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New Paradigmatic Framework of Entropy Computing in Benzenoids Octahedral Structures

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Abstract Network entropy is a potent quantitative approach to the analysis of the structural complexity of connected systems, derived out of information theory and has received significant interest in computer science, the biological sciences, and molecular chemistry because of its capacity to reflect high structural diversity and low symmetry. Topological indices give a graph entropy measurement which is also an efficient and systematic set of indices to study the structure of molecules and predict their behaviour. This work is a research on the K-Banhatti entropy of three benzenoid octahedral structures, i.e. BPOS, BDPOS, and BHPOS, and the purpose of this investigation is to use the data on the entropy to point out the structural features of these structures. Topological descriptors of molecular structures are an important part of the chemical graph theory and are widely used in cheminformatics, information technology, biological research, and other areas. There has also been a broad selection of topological indices designed to represent the behavior of molecules especially non-regular graphs where the irregularity measures are able to provide a better insight into the structural heterogeneity. Inevitably, we analyse a few indices of irregularity in order to describe the non-uniformity of benzenoid networks and aid quantitative structure-activity relationship (QSAR) analysis. A more detailed insight into structural organization of benzenoid octahedral structures is made possible through combined application of entropy measures and irregularity indices. Further, we compute the first and second kinds of modified Zagreb entropies for BPOS, BDPOS, and BHPOS structures. The findings reveal that the suggested descriptors are robust, informative and computationally efficient measures used in examining complex molecular networks and thus, serve in the development of entropy-based measures in chemical graph theory.

Keywords: Topological indices, $K-$Banhatti entropy, $K-$hyper Banhatti entropy, $BPOS_n$, $BDPOS_n$, $BHPOS_n$, Molecular descriptors; First and second kinds of modified Zagreb entropies.

Introduction

In the context of benzenoids, topological indices are mathematical descriptors used to characterize the structural features of molecules [1-6]. These indices provide insights into the topology of molecular graphs and are widely used in quantitative structure-activity relationship (QSAR) studies [7-12], which aim to correlate the structure of chemical compounds with their biological or physical activities. Planar octahedral structures are more commonly associated with coordination compounds and transition metal complexes than with benzenoids. In the context of coordination chemistry, indices such as coordination number, connectivity indices and various descriptors related to the geometry of the octahedral coordination sphere maybe relevant. The investigation of Benzenoids planar octahedron structures holds promise for expanding our understanding of molecular design principles and may pave the way for applications in diverse fields, including materials science and catalysis [13-17]. As we delve into this unexplored territory, the potential for discovering new reactivity patterns and properties remains an exciting prospect in the realm of chemical research. The application of topological indices, coherence and robustness analysis for a family of unbalanced networks is discussed and many others computes based problems are discussed in [28-33]. Many algebraic and chemical structures-based entropies are discussed in [34-40].

Graph-based molecular structure descriptors are widely termed topological indices in chemical graph theory [18-20]. Where $V_{\mathcal{E}_i}$, $V_{\mathcal{E}_j}$ represents the degree of an arbitrary vertex u in $\mathcal{G}$ and uv is the edge between the vertices $V_{\mathcal{E}_i}$, $V_{\mathcal{E}_j}$ [15].The connectivity index was modified by taking into consideration not only the degree of the end-vertices of the edge uv but also the degree $(V_{\mathcal{E}_i}+V_{\mathcal{E}_j})$ of this edge. The resulting index was called the 1st valency-based K –Banhatti index [16]. Later, Chen et. al. computed some bounds for this index [17]. Accordingly, the 1st, 2nd K –Banhatti index & 1st, 2nd hyper K –Banhatti index [17-20] & polynomial are as follows: 0474

$$B_1(\mathcal{G},\sigma)=\sum_{\mathcal{E}_i\sim\mathcal{E}_j}\sigma^{(V_{\mathcal{E}_i}+V_{\mathcal{E}_j})} \quad \& \quad B_{1(\mathcal{G})}=\sum_{\mathcal{E}_1\sim\mathcal{E}_j}(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}). \tag{1}$$

$$B_2(\mathcal{G},\sigma)=\sum_{\mathcal{E}_i\sim\mathcal{E}_j}\sigma^{(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j})} \quad \& \quad B_{2(\mathcal{G})}=\sum_{\mathcal{E}_1\sim\mathcal{E}_j}(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}). \tag{2}$$

$$HB_1(\mathcal{G},\sigma)=\sum_{\mathcal{E}_i\sim\mathcal{E}_j}\sigma^{\left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)^2} \quad \& \quad HB_{1(\mathcal{G})}=\sum_{\mathcal{E}_1\sim\mathcal{E}_j}(V_{\mathcal{E}_i}+V_{\mathcal{E}_j})^2 \tag{3}$$

$$HB_2(\mathcal{G},\sigma)=\sum_{\mathcal{E}_i\sim\mathcal{E}_j}\sigma^{\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)^2} \quad \& \quad HB_{2(\mathcal{G})}=\sum_{\mathcal{E}_1\sim\mathcal{E}_j}(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j})^2 \tag{4}$$

K − Banhatti Entropies

Following formula expresses the valency-based entropy

$$ENT_{\mu_{(\mathcal{G})}}=-\sum_{\mathcal{E}_i\sim\mathcal{E}_j}\frac{\mu(V_{\mathcal{E}_i},V_{\mathcal{E}_j})}{\sum_{\mathcal{E}_i\sim\mathcal{E}_j}\mu(V_{\mathcal{E}_i},V_{\mathcal{E}_j})}\log\left\{\frac{\mu(V_{\mathcal{E}_i},V_{\mathcal{E}_j})}{\sum_{\mathcal{E}_i\sim\mathcal{E}_j}\mu(V_{\mathcal{E}_i},V_{\mathcal{E}_j})}\right\} \tag{5}$$

The 1st K − Banhatti Entropies

By using equation (1), we get

$$B_{1(\mathcal{G})}=\sum_{\mathcal{E}_i\sim\mathcal{E}_j}\left\{V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right\}=\sum_{\mathcal{E}_i\sim\mathcal{E}_j}\mu(V_{\mathcal{E}_i}V_{\mathcal{E}_j})$$

By using (5), we get

$$ENT_{B_{1_{(\mathcal{G})}}}=\log(B_{1(\mathcal{G})})-\frac{1}{B_{1(\mathcal{G})}}\log\left\{\prod_{\mathcal{E}_i\sim\mathcal{E}_j}\left[V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right]^{\left[V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right]}\right\} \tag{6}$$

The 2nd K − Banhatti Entropies

Let $(V_{\mathcal{E}_i}V_{\mathcal{E}_j}) = V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}$. Therefore the 2nd K –Banhatti index (2) is presented by

$$B_{2(\mathcal{G})} = \sum_{\mathcal{E}_i \sim \mathcal{E}_j} \left\{ V_{\mathcal{E}_i} \times V_{\mathcal{E}_j} \right\} = \sum_{\mathcal{E}_i \sim \mathcal{E}_j} \mu(V_{\mathcal{E}_i} V_{\mathcal{E}_j})$$

By using (5), we get

$$ENT_{B_{2(\mathcal{G})}} = \log(B_{2(\mathcal{G})}) - \frac{1}{B_{2(\mathcal{G})}} \log \left\{ \prod_{\mathcal{E}_i \sim \mathcal{E}_j} \left[V_{\mathcal{E}_i} \times V_{\mathcal{E}_j} \right]^{\left[V_{\mathcal{E}_i} \times V_{\mathcal{E}_j} \right]} \right\} \quad (7)$$

The 1st $K-$ hyper Banhatti Entropies
By using equation (3), we get

$$HB_{1(\mathcal{G})} = \sum_{\mathcal{E}_i \sim \mathcal{E}_j} \left\{ \left\{ V_{\mathcal{E}_i} + V_{\mathcal{E}_j} \right\}^2 \right\} = \sum_{\mathcal{E}_i \sim \mathcal{E}_j} \mu(V_{\mathcal{E}_i} V_{\mathcal{E}_j})$$

By using (5), we get

$$ENT_{HB_{1(\mathcal{G})}} = \log(HB_{1(\mathcal{G})}) - \frac{1}{HB_{1(\mathcal{G})}} \log \left\{ \prod_{\mathcal{E}_i \sim \mathcal{E}_j} \left[V_{\mathcal{E}_i} + V_{\mathcal{E}_j} \right]^{2\left[V_{\mathcal{E}_i} + V_{\mathcal{E}_j} \right]^2} \right\} \quad (8)$$

The 2nd $K-$ Hyper Banhatti Entropies
By using equation (4), we get

$$HB_{2(\mathcal{G})} = \sum_{\mathcal{E}_i \sim \mathcal{E}_j} \left\{ \left\{ V_{\mathcal{E}_i} \times V_{\mathcal{E}_j} \right\}^2 \right\} = \sum_{\mathcal{E}_i \sim \mathcal{E}_j} \mu(V_{\mathcal{E}_i} V_{\mathcal{E}_j})$$

By using (5), we get

$$ENT_{B_{2(\mathcal{G})}} = \log(HB_{2(\mathcal{G})}) - \frac{1}{HB_{2(\mathcal{G})}} \log \left\{ \prod_{\mathcal{E}_i \sim \mathcal{E}_j} \left[V_{\mathcal{E}_i} \times V_{\mathcal{E}_j} \right]^{2\left[V_{\mathcal{E}_i} \times V_{\mathcal{E}_j} \right]^2} \right\} \quad (9)$$

Main Results and Discussions

Benzenoid Planar Octahedron Structures $(BPOS_n)$

The topological characteristics of the $BPOS$ are widely explored. The two-dimensional structure of a $BPOS$ depicts Figure 1. The graph of the BPOS is represented as $BPOS_n$, $n \geq 2$, where n is the dimension of the $BPOS$. Figure 1 displays the 2-dimensional structure of the molecular graph of $BPOS_n$ [21-23].

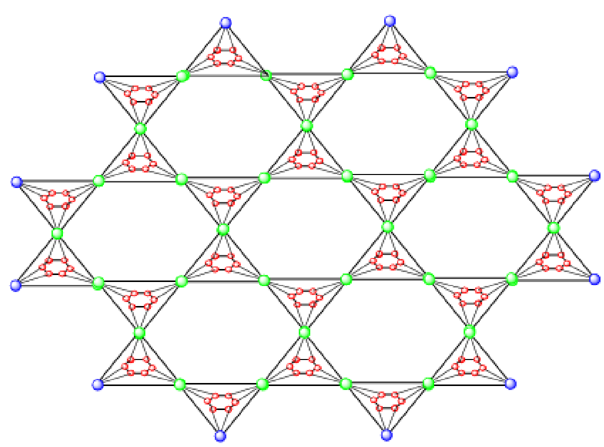

Figure 1. $BPOS$ Structures.

The $BPOS$ has a total of $45n^2 - 3n$ vertices (s) and $90n^2$ edges (t). The degree of end vertices divides the set of edges of the $BPOS$ into five divisions [24, 25]. There are $36n^2$ edges st in the first edge partition, where $s = 3$ and $t = 3$. There are $12n$ edges st in the second edge partition, where $s = 3$ and $t = 4$. There are $36n^2 - 12n$ edges st in the third edge partition, where $s = 3$ and $t = 8$. There are $12n$ edges st in the fourth edge partition, where $s = 4$ and $t = 8$. There are $18n^2 - 12n$ edges st in the fifth edge partition, where $s = 8$ and $t = 8$. The edge partition of a $BPOS$ is shown in Table 1

Table 1. Edge partition of $BPOS$.

S. No.	Class	Number of Appearance
1	$d_{(3,3)}$	$36n^2$
2	$d_{(3,4)}$	$12n$
3	$d_{(3,8)}$	$36n^2 - 12n$
4	$d_{(4,8)}$	$12n$
5	$d_{(8,8)}$	$18n^2 - 12n$

1st K –Banhatti Entropy of $BPOS_n$

Let $BPOS_n$ is a computational approach used to study the electronic structure and properties of materials. The 1st K –Banhatti polynomial is calculated the use of the Equation (1) and the Table 1.

$$B_1(BPOS_n) = \sum_{V_{(3\sim3)}} \sigma^{3+3} + \sum_{V_{(3\sim4)}} \sigma^{3+4} + \sum_{V_{(3\sim8)}} \sigma^{3+8} + \sum_{V_{(4\sim8)}} \sigma^{4+8} + \sum_{V_{(8\sim8)}} \sigma^{8+8}$$

$$= (36n^2)\sigma^6 + (12n)\sigma^7 + (36n^2 - 12n)\sigma^{11} + (12n)\sigma^{12} + (18n^2 - 12n)\sigma^{16}. \qquad (10)$$

Differentiate (10) $\sigma = 1$, we compute

$$B_1(BPOS_n) = 900n^2 - 96n \qquad (11)$$

By using Table 1 & Equation (11) in Equation (6), we get

$$ENT_{B_{1(BPOS_n)}} = \log(B_1) - \frac{1}{B_1}\log\left\{\prod_{V_{(3,3)}}\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)^{\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)} \times \prod_{V_{(3,4)}}\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)^{\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)} \times \prod_{V_{(3,8)}}\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)^{\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)} \times \prod_{V_{(4,8)}}\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)^{\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)} \times \prod_{V_{(8,8)}}\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)^{\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)}\right\}$$

$$= \log(900n^2 - 96n) - \frac{1}{(900n^2 - 96n)}\log\{(36n^2)(6)^6 \times (12n)(7)^7 \times (36n^2 - 12n)(11)^{11} \times (12n)(12)^{12} \times (18n^2 - 12n)(16)^{16}\}$$

2nd K –Banhatti Entropy of $BPOS_n$

Let $BPOS_n$ is a computational approach used to study the electronic structure and properties of materials. Then, by using Equation (2) & Table1, we get

$$B_2(BPOS_n) = \sum_{V_{(3\sim3)}} \sigma^{3\times3} + \sum_{V_{(3\sim4)}} \sigma^{3\times4} + \sum_{V_{(3\sim8)}} \sigma^{3\times8} + \sum_{V_{(4\sim8)}} \sigma^{4\times8} + \sum_{V_{(8\sim8)}} \sigma^{8\times8}$$

$$= (36n^2)\sigma^9 + (12n)\sigma^{12} + (36n^2 - 12n)\sigma^{24} + (12n)\sigma^{32} + (18n^2 - 12n)\sigma^{64}. \qquad (12)$$

Differentiate (12) at $\sigma = 1$, we compute

$$B_2(BPOS_n) = 2340n^2 - 528n \tag{13}$$

By using Table 1 & Equation (13) in Equation (7), we get

$$ENT_{B_{2(BPOS_n)}} = \log(B_2) - \frac{1}{B_2}\log\left\{\prod_{V_{(3,3)}}\left(V_{\Sigma i}\times V_{\Sigma j}\right)^{\left(V_{\Sigma i}\times V_{\Sigma j}\right)} \times \prod_{V_{(3,4)}}\left(V_{\Sigma i}\times V_{\Sigma j}\right)^{\left(V_{\Sigma i}\times V_{\Sigma j}\right)} \times \prod_{V_{(3,8)}}\left(V_{\Sigma i}\times V_{\Sigma j}\right)^{\left(V_{\Sigma i}\times V_{\Sigma j}\right)} \times \prod_{V_{(4,8)}}\left(V_{\Sigma i}\times V_{\Sigma j}\right)^{\left(V_{\Sigma i}\times V_{\Sigma j}\right)} \times \prod_{V_{(8,8)}}\left(V_{\Sigma i}\times V_{\Sigma j}\right)^{\left(V_{\Sigma i}\times V_{\Sigma j}\right)}\right\}$$

$$= \log(2340n^2 - 528n) - \frac{1}{(2340n^2 - 528n)}\log\{(36n^2)(9)^9 \times (12n)(12)^{12} \times (36n^2 - 12n)(24)^{24} \times (12n)(32)^{32} \times (18n^2 - 12n)(64)^{64}\}$$

1st K −Hyper Banhatti Entropy of $BPOS_n$

Let $BPOS_n$ is a computational approach used to study the electronic structure and properties of materials. Then by using Equation (3) and Table 1, we get

$$HB_1(BPOS_n) = \sum_{V_{(3\sim3)}} \sigma^{(3+3)^2} + \sum_{V_{(3\sim4)}} \sigma^{(3+4)^2} + \sum_{V_{(3\sim8)}} \sigma^{(3+8)^2} + \sum_{V_{(4\sim8)}} \sigma^{(4+8)^2} + \sum_{V_{(8\sim8)}} \sigma^{(8+8)^2}$$

$$= (36n^2)\sigma^{36} + (12n)\sigma^{49} + (36n^2 - 12n)\sigma^{121} + (12n)\sigma^{144} + (18n^2 - 12n)\sigma^{256}. \tag{14}$$

Differentiate (14) at $\sigma = 1$, we compute

$$HB_1(BPOS_n) = 10208n^2 - 2208n \tag{15}$$

By using Table 1 & Equation (15) in Equation (8), we get

$$ENT_{HB_{1(BPOS_n)}} = \log(HB_1) - \frac{1}{HB_1}\log\left\{\prod_{V_{(3,3)}}\left(V_{\Sigma i}+V_{\Sigma j}\right)^{2\left(V_{\Sigma i}+V_{\Sigma j}\right)^2} \times \prod_{V_{(3,4)}}\left(V_{\Sigma i}+V_{\Sigma j}\right)^{2\left(V_{\Sigma i}+V_{\Sigma j}\right)^2} \times \prod_{V_{(3,8)}}\left(V_{\Sigma i}+V_{\Sigma j}\right)^{2\left(V_{\Sigma i}+V_{\Sigma j}\right)^2} \times \prod_{V_{(4,8)}}\left(V_{\Sigma i}+V_{\Sigma j}\right)^{2\left(V_{\Sigma i}+V_{\Sigma j}\right)^2} \times \prod_{V_{(8,8)}}\left(V_{\Sigma i}+V_{\Sigma j}\right)^{2\left(V_{\Sigma i}+V_{\Sigma j}\right)^2}\right\}$$

$$= \log(10208n^2 - 2208n) - \frac{1}{(10208n^2 - 2208n)}\log\{(36n^2)(36)^{36} \times (12n)(49)^{49} \times (36n^2 - 12n)(121)^{121} \times (12n)(144)^{144} \times (18n^2 - 12n)(256)^{256}\}$$

2nd K −Hyper Banhatti Entropy of $BPOS_n$

Let $BPOS_n$ is a computational approach used to study the electronic structure and properties of materials. Then by using Equation (4) and Table 1, we get

$$HB_2(BPOS_n) = \sum_{V_{(3\sim3)}} \sigma^{(3\times3)^2} + \sum_{V_{(3\sim4)}} \sigma^{(3\times4)^2} + \sum_{V_{(3\sim8)}} \sigma^{(3\times8)^2} + \sum_{V_{(4\sim8)}} \sigma^{(4\times8)^2} + \sum_{V_{(8\sim8)}} \sigma^{(8\times8)^2}$$

$$= (36n^2)\sigma^{81} + (12n)\sigma^{144} + (36n^2 - 12n)\sigma^{576} + (12n)\sigma^{1024} + (18n^2 - 12n)\sigma^{4096}. \qquad (16)$$

Differentiate (16) at $\sigma = 1$, we compute

$$HB_2(BPOS_n) = 97380n^2 - 42048n. \qquad (17)$$

By using Table 1 & Equation (17) in Equation (9), we get

$$ENT_{HB_{2(BPOS_n)}} = \log(HB_2) - \frac{1}{HB_2}\log\left\{\prod_{V_{(3,3)}} \left(V_{\varepsilon_i} \times V_{\varepsilon_j}\right)^{2\left(V_{\varepsilon_i}\times V_{\varepsilon_j}\right)^2} \times \prod_{V_{(3,4)}} \left(V_{\varepsilon_i} \times V_{\varepsilon_j}\right)^{2\left(V_{\varepsilon_i}\times V_{\varepsilon_j}\right)^2} \times \prod_{V_{(3,8)}} \left(V_{\varepsilon_i} \times V_{\varepsilon_j}\right)^{2\left(V_{\varepsilon_i}\times V_{\varepsilon_j}\right)^2} \times \prod_{V_{(4,8)}} \left(V_{\varepsilon_i} \times V_{\varepsilon_j}\right)^{2\left(V_{\varepsilon_i}\times V_{\varepsilon_j}\right)^2} \times \prod_{V_{(8,8)}} \left(V_{\varepsilon_i} \times V_{\varepsilon_j}\right)^{2\left(V_{\varepsilon_i}\times V_{\varepsilon_j}\right)^2}\right\}$$

$$= \log(97380n^2 - 42048n) - \frac{1}{(97380n^2 - 42048n)}\log\{(36n^2)(81)^{81} \times (12n)(144)^{144} \times (36n^2 - 12n)(576)^{576} \times (12n)(1024)^{1024} \times (18n^2 - 12n)(4096)^{4096}\}$$

Comparison Topological Indices

In this section, we represent a numerical and graphical comparison of K –Banhatti indices (B_1, B_2, HB_1 and HB_2) in Table 2 and Figure 2, respectively.

Table 2. K –Banhatti indices of $BPOS_n$

n	B_1	B_2	HB_1	HB_2
2	3408	19476	154496	2224260
3	7812	35328	244160	3253392
4	12016	55860	354240	4477284
5	22020	81072	484736	5895936
6	31824	110964	635648	7509348
7	43428	145536	806976	9317520
8	56832	184788	998720	11320452
9	72036	228720	1210880	13518144
10	89040	277332	1443456	15910596

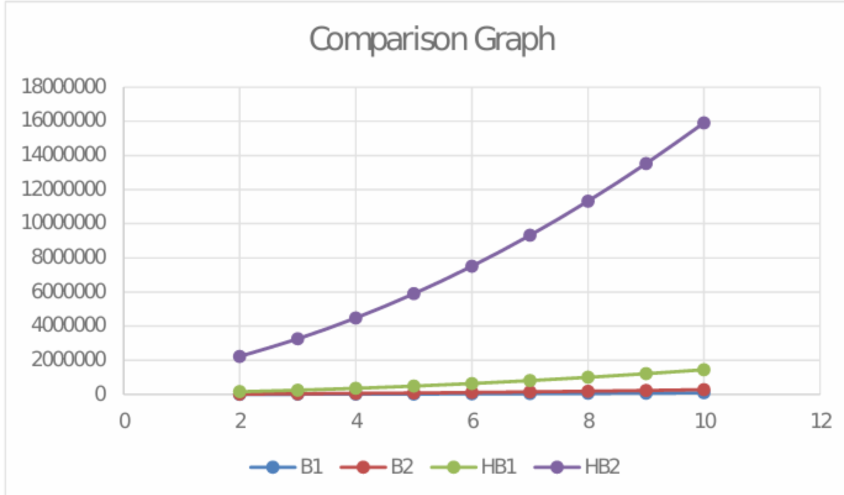

Figure 2. Graphical comparison of $BPOS_n$

Benzenoid Dominating Planar Octahedron Structures $(BDPOS_n)$

The topological features of a $BDPOS$ are well explained. Figure3 reflects the 2-dimensional structure of the $BDPOS$. $BDPOS_n$, $n \geq 2$ represents the graph of $BDPOS_n$, where n is the dimension of $BDPOS$.

The two-dimensional structure of the vital molecular graph of $BDPOS_n$, is expressed in Figure 3.

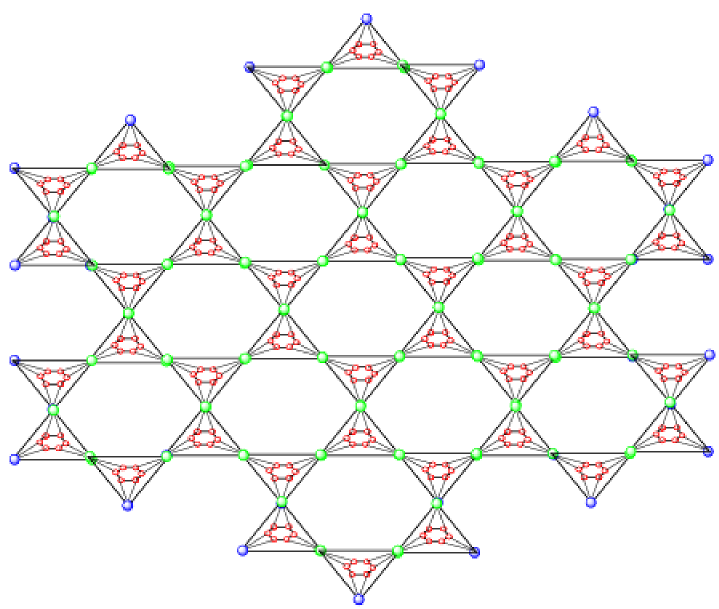

Figure 3. Benzenoid dominating planar octahedron structure

In the $BDPOS$, there are a total number of vertices (s) $27n^2 - 33n + 12$ and the edges (t) $270n^2 - 378n + 156$. The set of edges of the $BDPOS$ is divided into five parts according to the degree of end vertices [25-27]. The first edge partition consists of $108n^2 - 132n + 48$ edges st, where $s = 3$ and $t = 3$. The second edge partition consists of $12(2n - 1)$ edges st, where $s = 3$ and $t = 4$. The third edge partition consists of $108n^2 - 132n + 48$ edges st, where $s = 3$ and $t = 8$. The fourth edge partition consists of $12(2n - 1)$ edges st, where $s = 4$ and $t = 8$. The fifth edge partition consists of $54n^2 - 162n + 84$ edges st, where $s = 8$ and $t = 8$. The edge partition of the $BDPOS$ is presented in Table 3.

Table 3. Partitions of edges in $BDPOS_n$.

S. No.	Class	Number of Appearance
1	$d_{(3,3)}$	$108n^2 - 132n + 48$
2	$d_{(3,4)}$	$12(12n - 1)$
3	$d_{(3,8)}$	$108n^2 - 132n + 48$
4	$d_{(4,8)}$	$12(12n - 1)$
5	$d_{(8,8)}$	$54n^2 - 162n + 84$

1st K −Banhatti Entropy of $BDPOS_n$

Let $BPDOS_n$ is a computational approach used to study the electronic structure and properties of materials.

The 1st K −Banhatti polynomial is calculated the use of the Equation (1) and the Table 3.

$$B_1(BDPOS_n) = \sum_{V_{(3\sim3)}} \sigma^{3+3} + \sum_{V_{(3\sim4)}} \sigma^{3+4} + \sum_{V_{(3\sim8)}} \sigma^{3+8} + \sum_{V_{(4\sim8)}} \sigma^{4+8} + \sum_{V_{(8\sim8)}} \sigma^{8+8}$$

$$= (108n^2 - 132n + 48)\sigma^6 + 12(12n - 1)\sigma^7 + (108n^2 - 132n + 48)\sigma^{11} + 12(12n - 1)\sigma^{12} + (54n^2 - 162n + 84)\sigma^{16}. \quad (18)$$

Differentiate (18) at $\sigma = 1$, we compute

$$B_1(BDPOS_n) = 2700n^2 - 4380n + 1932 \quad (19)$$

By using Table 3 and the above derived Equation (19) in Equation (6), we get

$$ENT_{B_{1(BDPOS_n)}} = \log(B_1) - \frac{1}{B_1}\log\left\{\prod_{V_{(3,3)}} \left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)^{\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)} \times \prod_{V_{(3,4)}} \left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)^{\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)} \times \prod_{V_{(3,8)}} \left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)^{\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)} \times \prod_{V_{(4,8)}} \left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)^{\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)} \times \prod_{V_{(8,8)}} \left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)^{\left(V_{\varepsilon_i}+V_{\varepsilon_j}\right)}\right\}$$

$$= \log(2700n^2 - 4380n + 1932) - \frac{1}{(2700n^2 - 4380n + 1932)}\log\{(108n^2 - 132n + 48)(6)^6 \times 12(12n - 1)(7)^7 \times (108n^2 - 132n + 48)(11)^{11} \times 12(12n - 1)(12)^{12} \times (54n^2 - 162n + 84)(16)^{16}\}$$

2nd K −Banhatti Entropy of $BDPOS_n$

Let $BDPOS_n$ is a computational approach used to study the electronic structure and properties of materials. Then, by using Equation (2) & Table 3, we get

$$B_2(BDPOS_n) = \sum_{V_{(3\sim3)}} \sigma^{3\times3} + \sum_{V_{(3\sim4)}} \sigma^{3\times4} + \sum_{V_{(3\sim8)}} \sigma^{3\times8} + \sum_{V_{(4\sim8)}} \sigma^{4\times8} + \sum_{V_{(8\sim8)}} \sigma^{8\times8}$$

$$= (108n^2 - 132n + 48)\sigma^9 + 12(12n - 1)\sigma^{12} + (108n^2 - 132n + 48)\sigma^{24} + 12(12n - 1)\sigma^{32} + (54n^2 - 162n + 84)\sigma^{64}. \quad (20)$$

Differentiate (20) at $\sigma = 1$, we compute

$$B_2(BDPOS_n) = 7020n^2 - 13668n + 6432 \quad (21)$$

By using Table 3 and the related Equation (21) in Equation (7), we get

$$ENT_{B_{2(BDPOS_n)}} = \log(B_2) - \frac{1}{B_2}\log\Bigg\{\prod_{V_{(3,3)}}\left(V_{\mathcal{E}i}\times V_{\mathcal{E}j}\right)^{\left(V_{\mathcal{E}i}\times V_{\mathcal{E}j}\right)}\times\prod_{V_{(3,4)}}\left(V_{\mathcal{E}i}\times V_{\mathcal{E}j}\right)^{\left(V_{\mathcal{E}i}\times V_{\mathcal{E}j}\right)} \times\prod_{V_{(3,8)}}\left(V_{\mathcal{E}i}\times V_{\mathcal{E}j}\right)^{\left(V_{\mathcal{E}i}\times V_{\mathcal{E}j}\right)}\times\prod_{V_{(4,8)}}\left(V_{\mathcal{E}i}\times V_{\mathcal{E}j}\right)^{\left(V_{\mathcal{E}i}\times V_{\mathcal{E}j}\right)}\times\prod_{V_{(8,8)}}\left(V_{\mathcal{E}i}\times V_{\mathcal{E}j}\right)^{\left(V_{\mathcal{E}i}\times V_{\mathcal{E}j}\right)}\Bigg\}$$

$$= \log(7020n^2 - 13668n + 6432) - \frac{1}{(7020n^2 - 13668n + 6432)}\log\{(108n^2 - 132n + 48)(9)^9 \times 12(12n-1)(12)^{12} \times (108n^2 - 132n + 48)(24)^{24} \times 12(12n-1)(32)^{32} \times (54n^2 - 162n + 84)(64)^{64}\}$$

1st K –Hyper Banhatti Entropy of $BDPOS_n$

Let $BDPOS_n$ is a computational approach used to study the electronic structure and properties of materials.
Then by using Equation (3) and Table 3, we get

$$HB_1(BDPOS_n) = \sum_{V_{(3\sim3)}} \sigma^{(3+3)^2} + \sum_{V_{(3\sim4)}} \sigma^{(3+4)^2} + \sum_{V_{(3\sim8)}} \sigma^{(3+8)^2} + \sum_{V_{(4\sim8)}} \sigma^{(4+8)^2} + \sum_{V_{(8\sim8)}} \sigma^{(8+8)^2}$$

$$= (108n^2 - 132n + 48)\sigma^{36} + 12(12n-1)\sigma^{49} + (108n^2 - 132n + 48)\sigma^{121} + 12(12n-1)\sigma^{144} + (54n^2 - 162n + 84)\sigma^{256}. \quad (22)$$

Differentiate (22) at $\sigma = 1$, we compute

$$HB_1(BDPOS_n) = 30780n^2 - 57564n + 26724 \quad (23)$$

By using Table 3 & Equation (23) in Equation (8), we get

$$ENT_{HB_{1(BDPOS_n)}} = \log(HB_1) - \frac{1}{HB_1}\log\Bigg\{\prod_{V_{(3,3)}}\left(V_{\mathcal{E}i}+V_{\mathcal{E}j}\right)^{2\left(V_{\mathcal{E}i}+V_{\mathcal{E}j}\right)^2}\times\prod_{V_{(3,4)}}\left(V_{\mathcal{E}i}+V_{\mathcal{E}j}\right)^{2\left(V_{\mathcal{E}i}+V_{\mathcal{E}j}\right)^2} \times\prod_{V_{(3,8)}}\left(V_{\mathcal{E}i}+V_{\mathcal{E}j}\right)^{2\left(V_{\mathcal{E}i}+V_{\mathcal{E}j}\right)^2}\times\prod_{V_{(4,8)}}\left(V_{\mathcal{E}i}+V_{\mathcal{E}j}\right)^{2\left(V_{\mathcal{E}i}+V_{\mathcal{E}j}\right)^2}\times\prod_{V_{(8,8)}}\left(V_{\mathcal{E}i}+V_{\mathcal{E}j}\right)^{2\left(V_{\mathcal{E}i}+V_{\mathcal{E}j}\right)^2}\Bigg\}$$

$$= \log(30780n^2 - 57564n + 26724) - \frac{1}{(30780n^2 - 57564n + 26724)}\log\{(108n^2 - 132n + 48)(36)^{36} \times 12(12n-1)(49)^{49} \times (108n^2 - 132n + 48)(121)^{121} \times 12(12n-1)(144)^{144} \times (54n^2 - 162n + 84)(256)^{256}\}$$

2nd K –Hyper Banhatti Entropy of $BDPOS_n$

Let $BDPOS_n$ is a computational approach used to study the electronic structure and properties of materials including zeolites. Then by using Equation (4) and Table 3, we get

$$HB_2(BDPOS_n) = \sum_{V_{(3\sim3)}} \sigma^{(3\times3)^2} + \sum_{V_{(3\sim4)}} \sigma^{(3\times4)^2} + \sum_{V_{(3\sim8)}} \sigma^{(3\times8)^2} + \sum_{V_{(4\sim8)}} \sigma^{(4\times8)^2} + \sum_{V_{(8\sim8)}} \sigma^{(8\times8)^2}$$

$$= (108n^2 - 132n + 48)\sigma^{81} + 12(12n-1)\sigma^{144} + (108n^2 - 132n + 48)\sigma^{576} + 12(12n-1)\sigma^{1024} + (54n^2 - 162n + 84)\sigma^{4096}. \quad (24)$$

Differentiate (24) at $\sigma = 1$, we compute

$$HB_2(BDPOS_n) = 292140n^2 - 741444n + 373872. \quad (25)$$

By using Table 3 & Equation (25) in Equation (9), we get

$$ENT_{HB_{2(BDPOS_n)}} = \log(HB_2) - \frac{1}{HB_2}\log\left\{\prod_{V_{(3,3)}}\left(V_{\Sigma i}\times V_{\Sigma j}\right)^{2\left(V_{\Sigma i}\times V_{\Sigma j}\right)^2} \times \prod_{V_{(3,4)}}\left(V_{\Sigma i}\times V_{\Sigma j}\right)^{2\left(V_{\Sigma i}\times V_{\Sigma j}\right)^2} \times \prod_{V_{(3,8)}}\left(V_{\Sigma i}\times V_{\Sigma j}\right)^{2\left(V_{\Sigma i}\times V_{\Sigma j}\right)^2} \times \prod_{V_{(4,8)}}\left(V_{\Sigma i}\times V_{\Sigma j}\right)^{2\left(V_{\Sigma i}\times V_{\Sigma j}\right)^2} \times \prod_{V_{(8,8)}}\left(V_{\Sigma i}\times V_{\Sigma j}\right)^{2\left(V_{\Sigma i}\times V_{\Sigma j}\right)^2}\right\}$$

$$= \log(292140n^2 - 741444n + 373872) - \frac{1}{(292140n^2 - 741444n + 373872)}\log\{(108n^2 - 132n + 48)(81)^{81} \times 12(12n-1)(144)^{144} \times (108n^2 - 132n + 48)(576)^{576} \times 12(12n-1)(1024)^{1024} \times (54n^2 - 162n + 84)(4096)^{4096}\}$$

Comparison Topological Indices

In this section, we represent a numerical and graphical comparison of K –Banhatti indices (B_1, B_2,, HB_1 and HB_2) in Table 4 and Figure 4, respectively.

Table 4. K –Banhatti indices of $BDPOS_n$

n	B_1	B_2	HB_1	HB_2
2	3972	28608	288948	3870152
3	13092	64080	508404	6442248
4	27612	113492	789420	9498624
5	47532	177144	1131996	13139280
6	72852	254736	1536132	17354216
7	103572	346368	2001828	22173432
8	139692	452040	2529084	27566928
9	181212	571752	3117900	33544704
10	228132	705504	3768276	40106760

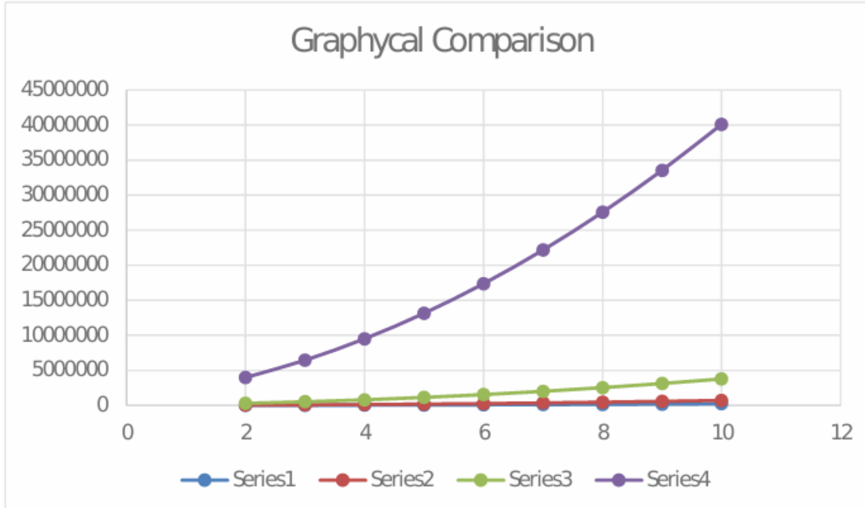

Figure 4. Graphical comparison of $BDPOS_n$

Benzenoid Hex Planar Octahedron Structures $(BHPOS_n)$

The $BHPOS$ is built and its topological features are thoroughly described [26, 27]. Figure 5 depicts the two-dimensional structure of a $BHPOS_n$ and $n \geq 2$, where n denotes the dimension of $BHPOS$. The 2-dimensional structure of the molecular graph of $BHPOS_n$ is seen in Figure 5.

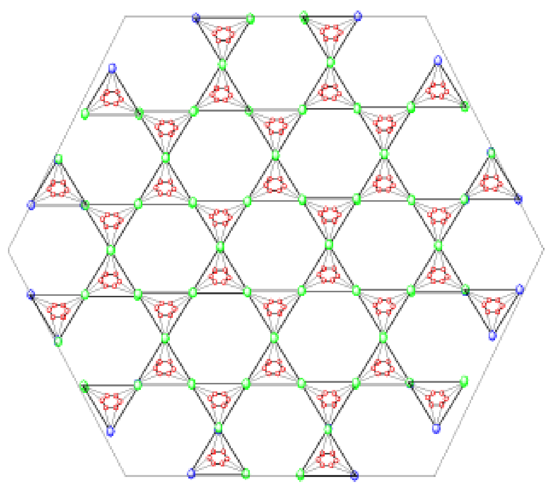

Figure 5. Benzenoid hex planar octahedron structure

The total number of vertices (s) and edges (t) in the $BHPOS_n$ are $45n^2 + 51n + 6$ and $90n^2 + 24n + 6$, respectively. The set of edges of the $BHPOS_n$ is divided into seven parts according to the degree of end vertices. The first edge partition consists of 12 edges st, where $s = 2$ and $t = 5$. The second edge partition consists of $36n(n-1)$ edges st, where $s = 3$ and $t = 3$. The third edge partition consists of $24n$ edges st, where $s = 3$ and $t = 5$. The fourth edge partition consists of $12n(3n-1)$ edges st, where $s = 3$ and $t = 8$. The fifth edge partition consists of $12n - 6$ edges st, where $s = 5$ and $t = 5$. The sixth edge partition consists of $12n$ edges st, where $s = 5$ and $t = 8$. The seventh edge partition consists of $18n^2$ edges st, where $s = 8$ and $t = 8$. The edge partition of the $BHPOS_n$ is shown in Table 5.

Table 5. Partitions of edges in $BHPOS_n$.

S. No.	Class	Number of Appearance
1	$d_{(2,5)}$	12
2	$d_{(3,3)}$	$36n(n-1)$
3	$d_{(3,5)}$	$24n$
4	$d_{(3,8)}$	$12n(3n-1)$
5	$d_{(5,5)}$	$12n-6$
6	$d_{(5,8)}$	$12n$
7	$d_{(8,8)}$	$18n^2$

1st K −Banhatti Entropy of $BHPOS_n$

Let $BHDOS_n$ is a computational approach used to study the electronic structure and properties of materials.

The 1st K −Banhatti polynomial is calculated the use of the Equation (1) and the Table 5.

$$B_1(BHPOS_n) = \sum_{V_{(2\sim5)}} \sigma^{2+5} + \sum_{V_{(3\sim3)}} \sigma^{3+3} + \sum_{V_{(3\sim5)}} \sigma^{3+5} + \sum_{V_{(3\sim8)}} \sigma^{3+8} + \sum_{V_{(5\sim5)}} \sigma^{5+5} + \sum_{V_{(5\sim8)}} \sigma^{5+8} + \sum_{V_{(8\sim8)}} \sigma^{8+8}$$

$$= 12\sigma^7 + 36n(n-1)\sigma^6 + (24n)\sigma^8 + 12n(3n-1)\sigma^{11} + (12n-6)\sigma^{10} + 12n\sigma^{13} + (18n^2)\sigma^{16}. \quad (26)$$

Differentiate (26) at $\sigma = 1$, we compute

$$B_1(BHPOS_n) = 900n^2 + 24 \quad (27)$$

By using Table 5 and the above derived Equation (27) in Equation (6), we get

$$ENT_{B_{1(BHPOS_n)}} = \log(B_1) - \frac{1}{B_1}\log\left\{\prod_{V_{(2,5)}} \left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)^{\left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)} \times \prod_{V_{(3,3)}} \left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)^{\left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)} \times \prod_{V_{(3,5)}} \left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)^{\left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)} \times \prod_{V_{(3,8)}} \left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)^{\left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)} \times \prod_{V_{(5,5)}} \left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)^{\left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)} \times \prod_{V_{(5,8)}} \left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)^{\left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)} \times \prod_{V_{(8,8)}} \left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)^{\left(V_{\mathcal{E}_i}+V_{\mathcal{E}_j}\right)}\right\}$$

$$= \log(900n^2+24) - \frac{1}{(900n^2+24)}\log\{12(7)^2 \times 36n(n-1)(6)^6 \times (24n)(8)^8 \times 12n(3n-1)(11)^{11} \times (12n-6)(10)^{10} \times 12n(13)^{13} \times (18n^2)(16)^{16}.\}$$

2nd K −Banhatti Entropy of $BHPOS_n$

Let $BHPOS_n$ is a computational approach used to study the electronic structure and properties of materials. Then, by using Equation (2) & Table 5, we get

$$B_2(BHPOS_n) = \sum_{V_{(2\sim5)}} \sigma^{2\times5} + \sum_{V_{(3\sim3)}} \sigma^{3\times3} + \sum_{V_{(3\sim5)}} \sigma^{3\times5} + \sum_{V_{(3\sim8)}} \sigma^{3\times8} + \sum_{V_{(5\sim5)}} \sigma^{5\times5} + \sum_{V_{(5\sim8)}} \sigma^{5\times8} + \sum_{V_{(8\sim8)}} \sigma^{8\times8}$$

$$= 12\sigma^{10} + 36n(n-1)\sigma^{9} + (24n)\sigma^{15} + 12n(3n-1)\sigma^{24} + (12n-6)\sigma^{25} + 12n\sigma^{40} + (18n^2)\sigma^{64}. \quad (28)$$

Differentiate (28) at $\sigma = 1$, we compute

$$B_2(BHPOS_n) = 2340n^2 + 528n - 30 \quad (29)$$

By using Table 5 and the related Equation (29) in Equation (7), we get

$$ENT_{B_{2(BHPOS_n)}} = \log(B_1) - \frac{1}{B_1}\log\left\{\prod_{V_{(2,5)}}\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)^{\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)} \times \prod_{V_{(3,3)}}\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)^{\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)} \times \prod_{V_{(3,5)}}\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)^{\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)} \times \prod_{V_{(3,8)}}\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)^{\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)} \times \prod_{V_{(5,5)}}\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)^{\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)} \times \prod_{V_{(5,8)}}\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)^{\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)} \times \prod_{V_{(8,8)}}\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)^{\left(V_{\mathcal{E}_i}\times V_{\mathcal{E}_j}\right)}\right\}$$

$$= \log(2340n^2 + 528n - 30\ ) - \frac{1}{(2340n^2 + 528n - 30\ )}\log\{12(10)^{10} \times 36n(n-1)(9)^{9} \times (24n)(15)^{15} \times 12n(3n-1)(24)^{24} \times (12n-6)(25)^{25} \times 12n(40)^{40} \times (18n^2)(64)^{64}.\}$$

1st K −Hyper Banhatti Entropy of $BHPOS_n$

Let $BHPOS_n$ is a computational approach used to study the electronic structure and properties of materials. Then by using Equation (3) and Table 5, we get

$$HB_1(BHPOS_n) = \sum_{V_{(2\sim5)}}\sigma^{(2+5)^2} + \sum_{V_{(3\sim3)}}\sigma^{(3+3)^2} + \sum_{V_{(3\sim5)}}\sigma^{(3+5)^2} + \sum_{V_{(3\sim8)}}\sigma^{(3+8)^2} + \sum_{V_{(5\sim5)}}\sigma^{(5+5)^2} + + \sum_{V_{(5\sim8)}}\sigma^{(5+8)^2} + \sum_{V_{(8\sim8)}}\sigma^{(8+8)^2}$$

$$= 12\sigma^{49} + 36n(n-1)\sigma^{36} + (24n)\sigma^{64} + 12n(3n-1)\sigma^{121} + (12n-6)\sigma^{100} + 12n\sigma^{169} + (18n^2)\sigma^{256}. \quad (30)$$

Differentiate (30) at $\sigma = 1$, we compute

$$HB_1(BHPOS_n) = 10260n^2 + 2016n - 12 \quad (31)$$

By using Table 5 & Equation (31) in Equation (8), we get

$$ENT_{HB_{1(BHPOS_n)}} = \log(HB_1) - \frac{1}{HB_1}\log\left\{\prod_{V_{(2,5)}}\left(V_{\Sigma_i}+V_{\Sigma_j}\right)^{2\left(V_{\Sigma_i}+V_{\Sigma_j}\right)^2} \times \prod_{V_{(3,3)}}\left(V_{\Sigma_i}+V_{\Sigma_j}\right)^{2\left(V_{\Sigma_i}+V_{\Sigma_j}\right)^2} \times \prod_{V_{(3,5)}}\left(V_{\Sigma_i}+V_{\Sigma_j}\right)^{2\left(V_{\Sigma_i}+V_{\Sigma_j}\right)^2} \times \prod_{V_{(3,8)}}\left(V_{\Sigma_i}+V_{\Sigma_j}\right)^{2\left(V_{\Sigma_i}+V_{\Sigma_j}\right)^2} \times \prod_{V_{(5,5)}}\left(V_{\Sigma_i}+V_{\Sigma_j}\right)^{2\left(V_{\Sigma_i}+V_{\Sigma_j}\right)^2} \times \prod_{V_{(5,8)}}\left(V_{\Sigma_i}+V_{\Sigma_j}\right)^{2\left(V_{\Sigma_i}+V_{\Sigma_j}\right)^2}\right\} \times \prod_{V_{(8,8)}}\left(V_{\Sigma_i}+V_{\Sigma_j}\right)^{2\left(V_{\Sigma_i}+V_{\Sigma_j}\right)^2}$$

$$= \log(10260n^2 + 2016n - 12) - \frac{1}{(10260n^2 + 2016n - 12\,)}\log\{12(49)^{49} \times 36n(n-1)(36)^{36} \times (24n)(64)^{64} \times 12n(3n-1)(121)^{121} \times (12n-6)(100)^{100} \times (12n)(169)^{169} \times (18n^2)(256)^{256}.\}$$

2nd K −Hyper Banhatti Entropy of $BHPOS_n$

Let $BDPOS_n$ is a computational approach used to study the electronic structure and properties of materials including zeolites. Then by using Equation (4) and Table 5, we get

$$HB_2(BHPOS_n) = \sum_{V_{(2\sim5)}} \sigma^{(2\times5)^2} + \sum_{V_{(3\sim3)}} \sigma^{(3\times3)^2} + \sum_{V_{(3\sim5)}} \sigma^{(3\times5)^2} + \sum_{V_{(3\sim8)}} \sigma^{(3\times8)^2} + \sum_{V_{(5\sim5)}} \sigma^{(5\times5)^2} + \sum_{V_{(5\sim8)}} \sigma^{(5\times8)^2} + \sum_{V_{(8\sim8)}} \sigma^{(8\times8)^2}$$

$$= (12)\sigma^{100} + 36n(n-1)\sigma^{81} + (24n)\sigma^{225} + 12n(3n-1)\sigma^{576} + (12n-6)\sigma^{625} + (12n)\sigma^{1600} + (18n^2)\sigma^{4096}. \quad (32)$$

Differentiate (32) at $\sigma = 1$, we get

$$HB_2(BHPOS_n) = 97380n^2 + 22270n - 2550\,. \quad (33)$$

The Table 5 & Equation (33) in Equation (9), we get

$$ENT_{HB_{2(BHPOS_n)}} = \log(HB_2) - \frac{1}{HB_2}\log\left\{\prod_{V_{(2,5)}}\left(V_{\Sigma_i}\times V_{\Sigma_j}\right)^{2\left(V_{\Sigma_i}\times V_{\Sigma_j}\right)^2} \times \prod_{V_{(3,3)}}\left(V_{\Sigma_i}\times V_{\Sigma_j}\right)^{2\left(V_{\Sigma_i}\times V_{\Sigma_j}\right)^2} \times \prod_{V_{(3,5)}}\left(V_{\Sigma_i}\times V_{\Sigma_j}\right)^{2\left(V_{\Sigma_i}\times V_{\Sigma_j}\right)^2} \times \prod_{V_{(3,8)}}\left(V_{\Sigma_i}\times V_{\Sigma_j}\right)^{2\left(V_{\Sigma_i}\times V_{\Sigma_j}\right)^2} \times \prod_{V_{(5,5)}}\left(V_{\Sigma_i}\times V_{\Sigma_j}\right)^{2\left(V_{\Sigma_i}\times V_{\Sigma_j}\right)^2} \times \prod_{V_{(5,8)}}\left(V_{\Sigma_i}\times V_{\Sigma_j}\right)^{2\left(V_{\Sigma_i}\times V_{\Sigma_j}\right)^2} \times \prod_{V_{(8,8)}}\left(V_{\Sigma_i}\times V_{\Sigma_j}\right)^{2\left(V_{\Sigma_i}\times V_{\Sigma_j}\right)^2}\right\}$$

$$= \log(97380n^2 + 22270n - 2550) - \frac{1}{(97380n^2 + 22270n - 2550)}\log\{(12)(100)^{100} + 36n(n-1)(81)^{81} + (24n)(225)^{225} + 12n(3n-1)(576)^{576} + (12n-6)(625)^{625} + (12n)(1600)^{1600} + (18n^2)(4096)^{4096}\}$$

Comparison Topological Indices

In this section, we represent a numerical and graphical comparison of K −Banhatti indices (B_1, B_2,, HB_1 and HB_2) in Table 6 and Figure 6, respectively.

Table 4. K –Banhatti indices of $BHPOS_n$

n	B_1	B_2	HB_1	HB_2
2	3624	22614	45060	431510
3	8124	39522	98376	940680
4	14424	61110	172212	1644610
5	22524	87378	266568	2543300
6	32424	118326	381444	3636750
7	44124	153954	516840	4924960
8	57624	194262	672756	6407930
9	72924	239250	849192	8085660
10	90024	288918	1046148	9958150

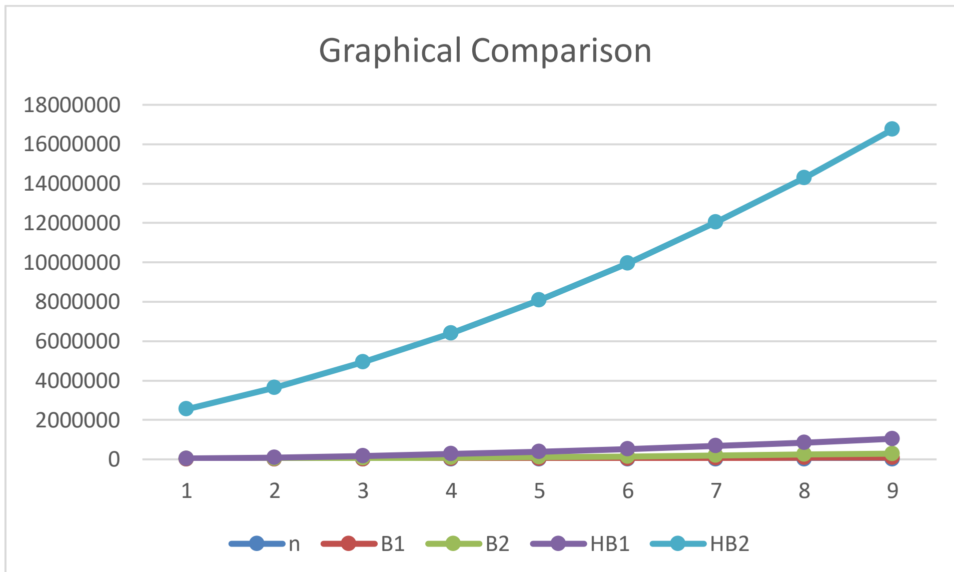

Figure 6. Graphical comparison of $BHPOS_n$

First and Second Kinds of Modified Zagreb Entropies

In this section, we will discuss the two well-known kinds of modified Zagreb entropies for $BPOS_n$, $BPOS_n$, and $BPOS_n$ networks. In Table 5, the mathematical expressions of modified Zagreb entropies of first and second kinds [41, 42].

Table 5. Some well-known entropies with mathematical expressions.

Entropies	Mathematical Expression
$ENT_{ReZE_1(G)}$	$\log(ReZG_1) - \frac{1}{ReZG_1}\log\left\{\prod_{\mathfrak{b}_i\mathfrak{f}_j \in E(G_1)} \left[\frac{\mathfrak{z}_{\mathfrak{b}_i} + \mathfrak{z}_{\mathfrak{f}_j}}{\mathfrak{z}_{\mathfrak{b}_i}\mathfrak{z}_{\mathfrak{f}_j}}\right]^{\left[\frac{\mathfrak{z}_{\mathfrak{b}_i} + \mathfrak{z}_{\mathfrak{f}_j}}{\mathfrak{z}_{\mathfrak{b}_i}\mathfrak{z}_{\mathfrak{f}_j}}\right]}\right\}$
$ENT_{ReZE_2(G)}$	$\log(ReZG_2) - \frac{1}{ReZG_2}\log\left\{\prod_{\mathfrak{b}_i\mathfrak{f}_j \in E(G_2)} \left[\frac{\mathfrak{z}_{\mathfrak{b}_i}\mathfrak{z}_{\mathfrak{f}_j}}{\mathfrak{z}_{\mathfrak{b}_i} + \mathfrak{z}_{\mathfrak{f}_j}}\right]^{\left[\frac{\mathfrak{z}_{\mathfrak{b}_i}\mathfrak{z}_{\mathfrak{f}_j}}{\mathfrak{z}_{\mathfrak{b}_i} + \mathfrak{z}_{\mathfrak{f}_j}}\right]}\right\}$

where

$$ReZG_1(G) = \sum_{b_i, f_j \in E(G)} \left\{ \frac{\mathfrak{z}_{b_i} + \mathfrak{z}_{f_j}}{\mathfrak{z}_{b_i} \mathfrak{z}_{f_j}} \right\}$$

$$ReZG_2(G) = \sum_{b_i, f_j \in E(G)} \left\{ \frac{\mathfrak{z}_{b_i} \mathfrak{z}_{f_j}}{\mathfrak{z}_{b_i} + \mathfrak{z}_{f_j}} \right\}$$

Lemma 1: Let $(BPOS_n)$ be a Benzenoid Planar Octahedron Structures network, then we have

$$RZE_1(BPOS_n) = 3n + 51n^2$$

$$RZE_2(BPOS_n\ ) = -\frac{1664n}{77} + \frac{10656n^2}{55}$$

Proof: Let $(BPOS_n)$ be a Benzenoid Planar Octahedron Structures network then the partition mapping of set of edges with respect to the degree of endpoints of edges is

$$\rho(\alpha, \beta) = \begin{cases} 36n^2, & \alpha = 2,\ \beta = 3 \\ 12n, & \alpha = 3,\ \beta = 4 \\ 36n^2 - 12n\,, & \alpha = 3,\ \beta = 8 \\ 12n, & \alpha = 4,\ \beta = 8 \\ 18n^2 - 12n, & \alpha = 8,\ \beta = 8 \end{cases}$$

$$RZE_1(BPOS_n)\ ) = \sum_{\alpha_i \beta_j \in E} \frac{\mathfrak{D}_{\alpha_i} + \mathfrak{D}_{\beta_j}}{\mathfrak{D}_{\alpha_i} \mathfrak{D}_{\beta_j}}$$

$$= (36n^2)\frac{5}{6} + (12n)\frac{7}{12} + \frac{(36n^2 - 12n)11}{24} + \frac{(12n)12}{32} + \frac{(18n^2 - 12n)16}{64} = 3n + 51n^2$$

$$RZE_2(BPOS_n)\ ) = \sum_{\alpha_i \beta_j \in E} \frac{\mathfrak{D}_{\alpha_i} \mathfrak{D}_{\beta_j}}{\mathfrak{D}_{\alpha_i} + \mathfrak{D}_{\beta_j}}$$

$$= (36n^2)\frac{6}{5} + (12n)\frac{12}{7} + \frac{(36n^2 - 12n)24}{11} + \frac{(12n)32}{12} + \frac{(18n^2 - 12n)64}{16}$$

$$= -\frac{1664n}{77} + \frac{10656n^2}{55}$$

Proposition 2. Let $(BPOS_n)$ be a Benzenoid Planar Octahedron Structures network, then we have

$$\boldsymbol{ENT_{RZE_1}}(BPOS_n)\ ) = -\frac{1}{3n + 51n^2} \mathrm{Log}[\mathrm{A}] + \mathrm{Log}[3n + 51n^2]$$

$$\boldsymbol{ENT_{RZE_2}}(BPOS_n)\ ) = -\frac{1}{-9840n + 29016n^2} \mathrm{Log}[B] + \mathrm{Log}(-9840n + 29016n^2)$$

where,

$$A = 2^{-\frac{9n}{2} + 30n^2 + \frac{1}{2}(12n - 18n^2) - \frac{11}{8}(-12n + 36n^2)} 3^{9n + 30n^2 - \frac{11}{24}(-12n + 36n^2)} 5^{30n^2} 7^{7n} 11^{\frac{11}{24}(-12n + 36n^2)}$$
$$n^{23n/2} (n^2)^{30n^2} (-12n + 18n^2)^{\frac{1}{4}(-12n + 18n^2)} (-12n + 36n^2)^{\frac{11}{24}(-12n + 36n^2)}$$

$$B = 2^{\frac{1696n}{7} + \frac{648n^2}{5} + 8(-12n + 18n^2) + \frac{72}{11}(-12n + 36n^2)} 3^{\frac{288n}{7} + \frac{648n^2}{5} + \frac{24}{11}(-12n + 36n^2)} 5^{-\frac{216n^2}{5}} 7^{-144n/7} 11^{-\frac{24}{11}(-12n + 36n^2)}$$
$$n^{368n/7} (n^2)^{\frac{216n^2}{5}} (-12n + 18n^2)^{4(-12n + 18n^2)} (-12n + 36n^2)^{\frac{24}{11}(-12n + 36n^2)}$$

Lemma 3. Let $(BDPOS_n)$ be a Benzenoid Dominating Planar Octahedron Structures network, then we have

$$RZE_1(BDPOS_n) = \frac{143}{2} - 73n + 246n^2$$

$$RZE_2(BDPOS_n) = \frac{171616}{385} - \frac{16224n}{35} + \frac{9072n^2}{11}$$

Proof: Let $(BDPOS_n)$ be a Benzenoid Dominating Planar Octahedron Structures network then the partition mapping of set of edges with respect to the degree of endpoints of edges is

$$\rho(\alpha,\beta) = \begin{cases} 108n^2 - 132n + 48, & \alpha = 2,\ \beta = 3 \\ 12(12n-1), & \alpha = 3,\ \beta = 4 \\ 108n^2 - 132n + 48\,, & \alpha = 3,\ \beta = 8 \\ 12(12n-1), & \alpha = 4,\ \beta = 8 \\ 54n^2 - 162n + 84, & \alpha = 8,\ \beta = 8 \end{cases}$$

$$\begin{aligned} RZE_1(BDPOS_n) &= \sum_{\alpha_i\beta_j \in E} \frac{\mathfrak{D}_{\alpha_i} + \mathfrak{D}_{\beta_j}}{\mathfrak{D}_{\alpha_i}\mathfrak{D}_{\beta_j}} \\ &= (108n^2 - 132n + 48)\frac{5}{6} + (12(12n-1))\frac{7}{12} + (108n^2 - 132n + 48)\frac{11}{24} \\ &\quad + \frac{(12(12n-1))12}{32} + \frac{(54n^2 - 162n + 84)16}{64} = \frac{143}{2} - 73n + 246n^2 \end{aligned}$$

$$\begin{aligned} RZE_2(BDPOS_n) &= \sum_{\alpha_i\beta_j \in E} \frac{\mathfrak{D}_{\alpha_i}\mathfrak{D}_{\beta_j}}{\mathfrak{D}_{\alpha_i} + \mathfrak{D}_{\beta_j}} \\ &= (108n^2 - 132n + 48)\frac{6}{5} + (12(12n-1))\frac{12}{7} + (108n^2 - 132n + 48)\frac{24}{11} \\ &\quad + \frac{(12(12n-1))32}{12} + \frac{(54n^2 - 162n + 84)64}{16} = \frac{171616}{385} - \frac{16224n}{35} + \frac{9072n^2}{11} \end{aligned}$$

Proposition 4. Let $(BDPOS_n)$ be a Benzenoid Dominating Planar Octahedron Structures network, then we have

$$ENT_{RZE_1}(BDPOS_n) = -\frac{1}{143 - 146n + 492n^2} 2\mathrm{Log}[C] + \mathrm{Log}[\frac{143}{2} - 73n + 246n^2]$$

$$ENT_{RZE_2}(BDPOS_n) = -\frac{1}{\frac{171616}{385} - \frac{16224n}{35} + \frac{9072n^2}{11}} \mathrm{Log}[D] + \mathrm{Log}[\frac{171616}{385} - \frac{16224n}{35} + \frac{9072n^2}{11}]$$

where

$$\begin{aligned} C = {} & 2^{-\frac{9}{2}(-1+12n)+\frac{1}{2}(-84+162n-54n^2)-\frac{53}{24}(48-132n+180n^2)} 3^{9(-1+12n)-\frac{31}{24}(48-132n+180n^2)} \\ & 5^{\frac{5}{6}(48-132n+180n^2)} 7^{7(-1+12n)} 11^{\frac{11}{24}(48-132n+180n^2)} (-1+12n)^{\frac{23}{2}(-1+12n)} (84-162n \\ & + 54n^2)^{\frac{1}{4}(84-162n+54n^2)} (48-132n+180n^2)^{\frac{31}{24}(48-132n+180n^2)} \end{aligned}$$

$$\begin{aligned} D = {} & 2^{\frac{1696}{7}(-1+12n)+8(84-162n+54n^2)+\frac{426}{55}(48-132n+180n^2)} 3^{\frac{288}{7}(-1+12n)+\frac{186}{55}(48-132n+180n^2)} \\ & 5^{-\frac{6}{5}(48-132n+180n^2)} 7^{-\frac{144}{7}(-1+12n)} 11^{-\frac{24}{11}(48-132n+180n^2)} (-1+12n)^{\frac{368}{7}(-1+12n)} (84-162n+ \\ & 54n^2)^{4(84-162n+54n^2)} (48-132n+180n^2)^{\frac{186}{55}(48-132n+180n^2)} \end{aligned}$$

Lemma 5. Let $(BHPOS_n)$ be a Benzenoid Hex Planar Octahedron Structures network, then we have

$$RZE_1(BDPOS_n) = 6 - \frac{73n}{10} + \frac{201n^2}{5}$$

$$RZE_2(BDPOS_n) = \frac{15}{7} + \frac{417n}{13} + \frac{3078n^2}{13}$$

Proof: Let $(BHPOS_n)$ be a Benzenoid Hex Planar Octahedron Structures network then the partition mapping of set of edges with respect to the degree of endpoints of edges is

$$\rho(\alpha,\beta) = \begin{cases} 12, & \alpha = 2,\ \beta = 5 \\ 36n(n-1), & \alpha = 3,\ \beta = 3 \\ 24n\,, & \alpha = 3,\ \beta = 5 \\ 12n(3n-1), & \alpha = 3,\ \beta = 8 \\ 12n-6, & \alpha = 5,\ \beta = 5 \\ 12n, & \alpha = 5,\ \beta = 8 \\ 18n^2, & \alpha = 8,\ \beta = 8 \end{cases}$$

$$RZE_1(BHPOS_n) = \sum_{\alpha_i\beta_j \in E} \frac{\mathfrak{D}_{\alpha_i} + \mathfrak{D}_{\beta_j}}{\mathfrak{D}_{\alpha_i}\mathfrak{D}_{\beta_j}}$$

$$= (12)\frac{7}{10} + \big(36n(n-1)\big)\frac{6}{9} + (24n)\frac{8}{15} + \frac{\big(12n(3n-1)\big)11}{24} + \frac{(12n-6)10}{25} + \frac{(12n)13}{40} + \frac{(18n^2)16}{64} = 6 - \frac{73n}{10} + \frac{201n^2}{5}$$

$$RZE_2(BHPOS_n) = \sum_{\alpha_i\beta_j \in E} \frac{\mathfrak{D}_{\alpha_i}\mathfrak{D}_{\beta_j}}{\mathfrak{D}_{\alpha_i} + \mathfrak{D}_{\beta_j}}$$

$$= (12)\frac{10}{7} + \big(36n(n-1)\big)\frac{9}{6} + (24n)\frac{15}{8} + \frac{\big(12n(3n-1)\big)24}{11} + \frac{(12n-6)25}{10} + \frac{(12n)40}{13} = \frac{15}{7} + \frac{417n}{13} + \frac{3078n^2}{13}$$

Proposition 6. Let $(BHPOS_n)$ be a Benzenoid Hex Planar Octahedron Structures network, then we have

$$ENT_{RZE_1}(BHPOS_n)\,) - \frac{1}{6 - \frac{73n}{10} + \frac{201n^2}{5}}\mathrm{Log[E]} + \mathrm{Log}[6 - \frac{73n}{10} + \frac{201n^2}{5}]$$

$$ENT_{RZE_2}(BHPOS_n\,) = -\frac{1}{\frac{15}{7} + \frac{417n}{13} + \frac{3078n^2}{13}}\mathrm{Log}[F] + \mathrm{Log}[\frac{15}{7} + \frac{417n}{13} + \frac{3078n^2}{13}]$$

where

$$E = 57648012^{\frac{42}{5}+\frac{384n}{5}+72(-1+n)n-\frac{9n^2}{2}-\frac{39}{10}n(-1+3n)+\frac{2}{5}(-6+12n)} 3^{\frac{42}{5}+3n+24(-1+n)n+9n^2+\frac{39}{10}n(-1+3n)} 5^{-\frac{42}{5}-\frac{64n}{5}-\frac{39}{10}n(-1+3n)-\frac{2}{5}(-6+12n)} 7^{2/5} 13^{\frac{39}{10}n(-1+3n)} n^{79n/5} \big((-1+n)n\big)^{24(-1+n)n} (n^2)^{\frac{9n^2}{2}} \big(n(-1+3n)\big)^{\frac{39}{10}n(-1+3n)} (-6+12n)^{\frac{2}{5}(-6+12n)}$$

$$F = \frac{1}{2326305139872077^{1/7}} \times 2^{\frac{360}{7}+192n+54(-1+n)n+216n^2+\frac{2400}{13}n(-1+3n)-\frac{5}{2}(-6+12n)} 3^{\frac{120}{7}+138n+162(-1+n)n+144n^2+\frac{480}{13}n(-1+3n)} 5^{\frac{120}{7}+45n+\frac{480}{13}n(-1+3n)+\frac{5}{2}(-6+12n)} 13^{-\frac{480}{13}n(-1+3n)} n^{93n} \big((-1+n)n\big)^{54(-1+n)n} (n^2)^{72n^2} \big(n(-1+3n)\big)^{\frac{480}{13}n(-1+3n)} (-6+12n)^{\frac{5}{2}(-6+12n)}$$

Conclusions

Experimentally investigating a chemical structure takes a lot of effort and money. Finding the molecular descriptors of the chemical structure makes the process easier and is approved method of structure analysis. Using a compelling method called the quotient graph approach, the distance-based molecular descriptors for symmetrically configured $BPOS_s$ $BPOS_n$, symmetrically configured Benzenoid dominant planar octahedron structures $BDPOS_n$, and $BHPOS_s$ $BHPOS_n$ are found in this study. Bye stablishing the foundation for comprehending the deep topology of dominant oxide networks, our findings also provide a substantial contribution to network research. These findings could aid scientists in understanding how these molecules interact with other materials in manufacturing and electronics.

Conflicts of Interest

The authors declare that there is no conflict of interest regarding the publication of this paper.

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