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 $SO_{red}(G) = \sum_{uv \in E(G)} \sqrt{(d_G(u) - 1)^2 + (d_G(v) - 1)^2}$, 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 $C_nH_{2n+1}$ 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 \( C_n \text{H}_{2n+2} \) [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 \( M(C_n \text{H}_{2n+2}) = 14.026n + 2.016 \) 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:

\[
\begin{align*}
\text{SO}(C_n \text{H}_{2n+2}) & = (4\sqrt{2} + 2\sqrt{17})n + (2\sqrt{17} - 4\sqrt{2}), \\
\text{SO}_{\text{red}}(C_n \text{H}_{2n+2}) & = (3\sqrt{2} + 6)n + (6 - 3\sqrt{2}).
\end{align*}
\]

(1)

The limit of the sequence is approximately 1.009 because

\[
\lim_{{n \to \infty}} a_n = \lim_{{n \to \infty}} \frac{14.026n + 2.016}{(4\sqrt{2} + 2\sqrt{17})n + (2\sqrt{17} - 4\sqrt{2})} = \frac{14.026}{4\sqrt{2} + 2\sqrt{17}} \approx 1.0088 \approx 1.009.
\]

(2)

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

The reduced Sombor index \( \text{SO}_{\text{red}}(\text{G}) \) and the Sombor index \( \text{SO}(\text{G}) \) 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, Table 2 shows that after the fourth alkane, the molecular mass is more than the Sombor index.

\[
\begin{align*}
\text{SO}(C_n \text{H}_{2n+1}) & = \begin{cases} 
3\sqrt{10}, & n = 1, \\
(2\sqrt{10} + 4\sqrt{2})n + (2\sqrt{10} - \sqrt{17} - 8\sqrt{2} + 5), & n \geq 2,
\end{cases} \\
\text{SO}_{\text{red}}(C_n \text{H}_{2n+1}) & = \begin{cases} 
6, & n = 1, \\
(6 + 3\sqrt{2})n + (1 - 6\sqrt{2} + \sqrt{13}), & n \geq 2.
\end{cases}
\end{align*}
\]

(3)

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

Note that \( \lim_{{n \to \infty}} M(C_n \text{H}_{2n+2}) - \text{SO}(C_n \text{H}_{2n+2}) = \lim_{{n \to \infty}} 0.123n - 0.573 = +\infty \).

Theorem 3. \( 0.972 < (M(C_n \text{H}_{2n+2})/\text{SO}(C_n \text{H}_{2n+2})) < 1.009 \).

Proof. It is easy to calculate that \( (M(\text{CH}_4)/\text{SO}(\text{CH}_4)) \approx 0.9727 \), and so \( 0.972 < (M(C_n \text{H}_{2n+2})/\text{SO}(C_n \text{H}_{2n+2})) \). Other terms of the sequence \( a_n = (M(C_n \text{H}_{2n+2})/\text{SO}(C_n \text{H}_{2n+2})) \) are as follows:

\[
\begin{align*}
a_1 & = 14.026 \approx 1.0088, \\
a_2 & = 0.123, \\
a_3 & = 0.123, \\
a_4 & = 0.123, \\
a_5 & = 0.123, \\
a_6 & = 0.123, \\
& \vdots
\end{align*}
\]

(4)

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 \( C_n \text{H}_{2n+1} \), and it is clear that the molecular mass general formula is computed as \( M(C_n \text{H}_{2n+1}) = 14.026n + 1.008 \), 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:
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:

$$1.227, 1.146, 1.109, 1.088, 1.074, 1.064, \ldots$$

$$= \frac{14.026n + 1.008}{(2\sqrt{17} + 4\sqrt{2})n + (2\sqrt{10} - \sqrt{17} - 8\sqrt{2} + 5)}$$

(5)

The limit of this sequence is approximately 1.009 because

$$\lim_{n \to \infty} a_n = \lim_{n \to \infty} \frac{14.026n + 1.008}{(2\sqrt{17} + 4\sqrt{2})n + (2\sqrt{10} - \sqrt{17} - 8\sqrt{2} + 5)}$$

$$= \lim_{n \to \infty} \frac{14.026n}{(2\sqrt{17} + 4\sqrt{2})n} = \frac{14.026}{2\sqrt{17} + 4\sqrt{2}} \approx 1.0088 \approx 1.009.$$ 

(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
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 \( C_nH_m \) \((n = \text{odd} \geq 3)\) is 
\[ M(C_nH_m) = 13.018 n + 1.008, \]
and that for the annulenes with formula \( C_nH_m \) \((n = \text{even} \geq 4)\) is 
\[ M(C_nH_m) = 13.018 n. \] 
Tables 3 and 4 show the values of 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       | 32.488         | 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          |
| Octodecane    | 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 \((n = \text{odd} \geq 3)\).

| Name of annulene | \( SO_{red}(G) \) | \( SO(G) \) | Molecular mass \((g/mol)\) | \( Mass/So(G) \) |
|-----------------|----------------|----------------|-----------------|----------------|
| [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          |
Theorem 6. The Sombor and reduced Sombor indices of the annulenes are computed from the following formulas:

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

\[
SO_{\text{red}}(G) = \begin{cases} 
(6 + 6\sqrt{2})m + (6 + 3\sqrt{2}) & m = \frac{n-1}{2}, & n = \text{odd} \geq 3, \\
(6 + 6\sqrt{2})m + (6 + 6\sqrt{2}) & m = \frac{n-2}{2}, & n = \text{even} \geq 4.
\end{cases}
\]

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

| Name of alkyl | \(SO_{\text{red}}(G)\) | \(SO(G)\) | 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.
Proof. Induct on $m$.

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

Proof. It is easy to calculate that $\frac{M(C_2H_4)}{SO(C_2H_4)} = 1.1972$, and so $1.197 < \frac{M(C_2H_4)}{SO(C_2H_4)}$. Consider the sequence $a_n = \frac{M(C_nH_{n+1})}{SO(C_nH_{n+1})}$, $n = odd \geq 3$. The terms of this sequence are

$$1.197, 1.245, 1.269, 1.282, 1.290, 1.296, \ldots$$

which shows that

$$\lim_{n \to \infty} a_n = \lim_{n \to \infty} \frac{13.018n + 1.008}{(8\sqrt{2} + 2\sqrt{17})(n - 1/2) + (4\sqrt{2} + 2\sqrt{17})} = \frac{13.018}{(8\sqrt{2} + 2\sqrt{17}/2)} = 1.331.$$ (9)
The limit is 1.331, and hence 1.197 < \frac{M(C_nH_n)}{SO(C_nH_n)} < 1.331. Similarly, we define \( b_n = \frac{M(C_nH_n)}{SO(C_nH_n)} \), \( n = \text{even} \geq 4 \). Then, the terms of this sequence are
\[ 1.331, 1.331, 1.331, 1.331, 1.331, 1.331, \ldots, \]
and so
\[ \lim_{n \to \infty} a_n = \lim_{n \to \infty} \frac{13.018 n}{(8\sqrt{2} + 2\sqrt{17}) \cdot (n - 2)/2 + (8\sqrt{2} + 2\sqrt{17})} = \frac{13.018}{(8\sqrt{2} + 2\sqrt{17})/2} \approx 1.331. \] (10)

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 \( T_I \) and/or any homologous series of molecules, the relation between \( T_I \) 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.

### References

[1] I. Gutman, “Geometric approach to degree-based topological indices: Sombor indices,” MATCH Communication. Maths. Computer. Chemistry, vol. 86, pp. 11–16, 2021.
[2] R. Cruz, I. Gutman, and J. Rada, “Sombor index of chemical graphs,” Applied Mathematics and Computation, vol. 399, Article ID 126018, 2021.
[3] I. Gutman, “Sombor index—one year later,” Bulletin. Classe des Sciences Mathematiques et Naturelles, vol. 45, pp. 43–55, 2020.
[4] D. D. Ebbing and S. D. Gammon, General Chemistry, Charles Hartford, Boston, MA, USA, 9th edition, 2009.
[5] R. H. Petrucci, F. G. Herring, J. D. Madura, and C. Bissonnette, General Chemistry: Principles and Modern Applications, Prentice Hall PTR, Hoboken, NJ, USA, 10th edition, 2010.