Article

A Paradigmatic Approach to Find the Valency-Based K-Banhatti and Redefined Zagreb Entropy for Niobium Oxide and a Metal–Organic Framework

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Abstract: Entropy is a thermodynamic function in chemistry that reflects the randomness and disorder of molecules in a particular system or process based on the number of alternative configurations accessible to them. Distance-based entropy is used to solve a variety of difficulties in biology, chemical graph theory, organic and inorganic chemistry, and other fields. In this article, the characterization of the crystal structure of niobium oxide and a metal–organic framework is investigated. We also use the information function to compute entropies by building these structures with degree-based indices including the K-Banhatti indices, the first redefined Zagreb index, the second redefined Zagreb index, the third redefined Zagreb index, and the atom-bond sum connectivity index.

Keywords: molecular graph; niobium oxide; metal–organic framework; topological indices; K-Banhatti entropies; redefined Zagreb entropies; Atom–bond sum connectivity entropy

1. Introduction

The optical properties of metallic nanoparticles have drawn the attention of scientists and researchers. The heat created by the nanoparticles overwhelms cancer tissue while causing no harm to healthy cells. Niobium nanoparticles have the capacity to easily attach to ligands, making them ideal for optothermal cancer treatment. Chemical graph theory is a contemporary branch of applied chemistry, which has remained an attractive area of research for scientists during the past two decades, and significant contributions have been made by scientists in this area of research including [1–7]. We investigate the relationship between atoms and bonds using combinatorial approaches such as vertex and edge partitions. Topological indices are essential in providing directions for treating malignancies or tumors. These indices can be obtained experimentally or numerically. Although experimental data are valuable, they are also costly; therefore, computational analysis gives a cost-effective and time-efficient solution.

The transformation of a chemical structure into a number is used to generate a topological index. The topological index is a graph invariant that characterizes the graph’s topology while remaining invariant throughout graph automorphism. A topological index is a numerical number defined only by the graph. The eccentricity-based topological indices are crucial in chemical graph theory [8]. Wiener, a chemist, first used a topological index in 1947 while researching the relationship between the molecular structure and the physical and chemical
properties of certain hydrocarbon compounds [9]. In 2010, Damir et al. defined the redefined second Zagreb index as the same as the inverse sum indeg index [10].

We used the concept of valency-based entropies in this article, where $v_{a_1}$ and $v_{a_2}$ denote the valency of atoms, $a_1$ and $a_2$, within the molecule. Kulli started computing valency-based topological indices in 2016 using the valency of atom bonds and some Banhatti indices [11–13], each of which has the following definition:

The first valence-based K-Banhatti polynomial and the first K-Banhatti index are as follows:

$$B_1(G, x) = \sum_{a_1 \sim a_2} x^{v_{a_1} + v_{a_2}} \quad B_1(G) = \sum_{a_1 \sim a_2} (v_{a_1} + v_{a_2})$$ (1)

The second valence based K-Banhatti polynomial and the second K-Banhatti index are as follows, respectively:

$$B_2(G, x) = \sum_{a_1 \sim a_2} x^{v_{a_1} \times v_{a_2}} \quad B_2(G) = \sum_{a_1 \sim a_2} (v_{a_1} \times v_{a_2})$$ (2)

The first valence based hyper K-Banhatti polynomial and the firstst hyper K-Banhatti index are as follows, respectively:

$$HB_1(G, x) = \sum_{a_1 \sim a_2} x^{(v_{a_1} + v_{a_2})^2} \quad HB_1(G) = \sum_{a_1 \sim a_2} (v_{a_1} + v_{a_2})^2$$ (3)

$$HB_2(G, x) = \sum_{a_1 \sim a_2} x^{(v_{a_1} \times v_{a_2})^2} \quad HB_2(G) = \sum_{a_1 \sim a_2} (v_{a_1} \times v_{a_2})^2$$ (4)

In 2013, Ranjini [14] introduced a redefined version of the Zagreb indices $ReZG_1$, and in 2021, Shanmukha [15] defined them as

$$ReZG_1(G, x) = \sum_{a_1 \sim a_2} x^{\frac{v_{a_1} + v_{a_2}}{v_{a_1} \times v_{a_2}}} \quad ReZG_1 = \sum_{a_1 \sim a_2} \frac{v_{a_1} + v_{a_2}}{v_{a_1} \times v_{a_2}}$$ (5)

$$ReZG_2(G, x) = \sum_{a_1 \sim a_2} x^{\frac{v_{a_1} \times v_{a_2}}{v_{a_1} + v_{a_2}}} \quad ReZG_2 = \sum_{a_1 \sim a_2} \frac{v_{a_1} \times v_{a_2}}{v_{a_1} + v_{a_2}}$$ (6)

The third redefined Zagreb index was defined as

$$ReZG_3(G, x) = \sum_{a_1 \sim a_2} x^{\frac{(v_{a_1} \times v_{a_2})}{v_{a_1} + v_{a_2}}} \quad ReZG_3 = \sum_{a_1 \sim a_2} (v_{a_1} \times v_{a_2}) \left(\frac{v_{a_1} + v_{a_2}}{v_{a_1} \times v_{a_2}}\right)$$ (7)

Recently, Ali et al. amalgamated the atom-bond connectivity index and sum connectivity index and initiated the new molecular descriptor named the atom-bond sum-connectivity index [16], defined as:

$$ABS(G, x) = \sum_{a_1 \sim a_2} x^{\sqrt{\frac{(v_{a_1} + v_{a_2})^2}{v_{a_1} \times v_{a_2}}}} \quad ABS = \sum_{a_1 \sim a_2} \sqrt{\frac{(v_{a_1} + v_{a_2} - 2)}{(v_{a_1} + v_{a_2})}}$$ (8)

Shannon first popularized the concept of entropy in his 1948 work [17]. Entropy is the quantity of thermal energy per unit temperature in a system that is not accessible for meaningful work [18,19]. Because the work is derived from organized molecular motion, entropy is also a measure of a system’s molecular disorder or unpredictability [20,21]. In this article, we build the Niobium dioxide NbO$_2$ and the metal–organic framework (MOF) to compute the K-Banhatti and redefined Zagreb entropies using K-Banhatti indices [22–24], and redefined Zagreb indices, respectively. The idea of entropy is extracted from Shazia Manzoor’s paper [25].
2. Valency-Based Entropy

The idea of edge-weighted graph entropy was introduced in 2009 \[26\], \(G = (V_G, E_G, \phi(v_a, v_b))\) for an edge-weighted graph, where \(V_G\) is the vertex set, \(E_G\) the edge set, and the edge-weight of an edge \((v_a, v_b)\) is represented by \(\phi(v_a, v_b)\). The entropy of an edge-weighted graph is defined as

\[
ENT_{\phi(G)} = - \sum_{d_1 \sim d_2} \frac{\phi(v_{d_1}, v_{d_2})}{\sum_{d_1 \sim d_2} \phi(v_{d_1}, v_{d_2})} \log \left\{ \frac{\phi(v_{d_1}, v_{d_2})}{\sum_{d_1 \sim d_2} \phi(v_{d_1}, v_{d_2})} \right\}.
\]  \hspace{1cm} (9)

- **The first K-Banhatti entropy**

Let \(\phi(v_{d_1}, v_{d_2}) = v_{d_1} + v_{d_2}\). Then, the first K-Banhatti index (1) is given by

\[
B_1(G) = \sum_{d_1 \sim d_2} \left\{ v_{d_1} + v_{d_2} \right\} = \sum_{d_1 \sim d_2} \phi(v_{d_1}, v_{d_2}).
\]

Now, by inserting these values into Equation (9), the first K-Banhatti entropy is

\[
ENT_{B_1(G)} = \log (B_1(G)) - \frac{1}{B_1(G)} \log \left\{ \prod_{d_1 \sim d_2} [v_{d_1} + v_{d_2}]^{[v_{d_1} + v_{d_2}]} \right\}.
\]  \hspace{1cm} (10)

- **The second K-Banhatti entropy**

Let \(\phi(v_{d_1}, v_{d_2}) = v_{d_1} \times v_{d_2}\). Then, the second K-Banhatti index (2) is given by

\[
B_2(G) = \sum_{d_1 \sim d_2} \left\{ v_{d_1} \times v_{d_2} \right\} = \sum_{d_1 \sim d_2} \phi(v_{d_1}, v_{d_2}).
\]

Now, by inserting these values into Equation (9), the second K-Banhatti entropy is

\[
ENT_{B_2(G)} = \log (B_2(G)) - \frac{1}{B_2(G)} \log \left\{ \prod_{d_1 \sim d_2} [v_{d_1} \times v_{d_2}]^{[v_{d_1} \times v_{d_2}]} \right\}.
\]  \hspace{1cm} (11)

- **The first K-hyper Banhatti entropy**

Let \(\phi(v_{d_1}, v_{d_2}) = (v_{d_1} + v_{d_2})^2\). Then, the first K-hyper Banhatti index (3) is given by

\[
HB_1(G) = \sum_{d_1 \sim d_2} \left\{ (v_{d_1} + v_{d_2})^2 \right\} = \sum_{d_1 \sim d_2} \phi(v_{d_1}, v_{d_2}).
\]

Now, by inserting these values into Equation (9), the first K-hyper Banhatti entropy is

\[
ENT_{HB_1(G)} = \log (HB_1(G)) - \frac{1}{HB_1(G)} \log \left\{ \prod_{d_1 \sim d_2} [(v_{d_1} + v_{d_2})^2]^{[(v_{d_1} + v_{d_2})^2]} \right\}.
\]  \hspace{1cm} (12)

- **The second K-hyper Banhatti entropy**

Let \(\phi(v_{d_1}, v_{d_2}) = (v_{d_1} \times v_{d_2})^2\). Then the second K-hyper Banhatti index (4) is given by

\[
HB_2(G) = \sum_{d_1 \sim d_2} \left\{ (v_{d_1} \times v_{d_2})^2 \right\} = \sum_{d_1 \sim d_2} \phi(v_{d_1}, v_{d_2}).
\]

Now, by inserting these values into Equation (9), the second K-hyper Banhatti entropy is

\[
ENT_{HB_2(G)} = \log (HB_1(G)) - \frac{1}{HB_1(G)} \log \left\{ \prod_{d_1 \sim d_2} [(v_{d_1} \times v_{d_2})^2]^{[(v_{d_1} \times v_{d_2})^2]} \right\}.
\]  \hspace{1cm} (13)
• The first redefined Zagreb entropy
Let \( \phi(v_{a_1}v_{a_2}) = \frac{v_{a_1}v_{a_2}}{d_{v_{a_1}}d_{v_{a_2}}^2} \). Then, the first redefined Zagreb index (5) is given by
\[
\text{ReZG}_1 = \sum_{a_1 \sim a_2} \left\{ \frac{v_{a_1} + v_{a_2}}{v_{a_1}v_{a_2}} \right\} = \sum_{a_1 \sim a_2} \phi(v_{a_1}v_{a_2}).
\]
Now, by inserting these values into Equation (9), the first redefined Zagreb entropy is
\[
\text{ENT}_{\text{ReZG}_1} = \log(\text{ReZG}_1) - \frac{1}{\text{ReZG}_1} \log \left\{ \prod_{a_1 \sim a_2} \left[ \frac{v_{a_1} + v_{a_2}}{v_{a_1}v_{a_2}} \right]^{\frac{\phi(v_{a_1}v_{a_2})}{\phi(v_{a_1}v_{a_2})}} \right\}. \tag{14}
\]

• The second redefined Zagreb entropy
Let \( \phi(v_{a_1}v_{a_2}) = \frac{v_{a_1}d_{v_{a_2}}}{v_{a_1} + v_{a_2}} \). Then, the second redefined index (6) is given by
\[
\text{ReZG}_2 = \sum_{a_1 \sim a_2} \left\{ \frac{v_{a_1}v_{a_2}}{v_{a_1} + v_{a_2}} \right\} = \sum_{a_1 \sim a_2} \phi(v_{a_1}v_{a_2}).
\]
Now, by inserting these values into Equation (9), the second redefined Zagreb entropy is
\[
\text{ENT}_{\text{ReZG}_2} = \log(\text{ReZG}_2) - \frac{1}{\text{ReZG}_2} \log \left\{ \prod_{a_1 \sim a_2} \left[ \frac{v_{a_1} + v_{a_2}}{v_{a_1}v_{a_2}} \right]^{\frac{\phi(v_{a_1}v_{a_2})}{\phi(v_{a_1}v_{a_2})}} \right\}. \tag{15}
\]

• The third redefined Zagreb entropy
Let \( \phi(v_{a_1}v_{a_2}) = \left\{ (v_{a_1}v_{a_2})(v_{a_1} + v_{a_2}) \right\} \). Then, the third redefined Zagreb index (7) is given by
\[
\text{ReZG}_3 = \sum_{a_1 \sim a_2} \left\{ (v_{a_1}v_{a_2})(d_{v_{a_1}} + d_{v_{a_2}}) \right\} = \sum_{a_1 \sim a_2} \phi(v_{a_1}v_{a_2}).
\]
Now, by inserting these values into Equation (9), the third redefined Zagreb entropy is
\[
\text{ENT}_{\text{ReZG}_3} = \log(\text{ReZG}_3) - \frac{1}{\text{ReZG}_3} \log \left\{ \prod_{a_1 \sim a_2} \left[ (v_{a_1}v_{a_2})(v_{a_1} + v_{a_2}) \right]^{\frac{\phi(v_{a_1}v_{a_2})}{\phi(v_{a_1}v_{a_2})}} \right\}. \tag{16}
\]

• Atom-bond sum connectivity entropy
Let \( \phi(\ddot{a}_1\ddot{a}_2) = \left\{ \sqrt{\frac{v_{a_1} + v_{a_2} - 2}{v_{a_1} + v_{a_2}}} \right\} \). Then, the fourth atom-bond connectivity index (8) is given by
\[
\text{ABS}(G) = \sum_{\ddot{a}_1, \ddot{a}_2 \in E_G} \left\{ \sqrt{\frac{v_{a_1} + v_{a_2} - 2}{v_{a_1} + v_{a_2}}} \right\} = \sum_{\ddot{a}_1, \ddot{a}_2 \in E_G} \phi(\ddot{a}_1\ddot{a}_2).
\]
By inserting the values of \( \text{ABS}(G) \) into Equation (9), the atom-bond sum connectivity (\( \text{ENT}_{\text{ABC}(G)} \)) entropy is
\[
\text{ENT}_{\text{ABS}(G)} = \log(\text{ABS}(G)) - \frac{1}{\text{ABS}(G)} \log \left\{ \prod_{\ddot{a}_1, \ddot{a}_2 \in E_G} \left( \sqrt{\frac{v_{a_1} + v_{a_2} - 2}{v_{a_1} + v_{a_2}}} \right) \left( \sqrt{\frac{v_{a_1} + v_{a_2} - 2}{v_{a_1} + v_{a_2}}} \right)^{\frac{\phi(\ddot{a}_1\ddot{a}_2)}{\phi(\ddot{a}_1\ddot{a}_2)}} \right\}. \tag{17}
\]

3. Niobium Dioxide NbO₂
Niobium Nb, a refractory metal, is a good choice for the initial shell of nuclear fusion reactors. It does, however, have a strong attraction for O₂ and C, both of which are available
in pyrotechnics and refrigerant-like liquids. As part of the first barrier, Nb is well known for its ability to interact very effectively with O\textsubscript{2} [27]. As a result, reliable thermodynamic data on NbO, NbO\textsubscript{2}, Nb\textsubscript{2}O\textsubscript{5}, and other intermediate phases, such as Nb\textsubscript{12}O\textsubscript{29}, are very effective. In transistors, niobium monoxide is used as a gate electrode, and a (NbO/NbO\textsubscript{2}) junction may be used in robust switching devices. In this article, we will attempt to explain NbO\textsubscript{2}, which has a total atom count of 2 + 5s + 5t + 9st; see Figure 1.

Figure 1. Niobium dioxide 3D structure.

There are three types of atoms in NbO\textsubscript{2} based on their valency: eight atoms with valency 2, 8s + 8t + 4st − 8 atoms with valency 3, and 2 − 3s − 3t + 5st atoms with valency 4. Table 1 shows the atom-bond partitions of NbO\textsubscript{2} derived from these results.

Table 1. Atom-bond partition of NbO\textsubscript{2}.

| Types of Atom Bonds | E\textsubscript{(2~3)} | E\textsubscript{(3~3)} | E\textsubscript{(3~4)} | E\textsubscript{(4~4)} |
|---------------------|----------------|----------------|----------------|----------------|
| Cardinality of Atom bonds | 16 | 8(2s + 2t − 3) | 4(3st − 2s − 2t + 2) | 2(2st + s + t) |

• The first K-Banhatti entropy of NbO\textsubscript{2}

Let NbO\textsubscript{2} be a network of a niobium dioxide molecule. Then, by using Equation (1) and Table 1, the first K-Banhatti polynomial is

\[ B_1(\text{NbO}_2, x) = \sum_{E_{(2~3)}} x^{2+3} + \sum_{E_{(3~3)}} x^{3+3} + \sum_{E_{(3~4)}} x^{3+4} + \sum_{E_{(4~4)}} x^{4+4} \]

\[ = 16x^5 + 8(2s + 2t − 3)x^6 + 4(3st − 2s − 2t + 2)x^7 + 2(2st + s + t)x^8. \] (18)

After simplifying Equation (18), we obtain the first K-Banhatti index by taking the first derivative at \( x = 1 \).

\[ B_1(\text{NbO}_2) = 116st + 24s + 24t − 8. \] (19)
Now, we compute the first K-Banhatti entropy of NbO₂ by using Table 1 and Equation (19) in Equation (10) in the following way:

\[ ENT_{B_1}(\text{NbO}_2) = \log(B_1) - \frac{1}{B_2} \log \left\{ \prod_{E(2,3)} (v_{u_1} + v_{u_2})^{(v_{u_1} + v_{u_2})} \times \prod_{E(3,3)} (v_{u_1} + v_{u_2})^{(v_{u_1} + v_{u_2})} \times \prod_{E(3,4)} (v_{u_1} + v_{u_2})^{(v_{u_1} + v_{u_2})} \right\} \]

\[ = \log(116st + 24s + 24t - 8) - \frac{1}{116st + 24s + 24t - 8} \log \left\{ 16(4)^4 \times 8(2s + 2t - 3)(5)^5 \times 4(3st - 2s - 2t + 2)(6)^6 \times 2(2st - s - t)(8)^8 \right\}. \]

- The second K-Banhatti entropy of NbO₂
Let NbO₂ be a network of a niobium dioxide molecule. Then, by using Equation (2) and Table 1, the second K-Banhatti polynomial is

\[ B_2(\text{NbO}_2) = 208st + 16s + 16t - 24. \]

Now, we compute the second K-Banhatti entropy of NbO₂ by using Table 1 and Equation (21) in Equation (11) in the following way:

\[ ENT_{B_2}(\text{NbO}_2) = \log(B_2) - \frac{1}{B_2} \log \left\{ \prod_{E(2,3)} (v_{u_1} \times v_{u_2})^{(v_{u_1} \times v_{u_2})} \times \prod_{E(3,3)} (v_{u_1} \times v_{u_2})^{(v_{u_1} \times v_{u_2})} \times \prod_{E(3,4)} (v_{u_1} \times v_{u_2})^{(v_{u_1} \times v_{u_2})} \right\} \]

\[ = \log(208st + 16s + 16t - 24) - \frac{1}{208st + 16s + 16t - 24} \log \left\{ 16(6)^6 \times 8(2s + 2t - 3)(5)^9 \times 4(3st - 2s - 2t + 2)(6)^{12} \times 2(2st - s - t)(8)^{16} \right\}. \]

- The first K-hyper Banhatti entropy of NbO₂
Let NbO₂ be a network of a niobium dioxide molecule. Then, by using Equation (3) and Table 1, the first K-hyper Banhatti polynomial is

\[ HB_1(\text{NbO}_2) = \sum_{E(2,3)} x^{(2+3)^2} + \sum_{E(3,3)} x^{(3+3)^2} + \sum_{E(3,4)} x^{(3+4)^2} + \sum_{E(4,4)} x^{(4+4)^2} \]

\[ = 16x^{25} + 8(2s + 2t - 3)x^{36} + 4(3st - 2s - 2t + 2)x^{49} + 2(2st - s - t)x^{64}. \]

Taking the first derivative of Equation (22) at \( x = 1 \), we obtain the first K-hyper Banhatti index

\[ HB_1(\text{NbO}_2) = 844st + 56s + 56t - 72. \]

Now, we compute the first K-hyper Banhatti entropy of NbO₂ by using Table 1 and Equation (23) in Equation (13) in the following way:
\[
\text{ENT}_{HB_1}(\text{NbO}_2) = \log (HB_1) - \frac{1}{\text{ENT}} \log \left\{ \prod_{E(2,3)} (v_a_1 + v_a_2)^2(v_u_1 + v_u_2)^2 \times \prod_{E(3,4)} (v_a_1 + v_a_2)^2(v_u_1 + v_u_2)^2 \right\}
\]

\[
\times \prod_{E(3,4)} (v_a_1 + v_a_2)^2(v_u_1 + v_u_2)^2 \times \prod_{E(3,3)} (v_a_1 + v_a_2)^2(v_u_1 + v_u_2)^2
\]

\[
= \log \left( \frac{944st + 136s + 200t}{944st + 136s + 200t} \right) \log \left\{ 16(5^{50}) \right\}
\]

\[\times 8(2s + 2t - 3) \times 4(3st - 2s - 2t + 2) (798) \times 2(2st - s - t)(8^{128}).\]

### The second K-hyper Banhatti entropy of \(\text{NbO}_2\)

Let \(\text{NbO}_2\) be a network of a niobium dioxide molecule. Then, by using Equation (4) and Table 1, the second K-hyper Banhatti polynomial is

\[
HB_2(\text{NbO}_2) = \sum_{E(2-3)} x^{2(x-3)^2} + \sum_{E(3-3)} x^{(3 \times 3)^2} + \sum_{E(3-4)} x^{(3 \times 4)^2} + \sum_{E(4-4)} x^{(4 \times 4)^2}
\]

\[
= 16x^{36} + 8(2s + 2t - 3)x^{81} + 4(3st - 2s - 2t + 2)x^{144}
\]

\[+ 2(2st - s - t)x^{256}.\]

Taking the first derivative of Equation (24) at \(x = 1\), we obtain the second K-hyper Banhatti index

\[
HB_2(\text{NbO}_2) = 2752st - 368s - 368t - 216.
\]  

(25)

Now, we compute the second K-hyper Banhatti entropy of \(\text{NbO}_2\) by using Table 1 and Equation (25) in Equation (13) in the following way:

\[
\text{ENT}_{HB_1}(\text{NbO}_2) = \log (HB_1) - \frac{1}{\text{ENT}} \log \left\{ \prod_{E(2,3)} (v_a_1 \times v_a_2)^2(v_u_1 \times v_u_2)^2 \times \prod_{E(3,4)} (v_a_1 \times v_a_2)^2(v_u_1 \times v_u_2)^2 \right\}
\]

\[\times \prod_{E(3,4)} (v_a_1 \times v_a_2)^2(v_u_1 \times v_u_2)^2 \times \prod_{E(3,3)} (v_a_1 \times v_a_2)^2(v_u_1 \times v_u_2)^2
\]

\[
= \log \left( \frac{2752st - 368s - 368t - 216}{2752st - 368s - 368t - 216} \right) \log \left\{ 16(6)^{72} \right\}
\]

\[\times 8(2s + 2t - 3)9^{91} \times 4(3st - 2s - 2t + 2)12^{288} \times 2(2st - s - t)16^{112}.\]

### The first redefined Zagreb entropy of \(\text{NbO}_2\)

Let \(\text{NbO}_2\) be a network of a niobium dioxide molecule. Then, by using Equation (5) and Table 1, the first redefined Zagreb polynomial is

\[
\text{ReZG}_1(\text{NbO}_2) = \sum_{E(2-3)} x^{\frac{1}{3} + \frac{1}{3}} + \sum_{E(3-3)} x^{\frac{1}{3} + \frac{1}{3}} + \sum_{E(3-4)} x^{\frac{1}{3} + \frac{1}{3}} + \sum_{E(4-4)} x^{\frac{1}{3} + \frac{1}{3}}
\]

\[
= 16x^6 + 8(2s + 2t - 3)x^2 + 4(3st - 2s - 2t + 2)x^2
\]

\[+ 2(2st - s - t)x^2.\]

Taking the first derivative of Equation (26) at \(x = 1\), we obtain the first redefined Zagreb index

\[
\text{ReZG}_1(\text{NbO}_2) = 9st + 5s + 5t + 2.
\]  

(27)
Now, we compute the first redefined Zagreb entropy by using Table 1 and Equation (27) in Equation (14) in the following way:

\[
\text{ENT}_{\text{ReZG}}(\text{NbO}_2) = \log \left( \text{ReZG}_1 \right) - \frac{1}{\text{ReZG}_1} \log \left\{ \prod_{E(3,3)} \left( \frac{\nu_{i_1} + \nu_{i_2}}{\nu_{i_1} \nu_{i_2}} \right)^{\nu_{i_1} + \nu_{i_2}} \right\} \\
\times \prod_{E(3,4)} \left( \frac{\nu_{i_1} + \nu_{i_2}}{\nu_{i_1} \nu_{i_2}} \right)^{\nu_{i_1} + \nu_{i_2}} \times \prod_{E(4,4)} \left( \frac{\nu_{i_1} + \nu_{i_2}}{\nu_{i_1} \nu_{i_2}} \right)^{\nu_{i_1} + \nu_{i_2}} \right\} \\
= \log 8(9st + 5s + 5t + 2) - \frac{1}{8(9st + 5s + 5t + 2)} \log \left\{ 16\left( \frac{9}{8} \right)^{\frac{5}{8}} \right\} \\
\times 8(2s + 2t - 3)\left( \frac{2}{3} \right)^3 \\
\times 4(3st - 2s - 2t + 2)\left( \frac{2}{3} \right)^2 \times 2(2st - s - t)\left( \frac{8}{16} \right)^{\frac{5}{16}} \right\}.
\]

- The second redefined Zagreb entropy of \(\text{NbO}_2\)

Let \(\text{NbO}_2\) be a network of a niobium dioxide molecule. Then, by using Equation (6) and Table 1, the second redefined Zagreb polynomial is

\[
\text{ReZG}_2(\text{NbO}_2) = \sum_{E(2,3)} x^{\frac{2s}{3}} + \sum_{E(3,3)} x^{\frac{3s}{3}} + \sum_{E(3,4)} x^{\frac{3t}{4}} + \sum_{E(4,4)} x^{\frac{4t}{4}}
= 16x^5 + 8(2s + 2t - 3)x^3 + 4(3st - 2s - 2t + 2)x^{\frac{12}{7}} + 2(2st - s - t)x^2.
\]  

Taking the first derivative of Equation (28) at \(x = 1\), we obtain the second redefined Zagreb index

\[
\text{ReZG}_2(\text{NbO}_2) = \frac{4}{7}(25st + 11s + 11t - 27).
\]  

Now, we compute the second redefined Zagreb entropy by using Table 1 and Equation (29) in Equation (15) in the following way:

\[
\text{ENT}_{\text{ReZG}}(\text{NbO}_2) = \log \left( \text{ReZG}_2 \right) - \frac{1}{\text{ReZG}_2} \log \left\{ \prod_{E(2,3)} \left( \frac{\nu_{i_1} + \nu_{i_2}}{\nu_{i_1} \nu_{i_2}} \right)^{\nu_{i_1} + \nu_{i_2}} \right\} \\
\times \prod_{E(3,4)} \left( \frac{\nu_{i_1} + \nu_{i_2}}{\nu_{i_1} \nu_{i_2}} \right)^{\nu_{i_1} + \nu_{i_2}} \times \prod_{E(4,4)} \left( \frac{\nu_{i_1} + \nu_{i_2}}{\nu_{i_1} \nu_{i_2}} \right)^{\nu_{i_1} + \nu_{i_2}} \right\} \\
= \log \left( \frac{4}{7}(25st + 11s + 11t - 27) \right) - \frac{7}{4(25st + 11s + 11t - 27)} \log \left\{ 16\left( \frac{9}{8} \right)^{\frac{5}{8}} \right\} \\
\times 8(2s + 2t - 3)\left( \frac{2}{3} \right)^3 \times 4(3st - 2s - 2t + 2)\left( \frac{12}{7} \right)^{\frac{12}{7}} \\
\times 2(2st - s - t)\left( \frac{8}{16} \right)^{\frac{5}{16}} \right\}.
\]

- The third redefined Zagreb entropy of \(\text{NbO}_2\)

Let \(\text{NbO}_2\) be a network of a niobium dioxide molecule. Then, by using Equation (7) and Table 1, the third redefined Zagreb polynomial is
\[
\text{ReZG}_3(\text{NbO}_2) = \sum_{E_{(2-3)}} x^{(2 \times 3)(2+3)} + \sum_{E_{(3-3)}} x^{(3 \times 3)(3+3)} + \sum_{E_{(3-4)}} x^{(3 \times 4)(3+4)} + \sum_{E_{(4-4)}} x^{(4 \times 4)(4+4)}
\]

\[
= 16x^{30} + 8(2s + 2t - 3)x^{54} + 4(3st - 2s - 2t + 2)x^{84} + 2(2st - s - t)x^{128}.
\]  

Taking the first derivative of Equation (30) at \(x = 1\), we obtain the third redefined Zagreb index

\[
\text{ReZG}_3(\text{NbO}_2) = 8(95st - 4s - 4t - 9).
\]

Now, we compute the third redefined Zagreb entropy by using Table 1 and Equation (31) in Equation (16) in the following way:

\[
\text{ENT}_{\text{ReZG}_3}(\text{NbO}_2) = \log (\text{ReZG}_3) - \frac{1}{\text{ReZG}_3} \log \left\{ \prod_{E_{(2-3)}} [(d_u v_{d_2})(d_u + v_{d_2})][(v_{a_1} v_{d_2})(v_{a_1} + v_{d_2})] \right\}
\times \prod_{E_{(3-3)}} [(v_{a_1} v_{d_2})(v_{a_1} + v_{d_2})][(d_u v_{a_2})(d_u + v_{a_2})]
\times \prod_{E_{(3-4)}} [(v_{a_1} v_{d_2})(v_{a_1} + v_{d_2})][(v_{a_1} v_{a_2})(v_{a_1} + v_{a_2})]
\times \prod_{E_{(4-4)}} [(v_{a_1} v_{d_2})(v_{a_1} + v_{d_2})][(v_{a_1} v_{a_2})(v_{a_1} + v_{a_2})] \right\}
\]

\[
= \log 8(95st - 4s - 4t - 9) - \frac{1}{8(95st - 4s - 4t - 9)} \log \left\{ 16(30)^{30} \times 8(2s + 2t - 3)^{54} \times 4(3st - 2s - 2t + 2)^{84} \times 2(2st - s - t)^{128} \right\}.
\]

**Atom-bond sum connectivity entropy of NbO_2**

Let NbO_2 be a network of a niobium dioxide molecule. Then, using Equation (8) and Table 1, the atom-bond sum connectivity polynomial is

\[
\text{ABS}(\text{NbO}_2) = \sum_{E_{(2-3)}} x^{\sqrt{\frac{9}{5}}} + \sum_{E_{(3-3)}} x^{\sqrt{\frac{15}{5}}} + \sum_{E_{(3-4)}} x^{\sqrt{\frac{21}{5}}} + \sum_{E_{(4-4)}} x^{\sqrt{\frac{27}{5}}}
\]

\[
= 16x^{\sqrt{\frac{9}{5}}} + 8(2s + 2t - 3)x^{\sqrt{\frac{15}{5}}} + 4(3st - 2s - 2t + 2)x^{\sqrt{\frac{21}{5}}} + 2(2st - s - t)x^{\sqrt{\frac{27}{5}}}.
\]

Taking the first derivative of Equation (32) at \(x = 1\), we obtain the atom-bond sum connectivity index

\[
\text{ABS}(\text{NbO}_2) = 16 \sqrt{\frac{3}{5}} + 8(2s + 2t - 3) \frac{2}{\sqrt{6}} + 4(3st - 2s - 2t + 2) \sqrt{\frac{5}{7}} + 2(2st - s - t) \frac{\sqrt{7}}{2}.
\]  

Now, we compute the atom-bond sum connectivity entropy by using Table 1 and Equation (33) in Equation (17) in the following way:
\[ ENT_{ABS}(\text{NbO}_2) = \log(ABS) - \frac{1}{ABS} \log \left\{ \prod_{E(2,3)} \left\{ \frac{\sqrt{(v'_{a_1} + v'_{a_2} - 2)}}{v'_{a_1} + v'_{a_2}} \right\} \right\} \]

\[ \times \prod_{E(3,3)} \left\{ \frac{\sqrt{(v'_{a_1} + v'_{a_2} - 2)}}{v'_{a_1} + v'_{a_2}} \right\} \times \prod_{E(3,4)} \left\{ \frac{\sqrt{(v'_{a_1} + v'_{a_2} - 2)}}{v'_{a_1} + v'_{a_2}} \right\} \]

\[ \times \prod_{E(4,4)} \left\{ \frac{\sqrt{(v'_{a_1} + v'_{a_2} - 2)}}{v'_{a_1} + v'_{a_2}} \right\} \]

\[ = \log(ABS) - \frac{1}{ABS} \log \left\{ 16\left(\frac{\sqrt{3}}{5}\right)^2 \times 8(2s + 2t - 3)\left(\frac{\sqrt{5}}{6}\right)^2 \right\} \]

\[ \times 4(3st - 2s - 2t + 2)\left(\frac{\sqrt{7}}{2}\right)^2 \times 2(2st - s - t)\left(\frac{\sqrt{7}}{2}\right)^2 \].

Comparison

In this section, we compare the K-Banhatti indices namely \(B_1\) (first K-Banhatti index), \(B_2\) (second K-Banhatti index), \(HB_1\) (first hyper K-Banhatti index), \(HB_2\) (second hyper K-Banhatti index) and the redefined Zagreb indices (\(ReG_1\), \(ReG_2\), \(ReG_3\)) for \(\text{NbO}_2\) numerically and graphically in Table 2 and Figure 2, respectively.

Table 2. Numerical comparison of the K-Banhatti topological indices of \(\text{NbO}_2\).

| \((s, t)\) | \(B_1\) | \(B_2\) | \(HB_1\) | \(HB_2\) | \(ReG_1\) | \(ReG_2\) | \(ReG_3\) | \(ABS\) |
|-----------|--------|--------|--------|--------|--------|--------|--------|-------|
| (2,2)     | 552    | 872    | 3528   | 9320   | 58     | 136.34 | 5680   | 75.92117 |
| (3,3)     | 1180   | 1944   | 7860   | 22,344 | 113    | 291.77 | 13,152 | 160.40086 |
| (4,4)     | 2040   | 3432   | 13,880 | 408,872| 186    | 504.34 | 23,664 | 275.748201 |
| (5,5)     | 3132   | 5336   | 21,588 | 64,904 | 277    | 774.058| 23,664 | 421.962304 |
| (6,6)     | 4456   | 7656   | 30,984 | 94,440 | 386    | 1100.91| 37,216 | 599.043115 |
| (7,7)     | 6012   | 10,392 | 42,068 | 129,480| 513    | 1484.9 | 73,440 | 806.990632 |
| (8,8)     | 7800   | 13,544 | 54,840 | 170,024| 658    | 1926.1 | 96,112 | 1045.804857 |
| (9,9)     | 9820   | 17,112 | 69,300 | 216,072| 821    | 2424.3 | 121,824| 1315.48579 |
| (10,10)   | 12,072 | 21,096 | 85,448 | 267,624| 1002   | 2979.7 | 150,576| 1616.03343 |
| (11,11)   | 14,556 | 25,496 | 103,284| 324,680| 1201   | 3592.3 | 182,368| 1947.447777 |
| (12,12)   | 17,272 | 30,312 | 122,808| 387,240| 1418   | 4262.1 | 217,200| 2309.728831 |

Figure 2. Graphical comparison of TT’s of \(\text{NbO}_2\).
4. Metal–Organic Framework

Metal–organic frameworks are distinguished by their three-dimensional frameworks composed of metallic ions. This metal–organic framework has the molecular formula FeTPyP–Co, where Fe denotes iron, TPyP denotes tetrakis pyridyl porphyrin, and Co denotes cobalt \[28\]. All metal ions and organic molecules in the MOF \((s,t)\) network can accommodate a wide range of guest molecules. Metal–organic frameworks have several uses, including as energy storage devices, gas storage, heterogeneous catalysis, and chemical evaluation. We will examine a 2D structure of a metal–organic framework called MOF \((s,t)\), where \(s\) and \(t\) are the unit cells in a row and column, respectively. The MOF \((2,2)\) is shown in Figure 3. There are 74 atoms in the MOF \((s,t)\), and \(2(44s - s - t + 1)\) atom-bonds are used, as Figure 3 of MOF \((2,2)\) demonstrates.

Figure 3. Two-dimensional MOF\(_{(2,2)}\) structure.

The atom-bonds partition of the MOF\(_{(s,t)}\) is shown in Table 3.

\[
E_{(1\sim3)} = \{ e = v_{a_1} \sim v_{a_2}, \forall \ a_1, a_2 \in E(\text{MOF}_{(s,t)}), (v_{a_1}) = 1, (v_{a_2}) = 3 \},
\]

\[
E_{(2\sim3)} = \{ e = v_{a_1} \sim v_{a_2}, \forall \ a_1, a_2 \in E(\text{MOF}_{(s,t)}), (v_{a_1}) = 2, (v_{a_2}) = 3 \},
\]

\[
E_{(3\sim3)} = \{ e = v_{a_1} \sim v_{a_2}, \forall \ a_1, a_2 \in E(\text{MOF}_{(s,t)}), (v_{a_1}) = 3, (v_{a_2}) = 3 \},
\]

\[
E_{(3\sim4)} = \{ e = v_{a_1} \sim v_{a_2}, \forall \ a_1, a_2 \in E(\text{MOF}_{(s,t)}), (v_{a_1}) = 3, (v_{a_2}) = 4 \},
\]

| Types of Atom Bonds | \(E_{(1\sim3)}\) | \(E_{(2\sim3)}\) | \(E_{(3\sim3)}\) | \(E_{(3\sim4)}\) |
|---------------------|-----------------|-----------------|-----------------|-----------------|
| Cardinality of Atom bonds | \(1 + 24st\) | \(6(s + t - 1)\) | \(2(28st - 2s - 2t + 1)\) | \(4(2st - s + t + 1)\) |

- The first K-Banhatti entropy of MOF\(_{(s,t)}\)
Let MOF\(_{(s,t)}\) be a metal–organic framework. Then, using Equation (1) and Table 3, the first K-Banhatti polynomial is

\[
B_1(\text{MOF}_{(s,t)}, x) = \sum_{E(1-3)} x^{1+1} + \sum_{E(2-3)} x^{2+3} + \sum_{E(3-3)} x^{3+3} + \sum_{E(3-4)} x^{3+4}
\]

\[
= (24st + 1)x^4 + 6(s + t - 1)x^5 + 2(28st - 2s - 2t + 1)x^6
\]

\[
+ 4(2st - s - t + 1)x^7.
\]

Taking the first derivative of Equation (34) at \(x = 1\), we obtain the first K-Banhatti index

\[
B_1(\text{MOF}_{(s,t)}) = 2(244st - 11s - 11t + 2).
\]

Now, we compute the 1st K-Banhatti entropy of (MOF\(_{(s,t)}\)) by using Table 3 and Equation (35) in Equation (10) in the following way:

\[
\text{ENT}_{B_1}(\text{MOF}_{(s,t)}, x) = \log(B_1) - \frac{1}{B_1} \log\left\{ \prod_{E(1,2)} (v_{a_1} + v_{b_2})^{(v_{a_1} + v_{b_2})} \times \prod_{E(2,3)} (v_{a_1} + v_{b_1})^{(v_{a_1} + v_{b_1})} \times \prod_{E(1,3)} (v_{a_2} + v_{b_1})^{(v_{a_2} + v_{b_1})} \right\}
\]

After simplification, we obtain

\[
\text{ENT}_{B_1}(\text{MOF}_{(s,t)}, x) = \log 2(244st - 11s - 11t + 2)
\]

\[
- \frac{1}{2(244st - 11s - 11t + 2)} \log\left\{ (24st + 1)^4 \times 6(s + t - 1)^5 \times 2(28st - 2s - 2t + 1)^6 \right\}
\]

\[
\times 4(2st - s - t + 1)^7.
\]

- The second K-Banhatti entropy of MOF\(_{(s,t)}\)

Let MOF\(_{(s,t)}\) be a metal–organic framework. Then, using Equation (1) and Table 3, the second K-Banhatti polynomial is

\[
B_2(\text{MOF}_{(s,t)}, x) = \sum_{E(1-3)} x^{1\times3} + \sum_{E(2-3)} x^{2\times3} + \sum_{E(3-3)} x^{3\times3} + \sum_{E(3-4)} x^{3\times4}
\]

\[
= (24st + 1)x^3 + 6(s + t - 1)x^4 + 2(28st - 2s - 2t + 1)x^5
\]

\[
+ 4(2st - s - t + 1)x^6.
\]

Taking the first derivative of Equation (37) at \(x = 1\), we obtain the second K-Banhatti index

\[
B_2(\text{MOF}_{(s,t)}) = 3(224st - 16s - 16t + 11).
\]

Now, we compute the second K-Banhatti entropy of (MOF\(_{(s,t)}\)) by using Table 3 and Equation (38) in Equation (11) in the following way:
\[
\text{ENT}_{B_2} (\text{MOF}_{(s,t)}) = \log (B_2) - \frac{1}{B_2} \log \left\{ \prod_{E_{(1,3)}} (v_{a_1} \times v_{a_2})^{(v_{a_1} \times v_{a_2})} \times \prod_{E_{(2,3)}} (v_{a_1} \times v_{a_2})^{(v_{a_1} \times v_{a_2})} \right\} \\
\times \prod_{E_{(3,3)}} (v_{a_1} \times v_{a_2})^{(v_{a_1} \times v_{a_2})} \times \prod_{E_{(3,4)}} (v_{a_1} \times v_{a_2})^{(v_{a_1} \times v_{a_2})} \\
= \log (3(224st - 16s - 16t + 11)) \\
- \frac{1}{3(224st - 16s - 16t + 11)} \log \left\{ (24st + 1)^{3} \right\} \\
\times (6(s + t - 1)6^6 \times 2(28st - 2s - 2t + 1)^{90} \times 4(2st - s - t + 1)^{1212}) \right\}.
\]

**The first K-hyper Banhatti entropy of MOF\(_{(s,t)}\)**

Let MOF\(_{(s,t)}\) be a metal–organic framework. Then, using Equation (3) and Table 3, the first K-hyper Banhatti polynomial is

\[
HB_1 (\text{MOF}_{(s,t)}, x) = \sum_{E_{(1,3)}} x^{(1+3)^2} + \sum_{E_{(2,3)}} x^{(2+3)^2} + \sum_{E_{(3,3)}} x^{(3+3)^2} + \sum_{E_{(3,4)}} x^{(3+4)^2} \\
= (24st + 1)x^{16} + 6(s + t - 1)x^{25} + 2(28st - 2s - 2t + 1)x^{36} + 4(2st - s - t + 1)x^{49}.
\] (39)

Taking the first derivative of Equation (39) at \(x = 1\), we obtain the first K-hyper Banhatti index

\[
HB_1 (\text{MOF}_{(s,t)}) = 2(1396st - 95s - 95t + 67).
\] (40)

Now, we compute the first K-hyper Banhatti entropy of MOF\(_{(s,t)}\) by using Table 3 and Equation (40) in Equation (12) in the following way:

\[
\text{ENT}_{HB_1} (\text{MOF}_{(s,t)}, x) = \log (HB_1) - \frac{1}{HB_1} \log \left\{ \prod_{E_{(1,3)}} (v_{a_1} + v_{a_2})^{2(\text{v}_{a_1} + \text{v}_{a_2})^2} \right\} \\
\times \prod_{E_{(2,3)}} (v_{a_1} + v_{a_2})^{2(v_{a_1} + v_{a_2})^2} \times \prod_{E_{(3,3)}} (v_{a_1} + v_{a_2})^{2(v_{a_1} + v_{a_2})^2} \\
\times \prod_{E_{(3,4)}} (v_{a_1} + v_{a_2})^{2(v_{a_1} + v_{a_2})^2}.
\]

After simplification, we obtain

\[
= \log 2(1396st - 95s - 95t + 67) - \frac{1}{2(1396st - 95s - 95t + 67)} \log \left\{ (24st + 1)^{432} \right\} \\
\times 6(s + t - 1)^{50} \times 2(28st - 2s - 2t + 1)^{672} \times 4(2st - s - t + 1)^{998}. \]

**The second K-hyper Banhatti entropy of MOF\(_{(s,t)}\)**

Let MOF\(_{(s,t)}\) be a metal–organic framework. Then, by using Equation (4) and Table 3, the second K-Banhatti polynomial is

\[
HB_2 (\text{MOF}_{(s,t)}, x) = \sum_{E_{(1,3)}} x^{(1+3)^2} + \sum_{E_{(2,3)}} x^{(2+3)^2} + \sum_{E_{(3,3)}} x^{(3+3)^2} + \sum_{E_{(3,4)}} x^{(3+4)^2} \\
= (24st + 1)x^{89} + 6(s + t - 1)x^{36} + 2(28st - 2s - 2t + 1)x^{81} + 4(2st - s - t + 1)x^{144}.
\] (41)

Taking the first derivative of Equation (41) at \(x = 1\), we obtain the second K-hyper Banhatti index

\[
HB_2 (\text{MOF}_{(s,t)}) = 5904st - 684s - 684t + 693.
\] (42)
Now, we compute the second K-hyper Banhatti entropy of MOF\(_{(s,t)}\) by using Table 3 and Equation (42) in Equation (13) in the following way:

\[
ENT_{HBd}(\text{MOF}_{(s,t)}) = \log (HB_2) - \frac{1}{HB_2} \log \left\{ \prod_{E_{(1,3)}} (v_{d_1} \times v_{d_2})^2 (v_{t_1} \times v_{t_2})^2 \right\}
\]

After simplification, we obtain

\[
= \log \left( \frac{5904st - 684s - 684t + 693}{5904st - 684s - 684t + 693} \right) - \frac{1}{2} \log \left\{ \left( \frac{24st + 1}{2} \right)^{1/2} \left( \frac{2st - s - t + 1}{2} \right)^{1/2} \right\}
\]

\[
\times 6(s + t - 1)^{2} \times 2(28st - 2s - 2t + 1)^{9/16} \times 4(2st - s - t + 1)^{12/288}.
\]

**The first redefined Zagreb entropy of MOF\(_{(s,t)}\)**

Let MOF\(_{(s,t)}\) be a metal–organic framework. Then, using Equation (5) and Table 3, the first redefined Zagreb polynomial is

\[
ReZG_1(\text{MOF}_{(s,t)}, x) = \sum_{E_{(1-3)}} x^{1/3} + \sum_{E_{(2-3)}} x^{2/3} + \sum_{E_{(3-4)}} x^{3/4} + \sum_{E_{(4-4)}} x^{3/4}
\]

\[
= (24st + 1)x^{1/2} + 6(s + t - 1)x^{3/2} + 2(28st - 2s - 2t + 1)x^{7/2}
\]

\[
+ 4(2st - s - t + 1)x^{11/2}.
\]

Taking the first derivative of Equation (44) at \(x = 1\), we obtain the first redefined Zagreb index

\[
ReZG_1(\text{MOF}_{(s,t)}) = 2(37st + 2).
\]

Now, we compute the first redefined Zagreb entropy using Table 3 and Equation (45) in Equation (14) in the following way:

\[
ENT_{ReZG_1}(\text{MOF}_{(s,t)}, x) = \log (ReZG_1) - \frac{1}{ReZG_1} \log \left\{ \prod_{E_{(1,3)}} \left( \frac{v_{d_1} + v_{d_2}}{v_{d_1} v_{d_2}} \right)^{\frac{v_{d_1} + v_{d_2}}{v_{d_1} v_{d_2}}} \right\}
\]

\[
\times \prod_{E_{(2,3)}} \left( \frac{v_{d_1} + v_{d_2}}{v_{d_1} v_{d_2}} \right)^{\frac{v_{d_1} + v_{d_2}}{v_{d_1} v_{d_2}}} \times \prod_{E_{(3,4)}} \left( \frac{v_{d_1} + v_{d_2}}{v_{d_1} v_{d_2}} \right)^{\frac{v_{d_1} + v_{d_2}}{v_{d_1} v_{d_2}}}
\]

After simplification, we obtain

\[
= \log 2(37st + 2) - \frac{1}{2(37st + 2)} \log \left\{ (24st + 1) \left( \frac{4}{3} \right)^{1/2} \times 6(s + t - 1) \left( \frac{5}{6} \right)^{3/2} \right\}
\]

\[
\times 2(28st - 2s - 2t + 1) \left( \frac{6}{9} \right)^{3/2} \times 4(2st - s - t + 1) \left( \frac{7}{12} \right)^{11/2}.
\]
The second redefined Zagreb entropy of \( \text{MOF}_{(s,t)} \)

Let \( \text{MOF}_{(s,t)} \) be a metal–organic framework. Then, using Equation (6) and Table 3, the second redefined Zagreb polynomial is

\[
ReZG_2(\text{MOF}_{(s,t)}, x) = \sum_{E(1,3)} x^{3 \times 3} + \sum_{E(2,3)} x^{2 \times 4} + \sum_{E(3,3)} x^{3 \times 3} + \sum_{E(3,4)} x^{3 \times 4} \\
= (24st + 1)x^2 + 6(s + t - 1)x^2 + 2(28st - 2s - 2t + 1)x^2 + 4(2st - s - t + 1)x^{\frac{5}{2}}. 
\]  

(46)

Taking the first derivative of Equation (46) at \( x = 1 \), we obtain the second redefined Zagreb index

\[
ReZG_2(\text{MOF}_{(s,t)}) = \frac{810}{7}st - \frac{198}{35}(s + t) + \frac{198}{35}. 
\]  

(47)

Now, we compute the second redefined Zagreb entropy by using Table 3 and Equation (47) in Equation (15) in the following way:

\[
\text{ENT}_{ReZG_2}(\text{MOF}_{(s,t)}, x) = \log (ReZG_2) - \frac{1}{ReZG_2} \log \left( \prod_{E(1,3)} \frac{\nu_{a_1} \nu_{a_2}}{\nu_{a_1} + \nu_{a_2}} \right) - \prod_{E(2,3)} \frac{\nu_{a_1} \nu_{a_2}}{\nu_{a_1} + \nu_{a_2}} - \prod_{E(3,3)} \frac{\nu_{a_1} \nu_{a_2}}{\nu_{a_1} + \nu_{a_2}} - \prod_{E(3,4)} \frac{\nu_{a_1} \nu_{a_2}}{\nu_{a_1} + \nu_{a_2}}. 
\]

After simplification, we obtain

\[
= \log \left( \frac{810}{7}st - \frac{198}{35}(s + t) + \frac{198}{35} \right) - \frac{1}{\frac{810}{7}st - \frac{198}{35}(s + t) + \frac{198}{35}} \log \left( (24st + 1)(\frac{3}{4})^3 \times 6(s + t - 1)(\frac{6}{5})^5 \right. \\
\left. \times 2(28st - 2s - 2t + 1)(\frac{9}{6})^2 \times 4(2st - s - t + 1)(\frac{12}{7})^{\frac{5}{2}} \right). 
\]

The third redefined Zagreb entropy of \( \text{MOF}_{(s,t)} \)

Let \( \text{MOF}_{(s,t)} \) be a metal–organic framework. Then, using Equation (7) and Table 3, the third redefined Zagreb polynomial is

\[
ReZG_3(\text{MOF}_{(s,t)}, x) = \sum_{E(1,3)} x^{(1 \times 3)(1 + 3)} + \sum_{E(2,3)} x^{(2 \times 3)(2 + 3)} + \sum_{E(3,3)} x^{(3 \times 3)(3 + 3)} \\
+ \sum_{E(3,4)} x^{(3 \times 4)(3 + 4)} \\
= (24st + 1)x^{12} + 6(s + t - 1)x^{30} + 2(28st - 2s - 2t + 1)x^{54} + 4(2st - s - t + 1)x^{84}. 
\]

(48)

Taking the first derivative of Equation (48) at \( x = 1 \), we obtain the third redefined Zagreb index

\[
ReZG_2(\text{MOF}_{(s,t)}) = 3984st - 372(s + t) + 384. 
\]  

(49)

Now, we compute the third redefined Zagreb entropy by using Table 3 and Equation (49) in Equation (16) in the following way:
Let NbO be a network of a niobium II oxide molecule. Then, using Equation (8) and Table 1, the atom-bond sum connectivity polynomial is

\[
\text{ABS(MOF}_{(s,t)},x) = \sum_{E(1,3)} x^{\frac{1}{\sqrt{2}}} + \sum_{E(2,3)} x^{\frac{2}{\sqrt{2}}} + \sum_{E(3,3)} x^{\frac{3}{\sqrt{2}}} + \sum_{E(3,4)} x^{\frac{5}{\sqrt{2}}} = (24st + 1)x^{\frac{1}{\sqrt{2}}} + 6(s + t - 1)x^{\frac{3}{\sqrt{2}}} + 2(28st - 2s - 2t + 1)x^{\frac{3}{\sqrt{2}}} + 4(2st - s - t + 1)x^{\frac{5}{\sqrt{2}}}.
\] (50)

Taking the first derivative of Equation (50) at \( x = 1 \), we obtain the atom-bond sum connectivity index

\[
\text{ABS(MOF)} = (24st + 1)\frac{1}{\sqrt{2}} + 6(s + t - 1)\sqrt{\frac{3}{5}} + 2(28st - 2s - 2t + 1)\sqrt{\frac{7}{3}} + 4(2st - s - t + 1)\sqrt{\frac{5}{7}}.
\] (51)

Now, we compute the third redefined Zagreb entropy using Table 3 and Equation (51) in Equation (17) in the following way:

\[
\text{ENT}_{\text{ABS(MOF)}} = \log(\text{ABS(MOF)}) - \frac{1}{\text{ABS}} \log \left\{ \prod_{E(1,3)} \left( \frac{(v_{a1} + v_{b2} - 2)}{v_{a1} + v_{b2}^2} \right)^{\frac{(v_{a1} + v_{b2} - 2)}{v_{a1} + v_{b2}^2}} \right\} \times \prod_{E(2,3)} \left( \frac{(v_{a1} + v_{b2} - 2)}{v_{a1} + v_{b2}^2} \right)^{\frac{(v_{a1} + v_{b2} - 2)}{v_{a1} + v_{b2}^2}} \times \prod_{E(3,3)} \left( \frac{(v_{a1} + v_{b2} - 2)}{v_{a1} + v_{b2}^2} \right)^{\frac{(v_{a1} + v_{b2} - 2)}{v_{a1} + v_{b2}^2}} \times \prod_{E(3,4)} \left( \frac{(v_{a1} + v_{b2} - 2)}{v_{a1} + v_{b2}^2} \right)^{\frac{(v_{a1} + v_{b2} - 2)}{v_{a1} + v_{b2}^2}} \right\} \times \frac{1}{\text{ABS}} \log \left\{ (24st + 1)(\frac{1}{\sqrt{2}})^{\sqrt{\frac{3}{5}}} \times 6(s + t - 1)(\sqrt{\frac{3}{5}})^{\sqrt{\frac{3}{5}}} \right\} \times 2(28st - 2s - 2t + 1)(\sqrt{\frac{3}{5}})^{\sqrt{\frac{3}{5}}} \times 4(2st - s - t + 1)(\sqrt{\frac{5}{7}})^{\sqrt{\frac{5}{7}}}. 
\]
Comparison

In this section, we compare the K-Banhatti and redefined Zagreb indices for MOF\(_{(s,t)}\) numerically and graphically in Table 4 and Figure 4, respectively.

Table 4. Numerical comparison of the topological indices of MOF\(_{(s,t)}\):

| \((s, t)\) | \(B_1\) | \(B_2\) | \(HB_1\) | \(HB_2\) | \(ReG_1\) | \(ReG_2\) | \(ReG_3\) | \(ABS\) |
|----------|--------|--------|--------|--------|--------|--------|--------|--------|
| (2,2)    | 1868   | 2529   | 10,542 | 21,573 | 296    | 307.03 | 14832  | 27,339.22 |
| (3,3)    | 4264   | 5793   | 24,122 | 49,725 | 444    | 700.71 | 34008  | 27,686.67 |
| (4,4)    | 7636   | 10,401 | 43,286 | 89,685 | 592    | 1256.40| 61152  | 28,173.03 |
| (5,5)    | 11,984 | 16,353 | 68,034 | 141,453| 740    | 1974.09| 96,264 | 28,798.29 |
| (6,6)    | 17,308 | 23,649 | 98,366 | 205,029| 888    | 2853.77| 139,344| 29,562.45 |
| (7,7)    | 23,608 | 32,289 | 134,282| 280,413| 1036   | 3895.46| 190,392| 30,465.50 |
| (8,8)    | 30,884 | 42,273 | 175,782| 367,605| 1184   | 5099.14| 249,408| 31,507.46 |
| (9,9)    | 39,136 | 53,601 | 222,866| 466,605| 1332   | 6464.83| 316,392| 32,688.32 |
| (10,10)  | 48,364 | 66,273 | 275,534| 577,413| 1480   | 7992.51| 391,344| 34,008.08 |
| (11,11)  | 58,568 | 80,289 | 333,786| 700,029| 1628   | 9682.20| 474,264| 35,466.73 |
| (12,12)  | 69,748 | 95,649 | 397,622| 834,453| 1776   | 11,533.89| 565,152| 37,064.29 |

Figure 4. Graphical comparison of TI’s of metal–organic framework.

5. Conclusions

The remarkable optical properties of metallic nanoparticles have piqued the interest of scientists and researchers. In this article, two important molecules niobium dioxide NbO\(_2\) and the MOF\(_{(s,t)}\) were considered, and the accurate formulas of some important valency-based topological indices were calculated using the technique of atom-bond partitioning. We investigated the distance-based entropies associated with a new information function and evaluated the relationship between degree-based topological indices and degree-based entropies in this article using Shannon’s entropy and Chen et al.’s entropy definitions. The idea of distance-based entropy is widely ingrained in industrial chemistry. It is used to calculate the complexity of molecules and molecular ensembles, their electronic structure, signal processing, physicochemical processes, and so on. The K-Banhatti entropy, in conjunction with the chemical structure, thermodynamic entropy, energy, and computer sciences can play an essential role in bridging various domains and providing a foundation for new interdisciplinary research. In the future, we hope to expand this concept to include various chemical structures, allowing researchers to pursue new avenues in this field.
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