Therefore, $\quad ^{\varepsilon}ES(G) \leq \sqrt{n}\, ^{\varepsilon}ES(G).$ □

Theorem 4.11. *Let G be a connected graph. Then*

$$\frac{rad(G)}{\sqrt{2}}\, ^{\varepsilon}M_1^2(G)\, ^{\varepsilon}H(G) \leq\, ^{\varepsilon}ES(G) \leq \frac{diam(G)}{\sqrt{2}}\, ^{\varepsilon}M_1^2(G)\, ^{\varepsilon}H(G).$$

Proof. Let G be a connected graph. Then

$$\begin{aligned} ^{\varepsilon}ES(G) &= \sum_{uv \in E(G)} \big(\varepsilon_G(u) + \varepsilon_G(v)\big)\sqrt{\varepsilon_G^2(u) + \varepsilon_G^2(v)}. \\ &= \sum_{uv \in E(G)} \frac{\big[\varepsilon_G(u) + \varepsilon_G(v)\big]^2}{2} \frac{2}{\varepsilon_G(u) + \varepsilon_G(v)} \sqrt{\varepsilon_G^2(u_i) + \varepsilon_G^2(v_i)}. \\ &\leq \frac{1}{2}\, ^{\varepsilon}M_1^2(G)\, ^{\varepsilon}H(G)\, \sqrt{2} diam(G). \\ &\leq \frac{diam(G)}{\sqrt{2}}\, ^{\varepsilon}M_1^2(G)\, ^{\varepsilon}H(G). \end{aligned}$$

Similarly, we prove the lower bound

$$^{\varepsilon}ES(G) \geq \frac{rad(G)}{\sqrt{2}}\, ^{\varepsilon}M_1^2(G)\, ^{\varepsilon}H(G).$$

Therefore, we obtain the desired result. □

Corollary 4.3. *Let G be a connected graph. Then*

$$\frac{(n-\Delta)}{\sqrt{2}}\, ^{\varepsilon}M_1^2(G)\, ^{\varepsilon}H(G) \leq\, ^{\varepsilon}ES(G) \leq \frac{(n-\delta)}{\sqrt{2}}\, ^{\varepsilon}M_1^2(G)\, ^{\varepsilon}H(G).$$

Further, the inequality holds if and only if G is regular.

Theorem 4.12. *Let G be a connected graph. Then*

$$2rad^2(G)\, ^{\varepsilon}H(G)\, ^{\varepsilon}SO(G) \leq\, ^{\varepsilon}ES(G) \leq 2diam^2(G)\, ^{\varepsilon}H(G)\, ^{\varepsilon}SO(G).$$

Proof. By Theorem 4.11, we obtain the desired result. □

Corollary 4.4. *Let G be a connected graph. Then*

$$2(n-\Delta)^2\, ^{\varepsilon}H(G)\, ^{\varepsilon}SO(G) \leq\, ^{\varepsilon}ES(G) \leq 2(n-\delta)^2\, ^{\varepsilon}H(G)\, ^{\varepsilon}SO(G).$$

Further, the inequality holds if and only if G is regular.

Theorem 4.13. *For any connected graph G,*

$$^{\varepsilon}ES(G) \leq \frac{rad(G)+diam(G)}{\sqrt{rad^2(G)+diam^2(G)}}\ ^{\varepsilon}F(G).$$

Proof. For any connected graph G,

$$\begin{aligned} ^{\varepsilon}ES(G) &= \sum_{uv\in E(G)} \big(\varepsilon_G(u)+\varepsilon_G(v)\big)\sqrt{\varepsilon_G^2(u)+\varepsilon_G^2(v)}.\\ &= \sum_{uv\in E(G)} \frac{\varepsilon_G(u)+\varepsilon_G(v)}{\sqrt{\varepsilon_G^2(u)+\varepsilon_G^2(v)}}(\varepsilon_G^2(u)+\varepsilon_G^2(v)).\\ &\leq \frac{rad(G)+diam(G)}{\sqrt{rad^2(G)+diam^2(G)}}\ ^{\varepsilon}F(G). \end{aligned}$$

□

Corollary 4.5. *For any connected graph G,*

$$^{\varepsilon}ES(G) \leq \frac{2mn-(\Delta+\delta)}{\sqrt{2n^2-2n(\Delta+\delta)+\Delta^2+\delta^2}}\ ^{\varepsilon}F(G).$$

Next, we prove a single results we make use of the following definition:

Semi-regular graph: A graph G^* is considered as a semiregular graph, if every vertex in the graph G^* is exactly 2 distance away from the same number of other vertices. If each vertex is 2 distance away from n other vertices, the graph is referred to as n-semiregular.

Theorem 4.14. *For any connected graph G,*

$$^{\varepsilon}ES(G) \leq (2mn - M_1(G))\sqrt{F(G)-2nM_1(G)+2mn^2},$$

more over the inequality holds if and only if $G \cong P_4$ *or* K_4 *or* $(n-1, n-2)$*-semi-regular graph.*

Proof. By using equations (1.2) and (1.4), we have

$$\begin{aligned} ^{\varepsilon}ES(G) &= \sum_{uv\in E(G)} \big(\varepsilon_G(u)+\varepsilon_G(v)\big)\sqrt{\varepsilon_G^2(u)+\varepsilon_G^2(v)}.\\ &= (n-d_G(u)+n-d_G(v)) \sum_{uv\in E(G)} \sqrt{(n-d_G(u))^2+(n-d_G(v))^2}.\\ &\leq (2mn-M_1(G))\sqrt{F(G)-2nM_1(G)+2mn^2}. \end{aligned}$$

Hence, the proof. □

5. Chemical applicabilities for molecular graph of Heptane isomers

In this research work, we use molecular graph of nine heptane isomers. Heptane (C_7H_{16}) is an alkane consisting of seven carbon atoms as shown in Figure 1. It has several isomers, which are compounds with the same molecular formula but different structural arrangements. Heptane can exist as various structural isomers based on how the carbon atoms are connected. These are differ in the number of carbon atoms in the parent chain. The IUPAC names of heptane isomers are n-heptane (G_1), 2-methylhexane (G_2), 3-methylhexane (G_3), 2,2-dimethylpentane (G_4), 2,3-dimethylpentane (G_5), 2,4-dimethylpentane (G_6), 3,3-dimethylpentane (G_7), 3-ethylpentane (G_8) and 2,2,3-trimethylbutane (G_9). As many different isomers of n-heptane are used in organic syntheses and are ingredients of gasoline, rubber solvent naphtha, mixed isomers for use as thinners in paints and coatings, as pure n-heptane for research and development, as a precursor in pharmaceutical manufacturing, and as petroleum mixtures used as fuels. For more details on molecular graph of heptane isomers we refer to [26, 35].

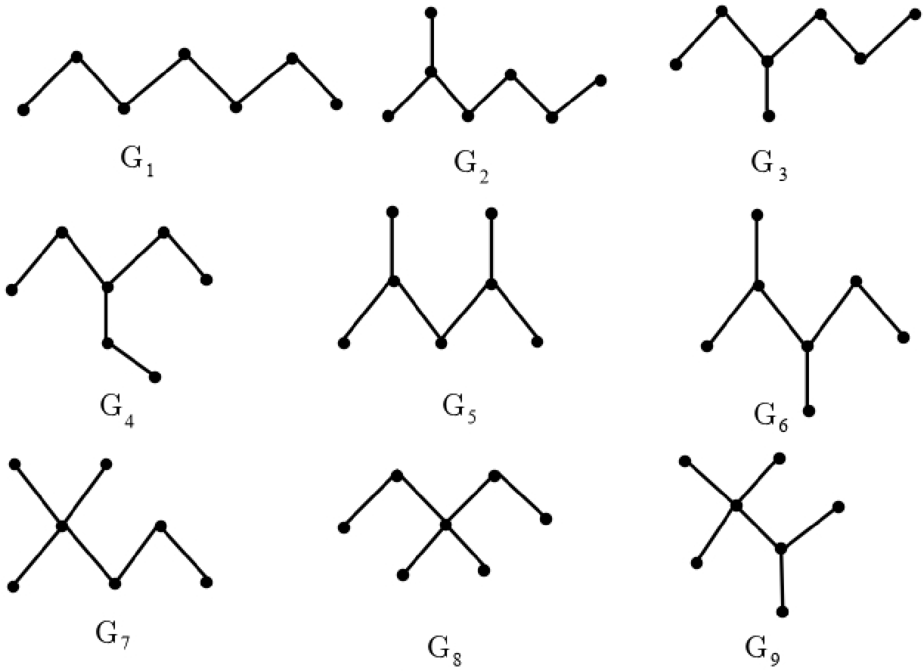

FIGURE 1. Molecular graph of heptane isomers

Heptane isomers	**Eccentricity based graphical indices**				
	${}^{\varepsilon}ES(G_i)$	${}^{\varepsilon}SO(G_i)$	${}^{\varepsilon}M_1(G_i)$	${}^{\varepsilon}M_2(G_i)$	${}^{\varepsilon}F(G_i)$
G_1	357.081	38.426	54	124	254
G_2	268.335	33.451	47	93	191
G_3	245.711	32.048	45	85	175
G_4	159.083	25.816	36	54	114
G_5	176.05	27.214	38	60	126
G_6	159.083	25.816	36	54	114
G_7	176.05	27.214	38	60	126
G_8	142.111	24.422	34	48	102
G_9	101.44	20.856	29	34	73

TABLE 3. The computed values of eccentricity based graphical indices of molecular graphs of heptane isomers

Comparative Analysis: The molecular graph of heptane isomers G_i for $1 \leq i \leq 9$ is compared. By comparing all the isomers n-heptane having more boiling point. The computed values of graphical indices and heptane isomers as shown in the Table 3. From this table we can easily analyse the more or less or equal or frequently changes their values of graphical indices for each isomers. The comparative analysis or graphical representation shows the variations between the graphical indies and heptane isomers are as shown in the Figure 2.

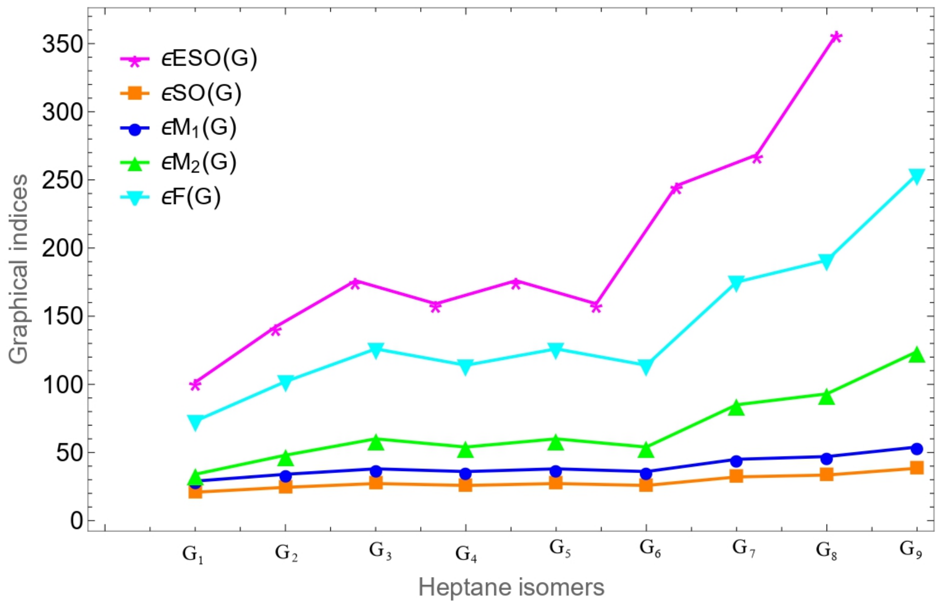

FIGURE 2. Comparative Analysis

By observation of Table 3 and Figure 2 the values of heptane isomers G_4 and G_6 are having the same value and also, G_5 and G_7. The remaining all the heptane isomers G_1, G_2, G_3, G_8 and G_9 are having different values. The ranges of eccentricity based graphical indices are decreasing or increasing their values. It is mathematically represented as

$$^{\varepsilon}ES(G_i) > {}^{\varepsilon}F(G_i) > {}^{\varepsilon}M_2(G_i) > {}^{\varepsilon}M_1(G_i) > {}^{\varepsilon}SO(G_i).$$

6. CONCLUSION AND FUTURE WORK

In this paper, we obtained the exact values for specific class graphs and found some bounds in terms order, size, minimum / maximum degrees, radius, and diameter. Also, the bounds and characterization of the elliptic-eccentric Sombor index and other eccentricity families of graphical indices were found. Finally, we show the relationship between the eccentricity families of graphical indices and molecular graphs of heptane isomers. For the comparative advantages, applications, and mathematical point of view, many questions are suggested by this research, including the following:

1. Find the extremal values and extremal graphs of the elliptic-eccentric Sombor index. Also, characterize the other eccentricity families of graphical indices.
2. Find the values of the elliptic-eccentric Sombor index of chemical graphs / product graph / derived graphs.
3. Determine the bounds and characterization of the elliptic-eccentric Sombor index in relation to other eccentric-based graphical indices.
4. Determine the elliptic-eccentric Sombor index values for the QSPR / QSAR / QSTR Model.

7. Declaration

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