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Research Article

Comparisons of the Sombor Index of Alkane, Alkyl, and Annulene Series with Their Molecular Mass

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Suppose G is an undirected simple graph. A topological index for G is a number with this property that it is invariant under all graph isomorphisms with applications in chemistry. The Sombor and reduced Sombor indices of G are defined as $SO(G) = \sum_{uv\in E(G)}\sqrt{d_G^2(u) + d_G^2(v)}$ and $SO_{\text{red}}(G) = \sum_{uv\in E(G)}\sqrt{(d_G(u) - 1)^2 + (d_G(v) - 1)^2}$, respectively. Here, $d_G(u)$ denotes the degree of the vertex u in G. In this paper, these invariants were computed for alkanes, alkyls, and annulenes. A comparison of our calculations with molecular mass is also presented. As a consequence, it is shown that there is a good correlation between Sombor index and molecular mass of these compounds.

1. Introduction

Suppose M is a molecule. The molecular graph of M is a graph with the set of all atoms as its vertex set and chemical bonds are the edges of this graph. We use the notation G (M), G for short, for this graph. For each vertex $u, d_G(u)$ denotes the degree of u. It is usual to use the notation $V(G)$ for the vertex set of G. Note that in molecular graphs, the degree of each vertex is assumed to be at most 4.

Gutman [1] proposed the degree-based topological index "Sombor index" as $SO(G) = \sum_{uv\in E(G)}\sqrt{d_G^2(u) + d_G^2(v)}$. In the mentioned paper, Gutman proved that the complete graph K_n has the maximum value of Sombor index in the set of all n-vertex graphs and the star graph S_n has the maximum value of Sombor index in the set of all n-vertex trees. The minimum values of Sombor index in the set of all n-vertex graphs and n-vertex trees are the n-vertex null graph $\varnothing_n$ and the n-vertex path graph P_n, respectively. We refer to [2, 3] and references therein for more information on this topic.

Alkanes are acyclic saturated hydrocarbons. They are important chemical structures consisting of carbon and hydrogen in a tree structure with the general chemical formula C_nH_{2n+2}. Alkyls are another chemical compounds with the same materials and general formula C_nH_{2n+1}. Annulenes are monocyclic hydrocarbons with the general chemical formula C_nH_{n+1} or C_nH_n, when n is odd or even, respectively. We refer to [4, 5] for more information on the importance of these compounds on chemistry.

The atomic mass of an atom is defined as the mass of this atom. It is calculated based on a single carbon-12 atom. It is usually expressed in terms of the unified mass (u). From the periodic table [4, 5], we know that the atomic mass of carbon is 12.0107u and that for hydrogen is 1.00794u. Furthermore, the molecular mass M for a molecule X is defined as the sum of the atomic masses of all atoms in X.

Redžepović [6] examined the predictive and discriminative potentials of the Sombor and reduced Sombor indices of chemical graphs and showed that these molecular descriptors have good predictive potential. In a recent paper [7], Liu et al. reviewed the existing bounds and extremal results related to the Sombor index and its variants.

2. Main Results and Discussion

The alkanes have the general formula C_nH_{2n+2} [4]. The structural formulas of the first four members of the chain of alkanes are depicted in Figure 1.

We also have a branched chain of alkanes like isobutane or 2-methylpropane with the graph structure depicted in Figure 2.

By our discussion about molecular mass on the last paragraph of Section 1, the atomic mass of alkanes can be calculated by $M(C_nH_{2n+2}) = 14.026n + 2.016$ where n is the number of carbon atoms in the alkane under consideration.

Theorem 1. *The Sombor and reduced Sombor indices of the alkanes with n carbon atoms can be calculated by the following formulas:*

$$SO(C_nH_{2n+2}) = (4\sqrt{2} + 2\sqrt{17})n + (2\sqrt{17} - 4\sqrt{2}),$$
$$SO_{red}(C_nH_{2n+2}) = (3\sqrt{2} + 6)n + (6 - 3\sqrt{2}). \quad (1)$$

Proof. Define an equivalence relation on the straight and branched-chain alkanes and then apply mathematical induction.

The absolute error of a calculation is defined as the amount of error in measurements. It is the difference between the measured and actual values. In what follows, we compare the Sombor index of alkanes with their molecular masses. To do this, its absolute error will be calculated. □

Theorem 2. *If* $a_n = M(C_nH_{2n+2}) - SO(C_nH_{2n+2})$, *then the absolute error can be evaluated as* $a_n = M(C_nH_{2n+2}) - SO(C_nH_{2n+2}) \approx 0.123n - 0.573$.

Note that $\lim_{n\longrightarrow+\infty} M(C_nH_{2n+2}) - SO(C_nH_{2n+2}) \approx \lim_{n\longrightarrow+\infty} 0.123n - 0.573 = +\infty$.

Theorem 3. $0.972 < (M(C_nH_{2n+2})/SO(C_nH_{2n+2})) < 1.009$.

Proof. It is easy to calculate that $(M(CH_4)/SO(CH_4)) \approx 0.9727$, and so $0.972 < (M(C_nH_{2n+2})/SO(C_nH_{2n+2}))$. Other terms of the sequence $a_n = (M(C_nH_{2n+2})/SO(C_nH_{2n+2}))$ are as follows:

$$0.973, 0.989, 0.995, 0.999, 1.001, 1.002, \ldots, \frac{14.026n + 2.016}{(4\sqrt{2} + 2\sqrt{17})n + (2\sqrt{17} - 4\sqrt{2})}. \quad (2)$$

The limit of the sequence is approximately 1.009 because

$$\begin{aligned} \lim_{n\longrightarrow+\infty} a_n &= \lim_{n\longrightarrow+\infty} \frac{14.026n + 2.016}{(4\sqrt{2} + 2\sqrt{17})n + (2\sqrt{17} - 4\sqrt{2})} \\ \% \\ &= \lim_{n\longrightarrow+\infty} \frac{14.026n}{(4\sqrt{2} + 2\sqrt{17})n} = \frac{14.026}{(4\sqrt{2} + 2\sqrt{17})} \approx 1.0088 \approx 1.009. \end{aligned} \quad (3)$$

This proves that $(M(C_nH_{n+2})/SO(C_nH_{n+2})) < 1.009$, and none of the sequence sentences are equal to the sequence limit. So, $0.972 < (M(C_nH_{2n+2})/SO(C_nH_{2n+2})) < 1.009$.

The reduced Sombor index $SO_{red}(G)$ and the Sombor index SO(G) of the first nineteen alkanes are shown in Table 1.

As shown in the graph of Figure 3, the equivalent values of the Sombor index and molecular mass, based on the number of carbons, are approximately equal or close to each other. Also, Table2 shows that after the fourth alkane, the molecular mass is more than the Sombor index.

If a hydrogen atom is removed from an end carbon atom of a straight-chain alkane, then the resulting compound is called alkyl. For example, removing a hydrogen atom from methane gives the methyl group, OCH_3 [4]. The general formula of the straight-chain and the branched-chain alkyls is C_nH_{2n+1}, and it is clear that the molecular mass general formula is computed as $M(C_nH_{n+1}) = 14.026n + 1.008$, where n is the number of the carbon in the alkane. □

Theorem 4. *The Sombor and reduced Sombor indices of the alkyls are computed from the following formulas:*

$$SO(C_nH_{n+1}) = \begin{cases} 3\sqrt{10}, & n = 1, \\ (2\sqrt{17} + 4\sqrt{2})n + (2\sqrt{10} - \sqrt{17} - 8\sqrt{2} + 5), & n \geq 2, \end{cases}$$
$$SO_{red}(C_nH_{n+1}) = \begin{cases} 6, & n = 1, \\ (6 + 3\sqrt{2})n + (1 - 6\sqrt{2} + \sqrt{13}), & n \geq 2. \end{cases} \quad (4)$$

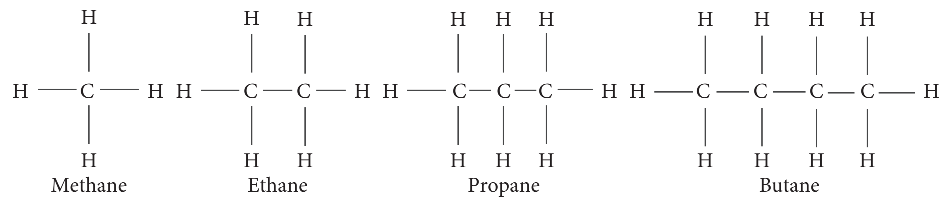

Figure 1: Straight chain of some alkanes.

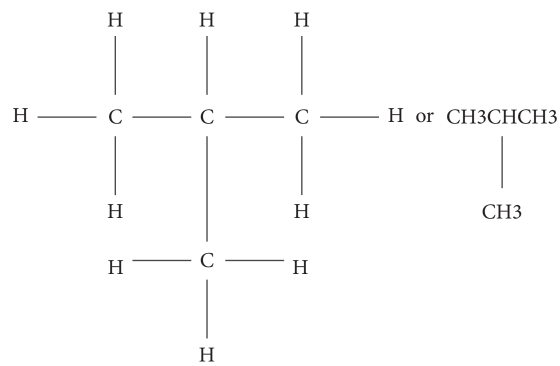

Figure 2: Branched chain of butane (isobutane) and its condensed structural formulas.

Proof. The result can be proved by defining an equivalence relation on straight and branched chain of alkyls and then applying the mathematical induction on n. □

Theorem 5. $1.009 < (M(C_nH_{2n+1})/SO(C_nH_{2n+1})) < 1.584$.

Proof. It is easy to see that $M(CH_3)/SO(CH_3) \approx 1.5846$, and so $1.548 > M(C_nH_{2n+1})/SO(C_nH_{2n+1})$. Consider the sequence with general formula $a_n = M(C_nH_{2n+1})/SO(C_nH_{2n+1})$. Then, approximately $a_1 = 1.585$, and for $n \geq 2$, the terms of the sequence are as follows:

$$1.227, 1.146, 1.109, 1.088, 1.074, 1.064, \ldots, \frac{14.026n + 1.008}{(2\sqrt{17} + 4\sqrt{2})n + (2\sqrt{10} - \sqrt{17} - 8\sqrt{2} + 5)}. \tag{5}$$

The limit of this sequence is approximately 1.009 because

$$\begin{aligned} \lim_{n \longrightarrow +\infty} a_n &\approx \lim_{n \longrightarrow +\infty} \frac{14.026n + 1.008}{(2\sqrt{17} + 4\sqrt{2})n + (2\sqrt{10} - \sqrt{17} - 8\sqrt{2} + 5)} \\ &= \lim_{n \longrightarrow +\infty} \frac{14.26n}{(2\sqrt{17} + 4\sqrt{2})n} = \frac{14.026}{(2\sqrt{17} + 4\sqrt{2})} \approx 1.0088 \approx 1.009. \end{aligned} \tag{6}$$

Since always $M(C_nH_{2n+1})/(SO(C_nH_{2n+1})) > 1.009$, none of the sequence terms are equal to the sequence limit. Therefore, $1.009 < (M(C_nH_{2n+1})/SO(C_nH_{2n+1})) < 1.584$.

Table 3 displays the Sombor index and molecular mass values of the first nineteen alkyls. In Figure 4, the upper line shows the molecular mass and the lower line is for the Sombor index.

Annulene belongs to a series of conjugated monocyclic hydrocarbons with chemical formulas C_nH_n, where n is even, and C_nH_{n+1}, where n is odd. Here, n denotes the

TABLE 1: Sombor index and molecular mass of some alkanes.

Name of alkane	$SO_{red}(G)$	SO (G)	Molecular mass (g/mol)	$Mass/So(G)$
Methane	12	16.492	16.042	0.973
Ethane	22.242	30.395	30.068	0.989
Propane	32.485	44.299	44.094	0.995
Butane	42.728	58.202	58.120	0.999
Pentane	52.971	72.105	72.146	1.001
Hexane	63.213	86.008	86.172	1.002
Heptane	73.456	99.911	100.198	1.003
Octane	83.698	113.814	114.224	1.004
Nonane	93.941	127.717	128.250	1.004
Decane	104.184	141.620	142.276	1.005
Undecane	114.426	155.523	156.302	1.005
Dodecane	124.669	169.426	170.328	1.005
Tridecane	134.912	183.329	184.354	1.006
Tetradecane	145.154	197.232	198.380	1.006
Pentadecane	155.397	211.135	212.406	1.006
Hexadecane	165.604	225.038	226.432	1.006
Heptadecane	175.882	238.941	240.458	1.006
Octadecane	186.125	252.845	254.484	1.006
Nonadecane	196.368	266.748	268.51	1.007

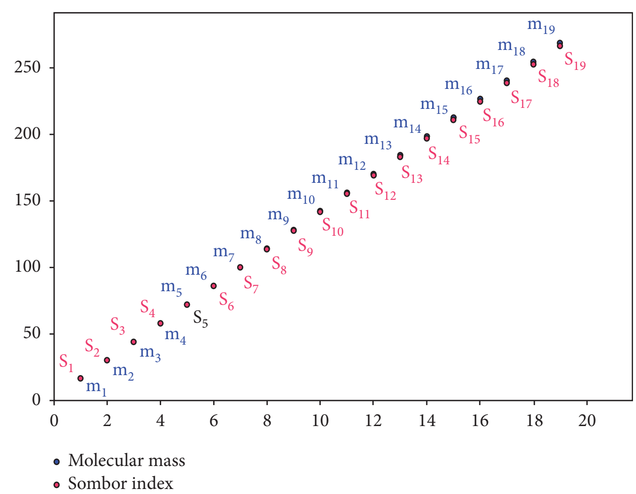

FIGURE 3: Sombor index and molecular mass of the first nineteen alkanes.

TABLE 2: Sombor index and molecular mass of some annulenes ($n = odd \geq 3$).

Name of annulene	$SO_{red}(G)$	SO (G)	Molecular mass (g/mol)	Mass/SO $(G)(n = \text{odd})$
[3]-Annulene	24.728	33.463	40.062	1.197
[5]-Annulene	39.213	53.023	66.098	1.246
[7]-Annulene	53.698	72.583	92.134	1.269
[9]-Annulene	68.184	92.143	118.170	1.282
[11]-Annulene	82.669	111.703	144.206	1.290
[13]-Annulene	97.154	131.263	170.242	1.296
[15]-Annulene	111.640	150.823	196.278	1.301
[17]-Annulene	126.125	170.382	222.314	1.304
[19]-Annulene	140.610	189.942	248.350	1.307

number of carbon atoms. Some of the most important members of this series are benzene ([6]-annulene), cyclobutadiene ([4]-annulene), cyclooctatetraene ([8]-annulene), and cyclotetradecaheptaene ([14]-annulene) [8]. It is clear that the molecular mass formula for annulenes with formula C_nH_{n+1} ($n = \text{odd} \geq 3$) is $M(C_nH_{n+1}) = 13.018n + 1.008$, and that for the annulenes with formula C_nH_n ($n = \text{even} \geq 4$) is $M(C_nH_n) = 13.018n$. Tables 3 and 4 show the values of the

Table 3: Sombor index and molecular mass values of some alkyls.

Name of alkyl	$SO_{red}(G)$	$SO(G)$	Molecular mass (g/mol)	Mass/$SO(G)$
Methyl	6	9.487	15.034	1.585
Ethyl	16.606	23.694	29.060	1.227
Propyl	26.848	37.597	43.086	1.146
Butyl	37.091	51.500	57.112	1.109
Pentyl	47.333	65.403	71.138	1.088
Hexyl	57.576	79.306	85.164	1.074
Heptyl	67.819	93.209	99.190	1.064
Octyl	78.061	107.112	113.216	1.057
Nonyl	88.304	121.015	127.242	1.052
Decyl	98.547	134.918	141.268	1.047
Undecyl	108.789	148.821	155.294	1.044
Dodecyl	119.032	162.725	169.320	1.041
Tridecyl	129.275	176.628	183.346	1.038
Tetradecyl	139.517	190.531	197.372	1.036
Pentadecyl	149.760	204.434	211.398	1.034
Hexadecyl	160.003	218.337	225.424	1.033
Heptadecyl	170.245	232.240	239.450	1.031
Octadecyl	180.488	246.143	253.476	1.030
Nonadecyl	190.730	260.046	267.502	1.029

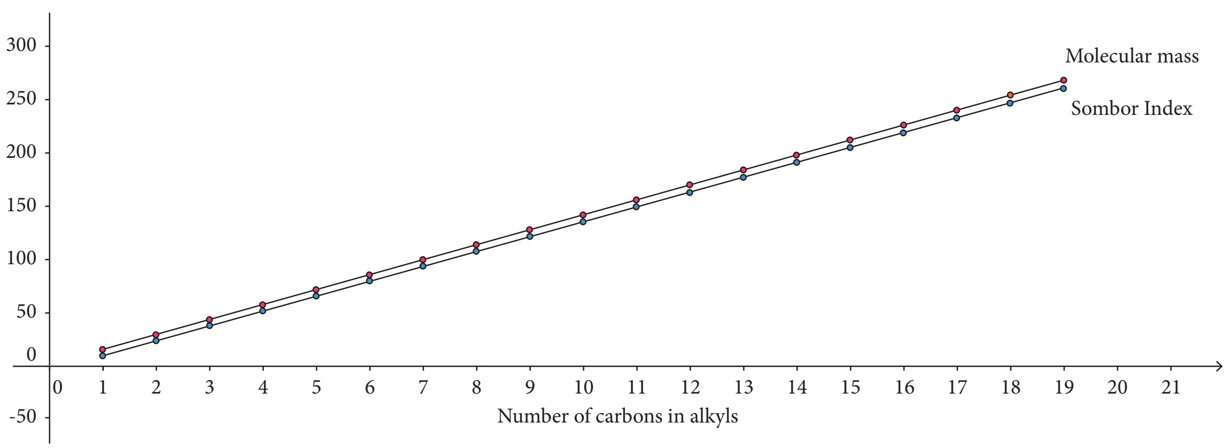

Figure 4: The Sombor index and molecular mass of nineteen alkyls with the correlation coefficient 1.

Sombor index and molecular mass of some annulenes. Their graphs are also drawn in Figures 5 and 6. □

Theorem 6. *The Sombor and reduced Sombor indices of the annulenes are computed from the following formulas:*

$$SO(G) = \begin{cases} (8\sqrt{2} + 2\sqrt{17})m + (4\sqrt{2} + 2\sqrt{17})m = \dfrac{n-1}{2}, & n = odd \geq 3, \\ (8\sqrt{2} + 2\sqrt{17})m + (8\sqrt{2} + 2\sqrt{17})m = \dfrac{n-2}{2}, & n = even \geq 4, \end{cases}$$

$$SO_{red}(G) = \begin{cases} (6 + 6\sqrt{2})m + (6 + 3\sqrt{2}) \quad m = \dfrac{n-1}{2}, & n = odd \geq 3, \\ (6 + 6\sqrt{2})m + (6 + 6\sqrt{2}) \quad m = \dfrac{n-2}{2}, & n = even \geq 4. \end{cases} \tag{7}$$

Table 4: Sombor index and molecular mass of some annulenes (n = even ≥ 4).

Name of annulene	$SO_{red}(G)$	SO (G)	Molecular Mass (gr/mol)	Mass/$SO(G)$ (n = even)
[4]-Annulene	28.971	39.120	52.072	1.331
[6]-Annulene	43.456	58.680	78.108	1.331
[8]-Annulene	57.941	78.240	104.144	1.331
[10]-Annulene	72.426	97.800	130.180	1.331
[12]-Annulene	86.912	117.360	156.216	1.331
[14]-Annulene	101.397	136.919	182.252	1.331
[16]-Annulene	115.882	156.479	208.288	1.331
[18]-Annulene	130.368	176.039	234.324	1.331

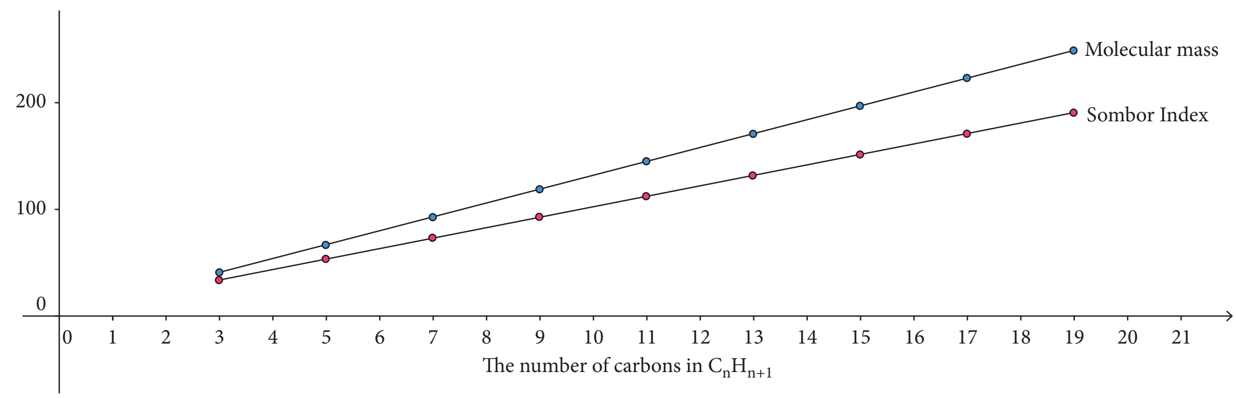

Figure 5: Diagram of Sombor index and molecular mass for some annulenes with odd n.

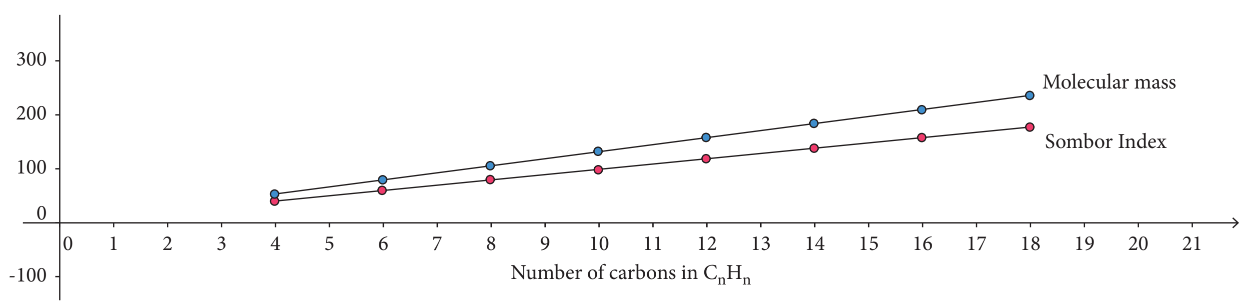

Figure 6: Diagram of Sombor index and molecular mass for some annulenes (n = even ≥ 4).

Proof. Induct on m. □

Theorem 7. $1.197 < (M(C_nH_{n+1})/SO(C_nH_{n+1})) < 1.331$.

Proof. It is easy to calculate that $(M(C_3H_4)/SO(C_3H_4)) \approx 1.1972$, and so $1.197 < (M(C_3H_4)/SO(C_3H_4))$. Consider the sequence $a_n = (M(C_nH_{n+1})/SO(C_nH_{n+1}))$, $n = odd \geq 3$. The terms of this sequence are

$$1.197, 1.245, 1.269, 1.282, 1.290, 1.296, \ldots, \frac{13.018\,n + 1.008}{(8\sqrt{2} + 2\sqrt{17})m + (4\sqrt{2} + 2\sqrt{17})}, \tag{8}$$

which shows that

$$\lim_{n \longrightarrow +\infty} a_n = \lim_{n \longrightarrow +\infty} \frac{13.018\,n + 1.008}{(8\sqrt{2} + 2\sqrt{17})((n-1)/2) + (4\sqrt{2} + 2\sqrt{17})} = \lim_{n \longrightarrow +\infty} \frac{13.018n}{(8\sqrt{2} + 2\sqrt{17}/2)n} = \frac{13.018}{(8\sqrt{2} + 2\sqrt{17}/2)} \approx 1.331. \tag{9}$$

The limit is 1.331, and hence $1.197 < (M(C_nH_{n+1})/SO(C_nH_{n+1})) < 1.331$. Similarly, we define $b_n = (M(C_nH_n)/SO(C_nH_n))$, $n = \text{even} \geq 4$. Then, the terms of this sequence are

$$1.331, 1.331, 1.331, 1.331, 1.331, 1.331, \ldots, \frac{13.018\,n}{(8\sqrt{2}+2\sqrt{17})((n-2)/2)+(8\sqrt{2}+2\sqrt{17})}, \tag{10}$$

and so

$$\lim_{n\longrightarrow+\infty} a_n = \lim_{n\longrightarrow+\infty} \frac{13.018\,n}{(8\sqrt{2}+2\sqrt{17})(n-2)/2+(8\sqrt{2}+2\sqrt{17})} = \lim_{n\longrightarrow+\infty} \frac{13.018n}{((8\sqrt{2}+2\sqrt{17})/2)n} = \frac{13.018}{((8\sqrt{2}+2\sqrt{17})/2)n} \approx 1.331. \tag{11}$$

This completes our argument. □

Theorem 8. *The Sombor index of the annulene series* ($n = \text{even} \geq 4$) *can be approximately written as* $M(C_nH_n) \approx 1.331 \times SO(C_nH_n)$.

Proof. Induct on n. □

3. Conclusion

In this article, the Sombor and reduced Sombor indices of the alkane, alkyl, and annulene groups were presented. We compare these values with the molecular mass of the first nineteen elements of these groups. It is shown that the fraction $M(G)/SO(G)$ has a good behavior which shows that Sombor index has good correlation with molecular mass. Finally, for any vertex degree-based topological index TI and/or any homologous series of molecules, the relation between TI and molecular mass is strictly linear.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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