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BOILING POINT MODELING OF EUGENOL COMPOUNDS AND ITS DERIVATIVES USING THE SOMBOR INDEX AND REDUCED SOMBOR INDEX APPROACHES

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Abstract. Eugenol and its derivatives, phenylpropanoid compounds derived from plants like *Syzygium aromaticum*, exhibit significant biological activities, including antimicrobial, antifungal, anti-inflammatory, antioxidant, analgesic, and anticancer properties. These attributes make them valuable in drug development and medical applications. In mathematical chemistry, chemical topology graphs are used to determine the topological indices of molecules, which help predict physical and chemical properties. Here, atoms are represented as nodes and bonds as edges. This study explores the relationship between the Sombor index, the reduced Sombor index, and the boiling points of eugenol and its derivatives. The methodology includes literature review and computational analysis of the indices, followed by correlation analysis with the boiling points. The findings reveal that the Sombor index negatively correlates with the boiling point, accounting for 84.8% of the variation. This implies that an increase in the Sombor index results in a lower boiling point. Conversely, the reduced Sombor index demonstrates a positive correlation, influencing 36.1% of the boiling point variations, indicating that higher reduced Sombor indices correspond to higher boiling points. When combined, the Sombor and reduced Sombor indices explain 86.4% of the boiling point variance, highlighting their significance as predictive parameters. These results provide insights into the thermal properties of eugenol-based compounds and their potential applications in material and pharmaceutical sciences. By leveraging these indices, researchers can better predict and tailor the physical properties of eugenol derivatives for specific purposes.
Keywords: Eugenol, Chemical Topology Graph, Sombor Index, Reduced Sombor Index.

I. INTRODUCTION

In recent years, studies related to graph theory in describing algebraic structures have become an increasingly intensive focus of research. These research studies are concerned with the construction and properties of graphs that underlie the structure of mathematical groups[1]. Graph theory has many uses in mathematics, for example in algebraic structures, graphs are used to represent a group or ring. In chemistry, graphs can be used to solve molecular problems. Furthermore, graphs are closely related to topological indices. A topological index is a numerical value that reflects the structural properties and connectivity of a graph. These values are used to numerically represent chemical structures, as well as help predict various chemical properties, the physical structure of molecules, and their chemical reactions[2]. In the field of chemical topological graphs, graph theory is used to represent models of chemical molecules, where atoms are treated as a set of corner points, and bonds between atoms form a set of edges in the graph[3].

One of the important topological indices in mathematical chemistry is the Sombor Index. This index was introduced by Ivan Gutman in 2021 and has a significant role in analyzing molecular structures. In graph theory, the Sombor Index is calculated based on the degree of connection between atoms in the molecule [4]. The Sombor Index is one of the topological parameters in quantum chemistry used to study molecular structures based on chemical graphs [5]. This index is useful for predicting physicochemical properties, molecular reactivity, and biological parameters in computational chemistry. The Sombor Index is known for considering the squared contribution of the vertex degree, which makes it different from other topological indices such as the Randić or Wiener Index [6]. The Reduced Sombor Index is a modification of the Sombor Index designed to provide a different perspective in molecular graph analysis. It calculates values based on the degree of vertices subtracted by one, making it more relevant for some chemical and molecular structure applications [7]. These two topological indices play an important role in predicting the physical properties of chemical molecular compounds by numerically calculating the molecular compounds by representing atoms as vertices and bonds between atoms as edges.

Eugenol is a natural phenolic compound found in various plants, especially in cloves (Syzygium aromaticum), bay leaves, cinnamon, and nutmeg. Eugenol has a distinctive aroma and various benefits that make it important in various fields [8]. Some derivatives of eugenol compounds are used in various specific fields such as the pharmaceutical field, perfume industry, cosmetics, food industry and agriculture [9]. The physical properties of eugenol compounds make it one of the important factors in its application, one of which is the boiling point. Usually, to find out the magnitude of the boiling point in chemical compounds, laboratory tests are carried out, but it can also be known by numerically calculating the compound using the calculation of the sombor index and the reduced sombor index [10]. This article aims to model the effect of sombor index and reduced sombor index on eugenol compounds and their derivatives so that the results of the modeling can be used to determine the boiling point of eugenol compound derivatives without conducting laboratory tests.

II. MAIN RESULT

This study aims to reveal the relationship pattern between molecular properties, such as boiling point with the Sombor index and the reduced Sombor index. Therefore, in this discussion, the results of the calculation of the Sombor index and the reduced Sombor index will be compared, and their relationship to the boiling point of eugenol compound derivatives will be analyzed. The following are the definitions of the Sombor index and the reduced Sombor index.

Definition 1. [11] Suppose given a graph G with vertex set $V(G)$ and edge set $E(G)$. Then the summory index of G, denoted by $SO(G)$ is

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

Definition 2. [11] Suppose a graph G with vertex set $V(G)$ and edge set $E(G)$ is given. Then the reduced Sombor index of G denoted by $SO_{red}(G)$ is

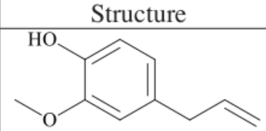
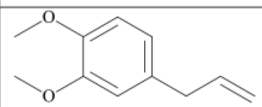
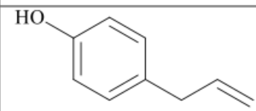
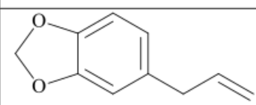
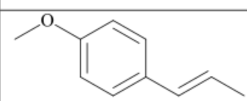
$$SO_{red}(G) = \sum_{(u,v)\in E(G)} \sqrt{(d(u)-1)^2 + (d(v)-1)^2}.$$

The definition above will be used in the calculation of the Chemical Topological Graph which is continued by analyzing the correlation between the values of the two indices with the boiling point of the eugenol compound derivatives. This analysis aims to understand the extent of the relationship between the structural parameters represented by the Sombor index and the reduced Sombor index with the physical properties of the compound, namely its boiling point. This section will present the results of research that discusses the boiling point model of five eugenol derivatives, with an approach using the Sombor index and the reduced Sombor index, as well as a comparison between the two models.

2.1 Compound Structure of Eugenol and its Derivatives

Eugenol and its derivatives are compounds of the phenylpropanoid pathway that have an aromatic ring-based structure (C6) with a three-carbon chain (C3), in which the hydroxyl (-OH) and methoxyl ($-OCH_3$) groups on the aromatic ring provide characteristic chemical properties and affect physical properties such as boiling point. These compounds are produced through the transformation of p-coumaryl-CoA which is a common precursor in the phenylpropanoid pathway through a series of specific enzymatic reactions producing compounds such as eugenol and its derivatives.

The following are the molecular structures and boiling points of 5 eugenol-derived compounds for which the Sombor index and reduced Sombor index will be calculated:

No.	Compound Name	Structure	Boiling Point (°C)
1.	Eugenol		254
2.	Methyl Eugenol		255
3.	4-Allylphenol		238
4.	Safrole		234
5.	Anethole		234

2.2 Modeling the Effect of Sombor Index on Eugenol Compound Derivatives

In this section we will discuss the calculation of the Sombor index of eugonol compound derivatives, the Sombor index on eugenol compound derivatives is calculated based on the groups in the chemical structure. Here is one of the calculation results of the eugenol compound:

$$
\begin{aligned}
SO\,(G) &= \sum_{(u,v)\in E(G)} \sqrt{d_u{}^2 + d_v{}^2} \\
&= \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{H\}}} \sqrt{d(u)^2 + d(v)^2} + \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{C*\}}} \sqrt{d(u)^2 + d(v)^2} \\
&\quad + \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{C**\}}} \sqrt{d(u)^2 + d(v)^2} + \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{O\}\\ u,v\in\{-OH\}}} \sqrt{d(u)^2 + d(v)^2} \\
&\quad + \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{O\}\\ u,v\in\{-OCH_3\}}} \sqrt{d(u)^2 + d(v)^2} \\
&= \sum_{\substack{(u,v)\in E(G)\\ u\in\{C\}\\ v\in\{H\}}} \sqrt{3^2 + 1^2} + \sum_{\substack{(u,v)\in E(\Gamma_{D_{2n}})\\ u\in\{C\}\\ v\in\{C*\}}} \sqrt{3^2 + 3^2} + \sum_{\substack{(u,v)\in E(\Gamma_{D_{2n}})\\ u\in\{C\}\\ v\in\{C**\}}} \sqrt{2^2 + 2^2} \\
&\quad + \sum_{\substack{(u,v)\in E(\Gamma_{D_{2n}})\\ u\in\{C\}\\ v\in\{O\}\\ u,v\in\{-OH\}}} \sqrt{3^2 + 1^2} + \sum_{\substack{(u,v)\in E(\Gamma_{D_{2n}})\\ u\in\{C\}\\ v\in\{O\}\\ u,v\in\{-OCH_3\}}} \sqrt{3^2 + 2^2} \\
&= 5\sqrt{10} + 6\sqrt{18} + \sqrt{8} + \sqrt{10} + \sqrt{13} \\
&= 50.8
\end{aligned}
$$

For the calculation results of the Sombor index on other eugenol compound derivatives, see table 2.2.1

.

Below are the boiling point values and Sombor index of five eugenol derivatives:

Table 2. 2. 1 Boiling Point Value and Sombor Index of Eugenol Derivative Compounds

Compound	Boiling Point (℃)	Sombor Index
Eugenol	254	50.8
Methyl Eugenol	249	57.1
4- Allylphenol	238	58.9
Safrole	234	62.9
Anethole	234	66.6

Based on the boiling point and Sombor index in table 2.2.1, a linear regression analysis can be performed to determine the relationship pattern. The correlation between the boiling point and the Sombor index value of the eugenol compound derivative is relatively strong, the following are the results of the linear regression analysis.

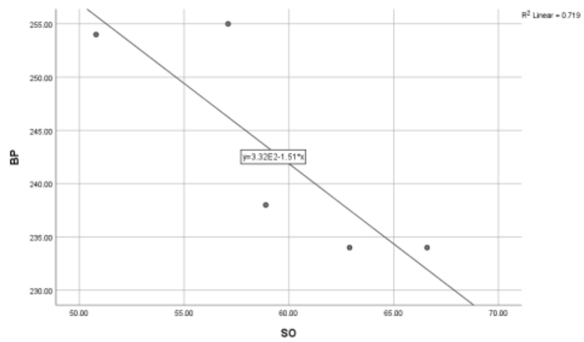


Figure 2.2. 1 Correlation Chart of Sombor Index to Boiling Point

Figure 2.2.1 is the result of correlation analysis between boiling point and Sombor index value, obtained R^2 value (coefficient of determination) of 0.719. This shows that the Sombor index gives an influence of 71,9% on the boiling point. Based on the figure, the correlation found is relatively strong, but negative. This means that the relationship between Sombor index and boiling point is inversely proportional, that is, if the value of Sombor index increases, the boiling point value will decrease, and vice versa.

In addition, the regression model to predict the boiling point using the independent variable is the Sombor index as follows:

$$Boiling\ Point\ (BP) = 3{,}32 \times 10^2 - 1{,}51 * (SO)$$

This regression model of the boiling point can be used to determine the boiling point of the latest Eugenol compound derivatives only by knowing the value of the Sombor index.

2.3 Modeling the effect of Reduced Sombor Index on 5 Eugenol derivatives

In this section will be discussed about the calculation of the reduced spear index of eugonol compound derivatives, the reduced spear index on eugenol derivatives is calculated based on the groups in the chemical structure. here is one of the calculation results of eugenol compounds:

For the calculation results of the reduced spear index on other eugenol compound derivatives, see table 3.1.

The following is the boiling point value and reduced Sombor index on 5 Eugenol derivatives:

Compound	Boiling Point (°C) (BP)	Indeks Sombor Tereduksi (SO_{red})
Eugenol	254	23.30
Methyl Eugenol	249	24.54
4- Allylphenol	238	20.07
Safrole	234	25.37

Anethole	234	20.70

Based on the linear regression analysis, it was found that the correlation between the boiling point and the value of the reduced Sombor index is relatively weak, here are the results of the linear regression analysis.

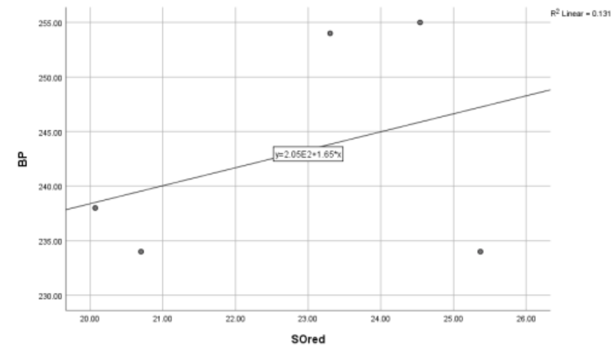


Figure 2.3. 1 Correlation Chart of Reduced Sombor Index to Boiling Point

In the figure above is the result of the correlation analysis between the boiling point and the value of the reduced Sombor index, the R value of the reduced Sombor index on the boiling point is 0.361 or 36.1%. The R value with a magnitude of 36.1% means that the effect of the reduced Sombor index on the boiling point of eugenol and its derivatives is relatively weak. In addition, the R^2 (coefficient of determination) value is 0.131, which shows the ability of the Sombor index to interpret the boiling point by 13.1%. Based on the figure, it is also found that the correlation is relatively weak, so that this reduced Sombor index has a weak influence on the boiling point of the 5 eugenol derivatives.

2.4 Modeling the effect of Sombor index and Reduced Sombor Index on Eugenol derivatives

Based on the explanation in points 1 and 2 above, it is found that the results of the analysis using linear regression get the result that the Sombor index is more influential on the 5 turnan of eugenol compounds compared to the reduced Sombor index.

The following are the results of regression analysis for both independent variables, namely Sombor index and reduced Sombor index to the boiling point:

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.864[a]	.747	.495	7.55630

a. Predictors: (Constant), SO, SOred

Figure 2.4. 1 Correlation of Sombor Index and Reduced Sombor Index at Boiling Point

In Figure 2.4.1, it is found that the correlation that occurs between the boiling point when using both variables, namely the Sombor index and the reduced Sombor index, has a very strong correlation because the R value is 0.864 or 86.4%, meaning that the Sombor index and the reduced Sombor index have an influence on the boiling point. It's just that for the reduced Sombor index there is a weak correlation of 13,1% and the Sombor index has a relatively strong correlation of 85.3%.

The following is a table to determine the regression model of the boiling point by the Sombor index and the reduced Sombor index:

Model		Unstandardized Coefficients B	Std. Error
1	(Constant)	310.076	60.147
	SOred	.785	1.667
	SO	-1.434	.649

Figure 2.4. 2 Estimation of the Relationship Pattern of Sombor Index and Sombor Index to Boiling Point

Figure 2.4.1 is used to estimate the relationship pattern/functional form between the Sombor index and the reduced Sombor index to the boiling point (BP) with the general model $Yi = \beta 0 + \beta 1\, Xi + \varepsilon i$ Estimating the regression equation means determining the parameter estimator so as to obtain an estimator with a line equation model $\hat{Y} = b0 + b1Xi$. The table above provides information on the constant value $(b0)$ of 310.076 while the regression coefficient value $(b1)$ is -1.434 and for the regression coefficient value $(b2)$ is 0.785 so that a linear regression equation is obtained, namely:

$$\hat{Y} = 310.076 - 1.434(SO) + 0.649(SOred)$$

The equation means that the constant value of the boiling point variable is 310.076 with a regression coefficient of the Sombor index of -1.434 which states that for every 1% increase in the boiling point of the Sombor index, it will decrease by 1.434 while there is a 1% increase in the boiling point of the reduced Sombor index which means an increase of 0.649. The regression coefficient on the Sombor index is negative, so it can be said that the direction of the influence of the Sombor index on the boiling point is negative. While the coefficient of the reduced Sombor index is positive, which means that it has a positive but very weak influence.

III. CONCLUSIONS

In this study, the following conclusions were obtained:

1. The effect of Sombor index on the boiling point of eugenol compound derivatives is 84.8% which is negatively correlated, meaning that the higher the Sombor index, the boiling point decreases, and vice versa. The regression model to predict the boiling point using the Sombor index is:
$$Titik\ Didih\ (BP) = 3{,}32 \times 10^2 - 1{,}51 * (SO)$$
2. The effect of the reduced Sombor index on the boiling point of eugenol compound derivatives has an effect of 36.1% which is positively correlated, meaning that the higher the reduced Sombor index, the boiling point increases, and vice versa.
3. The effect of Sombor index and reduced Sombor index on the boiling point of eugenol compound derivatives is 86.4% which has a strong influence on the boiling point. The regression model to predict the boiling point using the Sombor index and the reduced Sombor index is:
$$\hat{Y} = 310.076 - 1.434(SO) + 0.649(SOred)$$

These are the results obtained in this study related to the effect of Sombor index and reduced Sombor index and its regression model on the boiling point of eugenol and its derivatives.

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