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Article

Entropies via Various Molecular Descriptors of Layer Structure of H_3BO_3

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Abstract: Entropy is essential. Entropy is a measure of a system's molecular disorder or unpredictability, since work is produced by organized molecular motion. Entropy theory offers a profound understanding of the direction of spontaneous change for many commonplace events. A formal definition of a random graph exists. It deals with relational data's probabilistic and structural properties. The lower-order distribution of an ensemble of attributed graphs may be used to describe the ensemble by considering it to be the results of a random graph. Shannon's entropy metric is applied to represent a random graph's variability. A structural or physicochemical characteristic of a molecule or component of a molecule is known as a molecular descriptor. A mathematical correlation between a chemical's quantitative molecular descriptors and its toxicological endpoint is known as a QSAR model for predictive toxicology. Numerous physicochemical, toxicological, and pharmacological characteristics of chemical substances help to foretell their type and mode of action. Topological indices were developed some 150 years ago as an alternative to the Herculean, and arduous testing is needed to examine these features. This article uses various computational and mathematical techniques to calculate atom–bond connectivity entropy, atom–bond sum connectivity entropy, the newly defined Albertson entropy using the Albertson index, and the IRM entropy using the IRM index. We use the subdivision and line graph of the H_3BO_3 layer structure, which contains one boron atom and three oxygen atoms to form the chemical boric acid.

Keywords: entropies via various molecular descriptors; H_3BO_3 layer structure; subdivision of H_3BO_3; line graph of H_3BO_3

MSC: 05C07; 05C09; 05C31; 05C76; 05C99

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1. Introduction

Theoretical chemistry and graph theory are combined in chemical graph theory (CGT). It makes a contribution to the modeling of actual and fictitious chemical substances, examines the mathematical structure and connectedness, and then unifies the mathematical and chemical notions [1]. A chemical compound is modeled by displaying its structural formula as a chemical graph, in which atoms are represented by vertices and chemical bonds by edges [2].

We determine a structure's distance-based entropy by using some well-known topological indices, which are the numbers that help characterize its topological features after it has been reproduced. The many pharmacological, physicochemical (such as melting point, boiling temperature, volume, molecular weight, density, etc.), and toxicological properties of a chemical molecule have a link with these invariants [3–5]. Topological indices have the amazing feature of remaining constant over graph isomorphisms, making them typically graph-invariant [6–14]. Numerous topological indices based on chemical graphs that rely on the number of vertices have been discovered and studied [15–19]. The atom–bond connectivity index and its modified form, the atom–bond sum connectivity index, the Albertson index, and the IRM index, as well as their mathematical equations, are introduced and defined in this section. For more explanation, see [20–27].

The atom–bond connectivity index was established by Estrada et al. [28] and is a modified version of the connectivity index. It is described as

$$ABC(G,x) = \sum_{a_i \sim \dot{a}_2} x^{\sqrt{\frac{(V_{\dot{a}_1}+V_{\dot{a}_2}-2)}{(V_{\dot{a}_1}\times V_{\dot{a}_2})}}} \quad \& \quad ABC = \sum_{\dot{a}_1 \sim \dot{a}_2} \sqrt{\frac{(V_{\dot{a}_1}+V_{\dot{a}_2}-2)}{(V_{\dot{a}_1}\times V_{\dot{a}_2})}} \tag{1}$$

Zhou and Trinajstic [29] proposed the sum-connectivity index, $\sum_{u,v\in\xi_g} \frac{1}{\sqrt{V_{a_i}+V_{a_j}}}$, an alternative to the connectivity index. The atom–bond sum-connectivity (ABS) index is a recently proposed modification of the atom–bond connectivity index that makes use of the fundamental concept of the sum-connectivity index [30]. A definition of the ABS index is

$$ABS(G,x) = \sum_{a_i \sim a_j} x^{\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}} \quad \& \quad ABS = \sum_{a_i \sim a_j} \sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}} \tag{2}$$

To determine a graph's irregularity, the authors in [31] established the Albertson index A(G).

$$A(G,x) = \sum_{a_i \sim a_j} x^{|V_{a_i}-V_{a_j}|} \quad \& \quad A(G) = \sum_{a_i \sim a_j} |V_{a_i}-V_{a_j}| \tag{3}$$

The irregularities of the graph are gauged using the Albertson, Bell, and IRM indices [32]. The definition of IRM(G) is

$$IRM(G,x) = \sum_{a_i \sim a_j} x^{[V_{a_i}-V_{a_j}]^2} \quad \& \quad IRM(G) = \sum_{a_i \sim a_j} [V_{a_i}-V_{a_j}]^2 \tag{4}$$

In this paper, we work with Boric acid H_3BO_3. It is an acid made up of four oxygen atoms, one phosphorus atom, and three hydrogen atoms. Boric acid is sometimes referred to as orthoboric acid, boracic acid, hydrogen borate, or acidum boricum. It possesses antiviral, antifungal, and antiseptic qualities and is a weak acid. Figure 1 depicts the boric acid complex, which consists of one boron atom, three oxygen atoms, and three hydrogen atoms. The floral pattern structure (base unit) depicted in Figure 1 is created by polymerizing the H_3BO_3 unit structure, which consists of six repeating units of H_3BO_3.

The degree of unpredictability (or disorder) in a system is measured by entropy. It may also be considered a measurement of how evenly the molecules in the system distribute their energy. The number of alternative configurations of molecule position and the amount of kinetic energy at a specific thermodynamic state is known as a microstate.

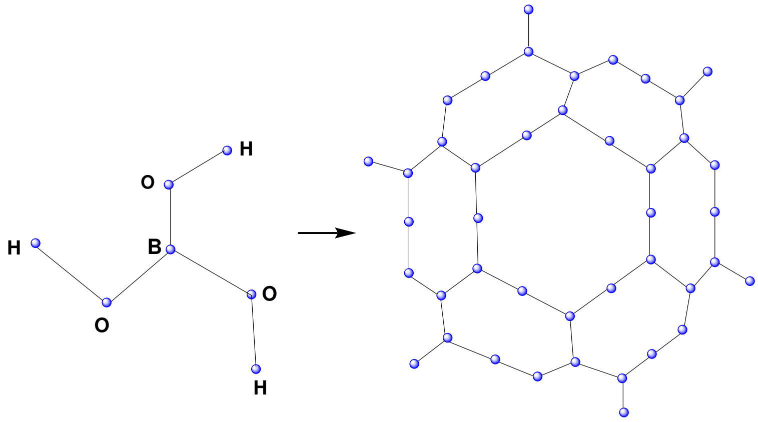

Figure 1. Boric acid H_3BO_3.

Entropies via Various Molecular Descriptors

Ghani et al. in [33] and Manzoor et al. in [34] recently offered another strategy that is a little bit novel in the literature: applying the idea of Shannon's entropy [35] in terms of topological indices. The following formula represents the graph entropy:

$$ENT_{\mu(G)} = -\sum_{a_i \sim a_j} \frac{\mu(V_{a_i}V_{a_j})}{\sum\limits_{a_i \sim a_j} \mu(V_{a_i}V_{a_j})} \log\left\{\frac{\mu(V_{a_i}V_{a_j})}{\sum\limits_{a_i \sim a_j} \mu(V_{a_i}V_{a_j})}\right\}. \tag{5}$$

where a_1, a_2 represents atoms, ξ_G represents the edge set, and $\mu(V_{a_i}V_{a_j})$ represents the edge weight of edge $(V_{a_i}V_{a_j})$.

- **Entropy related to ABC index**

Let $\mu((a_i)(a_j)) = \left\{\sqrt{\frac{V_{a_i}+V_{a_j}-2}{V_{\dot{a}_i}\times V_{\dot{a}_j}}}\right\}$. Then ABC index (1) is given by

$$ABC_G = \sum_{a_i,a_j \in \xi_G} \left\{\sqrt{\frac{V_{a_i}+V_{a_j}-2}{V_{a_i}\times V_{a_j}}}\right\} = \sum_{a_i,a_j \in \xi_G} \mu((a_i)(a_j)).$$

Adding the parameters of ABC_G into Equation (5), then the atom–bond connectivity (ENT_{ABC}) entropy is

$$ENT_{ABC_G} = \log(ABC_G) - \frac{1}{ABC_G} \log\left\{\prod_{a_i,a_j \in \xi_G} \left(\sqrt{\frac{V_{a_i}+V_{a_j}-2}{V_{a_i}\times V_{a_j}}}\right)^{\left(\sqrt{\frac{V_{a_i}+V_{a_j}-2}{V_{a_i}\times V_{a_j}}}\right)}\right\}. \tag{6}$$

- **Entropy related to ABS index**

Let $\mu((a_i)(a_j)) = \left\{\sqrt{\frac{V_{a_i}+V_{a_j}-2}{V_{a_i}+V_{a_j}}}\right\}$. Then the ABS index (2) is given by

$$ABS_G = \sum_{a_i,a_j \in \xi_G} \left\{\sqrt{\frac{V_{a_i}+V_{a_j}-2}{V_{a_i}+V_{a_j}}}\right\} = \sum_{a_i,a_j \in \xi_G} \mu((a_i)(a_j)). \tag{7}$$

Adding the parameters of ABS_G into Equation (5), then the atom–bond sum connectivity $(ENT_{ABC(G)})$ entropy is

$$ENT_{ABS_G} = \log(ABS_G) - \frac{1}{ABS_G} \log\left\{\prod_{a_i,a_j \in \xi_G} \left(\sqrt{\frac{V_{a_i}+V_{a_j}-2}{V_{a_i}+V_{a_j}}}\right)^{\left(\sqrt{\frac{V_{a_i}+V_{a_j}-2}{V_{a_i}+V_{a_j}}}\right)}\right\}. \tag{8}$$

- **Entropy related to Albertson index**

Let $\mu((a_i)(a_j)) = \left\{|V_{a_i} - V_{a_j}|\right\}$. Then the Alberston entropy (3) is given by

$$A_{(G)} = \sum_{a_i, a_j \in \xi_G} \left\{|V_{a_i} - V_{a_j}|\right\} = \sum_{a_i, a_j \in \xi_G} \mu((a_i)(a_j)).$$

Adding the parameters of $A_{(G)}$ into Equation (5), then the Alberston $(ENT_{A)})$ entropy is

$$ENT_{A_{(G)}} = \log\left(A_{(G)}\right) - \frac{1}{A_{(G)}} \log\left\{ \prod_{a_i, a_j \in \xi_G} \left(|V_{a_i} - V_{a_j}|\right)^{\left(|V_{a_i} - V_{a_j}|\right)} \right\}. \quad (9)$$

- **Entropy related to IRM index**

Let $\mu((a_i)(a_j)) = \left\{[V_{a_i} - V_{a_j}]^2\right\}$. Then the IRM entropy (4) is given by

$$IRM_{(G)} = \sum_{a_i, a_j \in \xi_G} \left\{[V_{a_i} - V_{a_j}]^2\right\} = \sum_{a_i, a_j \in \xi_G} \mu((a_i)(a_j)).$$

Adding the parameters of $IRM_{(G)}$ into Equation (5), then the IRM (ENT_{IRM}) entropy is

$$ENT_{IRM_{(G,x)}} = \log IRM_{(G)} - \frac{1}{IRM_{(G,x)}} \log\left\{ \prod_{a_i, a_j \in \xi_G} \left([V_{a_i} - V_{a_j}]^2\right)^{\left([V_{a_i} - V_{a_j}]^2\right)} \right\}. \quad (10)$$

2. Layer Structure of $H_3BO_3(s,t)$

In this section, we discuss the $H_3BO_3(s,t)$ layer structure, which serves as the foundation for its subdivision and line graph. The $H_3BO_3(s,t)$ unit structure polymerizes to generate the floral pattern structure (base unit) seen in Figure 2, which is made up of six repeating H_3BO_3 units. This layer structure may be stretched to whatever number of rows and columns is desired. The horizontal lines of floral pattern structures are characterized as rows "s", while the vertical lines are designated as columns "t". Figure 2 depicts $H_3BO_3(s,t)$ with one row and two columns, s = 1 and t = 2.

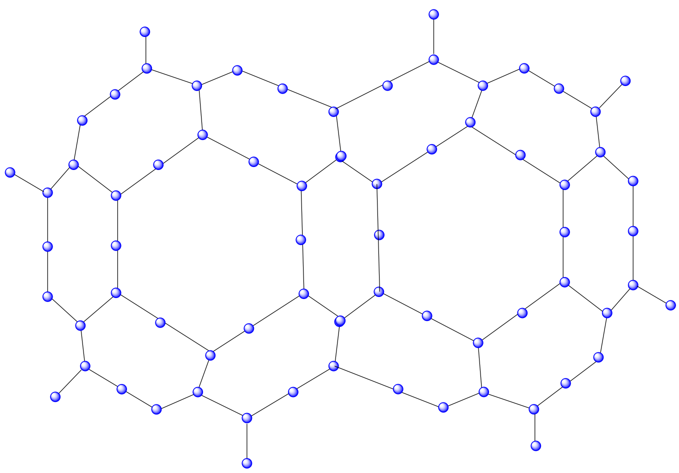

Figure 2. Layer structure of H_3BO_3.

2.1. *Subdivision of the Layer Structure $H_3BO_3(s,t)$*

Figure 3 shows the subdivision of $H_3BO_3(s,t)$, the layer structure achieved by installing one atom between each atom–bond of Figure 2.

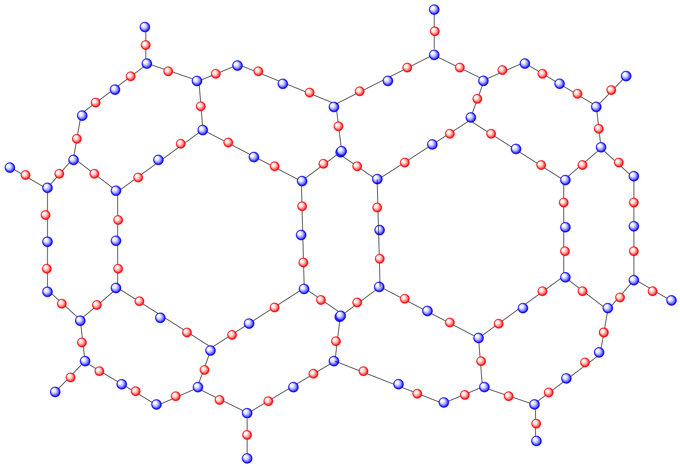

Figure 3. Subdivision of H_3BO_3.

Result and Discussion

In subdivision of the layer structure $H_3BO_3(s,t)$, the atom–bond $E(G)$ is divided into three groups based on the degree of each edge's end vertices. The set that is disjointed is shown by the symbols $\xi_{(d(u_i),d(V_j))}$. The first set that is disjointed is $\xi_{(1,2)}$, the second set that is disjointed is $\xi_{(2,2)}$, and the third set that is disjointed is $\xi_{(2,3)}$. The table below describes the different types of edges as well as the equations for calculating the number of edges in each type of the $SH_3BO_3(s,t)$ layer structure.

- **Entropy related to the ABC index of subdivision H_3BO_3**

Let $S(H_3BO_3)$ be a subdivision of $H_3BO_3(s,t)$. Then by using Equation (1) and Table 1, the atom–bond connectivity index is

$$\begin{aligned} ABC(S(H_3BO_3)) &= \sum_{\xi_{(1\sim 2)}} x^{\sqrt{\frac{1+2-2}{1\times 2}}} + \sum_{\xi_{(2\sim 2)}} x^{\sqrt{\frac{2+2-2}{2\times 2}}} + \sum_{\xi_{(2\sim 3)}} x^{\sqrt{\frac{2+3-2}{2\times 3}}} \\ &= 2(s+t+1)x^{\sqrt{\frac{1}{2}}} + 12(st+s+t)x^{\sqrt{\frac{1}{2}}} \\ &+ 6(3s+3t+4st-1)x^{\sqrt{\frac{1}{2}}} \end{aligned} \tag{11}$$

Differentiate (11) at $x = 1$; we get the atom–bond connectivity index

$$ABCS(H_3BO_3) = \sqrt{\frac{1}{2}}(32s + 32t + 36st - 4) \tag{12}$$

Here, we determine the atom–bond connectivity entropy by using Table 1 and Equation (12) in Equation (6) according to the following:

Table 1. Edge division based on vertices in the layer structure of subdivision $H_3BO_3(s,t)$.

Atomic bond type	$\xi_{(1,2)}$	$\xi_{2\sim 2}$	$\xi_{2\sim 3}$
Number of atom bonds	$2(s+t+1)$	$12(st+s+t)$	$6(3s+3t+4st-1)$

$$\begin{aligned} ENT_{ABC}S(H_3BO_3) &= \log(ABC) - \frac{1}{ABC}\log\Big\{\prod_{\xi_{(1,2)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]} \\ &\times \prod_{\xi_{(2,2)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]} \times \prod_{\xi_{(2,3)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]}\Big\} \\ &= \log(\sqrt{\frac{1}{2}}(32s+32t+36st-4) - \frac{1}{\sqrt{\frac{1}{2}}(32s+32t+36st-4)} \\ &\times \log\Big\{2(s+t+1)(\sqrt{\frac{1}{2}})^{\sqrt{\frac{1}{2}}} \times 12(st+s+t)(\sqrt{\frac{1}{2}})^{\sqrt{\frac{1}{2}}} \\ &\times 6(3s+3t+4st-1)(\sqrt{\frac{1}{2}})^{\sqrt{\frac{1}{2}}}\Big\}. \end{aligned} \tag{13}$$

- **Entropy related to the ABS index of subdivision H_3BO_3**

Let $S(H_3BO_3)$ be a subdivision of $H_3BO_3(s,t)$. Then by using Equation (2) and Table 1, the atom–bond sum connectivity is

$$\begin{aligned} ABSS(H_3BO_3) &= \sum_{\xi_{(1\sim2)}} x^{\sqrt{\frac{1+2-2}{1+2}}} + \sum_{\xi_{(2\sim2)}} x^{\sqrt{\frac{2+2-2}{2+2}}} + \sum_{\xi_{(2\sim3)}} x^{\sqrt{\frac{2+3-2}{2+3}}} \\ &= 2(s+t+1)x^{\sqrt{\frac{1}{3}}} + 12(st+s+t)x^{\sqrt{\frac{1}{2}}} \\ &+ 6(3s+3t+4st-1)x^{\sqrt{\frac{3}{5}}} \end{aligned} \tag{14}$$

Taking the first derivative of Equation (14) at $x=1$, we get the atom–bond sum connectivity index

$$ABS(S(H_3BO_3)) = 2(s+t+1)\sqrt{\frac{1}{3}} + 12(st+s+t)\sqrt{\frac{1}{2}} + 6(3s+3t+4st-1))\sqrt{\frac{3}{5}}. \tag{15}$$

Here, we determine the atom–bond sum connectivity entropy by using Table 1 and Equation (15) in Equation (6) according to the following:

$$\begin{aligned} ENT_{ABS}(S(H_3BO_3)) &= \log(ABS) - \frac{1}{ABS}\log\Big\{\prod_{\xi_{(1,2)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]} \\ &\times \prod_{\xi_{(2,2)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]} \times \prod_{\xi_{(2,3)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]}\Big\} \\ &= \log(ABS) - \frac{1}{ABS}\log\Big\{2(s+t+1)(\sqrt{\frac{1}{3}})^{\sqrt{\frac{1}{3}}} \times 12(st+s+t)(\sqrt{\frac{1}{2}})^{\sqrt{\frac{1}{2}}} \\ &\times 6(3s+3t+4st-1)(\sqrt{\frac{3}{5}})^{\sqrt{\frac{3}{5}}}\Big\}. \end{aligned} \tag{16}$$

- **Entropy related to the Albertson index $S(H_3BO_3)$**

Let $S(H_3BO_3)$ be a subdivision of $H_3BO_3(s,t)$. Then by using Equation (3) and Table 1, the atom–bond connectivity index is

$$\begin{aligned} A_{(G,x)}(S(H_3BO_3)) &= \sum_{\xi_{(1\sim 2)}} x^{|1-2|} + \sum_{\xi_{(2\sim 2)}} x^{|2-2|} + \sum_{\xi_{(2\sim 3)}} x^{|2-3|} \\ &= 2(s+t+1)x + 12(st+s+t) + 6(3s+3t+4st-1)x \end{aligned} \quad (17)$$

Differentiate (17) at $x = 1$; we get the atom–bond connectivity index

$$A_{(G,x)}S(H_3BO_3) = 32s + 32t + 36st - 4 \quad (18)$$

Here, we determine the atom–bond connectivity entropy by using Table 1 and Equation (18) in Equation (9) according to the following:

$$\begin{aligned} ENT_{A_{(G,x)}}S(H_3BO_3) &= \log\left(A_{(G,x)}\right) - \frac{1}{A_{(G,x)}} \log\left\{ \prod_{\xi_{(1,2)}} [|V_{a_i} - V_{a_j}|]^{[|V_{a_i} - V_{a_j}|]} \right. \\ &\times \left. \prod_{\xi_{(2,2)}} [|V_{a_i} - V_{a_j}|]^{[|V_{a_i} - V_{a_j}|]} \times \prod_{\xi_{(2,3)}} [|V_{a_i} - V_{a_j}|]^{[|V_{a_i} - V_{a_j}|]} \right\} \\ &= \log(32s + 32t + 36st - 4) - \frac{1}{32s + 32t + 36st - 4} \log\Big\{ 2(s+t+1) \\ &+ 12(st+s+t) + 6(3s+3t+4st-1) \Big\}. \end{aligned} \quad (19)$$

- **Entropy related to the *IRM* index of subdivision H_3BO_3**

Let $S(H_3BO_3)$ be a subdivision of $H_3BO_3(s,t)$. Then by using Equation (4) and Table 1, the atom–bond connectivity index is

$$\begin{aligned} IRM_{(G,x)}(S(H_3BO_3)) &= \sum_{\xi_{(1\sim 2)}} x^{[1-2]^2} + \sum_{\xi_{(2\sim 2)}} x^{[2-2]^2} + \sum_{\xi_{(2\sim 3)}} x^{[2-3]^2} \\ &= 2(s+t+1)x + 12(st+s+t) \\ &+ 6(3s+3t+4st-1)x \end{aligned} \quad (20)$$

Differentiate (20) at $x = 1$; we get the atom–bond connectivity index

$$IRM_{(G,x)})S(H_3BO_3) = 32s + 32t + 36st - 4 \quad (21)$$

Here, we determine the atom–bond connectivity entropy by using Table 1 and Equation (21) in Equation (10) according to the following:

$$\begin{aligned} ENT_{IRM_{(G,x)}}S(H_3BO_3) &= \log\left(IRM_{(G,x)})\right) - \frac{1}{IRM_{(G,x)}} \log\left\{ \prod_{\xi_{(1,2)}} [[V_{a_i} - V_{a_j}]^2]^{[[V_{a_i} - V_{a_j}]^2]} \right. \\ &\times \left. \prod_{\xi_{(2,2)}} [[V_{a_i} - V_{a_j}]^2]^{[[V_{a_i} - V_{a_j}]^2]} \times \prod_{\xi_{(2,3)}} [[V_{a_i} - V_{a_j}]^2]^{[[V_{a_i} - V_{a_j}]^2]} \right\} \\ &= \log(32s + 32t + 36st - 4) - \frac{1}{32s + 32t + 36st - 4} \log\Big\{ 2(s+t+1) \\ &+ 12(st+s+t) + 6(3s+3t+4st-1) \Big\}. \end{aligned} \quad (22)$$

2.2. Layer Structure of H_3BO_3 in the Form of a Line Graph

In the line graph of the layer structure $H_3BO_3(s,t)$, the atom–bond $E(G)$ is divided into five groups based on the degree of each edge's end vertices. The set that is disjointed is shown by the symbols $\xi_{(d(u_i),d(V_j))}$. The first set that is disjointed is $\xi_{(2,3)}$, the second set that is disjoint is $\xi_{(2,4)}$, the third set that is disjointed is $\xi_{(3,3)}$, the fourth set that is disjointed is $\xi_{(3,4)}$, and the fifth set that is disjointed is $\xi_{(4,4)}$.

Figure 4 displays the $H_3BO_3(s,t)$ layer structure as a line graph.

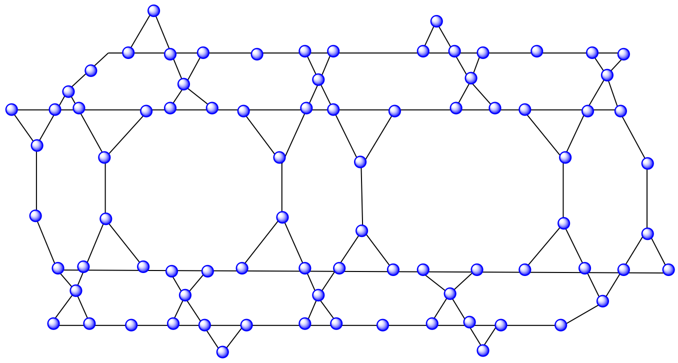

Figure 4. Line graph of H_3BO_3.

- **Entropy related to the ABC index of $L(H_3BO_3)$**

Let $L(H_3BO_3)$ be a line graph of $H_3BO_3(s,t)$). Then by using Equation (1) and Table 2, the ABC polynomial is

$$\begin{aligned} ABCL(H_3BO_3) &= \sum_{\xi_{(2\sim3)}} x^{\sqrt{\frac{2+3-2}{2\times3}}} + \sum_{\xi_{(2\sim4)}} x^{\sqrt{\frac{2+4-2}{2\times4}}} + \sum_{\xi_{(3\sim3)}} x^{\sqrt{\frac{3+3-2}{3\times3}}} + \sum_{\xi_{(3\sim4)}} x^{\sqrt{\frac{3+4-2}{3\times4}}} + \sum_{\xi_{(4\sim4)}} x^{\sqrt{\frac{4+4-2}{4\times4}}} \\ &= 6(1+t+s)x^{\sqrt{\frac{1}{2}}} + 2(s+t+1)x^{\frac{1}{2}} + 4(s+t+3st-2)x^{\frac{2}{3}} \\ &+ 2(5s+5t+6st-1)x^{\sqrt{\frac{5}{12}}} + 2(s+t+3st-2)x^{\sqrt{\frac{3}{8}}}. \end{aligned} \tag{23}$$

Taking the first derivative of Equation (23) at $x=1$, we get the ABC index

$$\begin{aligned} ABCL(H_3BO_3) &= 6(1+t+s)\sqrt{\frac{1}{2}} + \frac{2}{3}(24st+11s+11t-5) + 2(5s+5t+6st-1)\sqrt{\frac{5}{12}} \\ &+ 2(s+t+3st-2)\sqrt{\frac{3}{8}} \end{aligned} \tag{24}$$

Here, we determine the ABC entropy by using Table 2 and Equation (24) in Equation (6) according to the following:

$$\begin{aligned} ENT &= \log(ABC) - \frac{1}{ABC}\log\Big\{\prod_{\xi_{(2,3)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]} \\ &\times \prod_{\xi_{(2,4)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]} \times \prod_{\xi_{(3,3)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]} \\ &\times \prod_{\xi_{(3,4)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]} \times \prod_{\xi_{(4,4)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}\times V_{a_j})}}]}\Big\} \\ &= \log(ABC) - \frac{1}{ABS}\log\Big\{6(1+t+s)(\sqrt{\frac{1}{2}})^{\frac{1}{\sqrt{2}}} + 2(s+t+1)(\frac{1}{2})^{\frac{1}{2}} \\ &+ 4(s+t+3st-2)(\sqrt{\frac{2}{3}})^{\sqrt{\frac{2}{3}}} + 2(5s+5t+6st-1)(\sqrt{\frac{5}{12}})^{\sqrt{\frac{5}{12}}} \\ &+ 2(s+t+3st-2)(\sqrt{\frac{3}{8}})^{\sqrt{\frac{3}{8}}}\Big\}. \end{aligned} \tag{25}$$

Table 2. Edge division based on vertices in the line graph $H_3BO_3(s,t)$ layer structure.

Atomic bonds	$\xi_{2\sim3}$	$\xi_{2\sim4}$	$\xi_{3\sim3}$	$\xi_{3\sim4}$	$\xi_{4\sim4}$
Cardinality	$6(1+t+s)$	$2(s+t+1)$	$4(s+t+3st-2)$	$2(5s+5t+6st-1)$	$2(s+t+3st-2)$

- **Entropy related to the ABS index of $L(H_3BO_3)$**

Let $L(H_3BO_3)$ be a line graph of $H_3BO_3(s,t)$). Then by using Equation (2) and Table 2, the ABS polynomial is

$$\begin{aligned} ABSL(H_3BO_3) &= \sum_{\xi_{(2\sim3)}} x^{\sqrt{\frac{2+3-2}{2+3}}} + \sum_{\xi_{(2\sim4)}} x^{\sqrt{\frac{2+4-2}{2+4}}} + \sum_{\xi_{(3\sim3)}} x^{\sqrt{\frac{3+3-2}{3+3}}} + \sum_{\xi_{(3\sim4)}} x^{\sqrt{\frac{3+4-2}{3+4}}} + \sum_{\xi_{(4\sim4)}} x^{\sqrt{\frac{4+4-2}{4+4}}} \\ &= 6(1+t+s)x^{\sqrt{\frac{3}{5}}} + 2(s+t+1)x^{\sqrt{\frac{2}{3}}} + 4(s+t+3st-2)x^{\sqrt{\frac{2}{3}}} \\ &+ 2(5s+5t+6st-1)x^{\sqrt{\frac{5}{7}}} + 2(s+t+3st-2)x^{\sqrt{\frac{3}{4}}}. \end{aligned} \tag{26}$$

Taking the first derivative of Equation (26) at $x=1$, we get the ABS index

$$\begin{aligned} ABS(L(H_3BO_3)) &= 6(1+t+s)\sqrt{\frac{3}{5}} + 2(6st+3s+3t-3)\sqrt{\frac{2}{3}} + 2(5s+5t+6st-1)\sqrt{\frac{5}{7}} \\ &+ 2(s+t+3st-2)\sqrt{\frac{3}{4}}. \end{aligned} \tag{27}$$

Here, we determine the ABS entropy by using Table 2 and Equation (27) in Equation (6) according to the following:

$$\begin{aligned} ENT_{ABS}(L(H_3BO_3)) &= \log(ABS) - \frac{1}{ABS}\log\Big\{\prod_{\xi_{(2,3)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]} \\ &\times \prod_{\xi_{(2,4)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]} \times \prod_{\xi_{(3,3)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]} \\ &\times \prod_{\xi_{(3,4)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]} \times \prod_{\xi_{(4,4)}}[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]^{[\sqrt{\frac{(V_{a_i}+V_{a_j}-2)}{(V_{a_i}+V_{a_j})}}]}\Big\} \\ &= \log(ABS) - \frac{1}{ABS}\log\Big\{6(1+t+s)(\sqrt{\frac{3}{5}})^{\sqrt{\frac{3}{5}}} + 2(s+t+1)(\sqrt{\frac{2}{3}})^{\sqrt{\frac{2}{3}}} \\ &+ 4(s+t+3st-2)(\sqrt{\frac{2}{3}})^{\sqrt{\frac{2}{3}}} + 2(5s+5t+6st-1)(\sqrt{\frac{5}{7}})^{\sqrt{\frac{5}{7}}} \\ &+ 2(s+t+3st-2)(\sqrt{\frac{3}{4}})^{\sqrt{\frac{3}{4}}}\Big\}. \end{aligned} \tag{28}$$

- **Entropy related to the Albertson index of $L(H_3BO_3)$**

Let $L(H_3BO_3)$ be a line graph of $H_3BO_3(s,t)$). Then by using Equation (3) and Table 2, the Albertson index is

$$\begin{aligned} A_{(G,x)}L(H_3BO_3) &= \sum_{\xi_{(2\sim3)}} x^{|2-3|} + \sum_{\xi_{(2\sim4)}} x^{|2-4|} + \sum_{\xi_{(3\sim3)}} x^{|3-3|} + \sum_{\xi_{(3\sim4)}} x^{|3-4|} + \sum_{\xi_{(4\sim4)}} x^{|4-4|} \\ &= 6(1+t+s)x + 2(s+t+1)x^2 + 4(s+t+3st-2) \\ &+ 2(5s+5t+6st-1)x + 2(s+t+3st-2). \end{aligned} \tag{29}$$

Taking the first derivative of Equation (29) at $x = 1$, we get the Albertson index

$$A_{(G,x)}(L(H3BO3)) \quad = \quad 2(15st + 13s + 13t - 2) \tag{30}$$

Here, we determine the A entropy by using Table 2 and Equation (30) in Equation (9) according to the following:

$$\begin{aligned}
ENT_{A_{(G,x)}}(L(H_3BO_3)) &= \log(A) - \frac{1}{A}\log\Big\{\prod_{\xi_{(2,3)}}[|V_{a_i} - V_{a_j}|]^{[|V_{a_i}-V_{a_j}|]} \\
&\times \prod_{\xi_{(2,4)}}[|V_{a_i} - V_{a_j}|]^{[|V_{a_i}-V_{a_j}|]} \times \prod_{\xi_{(3,3)}}[|V_{a_i} - V_{a_j}|]^{[|V_{a_i}-V_{a_j}|]} \\
&\times \prod_{\xi_{(3,4)}}[|V_{a_i} - V_{a_j}|]^{[|V_{a_i}-V_{a_j}|]} \times \prod_{\xi_{(4,4)}}[|V_{a_i} - V_{a_j}|]^{[|V_{a_i}-V_{a_j}|]}\Big\} \\
&= \log 2(15st + 13s + 13t - 2) - \frac{1}{2(15st + 13s + 13t - 2)}\log\Big\{6(1 + t + s) \\
&+ 4(s + t + 1) + 4(s + t + 3st - 2) + 2(5s + 5t + 6st - 1) \\
&+ 2(s + t + 3st - 2)\Big\}.
\end{aligned} \tag{31}$$

- **Entropy related to the IRM index of $L(H_3BO_3)$**

Let $L(H_3BO_3)$ be a line graph of $H_3BO_3(s,t)$. Then by using Equation (4) and Table 2, the IRM index is

$$\begin{aligned}
IRM_{(G,x)}L(H_3BO_3) &= \sum_{\xi_{(2\sim3)}} x^{[2-3]^2} + \sum_{\xi_{(2\sim4)}} x^{[2-4]^2} + \sum_{\xi_{(3\sim3)}} x^{[3-3]^2} + \sum_{\xi_{(3\sim4)}} x^{[3-4]^2} + \sum_{\xi_{(4\sim4)}} x^{[4-4]^2} \\
&= 6(1 + t + s)x + 2(s + t + 1)x^4 + 4(s + t + 3st - 2) \\
&+ 2(5s + 5t + 6st - 1)x + 2(s + t + 3st - 2).
\end{aligned} \tag{32}$$

Taking the first derivative of Equation (32) at $x = 1$, we get the IRM index

$$IRM_{(G,x)}(L(H_3BO_3)) \quad = \quad 30s + 30t + 30st. \tag{33}$$

Here, we determine the IRM entropy by using Table 2 and Equation (33) in Equation (10) according to the following:

$$\begin{aligned}
ENT_{IRM}(L(H_3BO_3)) &= \log(IRM) - \frac{1}{IRM}\log\Big\{\prod_{\xi_{(2,3)}}[[V_{a_i} - V_{a_j}]^2]^{[[V_{a_i}-V_{a_j}]^2]} \\
&\times \prod_{\xi_{(2,4)}}[[V_{a_i} - V_{a_j}]^2]^{[[V_{a_i}-V_{a_j}]^2]} \times \prod_{\xi_{(3,3)}}[[V_{a_i} - V_{a_j}]^2]^{[[V_{a_i}-V_{a_j}]^2]} \\
&\times \prod_{\xi_{(3,4)}}[[V_{a_i} - V_{a_j}]^2]^{[[V_{a_i}-V_{a_j}]^2]} \times \prod_{\xi_{(4,4)}}[|V_{a_i} - V_{a_j}|]^{[|V_{a_i}-V_{a_j}|]}\Big\} \\
&= \log(30s + 30t + 30st) - \frac{1}{30s + 30t + 30st}\log\Big\{6(1 + t + s) + 8(s + t + 1) \\
&+ 4(s + t + 3st - 2) + 2(5s + 5t + 6st - 1) + 2(s + t + 3st - 2)\Big\}.
\end{aligned} \tag{34}$$

3. Comparison and Conclusions

Here, molecular descriptors for the subdivision and line graph of the layer structure of H_3BO_3 that are multiplicative and degree-based have been studied. Using these molecular descriptors, we compute the ABC entropy, ABS entropy, A entropy, and IRM entropy of the subdivision and line graph of the layer structure of H_3BO_3. Our results (entropies) help to describe the randomness and disorder of a molecule of H_3BO_3 based on the number of different arrangements available to it in a given system or reaction. For instance, the atom–bond connectivity (ABC) index offers excellent calculations of the strain energy of molecules via correlation. When the temperatures of the production of alkanes are described using the ABC-index, a good quantitative structure–property relationship (QSPR) model (r = 0.9970) is produced.

The values of four degree-based indices, namely, the ABC-index, ABS-index, A-index, and IRM-index, are presented in this work, numerically in Table 3 and graphically in Figure 5. As shown in Figure 5, the values of all indices are directly proportional to the values of (s, t), with the values of (s, t) along the x-axes and the resultant of the indices along the y-axes. The disparities between each topological index for a certain structure are revealed by these charts. The results of the computations demonstrate that the degree-based indices and entropy estimates depend greatly on the values of s and t or the molecular structure.

Table 3. Numerical comparison of molecular descriptors.

Values of (s,t)	ABC-Index	ABS-Index	Albertson Index	IRM-Index
(1, 2)	115.948	120.98	164	164
(2, 3)	263.004	275.844	372	372
(3, 4)	460.964	484.636	652	652
(4, 5)	709.828	747.356	1004	1004
(5, 6)	1009.596	1064.004	1428	1428
(6, 7)	1360.268	1434.58	1924	1924
(7, 8)	1761.844	1859.084	2492	2492
(8, 9)	2214.324	2337.516	3132	3132
(9, 10)	2717.708	2869.876	3844	3844
(10, 11)	3271.996	3456.164	4628	4628
(11, 12)	3877.188	4096.38	5484	5484
(12, 13)	4533.284	4790.524	6412	6412

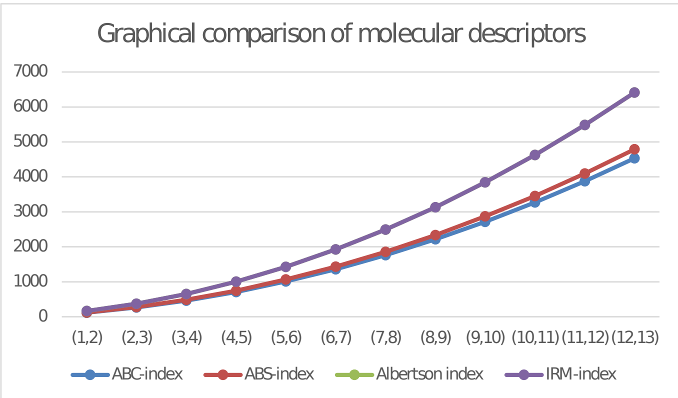

Figure 5. Graphical Comparison of ABC-index, ABS-index, Albertson index and IRM-index.

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