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STRUCTURAL ANALYSIS OF THE STATUS ELLIPTIC SOMBOR INDEX AND ITS CHEMICAL APPLICATIONS TO OCTANE ISOMERS

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Abstract : *In a graph G, the status $\sigma(\alpha)$ of a vertex α is given by $\sigma(\alpha) = \sum_{\beta\in V(G)} d(\alpha,\beta)$, where $V(G)$ represents the vertex set and $d(\alpha,\beta)$ denotes the distance between α and β in G. The status elliptic Sombor index (SESO) is defined as $SESO(G) = \sum_{\alpha\beta\in E(G)} (\sigma(\alpha) + \sigma(\beta))\sqrt{\sigma(\alpha)^2 + \sigma(\beta)^2}$, where $E(G)$ is the edge set of the graph G. In this paper, we investigate the comparative analysis of molecular graphs of octane isomers with status based indices, observing that status elliptic Sombor index attains the highest value among them. Additionally, we establish certain bounds for this index in terms of diameter and other status based indices. Furthermore, we compute exact values of the status elliptic Sombor index for specific graph classes.*

Mathematics Subject Classification (2020): *05C07, 05C12.*

Keywords : *Distance, status of a vertex, elliptic Sombor index, status elliptic Sombor index.*

1 Introduction

Topological indices are numerical numbers that represent a molecule's structural characteristics by taking into account the connections between its atoms. A graph with vertices representing atoms and edges representing covalent bonds can be used to model this. *QSPR* (quantitative structural property-property relation) and *QSAR* (quantitative structure-activity relationship) are mostly computed using these. The primary question in the study of topological indices is whether or not chemical properties can be identified using them. Octane isomers are typically the unique data used in these investigations.

In this paper, we focus on graphs that are connected, finite, and simple. Let G be such a graph, where $E(G)$ and $V(G)$ represent its edge and vertex sets, respectively. The edge connecting two vertices β and α is denoted as $\beta\ \alpha$. The degree of a vertex β, represented as $d(\beta)$, is the number of edges incident to it. The shortest path length between vertices β and α in G is denoted by $d(\beta,\alpha)$. The eccentricity of a vertex β, written as $e(\beta)$, is defined as the greatest distance between β and any other vertex in G. The diameter of G, represented by *diam(G)*, is the maximum eccentricity among all vertices in the graph. The status *or* transmission $\sigma(\alpha)$ of a vertex α is the sum of its distance from every other vertex in $V(G)$. That is

$$\sigma(\alpha) = \sum_{\beta\in V(G)} d(\alpha,\beta).$$

for other graph theoretic terminology, we refer [4, 20].

The total of the distances between each pair of vertices in a connected graph G is its Weiner index$W(G)$[21], that is

$$W(G) = \sum_{\beta,\alpha\in V(G)} d(\beta,\alpha) = \frac{1}{2}\sum_{\beta\in V(G)} \sigma(\beta).$$

In 2016, Ramane and Yalnaik introduced the status connectivity indices [15] of a graph G, defined as

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$$S_1(G) = \sum_{\beta\alpha \in E(G)} [\sigma(\beta) + \sigma(\alpha)], \quad S_2(G) = \sum_{\beta\alpha \in E(G)} \sigma(\beta)\sigma(\alpha).$$

The status Sombor index[7] and F-Status index [8] of a graph G were introduced by Kulli and are defined as

$$SSO(G) = \sum_{\beta\alpha \in E(G)} \sqrt{\sigma(\beta)^2 + \sigma(\alpha)^2}.$$

$$FS(G) = \sum_{\beta\alpha \in E(G)} [\sigma(\beta)^2 + \sigma(\alpha)^2].$$

For more information on other status graphical indices, we refer [3, 12, 13, 14, 17].

In 2024, Gutman *et. al.,*[6] introduced the vertex degree based topological index named as elliptic Sombor index, and defined as

$$ESO(G) = \sum_{\beta\alpha \in E(G)} (d(\beta) + d(\alpha))\sqrt{d(\beta)^2 + d(\alpha)^2}.$$

For more details on the elliptic Sombor index, we refer[5, 9, 10, 16, 19, 18]

Motivated by the works on elliptic Sombor index and above status based indices, very recently, Kulli initiated the Status elliptic Sombor index [11]of a graph G, defined as

$$SESO(G) = \sum_{\beta\alpha \in E(G)} (\sigma(\beta) + \sigma(\alpha))\sqrt{\sigma(\beta)^2 + \sigma(\alpha)^2}.$$

After the introductory section, this paper is organized into four main sections. In Section 2, we investigate the comparative analysis. Section 3 presents the bounds of the status elliptic Sombor index in relation to diameter and various other status-based graphical indices. In section 4, exact values of the status elliptic Sombor index for standard classes of graphs and graphs derived from complete graph are computed.

2 Chemical Applicability

We use molecular graphs of 18 octane isomers in our work. As seen in fig 1., octane (C_8H_{18}) is an alkane with eight carbon atoms. It has many isomers, which are molecules with different structural configurations but the same chemical formula. Depending on how the carbon atoms are joined, octane can exist in a variety of structural isomers. The IUPAC names of octane isomers are n- octane(G_1), 2-methyl heptane (G_2), 3-methyl heptane (G_3), 4-methyl heptane (G_4), 3-ethyl hexane (G_5), 2,2-dimethyl hexane (G_6), 2,3-dimethyl hexane (G_7), 2,4-dimethyl hexane (G_8), 2,5-di methyl hexane (G_9), 3,3-di methyl hexane (G_{10}), 3,4-dimethyl hexane (G_{11}), 2- methyl 3-ethylpentane (G_{12}), 3- methyl 3-ethylpentane (G_{13}), 2,2,3-trimethylpentane (G_{14}), 2,2,4-trimethylpentane (G_{15}), 2,3,3-trimethylpentane (G_{16}), 2,3,4-trimethylpentane (G_{17}) and 2,2,3,3-tetramethylbutane (G_{18}). As many different isomers of n-octane are used in understanding the molecular structure and properties of chemical compounds, developing algorithms for graph analysis and machine learning. Octane isomers are also used as a precursor in pharmaceutical manufacturing and as petroleum mixtures used as fuels.

Comparative Analysis : Here, the molecular graph of octane isomers G_i for $1 \leq i \leq 18$ is compared. The computed values of graphical indices and octane isomers as shown in table 1 From this table, it is observed that the more or less or frequently changes their values of graphical indices for each isomers. The comparative analysis shows the variation between the graphical indices and octane isomers are as shown in the Figure 2. From this figure it is observed that for all octane isomers status elliptic Sombor index gets the highest value and status Sombor index gets the least value compared to all other indices. We can represent this mathematically as

$$SSO(G_i) < S_1(G_i) < S_2(G_i) < FS(G_i) < SESO(G_i) \quad \text{for} \quad 2 \leq i \leq 18.$$

For n-octane, we get

$$SSO(G_1) < S_1(G_1) < FS(G_1) < S_2(G_1) < SESO(G_1).$$

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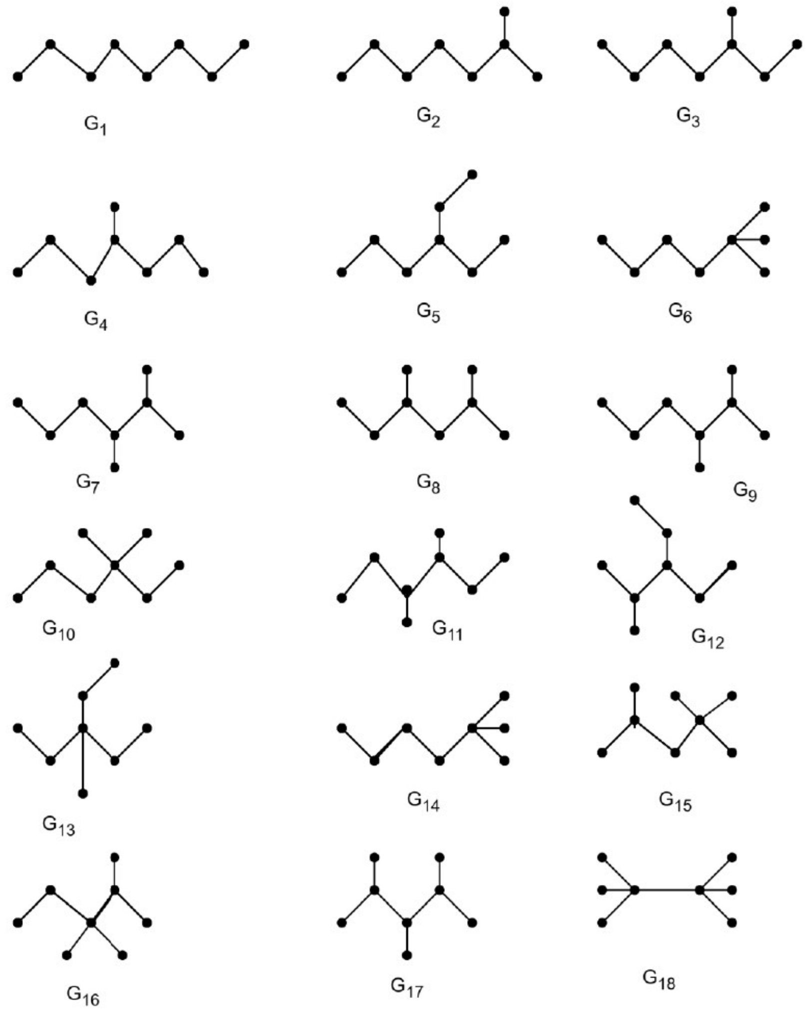

Figure 1: Molecular graph of octane isomers

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Table 1: The computed values of status based graphical indices of molecular graphs of octane isomers

Octane isomers	**Status based based graphical indices**				
	$SESO(G_i)$	$S_1(G_i)$	$S_2(G_i)$	$SSO(G_i)$	$SF(G_i)$
G_1	8196.66	280	2856	198.8625	2336
G_2	7043.988	260	2441	184.9815	5014
G_3	6442.901	248	2224	176.6908	4592
G_4	6257.625	244	2157	173.9367	4462
G_5	5656.552	232	1940	165.6485	4040
G_6	5448 .555	228	1865	162.9075	3894
G_7	5257.636	224	1796	160.1412	3760
G_8	5414.642	228	1853	162.8715	3870
G_9	5964.836	240	2052	171.1313	4256
G_{10}	4741.354	212	1609	151.936	3398
G_{11}	4892.715	216	1664	154.6431	3504
G_{12}	4707.454	212	1597	151.8889	3374
G_{13}	4219.439	200	1420	143.7212	3032
G_{14}	4022.746	196	1349	140.9582	2894
G_{15}	4493.799	208	1520	149.1358	3224
G_{16}	3865.741	192	1292	138.2408	2784
G_{17}	4331.149	204	1461	146.3941	3110
G_{18}	3226.245	176	1060	127.3499	2336

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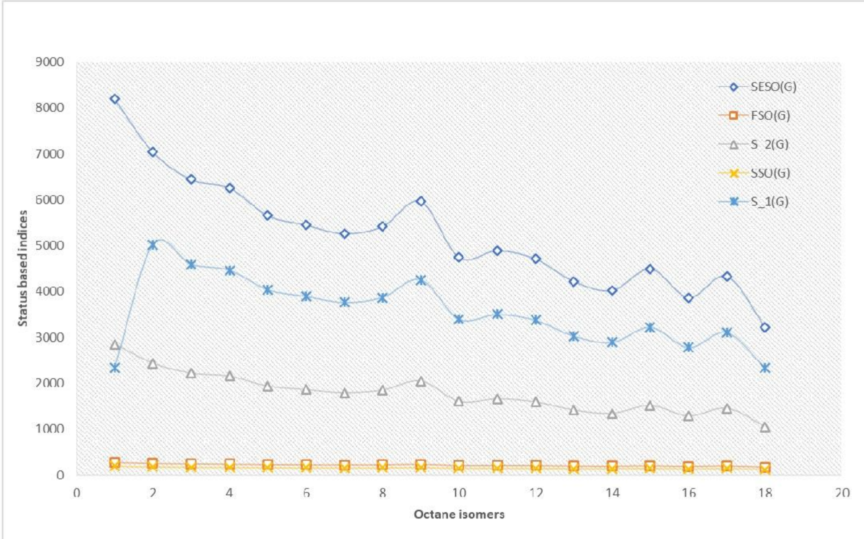

Figure 2: Comparative analysis

3 Bounds for Status elliptic Sombor index

3.1 Bounds in terms of diameter

Theorem 1 *Let G be graph with n vertices, and let $diam(G) = D$. Then*

$$SESO(G) \leq \sum_{\beta\alpha\in E(G)} [2D(n-1)-(D-1)q]\sqrt{2D^2(n-1)^2+(D-1)^2p-2D(D-1)(n-1)q}$$

and

$$SESO(G) \geq \sum_{\beta\alpha\in E(G)} [4(n-1)-q]\sqrt{8(n-1)^2+p-4(n-1)q}$$

where $p = d(\beta)^2 + d(\alpha)^2$ and $q = d(\beta) + d(\alpha)$. Equality in both holds if and only if $diam(G) \leq 2$.

Proof. **Upper bound :** For each vertex β in G, there are $n-1-d(\beta)$ vertices are having distance at most D and $d(\beta)$ vertices are having distance one from the vertex β, therefore $\sigma(\beta) \leq D(n-1-d(\beta)) + d(\beta)$. Hence by the status elliptic Sombor index

$$\begin{aligned} SESO(G) &= \sum_{\beta\alpha\in E(G)} (\sigma(\beta)+\sigma(\alpha))\sqrt{\sigma(\beta)^2+\sigma(\alpha)^2} \\ &\leq \sum_{\beta\alpha\in E(G)} [2D(n-1)-(D-1)q]\sqrt{2D^2(n-1)^2+(D-1)^2p-2D(D-1)(n-1)q}, \end{aligned}$$

where $p = d(\beta)^2 + d(\alpha)^2$ and $q = d(\beta) + d(\alpha)$.

Lower bound : For each vertex β in G, there are $n-1-d(\beta)$ vertices are having distance at least two and $d(\beta)$ vertices are having distance one from the vertex β. Therefore for any β in G, $\sigma(\beta) \geq D(n-1) - (D-1)d(\beta)$. Hence by the Status elliptic Sombor index, we have

$$\begin{aligned} SESO(G) &= \sum_{\beta\alpha\in E(G)} (\sigma(\beta)+\sigma(\alpha))\sqrt{\sigma(\beta)^2+\sigma(\alpha)^2} \\ &\geq \sum_{\beta\alpha\in E(G)} [4(n-1)-q]\sqrt{8(n-1)^2+p-4(n-1)q} \end{aligned}$$

where $p = d(\beta)^2 + d(\alpha)^2$ and $q = d(\beta) + d(\alpha)$.

Corollary 1 *Let G be a graph with m edges and n vertices. Let $diam(G) = D$ and let Δ and δ be the maximum and minimum vertex degrees, respectively. Then*

$$SESO(G) \leq 2m[D(n-1) - \Delta(D-1)]\sqrt{2D^2(n-1)^2 + 2\Delta^2(D-1)^2 - 4D(D-1)(n-1)\Delta}$$

and

$$SESO(G) \geq 2m[2(n-1) - \delta]\sqrt{8(n-1)^2 + 2\delta^2 - 8(n-1)\delta}.$$

Proof. $\delta \leq d(\beta) \leq \Delta$ for any vertex $\beta \in V(G)$. Thus, we obtain the necessary result by replacing $d(\beta)^2 + d(\alpha)^2 \leq 2\Delta^2$, $d(\beta) + d(\alpha) \leq 2\Delta$ in the upper bound and $d(\beta)^2 + d(\alpha)^2 \geq 2\delta^2$, $d(\beta) + d(\alpha) \geq 2\delta$ in the lower bound of Theorem 1.

Corollary 2 *Let G be an r- regular connected graph with m edges and n vertices. suppose $diam(G) = D$. Then*

$$SESO(G) \leq 2m[D(n-1) - (D-1)r]\sqrt{2D^2(n-1)^2 + 2(D-1)^2r^2 - 4D(D-1)(n-1)r}$$

and

$$SESO(G) \geq 2m[2(n-1) - r]\sqrt{8(n-1)^2 + 2r^2 - 8(n-1)r}.$$

Theorem 2 *Let $\overline{G}$ be the complement of the graph G, suppose $\overline{G}$ is connected. Then*

$$SESO(\overline{G}) \leq \sum_{\beta\alpha \in E(\overline{G})} [2(n-1) + (D-1)q]\sqrt{2(n-1)^2 + (D-1)^2p + 2(D-1)(n-1)q}$$

and

$$SESO(\overline{G}) \geq \sum_{\beta\alpha \in E(\overline{G})} [2(n-1) + q]\sqrt{2(n-1)^2 + p + 2(n-1)q},$$

where $D = diam(\overline{G}), p = d(\beta)^2 + d(\alpha)^2$ and $q = d(\beta) + d(\alpha)$.

Proof. There are $n - 1 - d_G(\beta)$ vertices at distance 1 for any vertex β in $\overline{G}$, whereas the remaining $d_G(\beta)$ vertices are at distance at least 2 and at most D. Therefore

$$\sigma_{\overline{G}}(\beta) \leq (n-1) + (D-1)d_G(\beta) \quad \text{and} \quad \sigma_{\overline{G}}(\beta) \geq n - 1 + d_G(\beta).$$

From the definition of Status elliptic Sombor index and above inequalities both upper and lower bound follows.

3.2 Bounds in terms of status based graphical indices

Theorem 3 *Let G be a connected graph. Then*

$$SESO(G) \leq S_1(G) \quad SSO(G).$$

Proof. Let G be a connected graph. Then

$$SESO(G) = \sum_{\beta\alpha \in E(G)} (\sigma(\beta) + \sigma(\alpha))\sqrt{\sigma(\beta)^2 + \sigma(\alpha)^2}.$$

$$\leq \sum_{\beta\alpha \in E(G)} (\sigma(\beta) + \sigma(\alpha)) \sum_{\beta\alpha \in E(G)} \sqrt{\sigma(\beta)^2 + \sigma(\alpha)^2}.$$

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Therefore, $SESO(G) \leq S_1(G) \quad SSO(G)$.

Lemma 1 *[2] Let κ_i and τ_i are real numbers. Then*

$$n\sum_{i=1}^{n} \kappa_i\tau_i \geq \sum_{i=1}^{n} \kappa_i \sum_{i=1}^{n} \tau_i,$$

with equality holds if and only if $\kappa_1 = \kappa_2 = \kappa_3 = \ldots = \kappa_n$ or $\tau_1 = \tau_2 = \tau_3 = \ldots = \tau_n$.

Theorem 4 *Let G be a connected graph. Then*

$$SESO(G) \geq \frac{1}{n}S_1(G)SSO(G).$$

Proof. Let $\kappa_i = (\sigma(\beta) + \sigma(\alpha))$ and $\tau_i = \sqrt{\sigma(\beta)^2 + \sigma(\alpha)^2}$ for i =1, 2, 3...,n. We have

$$SESO(G) = \sum_{\beta\alpha\in E(G)} (\sigma(\beta) + \sigma(\alpha))\sqrt{\sigma(\beta)^2 + \sigma(\alpha)^2}.$$

by the Lemma 1

$$n\sum_{\beta\alpha\in E(G)} (\sigma(\beta) + \sigma(\alpha))\sqrt{\sigma(\beta)^2 + \sigma(\alpha)^2} \geq \sum_{\beta\alpha\in E(G)} (\sigma(\beta) + \sigma(\alpha))\sum_{\beta\alpha\in E(G)} \sqrt{\sigma(\beta)^2 + \sigma(\alpha)^2}$$

$$SESO(G) \geq \frac{1}{n}S_1(G)SSO(G).$$

Hence, the result.

Lemma 2 *[2] For positive real numbers $\kappa_1 = \kappa_2 = \kappa_3, \ldots, \kappa_n$, we have*

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

Theorem 5 *Let G be a connected graph. Then*

$$SESO(G) \leq \sqrt{n}SESO(G).$$

Proof. Let $\kappa_i = (\sigma(\beta_i) + \sigma(\alpha_i))\sqrt{\sigma(\beta_i)^2 + \sigma(\alpha_i)^2}$, for $i = 1,2,3,\ldots,n$ in Lemma 2. We get

$$\frac{\sum_{i=1}^{n}(\sigma(\beta)+\sigma(\alpha))\sqrt{\sigma(\beta)^2+\sigma(\alpha)^2}}{n} \leq \sqrt{\frac{\sum_{i=1}^{n}(\sigma(\beta)+\sigma(\alpha))\sqrt{\sigma(\beta)^2+\sigma(\alpha)^2}}{n}}.$$

Therefore, $SESO(G) \leq \sqrt{n \cdot SESO(G)}$.

Lemma 3 *[1] (The Cauchy–Schwarz inequality) Let $\kappa = (\kappa_1, \kappa_2, \ldots, \kappa_n)$ and $\tau = (\tau_1, \tau_2, \ldots, \tau_n)$ are real n-vectors then*

$$\left(\sum_{i=1}^{n} \kappa_i\tau_i\right)^2 \leq \left(\sum_{i=1}^{n} \kappa_i^2\right)\left(\sum_{i=1}^{n} \tau_i^2\right).$$

Equality holds if and only if κ and τ are proportional.

Theorem 6 *Let G be a connected graph. Then*

$$SESO(G) \leq (FS(G) + 2S_2(G))FS(G).$$

Proof. By setting $\kappa_i = \sigma(\beta) + \sigma(\alpha)$ and $\tau_i = \sqrt{\sigma(\beta)^2 + \sigma(\alpha)^2}$ in the Lemma 3 and the

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definition of status elliptic Sombor index, we get the required result.

4 Status Elliptic Sombor index of some standard graphs and graphs derived from the complete graph

Proposition 1 *Let* K_n *be a complete graph with* $n \geq 2$*. Then* $SESO(K_n) = \sqrt{2}n(n-1)^3$.

Proposition 2 *Let* $K_{s,t}$ *be a complete bipartite graph with* $n = s + t \geq 3$ *vertices and* $m = st$ *edges. Then* $SESO(K_{s,t}) = m(3n-4)\sqrt{5n^2 - 12n - 2m + 8}$.

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

$$SESO(C_n) = \begin{cases} \dfrac{n^5}{\sqrt{24}} & \text{if } n \text{ is even} \\ \dfrac{n(n^2-1)^2}{\sqrt{24}} & \text{if } n \text{ is odd.} \end{cases}$$

Proposition 4 *Let* P_n *be a path graph with* $n \geq 2$*. Then*

$$SESO(P_n) = \sum_{i=1}^{n-1} [(n-i)^2 + i^2]\sqrt{((n-i)^2 + i^2)^2 - 2\left(\frac{n^2+n}{2} + i(i-n-1)\right)\left(\frac{n^2+n}{2} + (i+1)(i-1)\right)^2}.$$

Proposition 5 *The graph* $K_{b_m}(t)$ *is obtained from* K_m*, by deleting the edges belonging to a* t*-membered cycle. Then,*

$$SESO(K_{b_m}(t)) = \sqrt{2}t(t-3)(m+1)^2 + 2\sqrt{2}mt(m-t)\sqrt{(m^2+1)} + 2\sqrt{2}(m-t)(m-t-1)(m-1)^2.$$

Proposition 6 *Consider* V_t *as subset of* t*-vertices from the vertex set of complete graph* K_m*, where* $2 \leq t \leq m-1$ *and* $m \geq 3$*. The graph* $K_{g_m}(t)$ *is formed by removing all edges in* K_m *that connect pairs of vertices within* V_t*. Then,*

$$SESO(K_{g_m}(t)) = t(m-t)(2m+t-3)\sqrt{(m-t)(m+4t-5) + (m-t)^2} + \sqrt{2}(m-1)^2(m-t)(m-t-1).$$

Proposition 7 *Let* $f_j (j = 1,2,\ldots,t)$ *be* t *independent edges in the complete graph* K_m*, where* $1 \leq t \leq \lfloor\frac{m}{2}\rfloor$ *and* $m \geq 3$*. The graph* $Kb_m(t)$ *is obtained by removing the edges* f_j *for* $j = 1,2,\ldots,t$ *from* K_m*. Then*

$$SESO(Kb_m(t)) = \sqrt{2}(m-1)^2(m-2t)(m-2t-1) + 4\sqrt{2}m^2t(t-1) + 2t(m-2t)(2m-1)\sqrt{(m-1)(m+3) + (m-2)^2}.$$

Proposition 8 *Consider* K_m *as complete graph* $m \geq 3$ *vertices. Let* $e_j (j = 1,2,\ldots,t)$ *be* t *distinct edges in* K_m*, all sharing a common vertex where* $1 \leq t \leq m-2$*. The graph* $Kc_m(t)$ *is*

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formed by removing the edges e_j *for* $j = 1,2,\ldots,t$ *from* K_m. *Then*

$$\begin{aligned} SESO(Kc_m(t)) &= \sqrt{2}t(t-1)m^2 + \sqrt{2}(m-1)^2(m-t-1)(m-t-2) \\ &+t(2m-1)(m-t-1)\sqrt{(m-1)(m+3)+(m-2)^2} \\ &+(m-t-1)(2m-2+t)\sqrt{2(m-1)(m+k-1)+t^2}. \end{aligned}$$

5 Conclusion

In this study, we first investigated a comparative analysis of the molecular graphs of octane isomers using the Status elliptic Sombor index along with other status-based indices. Additionally, we obtained bounds for the Status elliptic Sombor index in terms of diameter and other status-based indices. Moreover, we computed the Status elliptic Sombor index for various standard graph classes and for graphs obtained from a complete graph.

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