



# Article Characterizations of Chemical Networks Entropies by K-Banhatii Topological Indices

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**Abstract:** Entropy is a thermodynamic function in physics that measures the randomness and disorder of molecules in a particular system or process based on the diversity of configurations that molecules might take. Distance-based entropy is used to address a wide range of problems in the domains of mathematics, biology, chemical graph theory, organic and inorganic chemistry, and other disciplines. We explain the basic applications of distance-based entropy to chemical phenomena. These applications include signal processing, structural studies on crystals, molecular ensembles, and quantifying the chemical and electrical structures of molecules. In this study, we examine the characterisation of polyphenylenes and boron ( $B_{12}$ ) using a line of symmetry. Our ability to quickly ascertain the valences of each atom, and the total number of atom bonds is made possible by the symmetrical chemical structures of polyphenylenes and boron  $B_{12}$ . By constructing these structures with degree-based indices, namely the *K* Banhatti indices,  $ReZG_1$ -index,  $ReZG_2$ -index, and  $ReZG_3$ -index, we are able to determine their respective entropies.

**Keywords:** boron  $B_{12}$ ; polyphenylenes  $\mathbf{P}_{[s,t]}$ ; entropy's related *K*-Banhatti indices; entropy's related redefined Zagreb indices

### 1. Introduction

In mathematical chemistry, topological indices are numerical values that describe the topology of molecular structures. The chemical process conceptual framework is a significant area of applied mathematics. This theory can be used to model issues in the real world. Since their inception, chemical networks have drawn the attention of researchers because of their widespread applications. The correlation coefficient (r) between the physicochemical characteristics and topological indices is determined in order to assess the utility of a topological index to forecast the physicochemical behavior of a chemical compound [1,2]. Additionally, it falls within a class of challenging chemical graph theory applications for precise molecular issue resolutions. In the fields of chemical sciences



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**Copyright:** © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). and chemical graph theory, this theory is crucial. The QSAR/QSPR analysis included physiochemical properties and topological indices such as the  $1^{st}$  multiple Zagreb index,  $2^{nd}$  multiple Zagreb index, and hyper Zagreb index [3,4]. Recently, Ali et al. defined the atom–bond sum–connectivity index in [5].

Let  $G(V_G, E_G)$  be a graph, with the vertices and edges denoted by  $V_G$  and  $E_G$ , respectively. In chemical graph theory, a molecular graph is a simple connected graph that contains chemical atoms and bonds, which are commonly referred to as atoms and atom-bonds, respectively [6,7].

The valency of atom bonds (line segments) and a few Banhatti indices, each of which had the following description [8], was used by Kulli to begin constructing valency-based topological indices in 2016 [9–11].

The 1<sup>st</sup> and 2<sup>nd</sup> K-Banhatti indices are as follows, respectively:

$$B_1(G) = \sum_{a_i, a_j \in E_G} (d_{a_i} + d_{a_j}) \qquad \& \qquad B_2(G) = \sum_{a_i, a_j \in E_G} (d_{a_i} \times d_{a_j}) \tag{1}$$

The 1<sup>st</sup> and 2<sup>nd</sup> hyper K-Banhatti indices are as follows, respectively:

$$HB_1(G) = \sum_{a_i, a_j \in E_G} (d_{a_i} + d_{a_j})^2 \qquad \& \qquad HB_2(G) = \sum_{a_i, a_j \in E_G} (d_{a_i} \times d_{a_j})^2 \qquad (2)$$

The 1<sup>st</sup> and 2<sup>nd</sup>K-generalized Banhatti indices are as follows, respectively:

$$GB_1(G) = \sum_{a_i, a_j \in E_G} (d_{a_i} + d_{a_j})^{\alpha} \qquad \& \qquad GB_2(G) = \sum_{a_i, a_j \in E_G} (d_{a_i} \times d_{a_j})^{\alpha}$$
(3)

The redefined Zagreb indices *ReZG1*, *ReZG2*, and *ReZG3* were 1<sup>st</sup> proposed by Ranjini [12] in 2013:

$$ReZG_1 = \sum_{a_i, a_j \in E_G} \frac{d_{a_i} + d_{a_j}}{d_{a_i} \times d_{a_j}} \qquad \& \qquad ReZG_2 = \sum_{a_i, a_j \in E_G} \frac{d_{a_i} \times d_{a_j}}{d_{a_i} + d_{a_j}}.$$
 (4)

The 3<sup>rd</sup> redefined Zagreb index is defined as

$$ReZG_3 = \sum_{a_i, a_j \in E_G} (d_{a_i} \times d_{a_j})(d_{a_i} + d_{a_j})$$
(5)

Entropy is the measurement of the amount of thermal energy per unit of temperature in a system that cannot be used for productive labour. Entropy is a measure of a system's molecular disorder or unpredictability since work is produced by organised molecular motion, see new works on graph theory in [13,14]. Entropy was initially discussed by Shannon in his well-known [15] from 1948. The entropy of a probability distribution measures the unpredictable nature of information content or the uncertainty of a system. Entropy was then used to analyse chemical networks and graphs in order to comprehend the structural information contained within these networks. Recently, graph entropies have become more well-liked in a variety of academic disciplines, including biology, chemistry, ecology, and sociology. Graph theory and network theory have both undertaken substantial study on invariants, which are utilised as information functionals in science and have been around for a long time. The degree of every atom is vitally crucial [16–18]. The following sections will discuss graph entropy measures that have been applied to analyse biological and chemical networks in chronological order for further information [19].

In this article, we construct the boron  $B_{12}$  and polyphenylenes  $\mathbf{P}_{[s,t]}$ . We determine the K-Banhatti entropies, redefined  $1^{st}$ ,  $2^{nd}$  and  $3^{rd}$  Zagreb entropies by using K-Banhatti indices [20–22],  $1^{st}$  Zagreb index,  $2^{nd}$  Zagreb index,  $3^{rd}$  Zagreb index and the concept of

entropy from Shazia Manzoor's article [23] and Ghani et al. [24,25]. Many researchers discussed several aspects of distance-based entropies in [26–33].

#### Entropy Related to Valency-Based Indices

The entropy of an edge-weighted graph G is defined in [34], which was published in 2009. Ghani et al. defined the modified definition of entropy in [35]. A network with lines that are weighted has the equation  $G = (V_G, E_G), \mu(a_i a_j))$ , where  $V_G, E_G$ , and the vertex set, edge set, and edge–weight of edge  $(a_i a_j)$  are each represented by  $\mu(a_i a_j)$ :

$$ENT_{\mu(G)} = -\sum_{a_i, a_j \in E_G} \frac{\mu(a_i a_j)}{\sum\limits_{a_i, a_j \in E_G} \mu(a_i a_j)} \log \left\{ \frac{\mu(a_i a_j)}{\sum\limits_{a_i, a_j \in E_G} \mu(a_i a_j)} \right\}$$
(6)

## • Entropy related to the 1<sup>st</sup> K-Banhatti index

Assume  $\mu(a_i a_j) = d_{a_i} + d_{a_j}$ . Then, the 1<sup>st</sup> *K*-Banhatti  $B_1$  index (1) is thus provided by

$$B_1(G) = \sum_{a_i, a_j \in E_G} \left\{ d_{a_i} + d_{a_j} \right\} = \sum_{a_i, a_j \in E_G} \mu(a_i a_j).$$

By putting these parameters into Equation (6), the  $1^{st}$  K-Banhatti entropy is

$$ENT_{B_1(G)} = \log\left(B_1(G)\right) - \frac{1}{B_1(G)}\log\left\{\prod_{a_i, a_j \in E_G} \left[d_{a_i} + d_{a_j}\right]^{\left[d_{a_i} + d_{a_j}\right]}\right\}.$$
(7)

### • Entropy related to the 2<sup>nd</sup> K-Banhatti index

Assume  $\mu(a_i a_j) = d_{a_i} \times d_{a_j}$ . Then, the 2<sup>*nd*</sup> *K*-Banhatti *B*<sub>2</sub> index (1) is thus provided by

$$B_2(G) = \sum_{a_i, a_j \in E_G} \left\{ (d_{a_i} \times d_{a_j}) \right\} = \sum_{a_i, a_j \in E_G} \mu(a_i a_j)$$

By putting these parameters into Equation (6), the  $2^{nd}$  K-Banhatti entropy is

$$ENT_{B_2(G)} = \log \left( B_2(G) \right) - \frac{1}{B_2(G)} \log \left\{ \prod_{a_i, a_j \in E_G} \left[ d_{a_i} \times d_{a_j} \right]^{\left[ d_{a_i} \times d_{a_j} \right]} \right\}.$$
(8)

## • Entropy related to the 1<sup>st</sup> K hyper Banhatti index

Assume  $\mu(a_i a_j) = (d_{a_i} + d_{a_j})^2$ . Then, the 1<sup>st</sup> K hyper Banhatti *HB*<sub>1</sub> index (2) is thus provided by

$$HB_1(G) = \sum_{a_i, a_j \in E_G} \left\{ (d_{a_i} + d_{a_j})^2 \right\} = \sum_{a_i, a_j \in E_G} \mu(a_i a_j).$$

By putting these parameters into Equation (6), the  $1^{st}$  K hyper Banhatti entropy is

$$ENT_{HB_1(G)} = \log\left(HB_1(G)\right) - \frac{1}{HB_1(G)}\log\left\{\prod_{a_i,a_j\in E_G} \left[d_{a_i} + d_{a_j}\right]^{2\left[d_{a_i} + d_{a_j}\right]^2}\right\}.$$
 (9)

## • Entropy related to the 2<sup>nd</sup>K hyper Banhatti index

Assume  $\mu(a_i a_j) = (d_{a_i} \times d_{a_j})^2$ . Then, the 2<sup>*nd*</sup> K hyper Banhatti index (2) is thus provided by

$$HB_{2}(G) = \sum_{a_{i},a_{j}\in E_{G}} \left\{ (d_{a_{i}} \times d_{a_{j}})^{2} \right\} = \sum_{a_{i},a_{j}\in E_{G}} \mu(a_{i}a_{j}).$$

By putting these parameters into Equation (6), the  $2^{nd}$  K hyper Banhatti entropy is

$$ENT_{HB_2(G)} = \log\left(HB_1(G)\right) - \frac{1}{HB_1(G)}\log\left\{\prod_{a_i,a_j\in E_G} [d_{a_i} \times d_{a_j}]^{2[d_{a_i} \times d_{a_j}]^2}\right\}.$$
 (10)

#### • The first redefined Zagreb entropy

Assume  $\mu(a_i a_j) = \frac{d_{a_i} + d_{a_j}}{d_{a_i} d_{a_j}}$ . Then, the 1<sup>st</sup> redefined Zagreb index (4) is thus provided by

$$ReZG_1 = \sum_{a_i, a_j \in E_G} \left\{ \frac{d_{a_i} + d_{a_j}}{d_{a_i} d_{a_j}} \right\} = \sum_{a_i, a_j \in E_G} \mu(a_i a_j)$$

By putting these parameters into Equation (6), the 1<sup>st</sup> redefined Zagreb entropy is

$$ENT_{ReZG_1} = \log\left(ReZG_1\right) - \frac{1}{ReZG_1}\log\left\{\prod_{a_i,a_j\in E_G}\left[\frac{d_{a_i}+d_{a_j}}{d_{a_i}d_{a_j}}\right]^{\left[\frac{d_{a_i}+d_{a_j}}{d_{a_i}d_{a_j}}\right]}\right\}.$$
 (11)

#### The second redefined Zagreb entropy

Assume  $\mu(a_i a_j) = \frac{d_{a_i} d_v}{d_{a_i} + d_{a_j}}$ . Then, the 2<sup>*nd*</sup> redefined index (4) is thus provided by

$$ReZG_2 = \sum_{a_i,a_j \in E_G} \left\{ \frac{d_{a_i}d_{a_j}}{d_{a_i} + d_{a_j}} \right\} = \sum_{a_i,a_j \in E_G} \mu(a_i a_j)$$

By putting these parameters into Equation (6), the  $2^{nd}$  redefined Zagreb entropy is

$$ENT_{ReZG_2} = \log (ReZG_2) - \frac{1}{ReZG_2} \log \left\{ \prod_{a_i, a_j \in E_G} \left[ \frac{d_{a_i} d_v}{d_{a_i} + d_{a_j}} \right]^{\left[ \frac{d_{a_i} d_{a_j}}{d_{a_i} + d_{a_j}} \right]} \right\}.$$
 (12)

### The third redefined Zagreb entropy

Assume  $\mu(a_i a_j) = \{ (d_{a_i} d_{a_j})(d_{a_i} + d_{a_j}) \}$ . Then, the 3<sup>*rd*</sup> redefined Zagreb index (5) is thus provided by

$$ReZG_{3} = \sum_{a_{i},a_{j}\in E_{G}} \left\{ (d_{a_{i}}d_{a_{j}})(d_{u}+d_{v}) \right\} = \sum_{a_{i},a_{j}\in E_{G}} \mu(a_{i}a_{j})$$

By putting these parameters into Equation (6), the  $3^{rd}$  redefined Zagreb entropy is

$$ENT_{ReZG_3} = \log\left(ReZG_3\right) - \frac{1}{ReZG_3}\log\left\{\prod_{a_i,a_j\in E_G}\left[(d_{a_i}d_{a_j})(d_{a_i}+d_{a_j})\right]^{\left[(d_{a_i}d_{a_j})(d_{a_i}+d_{a_j})\right]}\right\}.$$
 (13)

### 2. The Boron Network

We discuss the topological characteristics of boron  $B_{12}$  in this article. The icosahedral network of boron  $B_{12}$  has two dimensions. The existence of icosahedral structures containing  $B_{12}$  was confirmed by a recent investigation of high-pressure solid boron [36]. However, prior theoretical and practical investigations of multiple boron clusters have demonstrated that the  $B_{12}$  structure is unstable in the gas phase [37–39]. Figure 1 displays the molecular graph of boron  $B_{12}$ . The dotted line in Figure 1 represents the line of symmetry; using this line, we can easily obtain the edge-partition of  $B_{12}$ .



**Figure 1.** Boron *B*<sub>12</sub>.

#### 2.1. Results and Discussion

Now, (s, t) are the units of  $B_{12}$ , where s and t show the number of  $B_{12}$  in horizontal rows and vertical columns. In the boron network, the edge set E(G) is divided into seven groups based on the degree of each edge's end vertices. The set that is disjoint is shown by the symbols  $\xi_{(d(u_i),d(v_j))}$ . The 1<sup>st</sup> set that is disjoint is  $\xi_{(2,4)}$ , the 2<sup>nd</sup> set that is disjoint is  $\xi_{(2,5)}$ , the 3<sup>*rd*</sup> set that is disjoint is  $\xi_{(3,4)}$ , the 4<sup>*th*</sup> set that is disjoint is  $\xi_{(3,5)}$ , the 5<sup>*th*</sup> set that is disjoint is  $\xi_{(4,4)}$ , the 6<sup>th</sup> set that is disjoint is  $\xi_{(4,5)}$ , and the 7<sup>th</sup> set that is disjoint is  $\xi_{(5,5)}$ . From the symmetrical chemical structure of boron,  $B_{12}$ , we find the edge-partition of

 $B_{12}$  easily:

$$\begin{split} \xi_{(2,4)} &= \left\{ e = a_i \sim a_j, \forall a_i, a_j \in E(B_{12}) \middle| d_{a_i} = 2, d_{a_j} = 4 \right\} = 2(s+t), \\ \xi_{(2,5)} &= \left\{ e = a_i \sim a_j, \forall a_i, a_j \in E(B_{12}) \middle| d_{a_i} = 2, d_{a_j} = 5 \right\} = 2(s+t), \\ \xi_{(3,4)} &= \left\{ e = a_i \sim a_j, \forall a_i, a_j \in E(B_{12}) \middle| d_{a_i} = 3, d_{a_j} = 4 \right\} = 3st + s + 5, \\ \xi_{(3,5)} &= \left\{ e = a_i \sim a_j, \forall a_i, a_j \in E(B_{12}) \middle| d_{a_i} = 3, d_{a_j} = 5 \right\} = 3st + 2s + 3t + 4, \\ \xi_{(4,4)} &= \left\{ e = a_i \sim a_j, \forall a_i, a_j \in E(B_{12}) \middle| d_{a_i} = 4, d_{a_j} = 4 \right\} = s + 2t + 1, \\ \xi_{(4,5)} &= \left\{ e = a_i \sim a_j, \forall a_i, a_j \in E(B_{12}) \middle| d_{a_i} = 4, d_{a_j} = 5 \right\} = 9st + 7s + 6t + 5, \\ \xi_{(5,5)} &= \left\{ e = a_i \sim a_j, \forall a_i, a_j \in E(B_{12}) \middle| d_{a_i} = 5, d_{a_j} = 5 \right\} = 9st + 7s + 7t + 3. \end{split}$$

This partition provides

## • The 1<sup>st</sup> K-Banhatti entropy of B<sub>12</sub>

Assume that  $B_{12}$  is an icosahedral network of boron. Then, by using Equation (1) and the edge-partition of  $B_{12}$ , the 1<sup>st</sup> *K*-Banhatti index is

$$B_1(B_{12}) = 190s + 190t + 216st + 147$$

By using the edge-partition of  $B_{12}$  and Equation (7) as described below,

$$\begin{split} ENT_{B_1}(B_{12}) &= \log \left( B_1 \right) - \frac{1}{B_1} \log \left\{ \prod_{E_{(2,4)}} \left( d_{a_i} + d_{a_j} \right)^{(d_{a_i} + d_{a_j})} \times \prod_{E_{(2,5)}} \left( d_{a_i} + d_{a_j} \right)^{(d_{a_i} + d_{a_j})} \right. \\ & \times \left. \prod_{E_{(3,4)}} \left( d_{a_i} + d_{a_j} \right)^{(d_{a_i} + d_{a_j})} \times \prod_{E_{(3,5)}} \left( d_{a_i} + d_{a_j} \right)^{(d_{a_i} + d_{a_j})} \times \prod_{E_{(4,4)}} \left( d_{a_i} + d_{a_j} \right)^{(d_{a_i} + d_{a_j})} \right. \\ & \times \left. \prod_{E_{(4,5)}} \left( d_{a_i} + d_{a_j} \right)^{(d_{a_i} + d_{a_j})} \times \prod_{E_{(5,5)}} \left( d_{a_i} + d_{a_j} \right)^{(d_{a_i} + d_{a_j})} \right. \\ &= \left. \log \left( 190s + 190t + 216st + 147 \right) - \frac{1}{190s + 190t + 216st + 147} \log \left\{ 2(s+t)(6)^6 \right. \\ & \times \left. 2(s+t)(7)^7 \times \left( 3st + s + 5 \right)(7)^7 \times \left( 3st + 2s + 3t + 4 \right)(8)^8 \times (s+2t+1)(8)^8 \right. \\ & \times \left. \left( 9st + 7s + 6t + 5 \right)(9)^9 \times \left( 9st + 7s + 7t + 3 \right)(10)^{10} \right\}. \end{split}$$

After simplifying the preceding expression, the following equation yields the precise value of the 1<sup>st</sup> *K*-Banhatti entropy:

$$ENT_{B_1}(B_{12}) = \log (190s + 190t + 216st + 147) - \frac{1}{190s + 190t + 216st + 147} \log \left\{ 2(s+t)(6)^6 \times (3st + 3s + 2t + 5)(7)^7 \times (3st + 3s + 5t + 5)(8)^8 \times (9st + 7s + 6t + 5)(9)^9 \times (9st + 7s + 7t + 3)(10)^{10} \right\}.$$
(14)

### • The second *K*-Banhatti entropy of *B*<sub>12</sub>

Assume that  $B_{12}$  is an icosahedral network of boron. Then, by using Equation (1) and the edge-partition of  $B_{12}$ , the  $2^{nd}$  *K*-Banhatti entropy index is

$$B_2(B_{12}) = 409s + 408t + 486st + 311$$

By using the edge-partition of  $B_{12}$  and Equation (8) as described below,

$$ENT_{B_{2}}(B_{12}) = \log (B_{2}) - \frac{1}{B_{2}} \log \left\{ \prod_{E_{(2,4)}} (d_{a_{i}} \times d_{a_{j}})^{(d_{a_{i}} \times d_{a_{j}})} \times \prod_{E_{(2,5)}} (d_{a_{i}} \times d_{a_{j}})^{(d_{a_{i}} \times d_{a_{j}})} \right. \\ \times \prod_{E_{(3,4)}} (d_{a_{i}} \times d_{a_{j}})^{(d_{a_{i}} \times d_{a_{j}})} \times \prod_{E_{(3,5)}} (d_{a_{i}} \times d_{a_{j}})^{(d_{a_{i}} \times d_{a_{j}})} \times \prod_{E_{(4,4)}} (d_{a_{i}} \times d_{a_{j}})^{(d_{a_{i}} \times d_{a_{j}})} \\ \times \prod_{E_{(4,5)}} (d_{a_{i}} \times d_{a_{j}})^{(d_{a_{i}} \times d_{a_{j}})} \times \prod_{E_{(5,5)}} (d_{a_{i}} \times d_{a_{j}})^{(d_{a_{i}} \times d_{a_{j}})} \right\} \\ = \log (409s + 408t + 486st + 311) - \frac{1}{409s + 408t + 486st + 311} \log \left\{ 2(s+t)8^{8} \\ \times 2(s+t)10^{10} \times (3st+s+5)12^{12} \times (3st+2s+3t+4)15^{15} \times (s+2t+1)16^{16} \\ \times (9st+7s+6t+5)20^{20} \times (9st+7s+7t+3)25^{25} \right\}.$$

$$(15)$$

• The 1<sup>st</sup> hyper K-Banhatti entropy of B<sub>12</sub>

Assume that  $B_{12}$  is an icosahedral network of boron. Then, by using the Equation (2) and the edge-partition of  $B_{12}$ , the 1<sup>st</sup> K hyper Banhatti index is

$$HB_1(B_{12}) = 1678s + 1676t + 1968st + 1270$$

By using the edge-partition of  $B_{12}$  and Equation (9) as described below;

$$\begin{split} ENT_{HB_{1}}(B_{12}) &= \log\left(HB_{1}\right) - \frac{1}{HB_{1}}\log\left\{\prod_{E_{(2,4)}} \left(d_{a_{i}} + d_{a_{j}}\right)^{2\left(d_{a_{i}} + d_{a_{j}}\right)^{2}} \times \prod_{E_{(2,5)}} \left(d_{a_{i}} + d_{a_{j}}\right)^{2\left(d_{a_{i}} + d_{a_{j}}\right)^{2}} \\ &\times \prod_{E_{(3,4)}} \left(d_{a_{i}} + d_{a_{j}}\right)^{2\left(d_{a_{i}} + d_{a_{j}}\right)^{2}} \times \prod_{E_{(3,5)}} \left(d_{a_{i}} + d_{a_{j}}\right)^{2\left(d_{a_{i}} + d_{a_{j}}\right)^{2}} \\ &\times \prod_{E_{(4,5)}} \left(d_{a_{i}} + d_{a_{j}}\right)^{2\left(d_{a_{i}} + d_{a_{j}}\right)^{2}} \times \prod_{E_{(5,5)}} \left(d_{a_{i}} + d_{a_{j}}\right)^{2\left(d_{a_{i}} + d_{a_{j}}\right)^{2}} \\ &= \log\left(1678s + 1676t + 1968st + 1270\right) - \frac{1}{1678s + 1676t + 1968st + 1270} \\ &\times \log\left\{2(s+t)6^{72} \times 2(s+t)7^{98} \times (3st+s+5)7^{98} \times (3st+2s+3t+4)8^{128} \\ &\times (s+2t+1)8^{128} \times (9st+7s+6t+5)9^{162} \times (9st+7s+7t+3)10^{200}\right\}. \end{split}$$

After simplification, we obtain

$$ENT_{HB_{1}}(B_{12}) = \log (1678s + 1676t + 1968st + 1270) - \frac{1}{1678s + 1676t + 1968st + 1270} \\ \times \log \left\{ 2(s+t)6^{72} \times (3st + 3s + 3t + 5)7^{98} \times (3st + 3s + 5t + 5)8^{128} \\ \times (9st + 7s + 6t + 5)9^{162} \times (9st + 7s + 7t + 3)10^{200} \right\}.$$
(16)

# • The 2<sup>*nd*</sup> hyper *K*-Banhatti entropy of *B*<sub>12</sub>

Assume that  $B_{12}$  is an icosahedral network of boron. Then, by using Equation (2) and the edge-partition of  $B_{12}$ , the  $2^{nd}$  *K* hyper Banhatti index is

$$HB_2(B_{12}) = 8233s + 8290t + 9972st + 5151$$

By using the edge-partition of  $B_{12}$  and Equation (10) as described below,

$$ENT_{HB_{2}}(B_{12}) = \log (HB_{2}) - \frac{1}{HB_{2}} \log \Big\{ \prod_{E_{(2,4)}} (d_{a_{i}} \times d_{a_{j}})^{2(d_{a_{i}} \times d_{a_{j}})^{2}} \times \prod_{E_{(2,5)}} (d_{a_{i}} \times d_{a_{j}})^{2(d_{a_{i}} \times d_{a_{j}})^{2}} \\ \times \prod_{E_{(3,4)}} (d_{a_{i}} \times d_{a_{j}})^{2(d_{a_{i}} \times d_{a_{j}})^{2}} \times \prod_{E_{(3,5)}} (d_{a_{i}} \times d_{a_{j}})^{2(d_{a_{i}} \times d_{a_{j}})^{2}} \\ \times \prod_{E_{(4,5)}} (d_{a_{i}} \times d_{a_{j}})^{2(d_{a_{i}} \times d_{a_{j}})^{2}} \times \prod_{E_{(5,5)}} (d_{a_{i}} \times d_{a_{j}})^{2(d_{a_{i}} \times d_{a_{j}})^{2}} \\ = \log (8233s + 8290t + 9972st + 5151) - \frac{1}{8233s + 8290t + 9972st + 5151} \\ \times \log \Big\{ 2(s+t)8^{128} \times 2(s+t)10^{200} \times (3st+s+5)12^{288} \\ \times (3st+2s+3t+4)15^{450} \\ \times (s+2t+1)16^{512} \times (9st+7s+6t+5)20^{800} \times (9st+7s+7t+3)25^{1250} \Big\}.$$
(17)

• The 1<sup>st</sup> redefined Zagreb entropy of B<sub>12</sub>

Assume that  $B_{12}$  is an icosahedral network of boron. Then, by using Equation (4) and the edge-partition of  $B_{12}$ , the 1<sup>st</sup> redefined Zagreb index is

$$ReZG_1(B_{12}) = 11st + 11s + 11t + 9$$

By using the edge-partition of  $B_{12}$  and Equation (11) as described below,

$$ENT_{ReZG_{1}}(B_{12}) = \log \left(ReZG_{1}\right) - \frac{1}{ReZG_{1}} \log \left\{ \prod_{E_{(2,4)}} \left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \times \prod_{E_{(2,5)}} \left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \times \prod_{E_{(3,5)}} \left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \times \prod_{E_{(4,5)}} \left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \times \prod_{E_{(5,5)}} \left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \times \prod_{E_{(5,5)}} \left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \times \prod_{E_{(5,5)}} \left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \times \prod_{E_{(5,5)}} \left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \left]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \times \sum_{E_{(5,5)}} \left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \left]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \times \sum_{E_{(5,5)}} \left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{i}}}{d_{a_{i}}d_{a_{j}}} \right]}$$

# • The $2^{nd}$ redefined Zagreb entropy of $B_{12}$

Assume that  $B_{12}$  is an icosahedral network of boron. Then, by using Equation (4) and the edge-partition of  $B_{12}$ , the  $2^{nd}$  redefined Zagreb index is

$$ReZG_2(B_{12}) = \frac{1}{504}(26847st + 23210s + 23175t + 18488)$$

By using the edge-partition of  $B_{12}$  and Equation (12) as described below,

$$ENT_{ReZG_{2}}(B_{12} = \log(ReZG_{2}) - \frac{1}{ReZG_{2}}\log\Big\{\prod_{E_{(2,4)}} [\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}} \times \prod_{E_{(2,5)}} [\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}}]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}} \times \prod_{E_{(3,5)}} [\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}}]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}}]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}}]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}}^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}}\Big]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}} \times \prod_{E_{(5,5)}} [\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}}\Big]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}} \times \prod_{E_{(5,5)}} [\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}}\Big]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}}\Big]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}}} \times \prod_{E_{(5,5)}} [\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}}}\Big]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}}\Big]^{\frac{d_{a_{i}} \times d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}}}} = \log \frac{1}{504} (26847st + 23210s + 23175t + 18488) - \frac{504}{(26847st + 23210s + 23175t + 18488)} \times \log \Big\{ 2(s+t)(\frac{4}{3})^{\frac{4}{3}} \times 2(s+t)(\frac{7}{10})^{\frac{7}{10}} \times (3st+s+5)(\frac{12}{7})^{\frac{12}{7}} \times (3st+2s+3t+4)(\frac{15}{8})^{\frac{15}{8}} \times 4(s+2t+1) \times (9st+7s+6t+5)(\frac{20}{9})^{\frac{20}{9}} \times (9st+7s+7t+3)(\frac{5}{2})^{\frac{5}{2}} \Big\}.$$
(19)

## • The $3^{rd}$ redefined Zagreb entropy of $B_{12}$

Assume that  $B_{12}$  is a hexagonal grid of benzenoid. Then, by using Equation (5) and the edge-partition of  $B_{12}$ , the  $3^{rd}$  redefined Zagreb index is

$$ReZG_3(B_{12}) = 4482st + 3698s + 3682t + 2678$$

Now, we compute the  $3^{rd}$  redefined Zagreb entropy by using the edge-partition of  $B_{12}$  and Equation (13) as described below,

$$ENT_{ReZG_{3}}(B_{12}) = \log (ReZG_{3}) - \frac{1}{ReZG_{3}} \log \Big\{ \prod_{E_{(2,4)}} [(d_{a_{i}}d_{a_{j}})(d_{a_{i}} + d_{a_{j}})]^{[\frac{d_{a_{i}}+d_{a_{j}}}{d_{a_{i}}d_{a_{j}}}]} \times \prod_{E_{(3,4)}} [d_{a_{i}}d_{a_{j}})(d_{a_{i}} + d_{a_{j}}]^{[d_{a_{i}}d_{a_{j}})(d_{a_{i}} + d_{a_{j}}]} \\ \times \prod_{E_{(3,5)}} [(d_{a_{i}}d_{a_{j}})(d_{a_{i}} + d_{a_{j}}]^{[\frac{d_{a_{i}}+d_{a_{j}}}{d_{a_{i}}d_{a_{j}}}]} \times \prod_{E_{(4,4)}} [d_{a_{i}}d_{a_{j}})(d_{a_{i}} + d_{a_{j}}]^{[d_{a_{i}}d_{a_{j}})(d_{a_{i}} + d_{a_{j}}]} \\ \times \prod_{E_{(4,5)}} [(d_{a_{i}}d_{a_{j}})(d_{a_{i}} + d_{a_{j}}]^{[\frac{d_{a_{i}}}{d_{a_{j}}}](d_{a_{i}} + d_{a_{j}}]} \times \prod_{E_{(5,5)}} [d_{a_{i}}d_{a_{j}})(d_{a_{i}} + d_{a_{j}}]^{[d_{a_{i}}d_{a_{j}})(d_{a_{i}} + d_{a_{j}}]} \Big] \Big\} \\ = \log (4482st + 3698s + 3682t + 2678) - \frac{1}{4482st + 3698s + 3682t + 2678} \\ \times \log \Big\{ 2(s+t)48^{48} \times 2(s+t)70^{70} \times (3st+s+5)84^{84} \\ \times (3st+2s+3t+4)120^{120} \\ \times (s+2t+1)2^{896} \times (9st+7s+6t+5)180^{180} \times (9st+7s+7t+3)250^{250} \Big\}.$$
(20)

### 2.2. Comparison of K-Banhatti and Redefined Zagreb Indices of B<sub>12</sub>

Here, we present numerical and graphical comparison of *K*-Banhatti indices and redefined Zagreb indices of boron  $B_{12}$  for s = 2, 4, 6, ..., 16 and t = 3, 5, 7, ..., 17, in Table 1 and Figure 2 respectively.

(s,t)	$B_1$	<i>B</i> <sub>2</sub>	$HB_1$	$HB_2$	$ReZG_1$	$ReZG_2$	$ReZG_3$
(2, 3)	2393	5269	21,462	106,319	130	586.35	48,012
(4, 5)	6177	13,707	55,722	278,973	328	1516.20	125,520
(6,7)	11,689	26,033	105,726	531,403	614	2872.20	238,884
(8,9)	18,929	42,247	171,474	863,609	988	4654.36	388,104
(10, 11)	27,897	62,349	252,966	1,275,591	1450	6862.68	573,180
(12, 13)	38,593	86,339	350,202	1,767,349	2000	9497.16	794,112
(14, 15)	51,017	114,217	463,182	2,338,883	2638	12,557.80	1,050,900
(16, 17)	65,169	145,983	591,906	2,990,193	3364	16,044.60	1,343,544

**Table 1.** Comparison of *K*-Banhatti and redefined Zagreb indices of  $B_{12}$ .



**Figure 2.** Graphical representation indices of *B*<sub>12</sub>.

#### 3. The Polyphenylenes Network

Polyphenylenes include benzenoid aromatic nuclei that are linked together by a carbon-carbon bond [40]. Polyphenylenes have been the subject of research for many years. Up until 1979, there was a lot of interest in polyphenylenes because of its thermal and thermo-oxidative stability. The quest for a single group of polymers that can be converted to another, such as an electrical insulator that can be transformed into an electrical conductor by utilizing doping with an electron acceptor or donor, is a key ongoing subject in polyphenylene [41].

Figure 3 for polyphenylenes  $\mathbf{P}_{[s,t]}$  has been shown.



Figure 3. 2D-polyphenylenes molecular.

In 2011, Zhen Zhou [42] indicated that two-dimensional polyphenylene is a conventional semiconductor with a large band gap and that the porous structure gives it a remarkable selectivity for  $H_2$  permeability compared to  $CO_2$ , CO, and  $CH_4$ . This porous graphene, which has been tested, is likely to find use in a hydrogen-powered civilization. In Figure 3, the dot lines represent the line of symmetry, with 6s(t + 1) atoms on the left side and the same on the right. Here, in the  $\mathbf{P}_{[s,t]}$ , there are two sorts of atoms  $v_i$  and  $a_j$  such that  $d_{v_i} = 2$  and  $d_{a_j} = 3$ , where  $d_{v_i}$  and  $d_{a_j}$  mean the valency of atoms  $\forall v_i, v_j \in \mathbf{P}_{[s,t]}$ . The order and size of  $\mathbf{P}_{[s,t]}$ , is

$$|\mathbf{P}_{[s,t]}| = 12s(t+1)$$
  $S(\mathbf{P}_{[s,t]}) = (30t+13)s - t$ 

From the symmetrical chemical structure of polyphenylene,  $\mathbf{P}_{[s,t]}$ , we find the edgepartition of  $\mathbf{P}_{[s,t]}$  easily. The edge partition of polyphenylenes  $\mathbf{P}_{[s,t]}$  is shown in Table 2.

**Table 2.** Edge-partition of polyphenylenes  $P_{[s,t]}$ .

Edge-Partition	$E_{(2\sim 2)}$	$E_{(2\sim3)}$	$E_{(3\sim3)}$
Number of bonds	4(2s+t)	4(6st+s-t)	(6st + s - t)

# • Entropy related to the 1<sup>st</sup> K-Banhatti index of P<sub>[s,t]</sub>

Assume that  $\mathbf{P}_{[s,t]}$  is a network of benzenoid aromatic nuclei in polyphenylenes. Equation (1) and Table 2 are then used to calculate the 1<sup>st</sup> K Banhatti index:

$$B_1(\mathbf{P}_{[s,t]}) = 26s + 42t + 188st$$

By using Table 2 and Equation (7) as follows:

$$\begin{split} ENT_{B_1}(\mathbf{P}_{[s,t]}) &= \log \left(B_1\right) - \frac{1}{B_1} \log \left\{ \prod_{E_{(2,2)}} \left(d_{a_i} + d_{a_j}\right)^{\left(d_{a_i} + d_{a_j}\right)} \times \prod_{E_{(2,3)}} \left(d_{a_i} + d_{a_j}\right)^{\left(d_{a_i} + d_{a_j}\right)} \right. \\ &\times \prod_{E_{(3,3)}} \left(d_{a_i} + d_{a_j}\right)^{\left(d_{a_i} + d_{a_j}\right)} \\ &= \log \left(26s + 42t + 188st\right) - \frac{1}{26s + 42t + 188st} \log \left\{4(2st + t)(4)^4 \right. \\ &\times \left. 4(6st + s - t)(5)^5 \times (6st + s - t)(6)^6 \right. \end{split}$$

After simplification, we obtain

$$ENT_{B_1}(\mathbf{P}_{[s,t]}) = \log\left(26s + 42t + 188st\right) - \frac{1}{26s + 42t + 188st}\log\left\{356984st + 59156s - 58132t\right\}.$$
(21)

# • Entropy related to $2^{nd}$ K-Banhatti index of $P_{[s,t]}$

Assume that  $\mathbf{P}_{[s,t]}$  is a network of benzenoid aromatic nuclei in polyphenylenes. Then, by using Equation (1) and Table 2, the 2<sup>*nd*</sup> *K*-Banhatti index is

$$B_2(\mathbf{P}_{[s,t]}) = 33s + 49t + 230st$$

By using Table 2 and Equation (8) as described below:

$$ENT_{B_{2}}(\mathbf{P}_{[s,t]}) = \log (B_{2}) - \frac{1}{B_{2}} \log \left\{ \prod_{E_{(2,2)}} (d_{a_{i}} \times d_{a_{j}})^{(d_{a_{i}} \times d_{a_{j}})} \times \prod_{E_{(2,3)}} (d_{a_{i}} \times d_{a_{j}})^{(d_{a_{i}} \times d_{a_{j}})} \right\}$$
  

$$\times \prod_{E_{(3,3)}} (d_{a_{i}} \times d_{a_{j}})^{(d_{a_{i}} \times d_{a_{j}})} \left\}$$
  

$$= \log (33s + 49t + 230st) - \frac{1}{33s + 49t + 230st} \log \left\{ 4(2st + t)4^{4} \times 4(6st + s - t)6^{6} \times (6st + s - t)9^{9} \right\}.$$
(22)

# • Entropy related to the 1<sup>st</sup> K hyper Banhatti index of P<sub>[s,t]</sub>

Assume that  $\mathbf{P}_{[s,t]}$  is a network of benzenoid aromatic nuclei in polyphenylenes. The 1<sup>st</sup> hyper Banhatti index is then determined using Equation (2) and Table 2

$$HB_1(\mathbf{P}_{[s,t]}) = 8(118st + 17s + 25t)$$

By using Table 2 and Equation (10) as described below,

$$ENT_{HB_{1}}(\mathbf{P}_{[s,t]}) = \log (HB_{1}) - \frac{1}{HB_{1}} \log \left\{ \prod_{E_{(2,2)}} (d_{a_{i}} + d_{a_{j}})^{2(d_{a_{i}} + d_{a_{j}})^{2}} \times \prod_{E_{(2,3)}} (d_{a_{i}} + d_{a_{j}})^{2(d_{a_{i}} + d_{a_{j}})^{2}} \right.$$

$$\times \prod_{E_{(3,3)}} (d_{a_{i}} + d_{a_{j}})^{2(d_{a_{i}} + d_{a_{j}})^{2}}$$

$$= \log (8(118st + 17s + 25t)) - \frac{1}{8(118st + 17s + 25t)} \log \left\{ 4(2st + t)4^{32} \times 4(6st + s - t)5^{50} \times (6st + s - t)6^{72} \right\}$$
(23)

## • Entropy related to the $2^{nd}$ K hyper Banhatti index of $P_{[s,t]}$

Assume that  $\mathbf{P}_{[s,t]}$  is a network of benzenoid aromatic nuclei in polyphenylenes. The 2<sup>*nd*</sup> K hyper Banhatti index is then calculated using the Equation (2) and Table 2:

$$HB_2(\mathbf{P}_{[s,t]}) = 225s + 289t + 1478st$$

By using Table 2 and Equation (10) as described below,

$$ENT_{HB_{1}}(\mathbf{P}_{[s,t]}) = \log (HB_{1}) - \frac{1}{HB_{1}} \log \left\{ \prod_{E_{(2,2)}} (d_{a_{i}} + d_{a_{j}})^{2(d_{a_{i}} + d_{a_{j}})^{2}} \times \prod_{E_{(2,3)}} (d_{a_{i}} + d_{a_{j}})^{2(d_{a_{i}} + d_{a_{j}})^{2}} \right.$$

$$\times \prod_{E_{(3,3)}} (d_{a_{i}} + d_{a_{j}})^{2(d_{a_{i}} + d_{a_{j}})^{2}}$$

$$= \log (225s + 289t + 1478st) - \frac{1}{225s + 289t + 1478st} \log \left\{ 4(2st + t)4^{32} \times 4(6st + s - t)5^{50} \times (6st + s - t)6^{72} \right\}$$
(24)

# • Entropy related to the 1<sup>st</sup> redefined Zagreb index of P<sub>[s,t]</sub>

Assume that  $\mathbf{P}_{[s,t]}$  is a network of benzenoid aromatic nuclei in polyphenylenes. The  $1^{st}$  redefined Zagreb index is then obtained by using Equation (4) and Table 2

$$ReZG_1(\mathbf{P}_{[s,t]}) = 8(12st + s + 2t)$$

By using Table 2 and Equation (11) as described below,

$$ENT_{ReZG_{1}}(\mathbf{P}_{[s,t]}) = \log (ReZG_{1}) - \frac{1}{ReZG_{1}} \log \left\{ \prod_{E_{(2,2)}} \left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \times \prod_{E_{(2,3)}} \left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}} + d_{a_{j}}}{d_{a_{i}}d_{a_{j}}} \right]} \right\}$$

$$= \log 8(12st + s + 2t) - \frac{1}{8(12st + s + 2t)} \log \left\{ 4(2st + t) \times 4(6st + s - t)(\frac{5}{6})^{\frac{5}{6}} \times (6st + s - t)(\frac{2}{3})^{\frac{2}{3}} \right\}.$$
(25)

## • Entropy related to the $2^{nd}$ redefined Zagreb in the index of $P_{[s,t]}$

Assume that  $\mathbf{P}_{[s,t]}$  is a network of benzenoid aromatic nuclei in polyphenylenes. The 2<sup>*nd*</sup> redefined Zagreb index is then obtained by utilizing Equation (4) and Table 2:

$$ReZG_2(\mathbf{P}_{[s,t]}) = 158st + 13s + 27t$$

By using Table 2 and Equation (12) as described below,

$$ENT_{ReZG_{2}}(\mathbf{P}_{[s,t]}) = \log (ReZG_{2}) - \frac{1}{ReZG_{2}} \log \left\{ \prod_{E_{(2,2)}} \left[ \frac{d_{a_{i}}d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}}d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}} \right]} \times \prod_{E_{(2,3)}} \left[ \frac{d_{a_{i}}d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}}d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}} \right]} \right\}$$

$$\times \prod_{E_{(3,3)}} \left[ \frac{d_{a_{i}}d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}} \right]^{\left[ \frac{d_{a_{i}}d_{a_{j}}}{d_{a_{i}} + d_{a_{j}}} \right]} \right\}$$

$$= \log (158st + 13s + 27t)$$

$$- \frac{1}{158st + 13s + 27t} \log \left\{ 4(2st + t) \times 4(6st + s - t)(\frac{6}{5})^{\frac{6}{5}} \times (6st + s - t)(\frac{3}{2})^{\frac{3}{2}} \right\}.$$
(26)

# • Entropy related to the $3^{rd}$ redefined Zagreb index of $P_{[s,t]}$

Assume that  $\mathbf{P}_{[s,t]}$  is a network of benzenoid aromatic nuclei in polyphenylenes. The  $3^{rd}$  redefined Zagreb index is then obtained using Equation (5) and Table 2

$$ReZG_3(\mathbf{P}_{[s,t]}) = 1172st + 174s - 110t$$

By using Table 2 and Equation (13) as described below,

$$ENT_{ReZG_{3}}(\mathbf{P}_{[s,t]}) = \log (ReZG_{3}) - \frac{1}{ReZG_{3}} \log \left\{ \prod_{E_{(2,2)}} [(d_{u}d_{a_{j}})(d_{u} + d_{a_{j}})]^{[(d_{a_{i}}d_{a_{j}})(d_{a_{i}} + d_{a_{j}})]} \right. \\ \times \prod_{E_{(2,3)}} [(d_{a_{i}}d_{a_{j}})(d_{a_{i}} + d_{a_{j}})]^{[(d_{u}d_{a_{j}})(d_{a_{i}} + d_{a_{j}})]} \\ \times \prod_{E_{(3,3)}} [(d_{a_{i}}d_{a_{j}})(d_{a_{i}} + d_{a_{j}})]^{[(d_{a_{i}}d_{a_{j}})(d_{a_{i}} + d_{a_{j}})]} \right] \\ = \log (1172st + 174s - 110t) - \frac{1}{1172st + 174s - 110t} \log \left\{ 4(2st + t)2^{64} \\ \times 4(6st + s - t)30^{30} \times (6st + s - t)54^{54} \right\}.$$

$$(27)$$

Comparison of K-Banhatti and Redefined Zagreb Indices of  $\mathbf{P}_{(s,t)}$ 

In this section, we present numerical and graphical comparison of  $B_1, B_23, HB_1$ ,  $HB_1, ReZG_1, ReZG_2$  and  $ReZG_3$ , of polyphenylenes  $\mathbf{P}_{(s,t)}$  for s, t = 1, 2, 3, ..., 11, in Table 3 and Figure 4 respectively.

**Table 3.** *K*-Banhatti and redefined Zagreb indices of  $\mathbf{P}_{(s,t)}$ .

(s,t)	$B_1$	$B_2$	$HB_1$	$HB_2$	$ReZG_1$	$ReZG_2$	$ReZG_3$
(1, 1)	256	312	1280	1992	120	198	1236
(2, 2)	888	1084	4448	6940	432	712	4816
(3, 3)	1896	2316	9504	14,844	936	1542	10,740
(4, 4)	3280	4008	16,448	25,704	1632	2688	19,008
(5, 5)	5040	6160	25,280	39,520	2520	4150	29,620
(6, 6)	7176	8772	36,000	56,292	3600	5928	42,576
(7,7)	9688	11,844	48,608	76,020	4872	8022	57,876
(8, 8)	12,576	15,376	63,104	98,704	6336	10,432	75,520
(9,9)	15,840	19,368	79,488	124,344	7992	13,158	95 <i>,</i> 508
(10, 10)	19,480	23,820	97,760	152,940	9840	16,200	117,840
(11, 11)	23,496	28,732	117,920	184,492	11,880	19,558	142,516



**Figure 4.** Graphical representation of indices  $\mathbf{P}_{(s,t)}$ .

#### 4. Conclusions

We investigated a variety of imperative molecules, namely boron  $B_{12}$  and polyphenylenes  $\mathbf{P}_{[s,t]}$  and estimated their valency-based K Banhatti indices using four K Banhatti polynomials by a set partition using an atom-bonds approach. The acquired results are valuable in anticipating numerous molecular features of chemical substances, such as boiling point, electron energy, pi, pharmaceutical configuration, and many more concepts. Using Shannon's entropy and Chen et al. entropy's definitions, we looked into the graph entropies connected to a novel information function and assessed the link between degreebased topological indices and degree-based entropies in this work. Industrial chemistry has a strong foundation in the concept of distance-based entropy. It is employed to determine the electronic structure, signal processing, physicochemical reactions, and complexity of molecules and molecular ensembles. Together with chemical structure, thermodynamic entropy, energy, and computer sciences, the K-Banhatti entropy can be crucial in linking different fields and serving as the basis for future interdisciplinary research. We intend to extend this idea to different chemical structures in the future, opening up new directions for study in this area. Furthermore, we can compute more results by using the valency-based technique for these symmetrical chemical structures.

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