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Calculation of degree-based entropy measures for benzenoid planar octahedron networks

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Abstract: Chemical graph theory, a branch of graph theory, uses molecular graphs for its representation. In QSAR/QSPR studies, topological indices are employed to evaluate the bioactivity of chemicals. Degree-based entropy, derived from Shannon's entropy, is a functional statistic influenced by the graph and the probability distribution of its vertex set, with informational graphs forming the basis of entropy concepts. Planar octahedron networks have diverse applications in pharmacy hardware and system management. This article explores the Benzenoid Planar Octahedron Network ($BPOH(n)$), Benzenoid Dominating Planar Octahedron Network (BDPOH(n)), and Benzenoid Hex Planar Octahedron Network ($BHPOH(n)$). We compute degree-based entropies, including Randić entropy, atom bond connectivity (ABC), and geometric arithmetic (GA) entropy, for the Benzenoid planar octahedron network.

Keywords: topological indices; Randić entropy; ABC entropy; GA entropy; structural complexity; molecular stability; benzenoid networks.

MSC: 05C90; 05C70; 05C50; 05C10.

1. Introduction

In this article, all the graphs are finite and having no directions. Vertices in a network are known as nodes, whereas vertices in a chemical graph are known as atoms. Edges in a network are referred to as links or lines, whereas they are referred to as covalent bonds in a chemical graph. Topological indices are a subfield of chemical graph theory. Many papers are published on topological indexes. A topological index is a graphic, a polynomial, a sequence of integers, matrices, or a composite number that describes a molecular graph. As a result, these numeric numbers are distinct under graph isomorphism. Most of the time, molecular graphs are used to display molecules and molecular compounds for better comprehension.

F shows the graph data set $F(V, E)$, where V denotes vertices and E denotes edges. The topological index is a number that is used to represent a graph. In the fields of information technology, biological sciences, and chemical sciences, these indices are utilised. Two examples are quantitative structure-activity connections and quantitative structure-property relationships. There are many a lot of numerical values known as topological signifier that have been gained and examined over the past decennium to comprehend the characteristics and information of graph theory. Mathematical chemistry is a subset of chemical graph theory that deals with the use of topological indices.

In graph theory, we discuss the application and properties of cheminformatics. Cheminformatics is the branch of science. This field combines mathematics, information technology, and chemistry. It is about QSAR and QSPR, which predict compound biochemical and physical chemical activity. In chemical graph theory, vertices represent molecules or atoms, and edges indicate the bonds between them [1]. The Wiener index is a series of issues in statistics, computer science, biology, discrete mathematics, chemistry, information theory, and other domains that investigate and address structural entropy.

The developer of topological indices is Wiener [2]. It is defined as:

$$W(F) = \sum_{(x,y)\subseteq V(F)} d(x,y). \tag{1}$$

In 1975, [3] *Randić* was the first to introduce the vertex degree based topological index which is expressed as:

$$R_{\frac{-1}{2}}(F) = \sum_{xy\in E(F)} \frac{1}{\sqrt{d_x d_y}}. \tag{2}$$

In 1998, *Bollobás* and Erdos [4] and Ami et al. [5] independently computed the "general *Randić* index."

$$R_\alpha(F) = \sum_{xy\in E(F)} (d_x d_y)^\alpha, \tag{3}$$

where $\alpha = \frac{-1}{2}, \frac{1}{2}, 1, -1$. Estrada et al. [6] developed the ABC index in 1998. Its formula is:

$$ABC(F) = \sum_{xy\in E(F)} \sqrt{\frac{d_x + d_y - 2}{d_x d_y}}. \tag{4}$$

Vuki*čević* and Furtula were the first researchers to look GA index [7]. It's simplified as GA index and written as:

$$GA(F) = \sum_{xy\in E(F)} \frac{2\sqrt{d_x d_y}}{(d_x + d_y)}. \tag{5}$$

The instability in a random variable or number is known as entropy. In another sense, it is the information obtained through the discovery of unknown variables' values [8]. Information entropy in information theory, thermodynamic entropy in chemistry, and graph entropy in graph theory are all examples of entropy [9–14]. Entropy is described generally as the following:

Let $g \in G$ and ρ be the probability distribution of set G and g be a discrete random variable. Then g entropy is

$$H(g) = -\sum_{g\in G} \rho(g) log \rho(g). \tag{6}$$

Shannon proposed the concept of entropy in 1948 [15]. Rashevsky introduced the concept of graph entropy to graph theory in 1955 [16], and it has since been generally used to describe the design of graph-based systems in mathematical research [17–20]. The graph entropy is computed as follows: $V(F)$ is the finite vertex set for a graph F. Let ρ be the density of probability of vertex set and $V(\rho(F))$ be the vertex packing polytope of F. Then, entropy of F with respect to ρ is

$$H(F,\rho) = \min_{a\in V\rho(F)} \sum_{i=1}^{n} \rho_i log\left(\frac{1}{a_i}\right). \tag{7}$$

Natural diamond crystals, as well as many metal ions, are octahedrons, hence octahedron networks have their origins in the physical world. These networks can be utilized as circuits in physics. Manuel and Rajasingh [21] derived the silicate structure, and Simonraj and George [22] derived *BPOH*. For the complete construction of *BPOH*, see Figure 1, for Benzenoid dominating planar *BDPOH*, see Figure 2, and for Benzenoid Hex planar octahedron network, see Figure 3; we refer the reader to the article [23]. Entropy based on degrees is defined as

$$ENT_\psi(F) = -\sum_{i=1}^{p} \frac{d(x_i)}{\sum_{j=1}^{p} d(x_j)} log\left[\frac{d(x_i)}{\sum_{j=1}^{p} d(x_j)}\right]. \tag{8}$$

Edge-based entropy can be calculated by using equation (8),

$$ENT_d(F) = -\sum_{x'y' \epsilon E(F)} \frac{d(x'y')}{\sum_{xy \epsilon E(F)} d(xy)} log\left[\frac{d(x'y')}{\sum_{xy \epsilon E(F)} d(xy)}\right]. \tag{9}$$

Randić entropy can be calculated by using Equations (3) and (9).

$$ENT_{R_\alpha}(F) = log(R_\alpha) - \frac{1}{R_\alpha}\sum_{i=1}^{m}\sum_{xy \epsilon E_i(F)} log\left[(d(x) \times d(y))^\alpha\right]^{(d(x)\times d(y))^\alpha}. \tag{10}$$

ABC entropy can be calculated by using Equations (4) and (9).

$$ENT_{ABC}(F) = log(ABC) - \frac{1}{ABC}\sum_{i=1}^{m}\sum_{xy \epsilon E_i(F)} log\left[\sqrt{\frac{d(x)+d(y)-2}{d(x)\times d(y)}}\right]^{\sqrt{d(x)+d(y)-2/d(x)\times d(y)}}. \tag{11}$$

GA entropy can be calculated by using Equations (5) and (9).

$$ENT_{GA}(F) = log(GA) - \frac{1}{GA}\sum_{i=1}^{m}\sum_{xy \epsilon E_i(F)} log\left[\frac{2\sqrt{d(x)\times d(y)}}{d(x)+d(y)}\right]^{2\sqrt{d(x)\times d(y)/d(x)+d(y)}}. \tag{12}$$

2. Main Results

Benzenoid Inorganic structures utilized in chemistry include the planar octahedron network and its derivatives. In this article, we examine degree-based entropies for these networks. Entropies are presently the subject of a huge study activity. For further information, see [14,24–26]; for basic definitions and notations, see [27,28].

2.1. Result on Benzenoid Planar Octahedron Network

We compute Randić, ABC, and GA entropies for Benzenoied planar octahedron network in this section. Table 1 shows the edge partition of BPOH.

Table 1. The Edge partition

$(d(x), d(y))$	Number of Edges
(3,3)	$36n^2$
(3,4)	$12n$
(3,8)	$36n^2 - 12n$
(4,8)	$12n$
(8,8)	$18n^2 - 12n$

2.1.1. Randić Entropy. If $F_1 \cong BPOH(n)$, then from Table 1 and Equation (3), we have

$$\begin{aligned} R_\alpha(F_1) &= (36n^2)\times(9)^\alpha + (12n)\times(12)^\alpha + (36n^2-12n)\times(24)^\alpha + \\ &\quad (12n)\times(32)^\alpha + (18n^2-12n)\times(64)^\alpha. \end{aligned} \tag{13}$$

For $\alpha = 1$

$$R_1(F_1) = 2340n^2 - 528n. \tag{14}$$

For $\alpha = -1$

$$R_{-1}(F_1) = 5.78125n^2 + 0.6875n. \tag{15}$$

For $\alpha = \frac{1}{2}$

$$R_{\frac{1}{2}}(F_1) = 428.363n^2 - 45.3363n. \tag{16}$$

For $\alpha = -\frac{1}{2}$

$$R_{-\frac{1}{2}}(F_1) = 21.5985n^2 + 1.63593n. \tag{17}$$

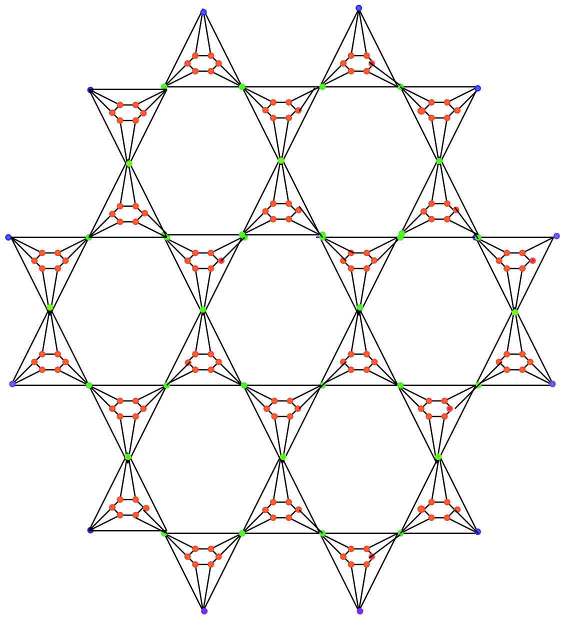

Figure 1. Benzenoid Planar Octahedron Network $BPOH(2)$

Using Equation (10) and Table 1, we have

$$ENT_{R_\alpha}(F_1) = log(R_\alpha) - \frac{1}{R_\alpha}\Big[(36n^2)\times log(9^\alpha)^{9^\alpha} + (12n)\times log(12^\alpha)^{12^\alpha} + (36n^2-12n)\times log(24^\alpha)^{24^\alpha} + (12n)\times log(32^\alpha)^{32^\alpha} + (18n^2-12n)\times log(64^\alpha)^{64^\alpha}\Big]. \quad (18)$$

For $\alpha = 1$

$$ENT_{R_1}(F_1) = log(R_1) - \frac{1}{R_1}\Big[(36n^2)\times log(9)^9 + (12n)\times log(12)^{12} + (36n^2-12n)\times log(24)^{24} + (12n)\times log(32)^{32} + (18n^2-12n)\times log(64)^{64}\Big],$$

$$ENT_{R_1}(F_1) = log(R_1) - \frac{1}{R_1}\left[\,3582.4n^2 - 105.27n\,\right]. \quad (19)$$

For $\alpha = -1$

$$ENT_{R_{-1}}(F_1) = log(R_{-1}) - \frac{1}{R_{-1}}\Big[(36n^2)\times log(1/9)^{1/9} + (12n)\times log(1/12)^{1/12} + (36n^2-12n)\times log(1/24)^{1/24} + (12n)\times log(1/32)^{1/32} + (18n^2-12n)\times log(1/64)^{1/64}\Big],$$

$$ENT_{R_{-1}}(F_1) = log(R_{-1}) - \frac{1}{R_{-1}}\left[\,-6.39528n^2 - 0.614848n\,\right]. \quad (20)$$

For $\alpha = \frac{1}{2}$

$$\begin{aligned} ENT_{R_{\frac{1}{2}}}(F_1) &= log(R_{\frac{1}{2}}) - \frac{1}{R_{\frac{1}{2}}}\Big[(36n^2) \times log(\sqrt{9})^{\sqrt{9}} + (12n) \times log(\sqrt{12})^{\sqrt{12}} + \\ &(36n^2 - 12n) \times log(\sqrt{24})^{\sqrt{24}} + (12n) \times log(\sqrt{32})^{\sqrt{32}} + \\ &(18n^2 - 12n) \times log(\sqrt{64})^{\sqrt{64}}\Big], \end{aligned}$$

$$ENT_{R_{\frac{1}{2}}}(F_1) = log(R_{\frac{1}{2}}) - \frac{1}{R_{\frac{1}{2}}}\left[\ 303.283n^2 - 53.7496n\ \right]. \tag{21}$$

For $\alpha = -\frac{1}{2}$

$$\begin{aligned} ENT_{R_{-\frac{1}{2}}}(F_1) &= log(R_{-\frac{1}{2}}) - \frac{1}{R_{-\frac{1}{2}}}\Bigg[(36n^2) \times log\left(\frac{1}{\sqrt{9}}\right)^{1/\sqrt{9}} + (12n) \times log\left(\frac{1}{\sqrt{12}}\right)^{1/\sqrt{12}} + \\ &(36n^2 - 12n) \times log\left(\frac{1}{\sqrt{24}}\right)^{1/\sqrt{24}} + (12n) \times log\left(\frac{1}{\sqrt{32}}\right)^{1/\sqrt{32}} + \\ &(18n^2 - 12n) \times log\left(\frac{1}{\sqrt{64}}\right)^{1/\sqrt{64}}\Bigg], \end{aligned}$$

$$ENT_{R_{-\frac{1}{2}}}(F_1) = log(R_{-\frac{1}{2}}) - \frac{1}{R_{-\frac{1}{2}}}\left[\ -12.8286n^2 - 0.420608n\ \right], \tag{22}$$

where R_α for α = 1, -1,$\frac{1}{2}$, $\frac{-1}{2}$ is written in (14), (15), (16), (17), respectively.

2.1.2 ABC Entropy. If $F_1 \cong$ BPOH(n), then from Table 1 and Equation (4), we have

$$\begin{aligned} ABC(F_1) &= (36n^2) \times \sqrt{\frac{3+3-2}{3\times 3}} + (12n) \times \sqrt{\frac{3+4-2}{3\times 4}} + (36n^2 - 12n) \times \sqrt{\frac{3+8-2}{3\times 8}} + \\ &(12n) \times \sqrt{\frac{4+8-2}{4\times 8}} + (18n^2 - 12n) \times \sqrt{\frac{8+8-2}{8\times 8}}, \end{aligned}$$

$$ABC(F_1) = 54.4641n^2 + 1.49322n. \tag{23}$$

Using Equation (11) and Table 1, we have

$$
\begin{aligned}
ENT_{ABC}(F_1) &= log(ABC) - \frac{1}{ABC}\Bigg[(36n^2)\times log\left(\sqrt{\frac{3+3-2}{3\times 3}}\right)^{\sqrt{3+3-2/3\times 3}} + \\
&(12n)\times log\left(\sqrt{\frac{3+4-2}{3\times 4}}\right)^{\sqrt{3+4-2/3\times 4}} + \\
&(36n^2-12n)\times log\left(\sqrt{\frac{3+8-2}{3\times 8}}\right)^{\sqrt{3+8-2/3\times 8}} + \\
&(12n)\times log\left(\sqrt{\frac{4+8-2}{4\times 8}}\right)^{\sqrt{4+8-2/4\times 8}} + \\
&(18n^2-12n)\times log\left(\sqrt{\frac{8+8-2}{8\times 8}}\right)^{\sqrt{8+8-2/8\times 8}}\Bigg],
\end{aligned}
$$

$$
ENT_{ABC}(F_1) = log(ABC) - \frac{1}{ABC}\left[\,-11.6999n^2 + 0.250499n\,\right]. \tag{24}
$$

Where ABC index is written in (24).

2.1.3 GA Entropy. If $F_1 \cong$ BPOH(n) then from Table 1 and Equation (5), we have

$$
\begin{aligned}
ENT_{GA}(F_1) &= (36n^2)\times\left(\frac{2\sqrt{3\times 3}}{(3+3)}\right) + (12n)\times\left(\frac{2\sqrt{3\times 4}}{(3+4)}\right) + (36n^2-12n)\times\left(\frac{2\sqrt{3\times 8}}{(3+8)}\right) + \\
&(12n)\times\left(\frac{2\sqrt{4\times 8}}{(4+8)}\right) + (18n^2-12n)\times\left(\frac{2\sqrt{8\times 8}}{(8+8)}\right),
\end{aligned}
$$

$$
ENT_{GA}(F_1) = 86.066n^2 + 0.501946n. \tag{25}
$$

Using Equation (12) and Table 1, we have

$$
\begin{aligned}
ENT_{GA}(F_1) &= log(GA) - \frac{1}{GA}\Bigg[(36n^2)\times log\left(\frac{2\sqrt{3\times 3}}{(3+3)}\right)^{2\sqrt{3\times 3}/(3+3)} + \\
&(12n)\times log\left(\frac{2\sqrt{3\times 4}}{(3+4)}\right)^{2\sqrt{3\times 4}/(3+4)} + (36n^2-12n)\times log\left(\frac{2\sqrt{3\times 8}}{(3+8)}\right)^{2\sqrt{3\times 8}/(3+8)} + \\
&(12n)\times log\left(\frac{2\sqrt{4\times 8}}{(4+8)}\right)^{2\sqrt{4\times 8}/(4+8)} + \\
&(18n^2-12n)\times log\left(\frac{2\sqrt{8\times 8}}{(8+8)}\right)^{2\sqrt{8\times 8}/(8+8)}\Bigg],
\end{aligned}
$$

$$
ENT_{GA}(F_1) = log(GA) - \frac{1}{GA}\left[\,-1.61155n^2 + 0.194642n\,\right]. \tag{26}
$$

2.2. Result on Benzenoid Dominating Planar Octahedron Network

we will compute Randić, ABC, and GA entropies for Benzenoid Dominating planar octahedron network in this section. Table 2 shows the *BDPOH* edge partition.

2.2.1 Randić Entropy. If $F_2 \cong BPOH(N)$ then from Table 2 and Equation (3), we have

Table 2. The Edge partition

$(d(x), d(y))$	Number of Edges
$(3,3)$	$108n^2 - 108n + 36$
$(3,4)$	$24n - 12$
$(3,8)$	$108n^2 - 132n + 48$
$(4,8)$	$24n - 12$
$(8,8)$	$54n^2 - 78n + 30$

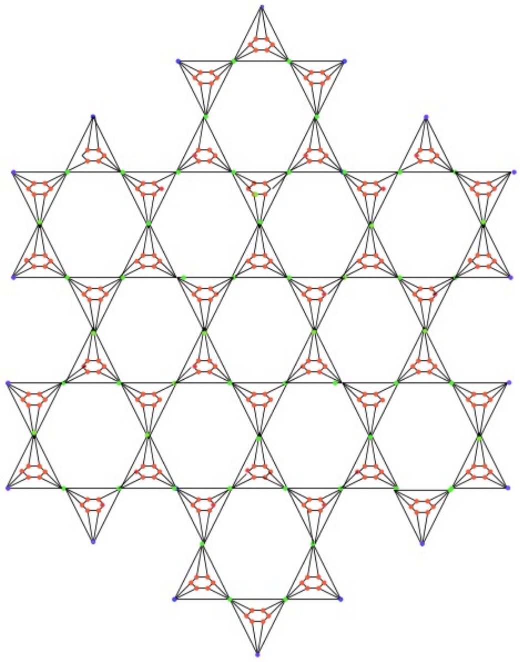

Figure 2. Benzenoid Dominating Planar Octahedron network *BDPOH*(2)

$$R_\alpha(F_2) = (108n^2 - 108n + 36) \times (9)^\alpha + (24n - 12) \times (12)^\alpha + (108n^2 - 132n + 48) \times (24)^\alpha + (24n - 12) \times (32)^\alpha + (54n^2 - 78n + 30) \times (64)^\alpha. \quad (27)$$

For $\alpha = 1$

$$R_1(F_2) = 7020n^2 - 8076n + 2868. \quad (28)$$

For $\alpha = -1$

$$R_{-1}(F_2) = 17.3438n^2 - 15.9688n + 5.09375. \quad (29)$$

For $\alpha = \frac{1}{2}$

$$R_{\frac{1}{2}}(F_2) = 1285.09n^2 - 1375.76n + 473.7. \quad (30)$$

For $\alpha = -\frac{1}{2}$

$$R_{-\frac{1}{2}}(F_2) = 64.7954n^2 - 61.5235n + 19.9625. \tag{31}$$

Using Equation (10) and Table 2, we have

$$\begin{aligned} ENT_{R_\alpha}(F_2) &= log(R_\alpha) - \frac{1}{R_\alpha}\Big[(108n^2 - 108n + 36) \times log(9^\alpha)^{9^\alpha} + (24n - 12) \times log(12^\alpha)^{12^\alpha} + \\ &(108n^2 - 132n + 48) \times log(24^\alpha)^{24^\alpha} + (24n - 12) \times log(32^\alpha)^{32^\alpha} + \\ &(54n^2 - 78n + 30) \times log(64^\alpha)^{64^\alpha}\Big]. \end{aligned} \tag{32}$$

For $\alpha = 1$

$$\begin{aligned} ENT_{R_1}(F_2) &= log(R_1) - \frac{1}{R_1}\Big[(108n^2 - 108n + 36) \times log(9)^9 + (24n - 12) \times log(12)^{12} + \\ &(108n^2 - 132n + 48) \times log(24)^{24} + (24n - 12) \times log(32)^{32} + \\ &(54n^2 - 78n + 30) \times log(64)^{64}\Big], \end{aligned}$$

$$ENT_{R_1}(F_2) = log(R_1) - \frac{1}{R_1}\left[\ 10747.2n^2 - 12849.7n + 4633.66\ \right]. \tag{33}$$

For $\alpha = -1$

$$\begin{aligned} ENT_{R_{-1}}(F_2) &= log(R_{-1}) - \frac{1}{R_{-1}}\Big[(108n^2 - 108n + 36) \times log(1/9)^{1/9} + (24n - 12) \times log(1/12)^{1/12} + \\ &(108n^2 - 132n + 48)) \times log(1/24)^{1/24} + (24n - 12) \times log(1/32)^{1/32} + \\ &(54n^2 - 78n + 30) \times log(1/64)^{1/64}\Big], \end{aligned}$$

$$ENT_{R_{-1}}(F_2) = log(R_{-1}) - \frac{1}{R_{-1}}\left[\ -19.1858n^2 + 17.9561n - 5.78043\ \right]. \tag{34}$$

For $\alpha = \frac{1}{2}$

$$\begin{aligned} ENT_{R_{\frac{1}{2}}}(F_2) &= log(R_{\frac{1}{2}}) - \frac{1}{R_{\frac{1}{2}}}\Big[(108n^2 - 108n + 36) \times log(\sqrt{9})^{\sqrt{9}} + (24n - 12) \times log(\sqrt{12})^{\sqrt{12}} + \\ &(108n^2 - 132n + 48) \times log(\sqrt{24})^{\sqrt{24}} + (24n - 12) \times log(\sqrt{32})^{\sqrt{32}} + \\ &(54n^2 - 78n + 30) \times log(\sqrt{64})^{\sqrt{64}}\Big], \end{aligned}$$

$$ENT_{R_{\frac{1}{2}}}(F_2) = log(R_{\frac{1}{2}}) - \frac{1}{R_{\frac{1}{2}}}\left[\ 909.85n^2 - 1017.35n + 357.033\ \right]. \tag{35}$$

For $\alpha = -\frac{1}{2}$

$$\begin{aligned} ENT_{R_{-\frac{1}{2}}}(F_2) &= log(R_{-\frac{1}{2}}) - \frac{1}{R_{-\frac{1}{2}}}\Bigg[(108n^2 - 108n + 36) \times log\left(\frac{1}{\sqrt{9}}\right)^{1/\sqrt{9}} + \\ &\quad (24n-12) \times log\left(\frac{1}{\sqrt{12}}\right)^{1/\sqrt{12}} + (108n^2 - 132n + 48) \times log\left(\frac{1}{\sqrt{24}}\right)^{1/\sqrt{24}} + \\ &\quad (24n-12) \times log\left(\frac{1}{\sqrt{32}}\right)^{1/\sqrt{32}} + \\ &\quad (54n^2 - 78n + 30) \times log\left(\frac{1}{\sqrt{64}}\right)^{1/\sqrt{64}}\Bigg], \end{aligned}$$

$$ENT_{R_{-\frac{1}{2}}}(F_2) = log(R_{-\frac{1}{2}}) - \frac{1}{R_{-\frac{1}{2}}}\left[\, -38.4859n^2 + 37.6447n - 12.408 \,\right]. \tag{36}$$

where R_α for $\alpha = 1, -1, \frac{1}{2}, \frac{-1}{2}$ is written in (28), (29), (30), and (31).

2.2.2. ABC Entropy. If $F_2 \cong$ BDPOH(n) then from Table 2 and Equation (4), we have

$$\begin{aligned} ABC(F_2) &= (108n^2 - 108n + 36) \times \sqrt{\frac{3+3-2}{3\times 3}} + (24n-12) \times \sqrt{\frac{3+4-2}{3\times 4}} + \\ &\quad (108n^2 - 132n + 48) \times \sqrt{\frac{3+8-2}{3\times 8}} + (24n-12) \times \sqrt{\frac{4+8-2}{4\times 8}} + \\ &\quad (54n^2 - 78n + 30) \times \sqrt{\frac{8+8-2}{8\times 8}}, \end{aligned}$$

$$ABC(F_2) = 163.392n^2 - 160.406n + 52.9709. \tag{37}$$

Using Equation (11) and Table 2, we have

$$\begin{aligned} ENT_{ABC}(F_2) &= log(ABC) - \frac{1}{ABC}\Bigg[(108n^2 - 108n + 36) \times log\left(\sqrt{\frac{3+3-2}{3\times 3}}\right)^{\sqrt{3+3-2/3\times 3}} + \\ &\quad (24n-12) \times log\left(\sqrt{\frac{3+4-2}{3\times 4}}\right)^{\sqrt{3+4-2/3\times 4}} + \\ &\quad (108n^2 - 132n + 48) \times log\left(\sqrt{\frac{3+8-2}{3\times 8}}\right)^{\sqrt{3+8-2/3\times 8}} + \\ &\quad (24n-12) \times log\left(\sqrt{\frac{4+8-2}{4\times 8}}\right)^{\sqrt{4+8-2/4\times 8}} + \\ &\quad (54n^2 - 78n + 30) \times log\left(\sqrt{\frac{8+8-2}{8\times 8}}\right)^{\sqrt{8+8-2/8\times 8}}\Bigg], \end{aligned}$$

$$ENT_{ABC}(F_2) = log(ABC) - \frac{1}{ABC}\left[\, -35.0997n^2 + 35.6007n - 11.9504 \,\right], \tag{38}$$

where ABC index is written in (37).

2.2.3. GA Entropy. If $F_2 \cong BDPOH(n)$ then from Table 2 and Equation (5), we have

$$
\begin{aligned}
ENT_{GA}(F_2) &= (108n^2-108n+36)\times\left(\frac{2\sqrt{3\times 3}}{(3+3)}\right)+(24n-12)\times\left(\frac{2\sqrt{3\times 4}}{(3+4)}\right)+\\
&\quad (108n^2-132n+48)\times\left(\frac{2\sqrt{3\times 8}}{(3+8)}\right)+(24n-12)\times\left(\frac{2\sqrt{4\times 8}}{(4+8)}\right)+\\
&\quad (54n^2-78n+30)\times\left(\frac{2\sqrt{8\times 8}}{(8+8)}\right),
\end{aligned}
$$

$$ENT_{GA}(F_2) = 258.198n^2 - 257.194n + 85.5641. \tag{39}$$

Using Equation (12) and Table 2, we have

$$
\begin{aligned}
ENT_{GA}(F_2) &= log(GA) - \frac{1}{GA}\Bigg[(108n^2-108n+36)\times log\left(\frac{2\sqrt{3\times 3}}{(3+3)}\right)^{2\sqrt{3\times 3}/(3+3)}+\\
&\quad (24n-12)\times log\left(\frac{2\sqrt{3\times 4}}{(3+4)}\right)^{2\sqrt{3\times 4}/(3+4)}+\\
&\quad (108n^2-132n+48)\times log\left(\frac{2\sqrt{3\times 8}}{(3+8)}\right)^{2\sqrt{3\times 8}/(3+8)}+\\
&\quad (24n-12)\times log\left(\frac{2\sqrt{4\times 8}}{(4+8)}\right)^{2\sqrt{4\times 8}/(4+8)}+\\
&\quad (54n^2-78n+30)\times log\left(\frac{2\sqrt{8\times 8}}{(8+8)}\right)^{2\sqrt{8\times 8}/(8+8)}\Bigg],
\end{aligned}
$$

$$ENT_{GA}(F_2) = log(GA) - \frac{1}{GA}\left[\,-4.83464n^2 + 5.22392n - 1.80619\,\right], \tag{40}$$

where GA index is written in (39).

2.3. Result on Benzenoid Hex Planar Octahedron Network

we will compute Randić, ABC, and GA entropies for benzenoid hex planar octahedron network in this section. Table 3 shows the edge partition of $BHPOH(n)$.

Table 3. Edge partition of benzenoid hex planar octahedron network based on degrees of end vertices

$(d(x),d(y))$	Number of Edges	$(d(x),d(y))$	Number of Edges
$(2,5)$	12	$(5,5)$	$12n-6$
$(3,3)$	$36n^2+36n$	$(5,8)$	$12n$
$(3,5)$	$24n$	$(8,8)$	$18n^2$
$(3,8)$	$36n^2+12n$		

2.3.1 Randić Entropy. If $F_3 \cong$ BHPOH(n), then from Table 3 and Equation (3), we have

$$
\begin{aligned}
R_\alpha(F_3) &= (12)\times(10)^\alpha+(36n^2+36n)\times(9)^\alpha+(24n)\times(15)^\alpha+(36n^2+12n)\times(24)^\alpha+\\
&\quad (12n-6)\times(25)^\alpha+(12n)\times(40)^\alpha+(18n^2)\times(64)^\alpha.
\end{aligned} \tag{41}
$$

For $\alpha = 1$

$$R_1(F_3) = 2340n^2 + 1752n - 30. \tag{42}$$

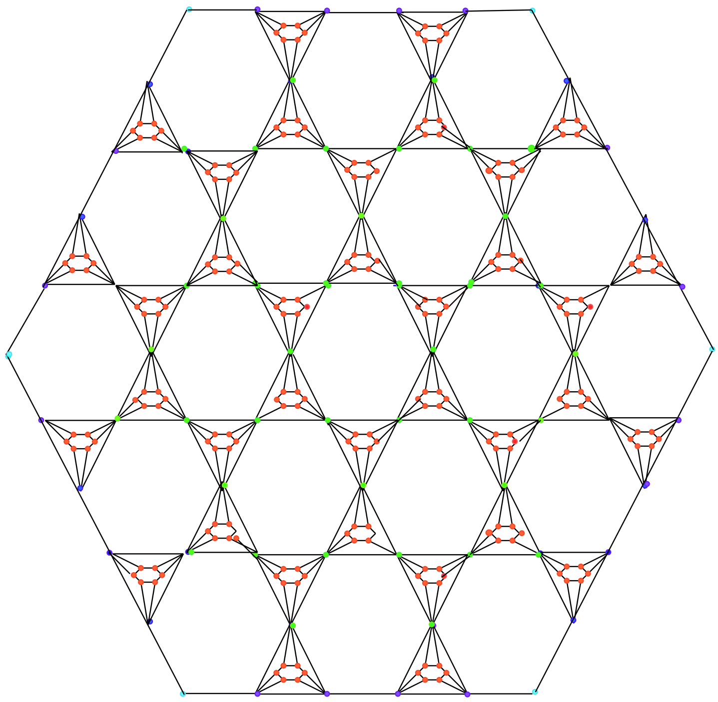

Figure 3. Benzenoid Hex Planar Octahedron network $BHPOH(2)$

For $\alpha = -1$

$$R_{-1}(F_3) = 5.78125n^2 + 6.88n + 0.96. \tag{43}$$

For $\alpha = \frac{1}{2}$

$$R_{\frac{1}{2}}(F_3) = 428.363n^2 + 395.634n + 7.94733. \tag{44}$$

For $\alpha = -\frac{1}{2}$

$$R_{-\frac{1}{2}}(F_3) = 21.5985n^2 + 24.9436n + 2.59473. \tag{45}$$

Using Equation (10) and Table 3, we have

$$\begin{aligned} ENT_{R_\alpha}(F_3) &= log(R_\alpha) - \frac{1}{R_\alpha}\Big[(12) \times log(10^\alpha)^{10^\alpha} + (36n^2 + 36n) \times log(9^\alpha)^{9^\alpha} + \\ & (24n) \times log(15^\alpha)^{15^\alpha} + (36n^2 + 12n) \times log(24^\alpha)^{24^\alpha} + (12n - 6) \times log(25^\alpha)^{25^\alpha} + \\ & (12n) \times log(40^\alpha)^{40^\alpha} + (18n^2) \times log(64^\alpha)^{64^\alpha}\Big]. \end{aligned} \tag{46}$$

For $\alpha = 1$

$$\begin{aligned} ENT_{R_1}(F_3) &= log(R_1) - \frac{1}{R_1}\Big[(12) \times log(10)^{10} + (36n^2 + 36n) \times log(9)^9 + (24n) \times log(15)^{15} + \\ & (36n^2 + 12n) \times log(24)^{24} + (12n - 6) \times log(25)^{25} + (12n) \times log(40)^{40} + \\ & (18n^2) \times log(64)^{64}\Big], \end{aligned}$$

$$ENT_{R_1}(F_3) = log(R_1) - \frac{1}{R_1}\left[\ 3582.4n^2 + 2318.44n - 89.691\ \right]. \tag{47}$$

For $\alpha = -1$

$$\begin{aligned} ENT_{R_{-1}}(F_3) &= log(R_{-1}) - \frac{1}{R_{-1}}\Big[(12) \times log(1/10)^{1/10} + (36n^2 + 36n) \times log(1/9)^{1/9} + \\ &(24n) \times log(1/15)^{1/15} + (36n^2 + 12n) \times log(1/24)^{1/24} + (12n - 6) \times log(1/25)^{1/25} + \\ &(12n) \times log(1/40)^{1/40} + (18n^2) \times log(1/64)^{1/64}\Big], \end{aligned}$$

$$ENT_{R_{-1}}(F_3) = log(R_{-1}) - \frac{1}{R_{-1}}\left[\ -6.39528n^2 - 7.54045n - 0.864494\ \right]. \tag{48}$$

For $\alpha = \frac{1}{2}$

$$\begin{aligned} ENT_{R_{\frac{1}{2}}}(F_3) &= log(R_{\frac{1}{2}}) - \frac{1}{R_{\frac{1}{2}}}\Big[(12) \times log(\sqrt{10})^{\sqrt{10}} + (36n^2 + 36n) \times log(\sqrt{9})^{\sqrt{9}} + \\ &(24n) \times log(\sqrt{15})^{\sqrt{15}} + (36n^2 + 12n) \times log(\sqrt{24})^{\sqrt{24}} + (12n - 6) \times log(\sqrt{25})^{\sqrt{25}} + \\ &(12n) \times log(\sqrt{40})^{\sqrt{40}} + (18n^2) \times log(\sqrt{64})^{\sqrt{64}}\Big], \end{aligned}$$

$$ENT_{R_{\frac{1}{2}}}(F_3) = log(R_{\frac{1}{2}}) - \frac{1}{R_{\frac{1}{2}}}\left[\ 303.283n^2 + 249.491n - 1.99543\ \right]. \tag{49}$$

For $\alpha = -\frac{1}{2}$

$$\begin{aligned} ENT_{R_{-\frac{1}{2}}}(F_3) &= log(R_{-\frac{1}{2}}) - \frac{1}{R_{-\frac{1}{2}}}\Bigg[(12) \times log\left(1/\sqrt{10}\right)^{1/\sqrt{10}} + (36n^2 + 36n) \times log\left(1/\sqrt{9}\right)^{1/\sqrt{9}} + \\ &(24n) \times log\left(1/\sqrt{15}\right)^{1/\sqrt{15}} + (36n^2 + 12n) \times log\left(1/\sqrt{24}\right)^{1/\sqrt{24}} + \\ &(12n - 6) \times log\left(1/\sqrt{25}\right)^{1/\sqrt{25}} + (12n) \times log\left(1/\sqrt{40}\right)^{1/\sqrt{40}} + \\ &(18n^2) \times log\left(1/\sqrt{64}\right)^{1/\sqrt{64}}\Bigg], \end{aligned}$$

$$ENT_{R_{-\frac{1}{2}}}(F_3) = log(R_{-\frac{1}{2}}) - \frac{1}{R_{-\frac{1}{2}}}\left[\ -12.8286n^2 - 14.2572n - 1.0586\ \right], \tag{50}$$

where R_α for $\alpha = 1, -1, \frac{1}{2}, \frac{-1}{2}$ is written in (42), (43), (44), and (45), respectively. **2.3.2. ABC Entropy.** If $F_3 \cong$ BHPOH(n), then from Table 3 and Equation (4), we have

$$\begin{aligned} ABC(F_3) &= (12) \times \sqrt{\frac{2+5-2}{2\times 5}} + (36n^2 + 36n) \times \sqrt{\frac{3+3-2}{3\times 3}} + (24n) \times \sqrt{\frac{3+5-2}{3\times 5}} + \\ &(36n^2 + 12n) \times \sqrt{\frac{3+8-2}{3\times 8}} + (12n - 6) \times \sqrt{\frac{5+5-2}{5\times 5}} + (12n) \times \sqrt{\frac{5+8-2}{5\times 8}} + \\ &(18n^2) \times \sqrt{\frac{8+8-2}{8\times 8}}, \end{aligned}$$

$$ABC(F_3) = 54.4641n^2 + 59.6085n + 5.09117. \tag{51}$$

Using Equation (11) and Table 3 we have

$$\begin{aligned} ENT_{ABC}(F_3) &= log(ABC) - \frac{1}{ABC}\Bigg[(12) \times log\left(\sqrt{\frac{2+5-2}{2\times 5}}\right)^{\sqrt{2+5-2/2\times 5}} + \\ &(36n^2+36n) \times log\left(\sqrt{\frac{3+3-2}{3\times 3}}\right)^{\sqrt{3+3-2/3\times 3}} + \\ &(24n) \times log\left(\sqrt{\frac{3+5-2}{3\times 5}}\right)^{\sqrt{3+5-2/3\times 5}} + \\ &(36n^2+12n) \times log\left(\sqrt{\frac{3+8-2}{3\times 8}}\right)^{\sqrt{3+8-2/3\times 8}} + \\ &(12n-6) \times log\left(\sqrt{\frac{5+5-2}{5\times 5}}\right)^{\sqrt{5+5-2/5\times 5}} + (12n) \times log\left(\sqrt{\frac{5+8-2}{5\times 8}}\right)^{\sqrt{5+8-2/5\times 8}} + \\ &(18n^2) \times log\left(\sqrt{\frac{8+8-2}{8\times 8}}\right)^{\sqrt{8+8-2/8\times 8}}\Bigg], \end{aligned}$$

$$ENT_{ABC}(F_3) = log(ABC) - \frac{1}{ABC}\left[\ -11.6999n^2 - 12.2551n - 0.437374\ \right]. \tag{52}$$

2.3.3. GA Entropy. If $F_3 \cong$ BHPOH(n), then from Table 3 and Equation (5), we have

$$\begin{aligned} ENT_{GA}(F_3) &= (12) \times \left(\frac{2\sqrt{2\times 5}}{(2+5)}\right) + (36n^2+36n) \times \left(\frac{2\sqrt{3\times 3}}{(3+3)}\right) + (24n) \times \left(\frac{2\sqrt{3\times 5}}{(3+5)}\right) + \\ &(36n^2+12n) \times \left(\frac{2\sqrt{3\times 8}}{(3+8)}\right) + (12n-6) \times \left(\frac{2\sqrt{5\times 5}}{(5+5)}\right) + (12n) \times \left(\frac{2\sqrt{5\times 8}}{(5+8)}\right) + \\ &(18n^2) \times \left(\frac{2\sqrt{8\times 8}}{(8+8)}\right), \end{aligned}$$

$$ENT_{GA}(F_3) = 86.066n^2 + 93.6027n + 4.84209. \tag{53}$$

Using equation (12) and Table (3), we have

$$\begin{aligned} ENT_{GA}(F_3) &= log(GA) - \frac{1}{GA}\Bigg[(12) \times log\left(\frac{2\sqrt{2\times 5}}{(2+5)}\right)^{2\sqrt{2\times 5}/(2+5)} + \\ &(36n^2+36n) \times log\left(\frac{2\sqrt{3\times 3}}{(3+3)}\right)^{2\sqrt{3\times 3}/(3+3)} + (24n) \times log\left(\frac{2\sqrt{3\times 5}}{(3+5)}\right)^{2\sqrt{3\times 5}/(3+5)} + \\ &(36n^2+12n) \times log\left(\frac{2\sqrt{3\times 8}}{(3+8)}\right)^{2\sqrt{3\times 8}/(3+8)} + (12n-6) \times log\left(\frac{2\sqrt{5\times 5}}{(5+5)}\right)^{2\sqrt{5\times 5}/(5+5)} + \\ &(12n) \times log\left(\frac{2\sqrt{5\times 8}}{(5+8)}\right)^{2\sqrt{5\times 8}/(5+8)} + (18n^2) \times log\left(\frac{2\sqrt{8\times 8}}{(8+8)}\right)^{2\sqrt{8\times 8}/(8+8)}\Bigg], \end{aligned}$$

$$ENT_{GA}(F_3) = log(GA) - \frac{1}{GA}\left[\ -1.61155n^2 - 1.0016n - 0.47779\ \right], \tag{54}$$

where GA index is written in (53).

Table 4. Comparison table of entropies for BPOH(n).

n	ENT_{R_1}	$ENT_{R_{-1}}$	$ENT_{R_{\frac{1}{2}}}$	$ENT_{R_{\frac{-1}{2}}}$	ENT_{ABC}	ENT_{GA}
2	2.219012	2.483488	2.528942	2.534295	2.553725	2.555703
3	2.650263	2.831281	2.879919	2.885152	2.905654	2.907856
4	2.937574	3.078956	3.129263	3.134387	3.155413	3.157713
5	3.153228	3.271454	3.322783	3.32782	3.349162	3.351531
6	3.325896	3.428943	3.480963	3.485926	3.507468	3.50989
7	3.469886	3.562202	3.614716	3.619642	3.641326	3.643776
8	3.593386	3.67772	3.730607	3.735499	3.757292	3.759758
9	3.701486	3.779657	3.832839	3.837696	3.859576	3.862061
10	3.797621	3.870879	3.924294	3.929127	3.951073	3.953568

Table 5. Comparison table of entropies for BDPOH(n).

n	ENT_{R_1}	$ENT_{R_{-1}}$	$ENT_{R_{\frac{1}{2}}}$	$ENT_{R_{\frac{-1}{2}}}$	ENT_{ABC}	ENT_{GA}
2	2.68845	2.724637	2.771439	2.776759	2.796656	2.798721
3	3.119482	3.153929	3.203977	3.209128	3.230059	3.232352
4	3.40804	3.441437	3.492986	3.498001	3.519405	3.521787
5	3.624744	3.657462	3.709881	3.714817	3.736468	3.738905
6	3.798208	3.830463	3.883446	3.888321	3.910146	3.912618
7	3.942807	3.974739	4.028118	4.032947	4.054878	4.057372
8	4.066781	4.098464	4.152125	4.156932	4.178941	4.181454
9	4.175264	4.206765	4.260652	4.265421	4.287498	4.29009
10	4.271711	4.303051	4.357115	4.361872	4.383995	4.386538

Table 6. Comparison table of entropies for BHPOH(n).

n	ENT_{R_1}	$ENT_{R_{-1}}$	$ENT_{R_{\frac{1}{2}}}$	$ENT_{R_{\frac{-1}{2}}}$	ENT_{ABC}	ENT_{GA}
2	2.64639	2.67529	2.719541	2.725073	2.743926	2.746066
3	2.936341	2.967727	3.014996	3.020292	3.040117	3.042365
4	3.152974	3.184967	3.233963	3.239117	3.259517	3.261834
5	3.326053	3.358172	3.408296	3.413352	3.434122	3.436491
6	3.470256	3.502307	3.553235	3.558228	3.579246	3.581651
7	3.593835	3.625795	3.677315	3.682252	3.703471	3.705906
8	3.701987	3.733838	3.785816	3.790714	3.812075	3.814537
9	3.798132	3.829879	3.882208	3.887081	3.908567	3.91104
10	3.88468	3.916318	3.968953	3.973803	3.995381	3.997869

3. Discussion and Conclusion

In this study, we generate several degree-based topological indices for Benzenoid planar octahedron networks and subsequently compute entropy values using Shannon's graph entropy concept. We compile numerical data for these networks in tables to analyze the variation in entropy values for the degree-based indices. Tables 4, 5, and 6 demonstrate that as the value of n increases, the entropy values for the Randić, ABC, and GA indices change proportionately. These equations and numerical values enable researchers to estimate the physiological and metabolic activity of these networks. Additionally, the entropy values can be used to determine the amount of energy in a chemical system that is unavailable for work. The results indicate that the degree-based entropies (Randić, ABC, GA) of Benzenoid Planar Octahedron Networks are linked to key chemical properties such as molecular stability, reactivity, and bioactivity. Higher entropy values suggest more stable and less reactive structures, while these metrics help predict the bioactivity potential in pharmaceutical applications. The entropies of other complicated networks will also be used in our future research.

Data Availability

No data were used to support this study.

Conflict of Interest

The authors declare no conflict of interest.

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