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Research Article

Extremal Sombor indices of cactus graphs: sparkle, sun, and broken sun graphs with chemical applications

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Abstract: In this paper, we consider a group of cactus graphs with specific pendant edge structures such as sparkle, sun, and broken sun graphs. We focus on calculating the extremal Sombor index of these graphs due to their importance in various scientific fields. The Sombor index, a topological index predicting physicochemical properties of molecules, was introduced by Ivan Gutman. This study extends previous work on Sombor indices for cactus graphs, presenting new findings on the Sombor index of these specialized graphs and their potential use in molecular property prediction.

Keywords: Sombor index, cactus graphs, sparkle, sun and broken sun graphs.

AMS Subject classification: 05C09, 05C90

1. Introduction

Topological indices are mathematical tools that have been extensively used to predict the physicochemical properties of molecular structures. Among these, the *Sombor index*, introduced by Ivan Gutman, has gained significant attention due to its affect in correlating molecular graphs with chemical properties. A molecular graph is a simple graph where vertices represent atoms and edges represent chemical bonds. The Sombor index, in particular, is a powerful predictor of various molecular characteristics and has been studied in numerous contexts such as references [6], [10] and [15], which include specific types of cactus graphs.
Cactus graphs represent a particular class of graphs for studying topological indices. Within this class, unicyclic graphs with pendant edges, such as sparkle, sun, and

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broken sun graphs, have particular importance. These graphs are not only significant in theoretical studies but also have practical applications in chemical science. Understanding the extremal properties of the Sombor index in these graphs can lead to better predictions and insights into molecular behavior and other systems.
This is to inform you that the section related to the sun and broken sun graphs has been made in the preprint at the following internet address (URL):
https://assets-eu.researchsquare.com/files/rs-4353166/v1_covered_bbacecd4-0c58-4c57-a0d1-4ea5007a0462.pdf?c=17152\69994
Let $G = (V(G), E(G))$ be a graph with the vertex set $V(G)$ ($|V(G)| = n$) and the edge set $E(G)$ ($|E(G)| = m$), then the *Sombor index, reduced Sombor index and average Sombor index* are defined as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d^2(u) + d^2(v)}, \tag{1.1}$$

$$SO_{red}(G) = \sum_{uv \in E(G)} \sqrt{(d(u)-1)^2 + (d(v)-1)^2} \tag{1.2}$$

and

$$SO_{avr}(G) = \sum_{uv \in E(G)} \sqrt{(d(u) - \frac{2m}{n})^2 + (d(v) - \frac{2m}{n})^2}, \tag{1.3}$$

where $d(u)$ is degree of vertex u in G.

2. The Sombor index of the sparkle graphs

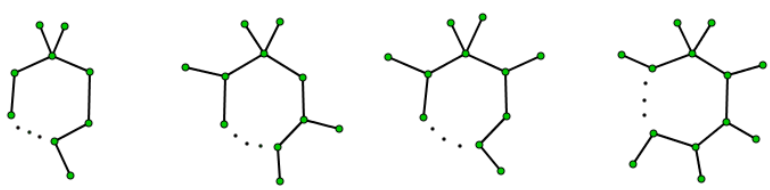

Figure 1. **Some sparkle graphs with p sides**

A unicyclic graph is a connected graph containing exactly one cycle. Some authors have studied the Sombor index and other indices in some articles such as [1], [10], [6],

and [14] for specific unicyclic graphs. Here, we have named a group of these unicyclic graphs as *sparkle graphs* and it is defined as a graph containing a cycle where one of its vertices has two pendent vertices and its other vertices could have one pendant vertex or not and we put the number of such vertices equal with r (see Figure 1). Sparkle graphs are denoted by $H_{1,r}$ and the set of all $H_{1,r}$s with n vertices is denoted by CY_n.
For an sparkle graph $H_{1,r}$, let n_d indicates the vertices number of degree d in the graph and $m_{d,d'}$ indicates the number of edges with ends vertices degree d and d'. Then $n_1 + n_2 + n_3 + n_4 = n$, $\Sigma m_{d,d'} = 2m$ and

$$\begin{aligned} SO(H_{1,r}) = 5m_{4,3} + 2\sqrt{5}m_{4,2} + 3\sqrt{2}m_{3,3} + \sqrt{13}m_{2,3} \\ +2\sqrt{2}m_{2,2} + \sqrt{10}r + 2\sqrt{17}, \end{aligned}$$

$$SO_{red}(H_{1,r}) = \sqrt{13}m_{4,3} + \sqrt{10}m_{4,2} + 2\sqrt{2}m_{3,3} + \sqrt{5}m_{2,3} + \sqrt{2}m_{2,2} + 2r + 6,$$

and

$$SO_{ave}(H_{1,r}) = \sqrt{5}m_{4,3} + 2m_{4,2} + m_{2,3} + \sqrt{2}m_{3,3} + \sqrt{2}r + 2\sqrt{5} \qquad (since\ \frac{2m}{n} = 2)$$

in which $m_{4,1} = 2$ and $m_{3,1} = r$.
It is easy to verify that for every $r \in \mathbb{N}_0$, the table of the vertex degree distribution for the graph $H_{1,r}$ corresponds to Table (1).

	n_4	n_3	n_2	n_1
$H_{1,r}$	1	$\forall\ r\ 0 \leq r \leq p-1$	$p-(1+r)$	$2+r$

Table 1. **Vertex degree distribution for graphs** $H_{1,r}$

In the following lemma, we show that the table of the edges distribution for the sparkle graphs is as Table (2).

$H_{1,r}$	$m_{4,3}$	$m_{4,2}$	$m_{4,1}$	$m_{3,3}$	$m_{3,2}$	$m_{3,1}$	$m_{2,2}$
	0	2	2	$m_{3,3}$	$2(r-m_{3,3})-0$	r	$n-(3r-m_{3,3}+4)$
$H_{1,r}$	1	1	2	$m_{3,3}$	$2(r-m_{3,3})-1$	r	$n-(3r-m_{3,3}+3)$
	2	0	2	$m_{3,3}$	$2(r-m_{3,3})-2$	r	$n-(3r-m_{3,3}+2)$

Table 2. **Edge distribution in graph** $H_{1,r} \in CY_n$ **for each** $r \in \mathbb{N}_0$ **and** $0 \leq m_{3,3} \leq r-1$.

Lemma 1. *The table of the edge distribution for the sparkle graphs is shown in Table* (2).

Proof. It is easily seen that $m_{4,3}$ can only take the values of 0, 1, or 2 and by having different values of $m_{4,3}$, one can easily obtain different values of $m_{4,1}$ and $m_{4,2}$. Now we show that for each $r \in \mathbb{N}_0$ and for values p with a fixed $m_{3,3}$ always $m_{3,2} = 2(r - m_{3,3}) - 0$ or $m_{3,2} = 2(r - m_{3,3}) - 1$ or $m_{3,2} = 2(r - m_{3,3}) - 2$. Indeed, at first, the problem is proved directly for $r = 0$ and $r = 1$:
If $r = 0$, then $m_{4,3} = 0$ and hence $m_{2,3} = 0 = 2(0 - 0) - 0$.
If $r = 1$ then $m_{4,3} = 0$ or $m_{4,3} = 0$ and hence $m_{2,3} = 2 = 2(1 - 0) - 0$ or $m_{2,3} = 1 = 2(1 - 0) - 1$, respectively.
Now the mathematical induction is applied on $r \geq 2$:
If $r = 2$, then for

$$m_{3,3} = 0, \quad \begin{cases} m_{2,3} = 4 = 2(2-0) - 0 \\ \textit{or} \\ m_{2,3} = 3 = 2(2-0) - 1 \\ \textit{or} \\ m_{2,3} = 2 = 2(2-0) - 2 \end{cases} \quad \text{and for} \quad m_{3,3} = 1,$$

$$\begin{cases} m_{2,3} = 2 = 2(2-1) - 0 \\ \textit{or} \\ m_{2,3} = 1 = 2(2-1) - 1 \\ \textit{or} \\ m_{2,3} = 0 = 2(2-1) - 2. \end{cases}$$ Now assume that the claim holds for $r - 1 (r \geq 3)$.

If $r = n - 1$, then $m_{4,3} = 2$ and $m_{3,3} = r - 1$ which deduces that $m_{2,3} = 0 = 2(r - m_{3,3}) - 2$. Now let $3 \leq r \leq n - 2$. So there exists at least one vertex of degree 2 such as u which is adjacent to a vertex of degree 3 such as v. We remove the pendant edge adjacent to the vertex v and we denote the new graph as G'. Two cases may occur.

Case 1. The vertex v is the ended of an edge of type $m_{3,3}$.
Then $m^{G'}_{3,3} = m^{G}_{3,3} - 1$, $r^{G'} = r^{G} - 1$ and $m^{G'}_{2,3} = m^{G}_{2,3}$. By the hypothesis $m^{G}_{2,3} = m^{G'}_{2,3} = 2(r^{G'} - m^{G'}_{3,3}) - i = 2((r^{G} - 1) - (m^{G}_{3,3} - 1)) - i = 2(r^{G} - m^{G}_{3,3}) - i$ for $i \in \{0, 1, 2\}$.

Case 2. The vertex v is not ended of an edge of type $m_{3,3}$. Then $m^{G'}_{3,3} = m^{G}_{3,3} - 1$, $r^{G'} = r^{G} - 1$ and $m^{G'}_{2,3} = m^{G}_{2,3}$. By the hypothesis $m^{G}_{2,3} = m^{G'}_{2,3} = 2(r^{G'} - m^{G'}_{3,3}) - i = 2((r^{G} - 1) - (m^{G}_{3,3} - 1)) - i = 2(r^{G} - m^{G}_{3,3}) - i$ for $i \in \{0, 1, 2\}$.
Also whereas $m_{4,3} + m_{4,2} + m_{4,1} + m_{3,3} + m_{3,2} + m_{3,1} + m_{2,2} = n$,
$m_{2,2} = n - m_{3,1} - m_{3,2} - m_{3,3} - m_{4,1} - m_{4,2} - m_{4,3}$ and so

$$m_{2,2} = \begin{cases} n-(3r-m_{3,3}+4) \\ or \\ n-(3r-m_{3,3}+3) \\ or \\ n-(3r-m_{3,3}+2). \end{cases}$$

for each $0 \leq m_{3,3} \leq r-1$. □

Equalities and inequalities for an index that make a good prediction of molecular physicochemical properties can be seen of them in [3], [13], [9], [10], and [2]. Here by applying (2.1), (2.1), (2.1) and Lemma 1 the following theorem is obtained.

Theorem 1. *For every $r \in \mathbb{N}_0$ $p \geq 3$ and each $0 \leq m_{3,3} \leq r-1$,*

$$SO(H_{1,r}) = \begin{cases} 2\sqrt{2}n + (2\sqrt{13}+\sqrt{10}-6\sqrt{2})r + (5\sqrt{2}-2\sqrt{13})m_{3,3} + 4\sqrt{5}+2\sqrt{17}-8\sqrt{2} \\ \qquad m_{4,3}=0 \\ 2\sqrt{2}n + (2\sqrt{13}+\sqrt{10}-6\sqrt{2})r + (5\sqrt{2}-2\sqrt{13})m_{3,3} + 5+2\sqrt{5}+2\sqrt{17}-6\sqrt{2}-\sqrt{13} \\ \qquad m_{4,3}=1 \\ 2\sqrt{2}n + (2\sqrt{13}+\sqrt{10}-6\sqrt{2})r + (5\sqrt{2}-2\sqrt{13})m_{3,3} + 10+2\sqrt{17}-2\sqrt{13}-4\sqrt{2} \\ \qquad m_{4,3}=2, \end{cases} \tag{2.1}$$

$$SO_{red}(H_{1,r}) = \begin{cases} \sqrt{2}n + (2\sqrt{5}+2-3\sqrt{2})r + (3\sqrt{2}-2\sqrt{5})m_{3,3} + (2\sqrt{10}+6-4\sqrt{2}) \qquad m_{4,3}=0 \\ \sqrt{2}n + (2\sqrt{5}+2-3\sqrt{2})r + (3\sqrt{2}-2\sqrt{5})m_{3,3} + (\sqrt{13}+\sqrt{10}+6-\sqrt{5}-3\sqrt{2}) \\ \qquad m_{4,3}=1 \\ \sqrt{2}n + (2\sqrt{5}+2-3\sqrt{2})r + (3\sqrt{2}-2\sqrt{5})m_{3,3} + (2\sqrt{13}+6-2\sqrt{5}-2\sqrt{2}) \\ \qquad m_{4,3}=2 \end{cases} \tag{2.2}$$

and

$$SO_{avr}(H_{1,r}) = \begin{cases} (\sqrt{2}+2)r + (\sqrt{2}-2)m_{3,3} + 4 + 2\sqrt{5} & m_{4,3}=0 \\ (\sqrt{2}+2)r + (\sqrt{2}-2)m_{3,3} + 3\sqrt{5}+1 & m_{4,3}=1 \\ (\sqrt{2}+2)r + (\sqrt{2}-2)m_{3,3} + 4\sqrt{5}-2 & m_{4,3}=2. \end{cases} \tag{2.3}$$

Theorem 2. *Let $H_{1,r}$ be a sparkle graph with $r \geq 2$ and for the constants p and r, $A_{p,r}$ be the set of all sparkle graphs with p vertices in the cycle and r pendent edges. In the following cases, $H_{1,r} \in A_{p,r}$ has the maximum (minimum) Sombor index if and only if $m_{3,3}=0$ ($m_{3,3}=r-1$).*
(i) $p \geq 2r+2$ *and* $m_{4,3}=0$.
(ii) $p \geq 2r+1$ *and* $m_{4,3}=1$.
(iii) $p \geq 2r$ *and* $m_{4,3}=2$.

Proof. Based on the equation (2.1), since $5\sqrt{2}-2\sqrt{13} < 0$, $H_{1,r} \in A_{p,r}$ has the maximum (minimum) Sombor index if and only if $m_{3,3}=0$ ($m_{3,3}=r-1$). □

Theorem 3. *Let $H_{1,r}$ be a sparkle graph with $r \geq 2$ and for the constants p and r, $A_{p,r}$ be the set of all sparkle graphs with p vertices in the cycle.*
(i) *If $r+3 \leq p < 2r+2$ and $m_{4,3} = 0$, then $H_{1,r} \in A_{p,r}$ has the maximum (minimum) Sombor index if and only if $m_{3,3} = 2r+2-p$ ($m_{3,3} = r-1$).*
(ii) *If $r+2 \leq p < 2r+1$ and $m_{4,3} = 1$, then $H_{1,r} \in A_{p,r}$ has the maximum (minimum) Sombor index if and only if $m_{3,3} = 2r+1-p$ ($m_{3,3} = r-1$).*
(iii) *$r+2 \leq p < 2r$ and $m_{4,3} = 2$, then $H_{1,r} \in A_{p,r}$ has the maximum (minimum) Sombor index if and only if $m_{3,3} = 2r-p$ ($m_{3,3} = r-1$).*

Proof. (i) Let $A \subseteq A_{p,r}$ be the set of sparkle graphs with $p = 2r+1$ and $m_{4,3} = 0$. It is not difficult to check that for each graph in A, $m_{3,3} \neq 0$. Now replace one edge $m_{3,3}$ of the cycle of each graph in A with a path of length two, the new set of sparkle graphs is denoted by A_1 with $p_0 = 2r+2$. Then by Theorem 2(i), the sparkle graph $G \in A_1$ has the maximum Sombor index if and only if $m_{3,3} = 0$. Now, we replace the same path of length 2 again with an edge so that the set A is obtained again. So the maximum (minimum) Sombor index occurs in A if and only if $m_{3,3} = 1 = p_0 - p$ ($m_{3,3} = r-1$). Now let $A \subseteq H_{1,r}$ be the set of sparkle graphs with $p = 2r$ and $m_{4,3} = 0$. By replacing two edges $m_{3,3}$ of the cycle of each graph in A with a path of length two, the new set of sparkle graphs is denoted by A_2 with $p_0 = 2r+2$. Then by Theorem 2(i), the sparkle graph $G \in A_2$ has the maximum Sombor index if and only if $m_{3,3} = 0$. Now, we replace each of the same paths of length 2 again with an edge so that the set A is obtained again such that for each graph in A, $m_{3,3} \geq 2$. So the maximum (minimum) Sombor index occurs in A if and only if $m_{3,3} = 2 = p_0 - p$ ($m_{3,3} = r-1$). Continuing this process and after a finite number, let $A \subseteq H_{1,r}$ be the set of sparkle graphs with $p = r+3$ and $m_{4,3} = 0$. Now replace $r-1$ edges $m_{3,3}$ of the cycle of each graph in A with a path of length two, the new set of sparkle graphs is shown by A_{r-1} with $p_0 = 2r+2$. Then by Theorem 2(i), the sparkle graph $G \in A_{r-1}$ has the maximum Sombor index if and only if $m_{3,3} = 0$. Now, by replacing each of the same paths of length 2 with an edge again, we obtain the set A such that for each graph in A, $m_{3,3} \geq r-1$. Thus the maximum (minimum) Sombor index occurs in A if and only if $m_{3,3} = r-1 = p_0 - p$ ($m_{3,3} = r-1$).
Similarly, using Theorems 2(ii) and 2(iii), parts (ii) and (iii) can be proven. □

2.1. Chemical application of sparkle graphs

In the references [6], [10], and [15], it is considered the Sombor index and other topological indices of trees and certain cactus chain graphs and desired conditions that would yield the maximum or minimum Sombor index. Also in the articles [3], [13], [9], [2] and [16] one can see some inequalities for the Sombor index which are a good prediction for molecular physicochemical properties.
Consider compounds in Figure 2, which are by substitution in the ring of the cycloalkanes. According to Theorem 1, the Table 4 is provided, and it can observed that as n increases, the Sombor index also increases. Additionally, for a fixed n and constant $m_{4,3}$, as $m_{3,3}$ increases the value of the Sombor index decreases.

To better understand Theorems 2 and 3, we have provided several different cases of $m_{i,j}$s in Table 3.

$H_{1,r}$	p	$n=p+r+2$	$m_{4,3}$	$m_{4,2}$	$m_{4,1}$	$m_{3,3}$	$m_{3,2}$	$m_{3,1}$	$m_{2,2}$
$H_{1,0}$	$3,\ 4,\ 5,\ldots$	$p+2$	0	2	2	0	0	0	$n-4$
$H_{1,1}$	$4,\ 5,\ 6,\ldots$	$p+3$	0	2	2	0	2	1	$n-7$
$H_{1,1}$	$3,\ 4,\ 5,\ldots$	$p+3$	1	1	2	0	1	1	$n-6$
$H_{1,2}$	$6,\ 7,\ 8,\ldots$	$p+4$	0	2	2	0	4	2	$n-10$
$H_{1,2}$	$5,\ 6,\ 7,\ldots$	$p+4$	1	1	2	0	3	2	$n-9$
$H_{1,2}$	$4,\ 5,\ 6,\ldots$	$p+4$	2	0	2	0	2	2	$n-8$
$H_{1,2}$	$5,\ 6,\ 7,\ldots$	$p+4$	0	2	2	1	2	2	$n-9$
$H_{1,2}$	$4,\ 5,\ 6,\ldots$	$p+4$	1	1	2	1	1	2	$n-8$
$H_{1,2}$	3	$p+4$	2	0	2	1	0	2	$n-7$
$H_{1,3}$	$8,\ 9,\ 10,\ldots$	$p+5$	0	2	2	0	6	3	$n-13$
$H_{1,3}$	$7,\ 8,\ 9,\ldots$	$p+5$	1	1	2	0	5	3	$n-12$
$H_{1,3}$	$6,\ 7,\ 8,\ldots$	$p+5$	2	0	2	0	4	3	$n-11$
$H_{1,3}$	$7,\ 8,\ 9,\ldots$	$p+5$	0	2	2	1	4	3	$n-12$
$H_{1,3}$	$6,\ 7,\ 8,\ldots$	$p+5$	1	1	2	1	3	3	$n-11$
$H_{1,3}$	$5,\ 6,\ 7,\ldots$	$p+5$	2	0	2	1	2	3	$n-10$
$H_{1,3}$	$6,\ 7,\ 8,\ldots$	$p+5$	0	2	2	2	2	3	$n-11$
$H_{1,3}$	$5,\ 6,\ 7,\ldots$	$p+5$	1	1	2	2	1	3	$n-10$
$H_{1,3}$	4	$p+5$	2	0	2	2	0	3	$n-9$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$H_{1,s-1}$	$2s, 2s+1,..$	$p+s+1$	0	2	2	0	$2(s-1)-0$	$s-1$	$n-(3s+1)$
$H_{1,s-1}$	$2s-1, 2s,\ldots$	$p+s+1$	1	1	2	0	$2(s-1)-1$	$s-1$	$n-3s$
$H_{1,s-1}$	$2s-2, 2s-1,\ldots$	$p+s+1$	2	0	2	0	$2(s-1)-2$	$s-1$	$n-(3s-1)$
$H_{1,s-1}$	$2s-1, 2s,\ldots$	$p+s+1$	0	2	2	1	$2(s-1-1)-0$	$s-1$	$n-3s$
$H_{1,s-1}$	$2s-2, 2s-1,\ldots$	$p+s+1$	1	1	2	1	$2(s-1-1)-1$	$s-1$	$n-(3s-1)$
$H_{1,s-1}$	$2s-3, 2s-2,\ldots$	$p+s+1$	2	0	2	1	$2(s-1-1)-2$	$s-1$	$n-(3s-2)$
$H_{1,s-1}$	$2s-2, 2s-1,\ldots$	$p+s+1$	0	2	2	2	$2(s-1-2)-0$	$s-1$	$n-(3s-1)$
$H_{1,s-1}$	$2s-3, 2s-2,\ldots$	$p+s+1$	1	1	2	2	$2(s-1-2)-1$	$s-1$	$n-(3s-2)$
$H_{1,s-1}$	$2s-4, 2s-3,\ldots$	$p+s+1$	2	0	2	2	$2(s-1-2)-2$	$s-1$	$n-(3s-3)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$H_{1,s-1}$	$s+3,\ s+4,\ldots$	$p+s+1$	0	2	2	$s-1-2$	4	$s-1$	$n-(2s+4)$
$H_{1,s-1}$	$s+2,\ s+3,\ldots$	$p+s+1$	1	1	2	$s-1-2$	3	$s-1$	$n-(2s+3)$
$H_{1,s-1}$	$s+1,\ s+2,\ldots$	$p+s+1$	2	0	2	$s-1-2$	2	$s-1$	$n-(2s+2)$
$H_{1,s-1}$	$s+2,\ s+3,\ldots$	$p+s+1$	0	2	2	$s-1-1$	2	$s-1$	$n-(2s+3)$
$H_{1,s-1}$	$s+1,\ s+2,\ldots$	$p+s+1$	1	1	2	$s-1-1$	1	$s-1$	$n-(2s+2)$
$H_{1,s-1}$	s	$p+s+1$	2	0	2	$s-1-1$	0	$s-1$	$n-(2s+1)$

Table 3. **Induction steps on r for $H_{1,r} \in CY_n$ $(n=p+r+2)$ and edge distribution.**

As illustrated in Table 4, increasing n results in a consistent average increase in both the Sombor index and the *boiling point*, as shown in each successive subtable in the column labeled *bp*. But considering each subtable for a fixed n and a fixed $m_{4,3} \in \{0,\ 1,\ 2\}$, the Sombor index is decreasing with increasing $m_{3,3}$ but the boiling point is increasing (The boiling points are sourced from [5], [8], [11], and [12], and statistical analysis (linear regression) presented in Figures 3 and 4).

Remark 1. Also, notice the two boiling points 184.7 ± 8 in the third subtable. If we approximate their values as 176 and 177, with attention to the process of their previous and next subtables, then the following diagrams are obtained.

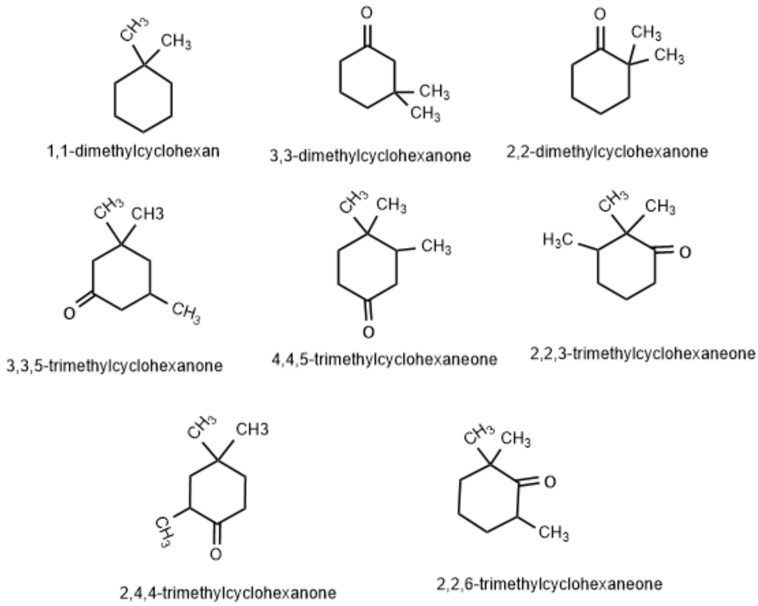

Figure 2. **Some compounds of cycloalkanes.**

$formula$	$H_{1,r}$	p	n	$m_{4,3}$	$m_{3,3}$	SO	SO_{red}	SO_{avr}	bp	SO/bp
C_8H_{16}	$H_{1,0}$	6	8	0	0	*28.504	4.761	8.473	119.5	$0.239 \approx 0.2$
$C_8H_{14}O$	$H_{1,1}$	6	9	0	0	*33.221	21.247	11.886	180	$0.185 \approx 0.2$
$C_8H_{14}O$	$H_{1,1}$	6	9	1	0	*32.971	19.247	11.122	172	$0.155 \approx 0.2$
$C_9H_{16}O$	$H_{1,2}$	6	10	0	0	*37.937	23.415	15.300	189	$0.201 \approx 0.2$
$C_9H_{16}O$	$H_{1,2}$	6	10	1	0	*37.688	24.889	14.536	$184.7 \pm 8 \cong 177$	$0.212 \approx 0.2$
$C_9H_{16}O$	$H_{1,2}$	6	10	2	0	*37.438	24.511	13.772	$184.7 \pm 8 \cong 176$	$0.211 \approx 0.2$
$C_9H_{16}O$	$H_{1,2}$	6	10	0	1	*37.797	23.186	14.714	191	$0.198 \approx 0.2$
$C_9H_{16}O$	$H_{1,2}$	6	10	1	1	*37.548	24.660	13.950	178.5	$0.210 \approx 0.2$

Table 4. (Reduced and average) Sombor index for cycloalkane compounds of Figure 2 without considering duble bond $C = C$ and single bond$-CH$

3. The Sombor index of sun graphs and broken sun graphs

The graph G is called a *sun graph* with $n = 2p$ vertices ($p \in \mathbb{N}$) when it is formed by adding one pendant vertex to each of the vertices of a p-cyclic graph. Also, it is named a *broken sun* graph when it is a unicyclic subgraph of a sun graph (see Figure 5). Here these graphs are shown by H_r such that r is the number of the pendant edges (if $r = p$, then H_r is a sun graph).
The set of all broken sun graphs H_r with n vertices and r pendant edges ($r \in \mathbb{N}_0$) is

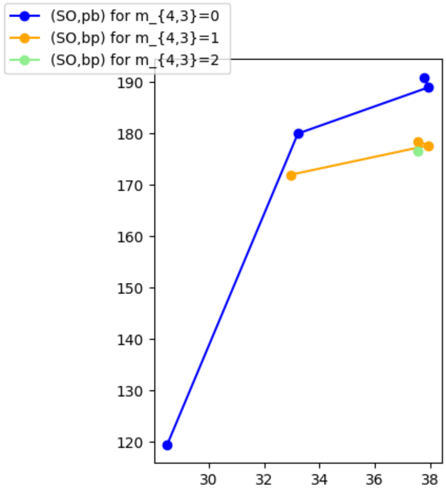

Figure 3. Sombor index versus boiling point of sparkle graphs of Table 4, with attention to values $m_{4,3} = 0, 1, 2$

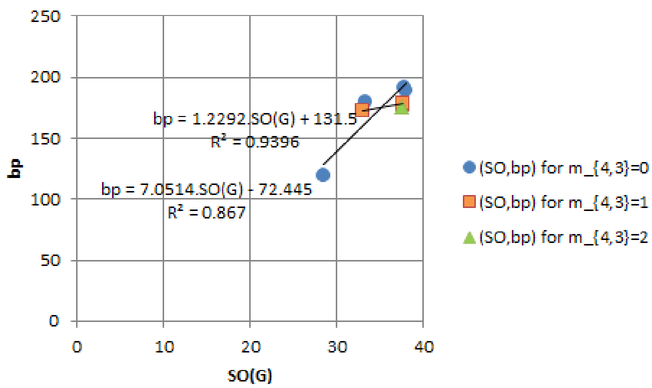

Figure 4. Sombor index versus boiling point of Table 4, with attention to values $m_{4,3} = 0, 1, 2$, shows rounded equations $bp = 7.0514.SO(G) - 72.445$ and $bp = 1.2292.SO(G) + 131.5$ with respective correlations $R^2 = 0.867$ and $R^2 = 0.9396$.

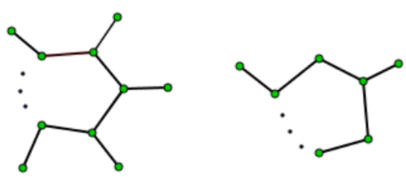

Figure 5. Sun graph and broken sun graph

denoted by CU_n. In this case, the vertex degree distribution table for these graphs is given in Table 5 and the edge distribution table is given in Table 6. So the formulas of the (reduced and averaged) Sombor index could be written as the following:

$$SO(H_r) = 3\sqrt{2}m_{3,3} + \sqrt{13}m_{2,3} + \sqrt{10}m_{1,3} + 2\sqrt{2}m_{2,2}, \tag{3.1}$$

$$SO_{red}(H_r) = 2\sqrt{2}m_{3,3} + \sqrt{5}m_{2,3} + 2m_{1,3} + \sqrt{2}m_{2,2}, \tag{3.2}$$

and since $\frac{2m}{n} = 2$, therefore

$$SO_{ave}(H_r) = (m_{3,3} + \sqrt{2}m_{1,3}) + m_{2,3}. \tag{3.3}$$

in which $m_{3,1} = r$.

n_d	n_1	n_2	n_3
H_r	r	$n-2r$	r

Table 5. **Vertex degree distribution in graphs** $H_r \in CU_n$.

$m_{d,d'}$	$m_{3,3}$	$m_{2,3}$	$m_{1,3}$	$m_{2,2}$
H_r	$m_{3,3}$	$2(r-m_{3,3})$	r	$n-(3r-m_{3,3})$

Table 6. **Table of edge distribution in graphs** $H_r \in CU_n$ **for each** $r \in \mathbb{N}_0$ **and** $0 \le m_{3,3} \le r$.

Lemma 2. *For each CU_n of broken sun graphs with n vertices, the table of the edge distribution with r -pendant vertices is as Table (6).*

Proof. First, we prove that for each graph $H_r \in CU_n$ with a fixed $m_{3,3}$, $m_{2,3} = 2(r-m_{3,3})$. To do this, note that every pending edge that is not adjacent to an edge of the kind $m_{3,3}$ is adjacent to two $m_{2,3}$ edges. Additionally, each set of edges of the type $m_{3,3}$ that are adjacent and their number is l can be attributed to $l+1$ pending edges and two $m_{2,3}$ -edges. Therefore, we can conclude $m_{2,3} = 2(r-m_{3,3})$.
Also since $m_{3,3}+m_{1,3}+m_{2,3}+m_{2,2} = n$, $m_{2,2} = n-m_{3,3}-m_{1,3}-m_{2,3} = n-m_{3,3}-r-2r+2m_{3,3} = n-(3r-m_{3,3})$. □

Now, we obtain the following theorem by using equations (3.1), (3.2), (3.3) and Lemma 2.

Theorem 4. *For each $r \in \mathbb{N}_0$, $p \geq 3$ and $0 \leq m_{3,3} \leq r$, we have*

$$SO(H_r) = 2\sqrt{2}n + (5\sqrt{2} - 2\sqrt{13})m_{3,3} + (2\sqrt{13} + \sqrt{10} - 6\sqrt{2})r, \tag{3.4}$$

$$SO_{red}(H_r) = \sqrt{2}n + (3\sqrt{2} - 2\sqrt{5})m_{3,3} + (2\sqrt{5} + 2 - 3\sqrt{2})r, \tag{3.5}$$

and

$$SO_{avr}(H_r) = (\sqrt{2} - 2)m_{3,3} + (\sqrt{2} + 2)r. \tag{3.6}$$

In Table 7, the edge distribution is given for the broken sun graphs based on the number of the graph's vertices. Also, to better understand Theorem 5, one could see Table 7.

Theorem 5. *Let H_r be a broken sun graph with $r \in \mathbb{N}_0$ such that for the constants p and r, $A_{p,r}$ be the set of all broken sun graphs with p vertices in the cycle and r pendant edges.*
(i) *For $0 \leq r \leq 1$ and $p \geq 3$, $H_r \in A_{p,r}$ has maximum (minimum) Sombor index if and only if $m_{3,3} = 0$ ($m_{3,3} = 0$).*
(ii) *For $r \geq 2$,*
a) If $p \geq 2r$, then $H_r \in A_{p,r}$ has maximum (minimum) Sombor index if and only if $m_{3,3} = 0$ ($m_{3,3} = r - 1$).
b) If $r < p < 2r$, then $H_r \in A_{p,r}$ has maximum (minimum) Sombor index if and only if $m_{3,3} = 2r - p$ ($m_{3,3} = r - 1$).
c) If $p = r$, then $H_r \in A_{p,r}$ has maximum (minimum) Sombor index if and only if $m_{3,3} = r$ ($m_{3,3} = r$).

Proof. (i) It is clear that if H_r be a broken sun graph with $r = 0$ or $r = 1$ then for $p \geq 3$ the graph $H_r \in A_{p,r}$ has both maximum Sombor index and minimum Sombor index if and only if $m_{3,3} = 0$ ($m_{3,3} = 0$).
(ii) For $r \geq 2$,
a) Since $p \geq 2r$, so $0 \leq m_{3,3} \leq r-1$. Now with attention to the equation (3.4) whereas the coefficient of $m_{3,3}$, $5\sqrt{2} - 2\sqrt{13}$, is a negative number, so $SO(H_r)$ is maximum (minimum) if and only if $m_{3,3} = 0$ ($m_{3,3} = r - 1$).
b) With attention to the part (i) if G is a broken sun graph with $p_0 = 2r$ and with maximum $SO(G)$, so $m_{3,3} = 0$, now if remove one vertex of the cycle, then the number of the cycle's vertices is $p = p_0 - 1 = 2r - 1$. So in a new graph G' two pendant edges would be adjacent and based on the relation (3.4) G' has the maximum (minimum) Sombor index if and only if $m_{3,3} = 1 = p_0 - p = 2r - (2r-1)$ ($m_{3,3} = r-1$). By keeping on this process and for other graphs, after a finite number, removing $r-1$ vertices and considering the new graph G' with $p = p_0 - (r-1) = 2r - (r-1) = r-1$, $r-1$ pendant edges also would be adjacent and necessarily the graph G' would have the maximum (minimum) Sombor index if and only if $m_{3,3} = r-1 = p_0 - p = 2r - (2r - (r-1)) = r-1$ ($m_{3,3} = r - 1$).
c) In this case, H_r is a sun graph and as a result $m_{3,3} = r$. □

To better understand Theorem 5, we have provided several different cases of $m_{i,j}$s in the following table.

H_r	$m_{3,3}$	p	$n=p+r$	$m_{2,3}$	$m_{1,3}$	$m_{2,2}$	$m_{1,4}$ ...
H_0	0	$3,\ 4,\ 5,...$	p	0	0	n	
H_1	0	$3,\ 4,\ 5,...$	$p+1$	2	1	$n-3$	
H_2	0	$4,\ 5,\ 6,...$	$p+2$	4	2	$n-6$	
H_2	1	$3,\ 4,\ 5,...$	$p+2$	2	2	$n-5$	
H_3	0	$6,\ 7,\ 8,...$	$p+3$	6	3	$n-9$	
H_3	1	$5,\ 6,\ 7,...$	$p+3$	4	3	$n-8$	
H_3	2	$4,\ 5,\ 6,...$	$p+3$	2	3	$n-7$	
H_3	3	3	$p+3$	0	3	$n-6$	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	
H_{r-1}	0	$2(r-1), 2(r-1)+1,...$	$p+r$	$2(r-1)$	$r-1$	$n-(3r-3)$	
H_{r-1}	1	$[2(r-1)-1], [2(r-1)],...$	$p+r$	$2(r-1)-2$	$r-1$	$n-(3r-4)$	
H_{r-1}	2	$[2(r-1)-2], [2(r-1)-1],...$	$p+r$	$2(r-1)-4$	$r-1$	$n-(3r-5)$	
H_{r-1}	3	$[2(r-1)-3], [2(r-1)-2],...$	$p+r$	$2(r-1)-6$	$r-1$	$n-(3r-6)$	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	
H_{r-1}	$r-1$	$[r-1]$	$p+r$	0	$r-1$	$n-(2r-2)$	
H_r	0	$2(r-1)+2, 2(r-1)+2+1,...$	$p+r$	$2(r-1)+2$	r	$n-3r$	
H_r	1	$[2(r-1)-1]+2, [2(r-1)-1]+2+1,...$	$p+r$	$2(r-1)$	r	$n-(3r-1)$	
H_r	2	$[2(r-1)-2]+2, [2(r-1)-2]+2+1,...$	$p+r$	$2(r-1)-2$	r	$n-(3r-2)$	
H_r	3	$[2(r-1)-3]+2, [2(r-1)-3]+2+1,...$	$p+r$	$2(r-1)-4$	r	$n-(3r-3)$	
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	
H_r	$r-1$	$[r-1]+2, [r-1]+2+1,...$	$p+r$	$2(r-1)-2r$	r	$n-(2r-1)$	
H_r	r	$[r-1]+1$	$p+r$	0	r	$n-2r$	

Table 7. **Induction table on number of pendant edges r for $H_r \in CU_n$**

3.1. Chemical applications of sun graphs and broken sun graphs

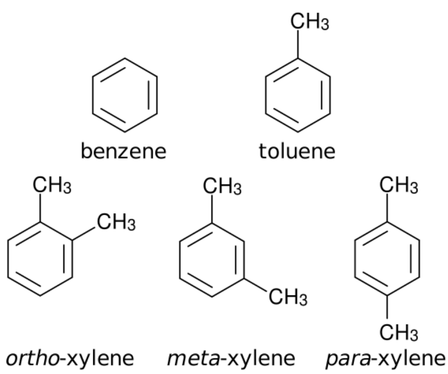

Figure 6. **Some aromatic hydrocarbons with distribution of pendant edge $-CH_3$**

In references [4] and [7], a category of chemical substances known as aromatic hydrocarbons is described. Aromatic hydrocarbons are hydrocarbons contain benzene

rings or similar features (Figure 6 shows some of them). Considering the distribution of single bonds $-CH_3$ in the benzene ring without considering the single bonds $-CH$ and double bonds $C = C$ (as explanations [16]) Tables 8 and 9 are provided (see Figures 7 and 8).
When considering $p = 6$, increasing r leads to a rise in both the Sombor index and boiling points. On the other hand, for a fixed r, as the Sombor index decreases, boiling points also continue to rise, following the earlier trend. This results in the ratio of the Sombor index to boiling point being approximately constant at 0.2.
Figuer 7 shows the variations n versus $SO(G)$, n versus bp and $SO(G)$ versus bp of the aromatics of Figure 6. Also Figure 8 shows the linear regression between $SO(G)$ and bp with the rounded equation $bp = 6.6593.SO(G) - 34.606$ and correlation $R^2 = 0.9936$.

$Name$	H_r	n	$m_{3,3}$	$m_{2,3}$	$m_{1,3}$	$m_{2,2}$	$SO(G)$	$SO_{red}(G)$	$SO_{avr}(G)$
$Benzene$	H_0	6	0	0	0	6	16.9705627485	8.4852813742	0
$Toluene$	H_1	7	0	2	1	4	21.6870887101	12.1289902045	3.4142135624
$Mata-xylene\ and\ para-xylene$	H_2	8	0	4	2	2	26.4036146717	15.7726990348	6.8284271247
$Ortho-xylene$	H_2	8	1	2	2	3	26.2635799327	15.5432037669	6.2426406871
$Mesitylene$	H_3	9	0	6	3	0	31.1201406333	19.416407865	10.2426406871
$Pseudocumene$	H_3	9	1	4	3	1	30.9801058942	19.1869125972	9.6568542495
$Hemellitol$	H_3	9	2	2	3	2	30.8400711551	18.9574173293	9.0710678119
$Durene$	H_4	10	2	4	4	0	35.5565971168	22.6011261595	12.4852813742
$Prehnitene$	H_4	10	3	2	4	1	35.4165623777	22.3716308916	11.8994949366
$Pentamethylbenzene$	H_5	11	4	2	5	0	39.9930536002	25.785844454	14.7279220614
$Hexamethylbenzene$	H_6	11	6	0	6	0	44.4295100838	28.9705627485	16.9705627485

Table 8. Sombor index for aromatic hydrocarbons introduced in Figure 6 without considering single bonds $-CH$ and double bounds $C = C$

H_r	n	$SO(G)$	$Boiling\ Point(°C)$	$SO(G)/P.B$
H_0	6	16.9705627485	80.1	$0.212 \approx 0.2$
H_1	7	21.6870887101	111	$0.195 \approx 0.2$
H_2	8	26.4036146717	138 to 139	0.190 to $0.191 \approx 0.2$
H_2	8	26.2635799327	144	$0.182 \approx 0.2$
H_3	9	31.1201406333	164.7	$0.189 \approx 0.2$
H_3	9	30.9801058942	169	$0.183 \approx 0.2$
H_3	9	30.8400711551	176	$0.175 \approx 0.2$
H_4	10	35.5565971168	195.9 to 197.9	0.182 to $0.180 \approx 0.2$
H_4	10	35.4165623777	204.4	$0.176 \approx 0.2$
H_5	11	39.9930536002	232	$0.172 \approx 0.2$
H_6	12	44.4295100838	265	$0.168 \approx 0.2$

Table 9. Comparison of Sombor index and boiling point of aromatic hydrocarbons under conditions of Table 8

Remark 2. Referring to the process of Table 6, the induction Table 7 and considering the single bonds $-CH$ and double bonds $C = C$, you have all the possible states only for $m_{3,3} = 0$ such that the Sombor index versus molecular mass has the rounded equation $SO(G) = 1.0088.(M.Mass) + 1.79$ and respective correlation $R^2 = 1$ (see Tables 10 and 11 and Figures 9, 10 and 11).

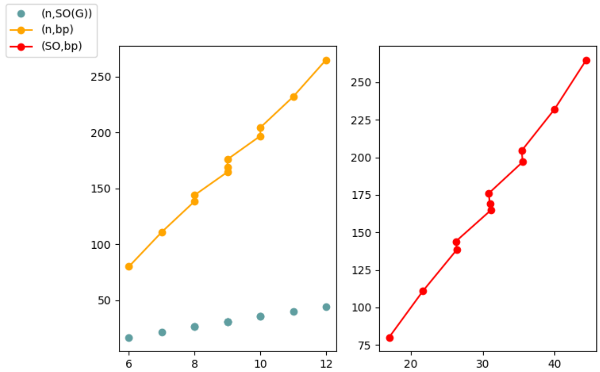

Figure 7. Variations for aromatic hydrocarbons of Tables 9

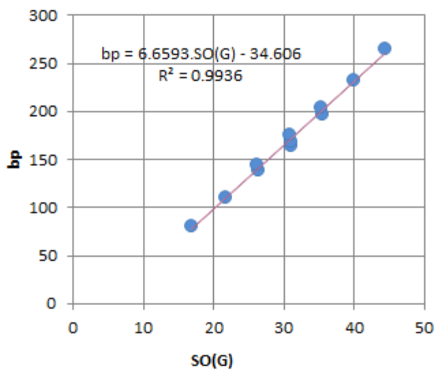

Figure 8. Linear regression for Sombor index versus boiling point for aromatic hydrocarbons of Table 9

So, we have

$$SO(G) = \sqrt{17}m_{4,1} + 4\sqrt{2}m_{4,4}, \tag{3.7}$$

$$SO_{red}(G) = 3m_{4,1} + 3\sqrt{2}m_{4,4}, \tag{3.8}$$

and

$$SO_{ave}(G) = m_{4,1}\sqrt{(4-\frac{2m}{n})^2 + (1-\frac{2m}{n})^2} + m_{4,4}\sqrt{2}(4-\frac{2m}{n})^2. \tag{3.9}$$

H_r	$m_{3,3}$	p	$m_{1,4}$	$m_{4,4}$	SO	SO_{red}	SO_{ave}
H_0	0	6	6	9	75.650	56.184	44.259
H_1	0	6	8	10	89.553	66.426	52.412
H_2	0	6	10	11	103.456	76.669	60.565
H_3	0	6	12	12	117.360	86.912	68.718
H_4	0	6	13	14	131.263	97.154	76.872
H_5	0	6	14	16	145.166	107.397	85.025
H_6	0	6	18	15	159.069	117.640	93.178

Table 10. Values $m_{4,1}$ versus Sombor index of aromatic hydrocarbons of Figure 6 by considering single bondes $C-H$ and double bonds $C=C$

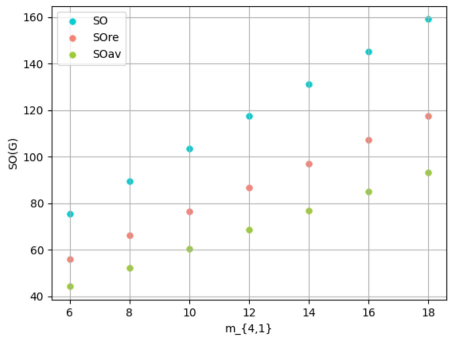

Figure 9. **Values $m_{4,1}$ versus Sombor index under conditions of Table 10**

Theorem 6. *In the aromatic hydrocarbons of the single benzene ring with the bonds $-CH3$ as the pendant edges r $(r \geq 0)$ the following relation holds:*

$$M \approx \begin{cases} 1.03.SO(H_r) & 0 \leq r \leq 2 \\ 1.02.SO(H_r) & 3 \leq r \leq 6 \end{cases} \tag{3.10}$$

where M is the molecular mass approximately.

Proof. Referring to Table 11 the result holds. □

4. Conclusions

The obtained results provide valuable insights into the behavior of the Sombor index in these specialized graph structures, demonstrating its effectiveness as a predictive tool.

For the compounds in Figure 2 named the sparkle graphs and with attention to Table 3, we constructed Table 2. Our findings indicate that with increasing n the Sombor

H_i	$m_{3,3}$	P	$m_{1,4}$	$m_{4,4}$	$SO(G)$	$M.Mass$	$M.Mass/SO(G)$	M
H_0	0	6	6	9	75.650	78.108	$1.033 \approx 1.03$	$77.920 \approx 78$
H_1	0	6	8	10	89.553	92.134	$1.029 \approx 1.03$	$92.240 \approx 92$
H_2	0	6	10	11	103.456	106.160	$1.026 \approx 1.03$	$106.560 \approx 106$
H_3	0	6	12	12	117.360	120.186	$1.024 \approx 1.02$	$119.712 \approx 120$
H_4	0	6	13	14	131.263	134.212	$1.022 \approx 1.02$	$133.888 \approx 134$
H_5	0	6	14	16	145.166	148.238	$1.021 \approx 1.02$	$148.069 \approx 148$
H_6	0	6	18	15	159.069	162.264	$1.020 \approx 1.02$	$162.250 \approx 162$

Table 11. $SO(G)$, $M.Mass$, and its approximation (M) of aromatic hydrocarbons introduced in Figure 6 by considering single bondes $-CH$ and double bonds $C = C$

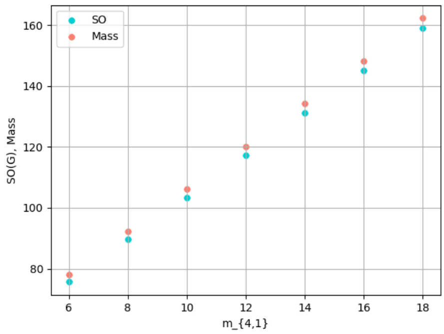

Figure 10. Values $m_{4,1}$ versus $SO(G)$ and $m_{4,1}$ versus $M.mass$ under conditions of Table 11.

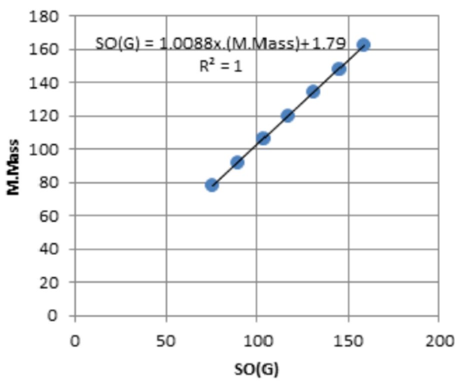

Figure 11. $SO(G)$ v.s $M.Mass$ under conditions of Table 11 with rounded equation $SO(G) = 1.0088.(M.Mass) + 1.79$ and respective correlation $R^2 = 1$

index is increasing. Additionally, for a fixed n and for a constant $m_{4,3}$ the Sombor index decreases with an increase in $m_{3,3}$.
Furthermore, it was demonstrated that for the sun and broken sun graphs and for

a number of the fixed pendant edges, increasing $m_{3,3}$ results in a decrease in the Sombor index while the boiling point increases as observed for the certain aromatic substances in Table 8. Also, in this group of graphs, the comparison between the molecular mass with the Sombor index reveals a strong correlation.
This work extends the understanding of the Sombor index beyond its previous applications, providing some theorems, plats and tables. These findings can be as a foundation for next studies on topological indices by continuing to explore and refine these indices, we can improve our ability to model and predict systems.

Conflict of Interest: We declare that we have no conflicts of interest to disclose related to the subject matter or findings presented in the manuscript. In the event that a conflict of interest arises during the peer review process or after publication, we will promptly disclose this information to the relevant parties.

Data Availability: Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

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