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Some Inequalities for the Entire Sombor Index

N. Harish and B. Chaluvaraju

(Department of Mathematics, Bangalore University, Jnana Bharathi Campus, Bangalore -560 056, India)

E-mail: harish.jaga16@gmail.com, bcrbub@gmail.com

Abstract: The entire Sombor index of a graph G was introduced by Movahedi and Akhbari [6]. By motivated their work, we obtained some properties, inequalities and characterization in terms of order, size, degree and other degree based graphical indices. Also, we present the computed values of certain families of graphs. In addition to that, we compare the statistical behaviour of Sombor based graphical indices such as KG-Sombor index, Reformulated Sombor index and Entire Sombor index of molecular graph of linear $[k]$- alkanes.

Key Words: Entire Sombor index, Sombor index, Kulli-Gutman Sombor index, topological indices.

AMS(2010): 05C05, 05C07, 05C09, 05C92.

§1. Introduction

A simple undirected graph $G = (V, E)$ is the set of all ordered pairs, such as the set of all vertices $V(G)$ are related to atoms and the set of all edges $E(G)$ are related to chemical bonds among atoms with $\mid V \mid= n$ and $\mid E \mid= m$. The vertices u and v are adjacent vertices if and only if they end vertices of a common edge $e = uv \in E(G)$. Let $(\delta(G), \Delta(G))$ be the set of all ordered pairs represented by the minimum and maximum number of adjacent edges incident on the vertex. Also, edge degree can be written as

$$d_G(e) = d_G(uv) = d_G(u) + d_G(v) - 2.$$

The entire Sombor index of a graph G is defined as the sum of the square root of the terms x and y are the two member of the set $B(G)$. Where $B(G)$ is the set of all subsets of two members $\{x, y\} \subseteq V(G) \cup E(G)$ such that x and y are adjacent or incident to each other. For more details on graph theoretical terminologies, we refer to [14,17].

Topological descriptors have made sure their essential importance, because of their easy formation and speed with which those tests may be accomplished. There are numerous graph associated numerical descriptors, that have proven their value in one-of-a-kind areas. Thereby, the system of finding the topological descriptors has emerge as a fascinating and appealing direction of research. We discussed in this paper are depicted in Table 1. For more details refer

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to [9, 10, 11, 23, 26, 27, 28, 29].

Graphical Indices	**Mathematical Representation**
First Zagreb index (Gutman and Trinajstic [12])	$M_1(G) = \sum_{uv \in E(G)} d_G(u) + d_G(v)$
Second Zagreb index (Gutman and Trinajstic [12])	$M_2(G) = \sum_{uv \in E(G)} d_G(u)\, d_G(v)$
Re-defined Zagreb index (Ranjini et al., [22])	$ReZG_3(G) = \sum_{uv \in E(G)} d_G(u) d_G(v) \big[d_G(u) + d_G(v)\big]$
First general Zagreb index (X.Li et al.,[20])	$M_4(G) = \sum_{u \in V(G)} (d_G(u))^4$
Forgotten index (Fortula and Gutman [7])	$F(G) = \sum_{uv \in E(G)} \big[d_G(u)^2 + d_G(v)^2\big]$
Sombor index (Gutman [8])	$SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}$
Reformulated Sombor index (Harish et al.,[15])	$RS(G) = \sum_{e \sim f} \sqrt{d_G(e)^2 + d_G(f)^2}$
KG Sombor index (Kulli et al.,[18])	$KG(G) = \sum_{ue} \sqrt{d_G(u)^2 + d_G(e)^2}$
First Entire Zagreb index (Alwardi et al.,[2])	$EM_1(G) = \sum_{\{x,y\} \subseteq B(G)} [d_G(x) + d_G(y)]$
Second Entire Zagreb index (Alwardi et al.,[2])	$EM_2(G) = \sum_{\{x,y\} \subseteq B(G)} [d_G(x)\, d_G(y)]$
Entire Forgotten index (Bharall et al.,[3])	$EF(G) = \sum_{\{x,y\} \subseteq B(G)} \big[d_G(x)^2 + d_G(y)^2\big]$
Entire Randic index (Saleh et al.,[25])	$ER(G) = \sum_{\{x,y\} \subseteq B(G)} \frac{1}{\sqrt{d_G(x) d_G(y)}}$
Entire ABC index (Saleh et al., [24])	$EABC(G) = \sum_{\{x,y\} \subseteq B(G)} \sqrt{\frac{d_G(x)+d_G(y)-2}{d_G(x) d_G(y)}}$
Platt index (Platt [21])	$Pl(G) = \sum_{u \in V(G)} d_G(u)(d_G(u) - 1)$

Table 1. Degree-based graphical indices and its representation

§2. Entire Sombor Index

The entire Sombor index of a graph G and is defined as

$$ES(G) = \sum_{\{x,y\}\subseteq B(G)} \sqrt{d_G(x)^2 + d_G(y)^2}.$$

2.1. Existing and Preliminary Results

Observation 2.1([6]) Let G be a connected graph with $n \geqslant 3$. Then

$$ES(G) = SO(G) + RS(G) + \sum_{u \text{ is incident to } e} \sqrt{d_G(u)^2 + d_G(e)^2}. \quad (2.1)$$

For edge $e = uv \in E(G)$, equation (2.1) can be expressed as

$$\begin{aligned} ES(G) &= SO(G) + RS(G) + \sum_{uv\in E(G)} \Big[\sqrt{d_G(u)^2 + (d_G(u) + d_G(v) - 2)^2} \\ &\quad + \sqrt{d_G(v)^2 + (d_G(u) + d_G(v) - 2)^2}\Big]. \end{aligned} \quad (2.2)$$

Observation 2.2([1, 13]) For any graph G with $n \geq 2$,

$$Pl(G) = M_1(G) - 2m.$$

Observation 2.3 Let G be a connected graph with $n \geqslant 3$. Then,

(i) $|B(G)| = 2m + \frac{M_1(G)}{2}$;
(ii) $|B(G)| = 3m + \frac{Pl(G)}{2}$.

Observation 2.4([5]) For any connected graph G with $n \geq 2$,

(i) $2m\,(\delta - 1) \leq Pl(G) \leq 2m\,(\Delta - 1)$;
(ii) $m \leq Pl(G) \leq 2m\,(n - 2)$.

Proposition 2.1([6]) *Let G be a r-regular graph with $n \geqslant 3$ and $r \geqslant 1$. Then*

$$ES(G) = nr\left[\frac{r}{\sqrt{2}} + \sqrt{2}(r-1)^2 + \sqrt{5r^2 - 8r + 4}\right].$$

Proposition 2.2([6]) *Let G be a complete graph K_n, cycle C_n, a complete bipartite graph $K_{r,s}$ or a path P_n.*

(i) *If $n \geq 2$ in K_n then*

$$ES(K_n) = n(n-1)\left[\frac{n-1}{\sqrt{2}} + \sqrt{2}(n-2)^2 + \sqrt{5n^2 - 18n + 17}\right].$$

(ii) *If $n \geqslant 3$ in C_n then*

$$ES(C_n) = 8\sqrt{2}\,n.$$

(iii) If $1 \leqslant r \leqslant s$ *in* $K_{r,s}$ *then*

$$\begin{aligned} ES(K_{r,s}) &= rs\left[\sqrt{r^2+s^2}+\frac{\sqrt{2}}{2}(r+s-2)^2+\sqrt{r^2+(r+s-2)^2}\right. \\ &\left.+\sqrt{s^2+(r+s-2)^2}\right]. \end{aligned}$$

(iv) If $n \geqslant 4$ *in* P_n *then*

$$ES(P_n) = 6\sqrt{5} + 8\sqrt{2}\,(n-3).$$

Proposition 2.3 *For any Wheel* W_n *with* $n \geqslant 4$*,*

$$\begin{aligned} ES(W_n) &= n\left[7\sqrt{2}+10\right]+n\sqrt{n^2+9}+2n\sqrt{n^2+2n+17} \\ &+n\left[\sqrt{n^2+2n+10}+\sqrt{2n^2+2n+1}\right]. \end{aligned}$$

Proof Let W_n be a Wheel with $n \geqslant 4$. Then $|V_{3,3}(G)| = n$, $|V_{3,n}(G)| = n$, $|E_{4,4}(G)| = n$, $|E_{4,n+1}(G)| = 2n$, $|E_{n+1,n+1}(G)| = n(n-1)/2$, $A_{3,4}(G) = 2n$, and $A_{3,n+1}(G) = A_{n,n+1} = n$. By Observation 2.1, we have

$$\begin{aligned} ES(W_n) &= n\sqrt{18}+n\sqrt{n^2+9}+n\sqrt{32}+2n\sqrt{16+(n+1)^2}+\frac{n(n-1)}{2} \\ &\times\sqrt{2(n+1)^2}+2n\sqrt{25}+n\sqrt{9+(n+1)^2}+n\sqrt{n^2+(n+1)^2}. \\ ES(W_n) &= n[7\sqrt{2}+10]+n\sqrt{n^2+9}+2n\sqrt{n^2+2n+17}+n[\sqrt{n^2+2n+10} \\ &+\sqrt{2n^2+2n+1}]. \end{aligned}$$

On simplification, we have the required result. □

Now, we obtain the relation between the Sombor index, reformulated Sombor index and KG Sombor index of a graph G as follows:

Theorem 2.1 *Let* G *be a connected graph with* $n \geqslant 3$*. Then*

$$ES(G) = SO(G) + RS(G) + KG(G).$$

Proof Let G be a connected graph with $n \geqslant 3$. Then

$$ES(G) = \sum_{\substack{x \text{ is either adjacent} \\ \text{or} \\ \text{incident to } y}} \sqrt{d_G(x)^2 + d_G(y)^2} = \sum_{xy \in E(G)} \sqrt{d_G(x)^2 + d_G(y)^2}$$

$$+\sum_{e,f\in E(G),\, e\sim f}\sqrt{d_G(e)^2+d_G(f)^2}+\sum_{x\ is\ incident\ to\ e}\sqrt{d_G(x)^2+d_G(e)^2}$$
$$=SO(G)+RS(G)+KG(G).$$

Thus, the result follows. □

2.2. Inequalities in Terms of Order, Size and Minimum/Maximum Degree

Theorem 2.2 *Let G be a connected graph with $n\geqslant 3$. Then*

$$\frac{\sqrt{2}m}{n}\left[n\delta+4(\delta-1)(2m-n)+\sqrt{2}n\sqrt{5\delta^2-8\delta+4}\right]\leq ES(G)$$
$$\leq\sqrt{2}\left[m\Delta+2(\Delta-1)(n\Delta^2-2m)+\sqrt{2}m\sqrt{5\Delta^2-8\Delta+4}\right].$$

The both left and right inequalities holds if and only if G is regular.

Proof Let G be a connected graph with $n\geqslant 3$. Then

$$ES(G)=\sum_{xy\in E(G)}\sqrt{d_G(x)^2+d_G(y)^2}+\sum_{e,f\in E(G),\, e\sim f}\sqrt{d_G(e)^2+d_G(f)^2}$$
$$+\sum_{x\ (e)}\sqrt{d_G(x)^2+d_G(e)^2}$$
$$\geqslant\sum_{xy\in E(G)}\sqrt{2}\delta+\sum_{e,f\in E(G),\, e\sim f}2\sqrt{2}(\delta-1)$$
$$+\sum_{x\in V(G)}\sum_{e\in E(G)}\sqrt{5\delta^2-8\delta+4}$$
$$\geq\sqrt{2}m\delta+2\sqrt{2}(\delta-1)\sum_{x\in V(G)}\binom{d_G(x)}{2}+\sum_{x\in V(G)}d_G(x)\sqrt{5\delta^2-8\delta+4}$$
$$\geq\sqrt{2}m\delta+2\sqrt{2}(\delta-1)(M_1(G)-2m)+2m\sqrt{5\delta^2-8\delta+4}$$
$$\geq\sqrt{2}m\delta+2\sqrt{2}(\delta-1)(\frac{4m^2}{n}-2m)+2m\sqrt{5\delta^2-8\delta+4}$$
$$\geq\sqrt{2}m\delta+4\frac{\sqrt{2}}{n}(\delta-1)(2m^2-mn)+2m\sqrt{5\delta^2-8\delta+4}$$

i.e.,

$$ES(G)\geq\frac{\sqrt{2}m}{n}\left[n\delta+4(\delta-1)(2m-n)+\sqrt{2}n\sqrt{5\delta^2-8\delta+4}\right].$$

Similarly, we have to prove the right inequality.

The both left and right inequalities holds if and only if G is regular. □

Theorem 2.3 *Let G be a connected graph with $n \geqslant 3$. Then*

$$\sqrt{2}m\big[\sqrt{2}\sqrt{5\delta^2-8\delta+4}+4(\delta-1)^2+\delta\big] \leqslant ES(G)$$
$$\leq \sqrt{2}m\left[\sqrt{2}\sqrt{5\Delta^2-8\Delta+4}+4(\Delta-1)^2+\Delta\right].$$

The both left and right inequalities holds if and only if G is regular.

Proof Let G be a connected graph with $n \geqslant 3$. By Theorem 2.2, Observations 2.2 and 2.4(i), we have

$$\begin{aligned} ES(G) &\geq \sqrt{2}m\delta + 2\sqrt{2}(\delta-1)(M_1(G)-2m) + 2m\sqrt{5\delta^2-8\delta+4} \\ &\geq \sqrt{2}m\delta + 2\sqrt{2}(\delta-1)2m(\delta-1) + 2m\sqrt{5\delta^2-8\delta+4} \\ &= \sqrt{2}m\delta + 4m\sqrt{2}(\delta-1)^2 + 2m\sqrt{5\delta^2-8\delta+4}. \end{aligned}$$

i.e.,

$$ES(G) \geqslant \sqrt{2}m\left[\sqrt{2}\sqrt{5\delta^2-8\delta+4}+4(\delta-1)^2+\delta\right].$$

Similarly, we have to prove the right inequality.

The both left and right inequalities holds if and only if G is regular. □

Theorem 2.4 *Let G be a connected graph with $n \geqslant 3$. Then*

$$\sqrt{2}m\left[\delta+2(\delta-1)+\sqrt{10\delta^2-16\delta+8}\right] \leqslant ES(G)$$
$$\leq \sqrt{2}m\left[\Delta+4(n-2)(\Delta-1)+\sqrt{10\Delta^2-16\Delta+8}\right].$$

The both left and right inequalities holds if and only if G is regular.

Proof Let G be a connected graph with $n \geqslant 3$. By Theorems 2.1 and 2.2, Observations 2.2 and 2.4(ii), we have

$$\begin{aligned} ES(G) &\leqslant \sqrt{2}m\Delta + 2\sqrt{2}(\Delta-1)(M_1(G)-2m) + 2m\sqrt{5\Delta^2-8\Delta+4} \\ &\leqslant \sqrt{2}m\Delta + 2\sqrt{2}(\Delta-1)2m(n-2) + 2m\sqrt{5\Delta^2-8\Delta+4} \end{aligned}$$
$$ES(G) \leqslant \sqrt{2}m\big[\Delta+4(n-2)(\Delta-1)+\sqrt{10\Delta^2-16\Delta+8}\big].$$

Similarly, we have to prove left inequality.

The both left and right inequalities holds if and only if G is regular. □

2.3. Inequalities in Terms of Other Degree Based Graphical Indices

Theorem 2.5 *Let G be a connected graph with $n \geqslant 3$. Then*

$$\frac{EM_1(G)}{\sqrt{2}} \leqslant ES(G) \leqslant EM_1(G).$$

The both left and right inequalities holds if and only if G is regular.

Proof Let G be a connected graph with $n \geqslant 3$. We have

$$\frac{d_G(x)+d_G(y)}{\sqrt{2}} \leqslant \sqrt{d_G(x)^2+d_G(y)^2} \leqslant d_G(x)+d_G(y).$$

Therefore, the above inequalities which satisfies for each members and also taking the summation of all the above inequalities, we have

$$\begin{aligned}\frac{1}{\sqrt{2}} \sum_{\{x,y\}\subseteq B(G)} [d_G(x)+d_G(y)] &\leqslant \sum_{\{x,y\}\subseteq B(G)} \sqrt{d_G(x)^2+d_G(y)^2} \\ &\leqslant \sum_{\{x,y\}\subseteq B(G)} d_G(x)+d_G(y).\end{aligned}$$

Thus,

$$\frac{EM_1(G)}{\sqrt{2}} \leqslant ES(G) \leqslant EM_1(G).$$

The both left and right inequalities holds if and only if G is regular. □

Theorem 2.6 *Let G be a connected graph with $n \geqslant 3$. Then*

$$EM_2(G)\frac{\sqrt{2}}{\Delta} \leqslant ES(G) \leqslant EM_2(G)\frac{\sqrt{2}}{\delta}.$$

The both left and right inequalities holds if and only if G is regular.

Proof Let G be a connected graph with $n \geqslant 3$. Then

$$\begin{aligned}ES(G) &= \sum_{\{x,y\}\subseteq B(G)} \sqrt{d_G(x)^2+d_G(y)^2} \\ &= \sum_{\{x,y\}\subseteq B(G)} d_G(x).d_G(y)\sqrt{\frac{1}{d_G(x)^2}+\frac{1}{d_G(y)^2}} \\ &\leq \sum_{\{x,y\}\subseteq B(G)} [d_G(x).d_G(y)]\Big(\sqrt{\frac{1}{\delta^2}+\frac{1}{\delta^2}}\Big) \\ &\leq EM_2(G)\frac{\sqrt{2}}{\delta}.\end{aligned}$$

Similarly, we have to prove the left inequality. Therefore,

$$EM_2(G)\frac{\sqrt{2}}{\Delta} \leqslant ES(G) \leqslant EM_2(G)\frac{\sqrt{2}}{\delta}.$$

The both left and right inequalities holds if and only if G is regular. □

To prove our next result, we make use of the definition of line graph following.

Any two vertices of a line graph $L(G)$ are adjacent if and only if the corresponding edges of a graph G are incident with the same vertex of G. The line graph $L(G)$ of a graph G is a graph whose vertices equal to the edges of G.

Theorem 2.7 *Let G be a connected graph with $n \geqslant 3$. Then,*

$$8\sqrt{2}m - 3\sqrt{2}|B(G)| + \sqrt{2}M_2(G) + \frac{F(G)}{\sqrt{2}}$$
$$\leqslant ES(G) \leqslant 16m - 6|B(G)| + 2M_2(G) + F(G).$$

The both left and right inequalities holds if and only if G is regular.

Proof Let G be a connected graph with $n \geqslant 3$. By Theorem 2.5, we have

$$\begin{aligned} EM_1(G) &= M_1(G) + M_1(L(G)) \\ &= \sum_{uv \in E(G)} \Big[d_G(u) + d_G(v) + (d_G(uv))^2 \Big] \\ &\leq 4m - 3M_1(G) + 2M_2(G) + \sum_{uv \in E(G)} [d_G(u)^2 + d_G(v)^2] \\ &\leq 4m - 3\big((2|B(G)| - 4m)\big) + 2M_2(G) + F(G) \\ &\leq 16m - 6|B(G)| + 2M_2(G) + F(G). \end{aligned}$$

Similarly, we have to prove the left inequality.

The both left and right inequalities holds if and only if G is regular. □

Theorem 2.8 *Let G be a connected graph with $n \geqslant 3$. Then*

$$\frac{EF(G)}{\sqrt{2}\,\Delta} \leqslant ES(G) \leq \frac{EF(G)}{\sqrt{2}\,\delta}.$$

The both left and right inequalities holds if and only if G is regular.

Proof Let G be a connected graph with $n \geqslant 3$. Then

$$\begin{aligned} ES(G) &= \sum_{\{x,y\} \subseteq B(G)} \sqrt{d_G(x)^2 + d_G(y)^2} \\ &= \sum_{\{x,y\} \subseteq B(G)} \frac{d_G(x)^2 + d_G(y)^2}{\sqrt{d_G(x)^2 + d_G(y)^2}} \\ &\leq \sum_{\{x,y\} \subseteq B(G)} [d_G(x)^2 + d_G(y)^2]\Big(\frac{1}{\sqrt{\delta^2 + \delta^2}}\Big) \\ &\leq \frac{EF(G)}{\sqrt{2}\,\delta}. \end{aligned}$$

Similarly, we have to prove the left inequality. Therefore,

$$\frac{EF(G)}{\sqrt{2}\,\Delta} \leqslant ES(G) \leqslant \frac{EF(G)}{\sqrt{2}\,\delta}.$$

The both left and right inequalities holds if and only if G is regular. □

Theorem 2.9 *Let G be a connected graph with $n \geqslant 3$. Then*

$$ER(G)\sqrt{2}\,\delta^2 \leqslant ES(G) \leqslant ER(G)\sqrt{2}\,\Delta^2.$$

The left and right inequalities holds if and only if G is regular.

Proof Let G be a connected graph with $n \geqslant 3$. Then,

$$\begin{aligned}
ES(G) &= \sum_{\{x,y\}\subseteq B(G)} \sqrt{d_G(x)^2 + d_G(y)^2} \\
&= \sum_{\{x,y\}\subseteq B(G)} \frac{1}{\sqrt{d_G(x).d_G(y)}} \left[\sqrt{d_G(x).d_G(y)\big(d_G(x)^2 + d_G(y)^2\big)}\right] \\
&\leq \sum_{\{x,y\}\subseteq B(G)} \frac{1}{\sqrt{d_G(x).d_G(y)}} \left[\sqrt{\Delta^2\, 2(\Delta)^2}\right] \\
&\leq ER(G)\,\sqrt{2}\,\Delta^2.
\end{aligned}$$

Similarly, we have to prove the left inequality. Therefore,

$$ER(G)\sqrt{2}\,\delta^2 \leqslant ES(G) \leqslant ER(G)\sqrt{2}\,\Delta^2.$$

The both left and right inequalities holds if and only if G is regular. □

Theorem 2.10 *Let G be a connected graph with $n \geqslant 3$. Then*

$$ES(G) \leqslant \sqrt{\frac{\Delta^2 + \delta^2}{\Delta\delta}}ER(G).$$

The inequality holds if and only if G is regular.

Proof Let G be a connected graph with $n \geqslant 3$. Then,

$$\begin{aligned}
ES(G) &= \sum_{\{x,y\}\subseteq B(G)} \sqrt{d_G(x)^2 + d_G(y)^2} \\
&= \sum_{\{x,y\}\subseteq B(G)} \sqrt{\left[\frac{d_G(x)}{d_G(y)} + \frac{d_G(y)}{d_G(x)}\right] d_G(x)\, d_G(y)} \\
&\leq \sqrt{\left[\frac{\Delta^2 + \delta^2}{\Delta\,\delta}\right]} \sum_{\{x,y\}\subseteq B(G)} \sqrt{d_G(x)\, d_G(y)} \\
&\leq \sqrt{\left[\frac{\Delta^2 + \delta^2}{\Delta\,\delta}\right]} ER(G).
\end{aligned}$$

The inequality holds if and only if G is regular. □

Corollary 2.1 *Let G be an r-regular connected graph with $n \geqslant 3$. Then*

$$ER(G) \leq ES(G) \leq \sqrt{2}ER(G).$$

Theorem 2.11 *Let G be a connected graph with $n \geqslant 3$. Then,*

(i) $ES(G) \leqslant \sqrt{\left(|B(G)|\right) EF(G)}$ *and*

(ii) $ES(G) \leqslant \sqrt{\left(|B(G)|\right) MEF^*(G)\ (EF(G))^2}$,

where,

$$MEF^*(G) = \sum_{\{x,y\}\subseteq B(G)} \frac{1}{d_G(x)^2 + d_G(y)^2}$$

is the modified forgotten index.

Proof Let G be a connected graph with $n \geq 3$.

(i) Consider

$$\begin{aligned} ES(G) &= \sum_{\{x,y\}\subseteq B(G)} \sqrt{d_G(x)^2 + d_G(y)^2} \\ &\leq \sqrt{\left(|B(G)|\right) \sum_{\{x,y\}\subseteq B(G)} d_G(x)^2 + d_G(y)^2} \leq \sqrt{\left(|B(G)|\right) EF(G)}. \end{aligned}$$

(ii) Consider

$$\begin{aligned} ES(G) &= \sum_{\{x,y\}\subseteq B(G)} \sqrt{d_G(x)^2 + d_G(y)^2} \\ &\leq \sqrt{(|B(G)|) \sum_{\{x,y\}\subseteq B(G)} \frac{\left[d_G(x)^2 + d_G(y)^2\right]^2}{d_G(x)^2 + d_G(y)^2}} \\ &\leq \sqrt{(|B(G)|) \sum_{\{x,y\}\subseteq B(G)} \frac{1}{d_G(x)^2 + d_G(y)^2} \sum_{\{x,y\}\subseteq B(G)} \left[d_G(x)^2 + d_G(y)^2\right]^2} \\ &\leq \sqrt{(|B(G)|)\ MEF^*(G)\ (EF(G))^2}. \end{aligned}$$

We obtained the desired results. □

Theorem 2.12 *Let G be a connected graph with $n \geqslant 3$. Then*

$$2\delta^2\sqrt{\left(|B(G)|\right) MEF^*(G)} \leqslant ES(G) \leqslant 2\Delta^2\sqrt{\left(|B(G)|\right) MEF^*(G)}.$$

The both left and right inequalities holds if and only if G is regular.

Proof Let G be a connected graph with $n \geqslant 3$. Then,

$$\begin{aligned} ES(G) &= \sum_{\{x,y\}\subseteq B(G)} \sqrt{d_G(x)^2 + d_G(y)^2} \\ &\leq \sqrt{(|B(G)|) \sum_{\{x,y\}\subseteq B(G)} \frac{1}{d_G(x)^2 + d_G(y)^2} (d_G(x)^2 + d_G(y)^2)^2} \\ &\leq \sqrt{(|B(G)|)\, 4\Delta^4 MEF^*(G)} \\ &\leq 2\Delta^2 \sqrt{(|B(G)|)\ MEF^*(G)}. \end{aligned}$$

Similarly, we have to prove the left inequality. Therefore,

$$2\delta^2 \sqrt{\Big(|B(G)|\Big)\ MEF^*(G)} \leqslant ES(G) \leqslant 2\Delta^2 \sqrt{\Big(|B(G)|\Big)\ MEF^*(G)}.$$

The both left and right inequalities holds if and only if G is regular. □

Corollary 2.2 *Let G be a connected graph with $n \geqslant 3$. Then,*

(*i*) $ES(G) \leqslant \sqrt{\left(\frac{Pl(G)}{2} + 3\,m\right) EF(G)}$ *and*

(*ii*) $ES(G) \leqslant \sqrt{\left(\frac{Pl(G)}{2} + 3\,m\right) MEF^*(G)\ (EF(G))^2}$.

Corollary 2.3 *Let G be a connected graph with $n \geqslant 3$. Then,*

(*i*) $ES(G) \leqslant \sqrt{\left(2m + \frac{M_1(G)}{2}\right) EF(G)}$ *and*

(*ii*) $ES(G) \leqslant \sqrt{\left(2m + \frac{M_1(G)}{2}\right) MEF^*(G)\ (EF(G))^2}$.

§3. Chemical Applicability of Linear $[k]$ Alkanes

Hydrocarbons are one of the major part of chemical graph theory. The hydrocarbons are the organic compounds containing carbon and hydrogen. For example alkane, alkene and alkynes. Alkanes are saturated, open chain hydrocarbons containing carbon-carbon single bonds. For example, methane (CH_4), ethane (C_2H_6), propane (C_3H_8), etc. These hydrocarbons are inert under normal conditions (i.e do not react with acids, bases and other reagents). Hence, they were earlier known as *paraffins*. The uses of alkanes depends on the quantity of carbon atoms. The first four alkanes are used largely for heating and culinary purposes. For more details, we refer to [4, 16, 19].

The molecular graph of alkane is a tree in which vertices coresoponds to atoms and edges to carbon-carbon or hydrogen-carbon bonds in a chemical alkane. The molecular formula for alkane C_nH_{2n+2} which contains $(3n+2)$ - vertices and $(3n+1)$ - edges and the linear $[k]$ alkanes can be represented as $A[k]$, see Figure 1. For partitioned of $A[k]$, the value of k represents the stages of alkanes $A[k]$. If $k = 1$ the number of pair of adjacent edges in $(3,3)$ is 6. For $k = 2$

the number of pair of adjacent edges in $(3,6)$ and $(6,6)$ are shown in Table 2.

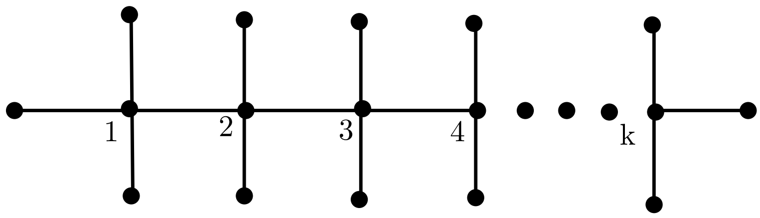

Figure 1. Linear [k] Alkanes

$\big(d_G(u), d_G(v)\big) : uv \in E(G)$	$(1,4)$ $(4,4)$
Number of edges	$(2k+2)$ $(k-1)$
$\big(d_G(e), d_G(f)\big) : e, f \in E(G)$	$(3,3)$ $(3,6)$ $(6,6)$
Number of pair of adjacent edges	$\big[(k-2)+6\big]$ $\big[4(k-1)+2\big]$ $(k-2)$
$\big(d_G(u), d_G(v)\big) : uv \in E(G)$	$(1,4)$ $(4,4)$
$d_G(e)$	3 6
Number of edges	$(2k+2)$ $(k-1)$

Table 2. Vertex-edges set partitions and their values.

Mathematically, the computed values of Sombor related indices of a graph can represents as, $SO(G) < KG(G) \leqslant RS(G) < ES(G)$. The computed values of graphical indices of different stages k for $1 \leq k \leq 4$ as shown in Table 3 and its comparative analysis as shown in Figure 2. This shows the highest and least value of Sombor related topological indices.

Indices	**Computed values**
$SO(G)$	$[2\sqrt{17}+4\sqrt{2}]k+[2\sqrt{17}-4\sqrt{2}]$
$RS(G)$	$[5+6\sqrt{2}]k+[24\sqrt{2}+6\sqrt{5}]$
$KG(G)$	$[2\sqrt{10}+4\sqrt{13}+10]k+[2\sqrt{10}-4\sqrt{13}+10]$
$ES(G)$	$[10\sqrt{2}+2\sqrt{17}+2\sqrt{10}+4\sqrt{13}+15]k$ $+[20\sqrt{2}+2\sqrt{17}+6\sqrt{5}+2\sqrt{10}-4\sqrt{13}+4]$

Table 3. The computed values of Sombor related indices

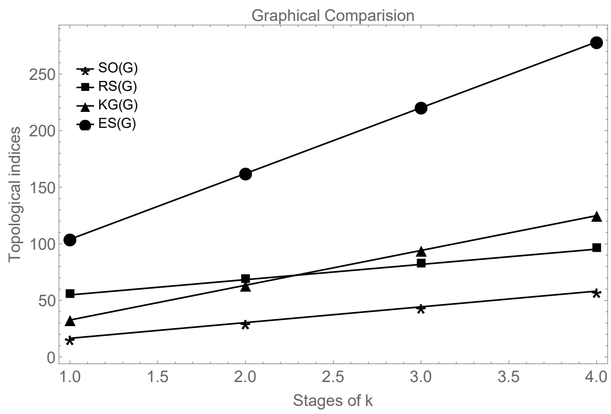

Figure 2. The computed values of Sombor related indices

Also, the computed values of graphical indices with respected to the particular values k for $1 \leq k \leq 4$ as shown in Table 4 and its comparative analysis as shown in Figure 3 as follows:

Stages of k	Sombor related indices			
	$SO(G)$	$RS(G)$	$KG(G)$	$ES(G)$
k=1	16.492	54.842	32.649	103.984
k=2	30.395	68.328	63.395	162.119
k=3	44.298	81.813	94.142	220.254
k=4	58.201	95.298	124.889	278.389

Table 4. The particular values of Sombor related indices

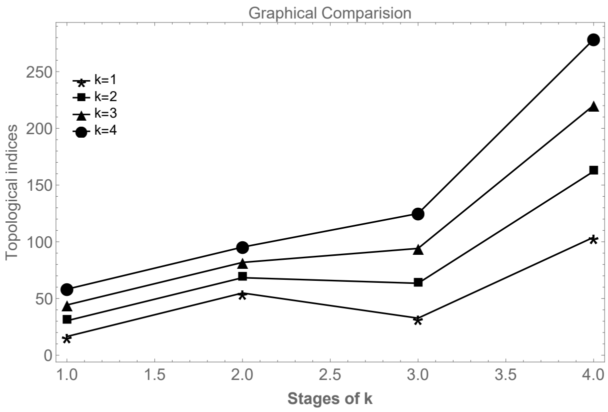

Figure 3. The particular values of Sombor related indices

§4. Conclusion

A topological descriptor can be assumed to be a function that provides the information in numerical form about any underline molecular structure. Topological descriptors capture the symmetry of chemical compounds and present the facts in the numerical form including the presence of heteroatoms, molecular size, multiple bonds, shape and branching.

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