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Review

Properties of Entropy-Based Topological Measures of Fullerenes

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Received: 8 April 2020; Accepted: 20 April 2020; Published: 7 May 2020

Abstract: A fullerene is a cubic three-connected graph whose faces are entirely composed of pentagons and hexagons. Entropy applied to graphs is one of the significant approaches to measuring the complexity of relational structures. Recently, the research on complex networks has received great attention, because many complex systems can be modelled as networks consisting of components as well as relations among these components. Information—theoretic measures have been used to analyze chemical structures possessing bond types and hetero-atoms. In the present article, we reviewed various entropy-based measures on fullerene graphs. In particular, we surveyed results on the topological information content of a graph, namely the orbit-entropy $I_a(G)$, the symmetry index, a degree-based entropy measure $I_\lambda(G)$, the eccentric-entropy $If_\sigma(G)$ and the Hosoya entropy $H(G)$.

Keywords: fullerene; graph entropy; automorphism group; eigenvalue; eccentricity

1. Introduction

In recent years, research on complex networks has been essential since many complex systems are modelled as networks consisting of components as well as relations among these components. Some studies focused on finding properties of real networks, such as degree distribution [1,2], degree correlation [3–5], and degree-based structure entropies [6,7]. Many significant properties of systems such as heterogeneity [1], assortative mixing [8,9], and self-similarity [10–12] are based on these statistics.

Entropy applied to graphs is one of two major approaches to measuring the complexity of relational structures. The origin of such measures goes back to Rashevsky who introduced the concept of topological information content; see [13]. Studies of graph complexity have been performed in many areas [8,11,14,15], such as chemistry to labeled chemical structures possessing bond types and hetero-atoms; see [16]. The aim of this paper was to review some selected entropy-based measures.

2. Definitions and Preliminaries

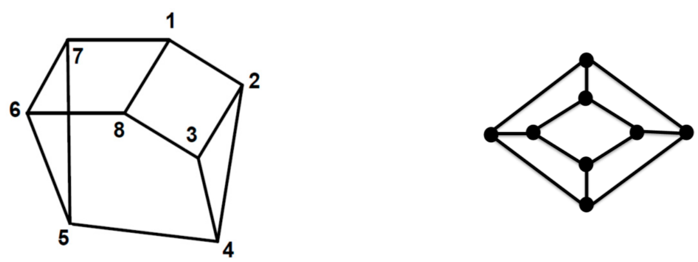
Here, we recall the definition of the automorphism group of a graph. It is a well-known fact that in a regular polyhedral graph such as a fullerene, the symmetry group and the automorphism group are the same; see [17]. A permutation π on the set of vertices of graph G, which preserves the adjacency of vertices of G, is called an automorphism. In other words, the permutation π is an automorphism if

$$uv \in E(G) \Leftrightarrow \pi(u)\pi(v) \in E(G).$$

The set of all automorphisms of G, denoted by $\mathrm{Aut}(G)$, forms a group under the composition of mappings called an automorphism group. Let the automorphism group Aut (G) act on vertex set V. This action yields an automorphism partition P = {V_1, V_2,..., V_k} in the which two vertices x and y are equivalent if and only if there exists g in Aut (G) such that $xg = y$. Each member of P is an orbit of Aut (G). The set of orbits of a graph enables us to investigate the heterogeneity of networks.

We say that Aut (G) acts transitively on the set of vertices, if for $u, v \in V(G)$, there is an automorphism $\beta \in \mathrm{Aut}(G)$, such that $\beta(u) = v$. In this case, we say that G is vertex-transitive. It is not difficult to see that every vertex-transitive graph has only one orbit whose size is equal to the number of vertices. For example, consider the rotation $\rho = (360/n)^{\circ}$ of cycle graph C_n; then, the corresponding permutation is $\rho = (1, 2, \ldots, n)$ which yields that C_n is vertex-transitive.

Measuring the heterogeneity of complex networks has been important in studies of the behaviour of complex networks. For example, existing heterogeneity measures [6,7] of complex networks are based on degree. Specifically, entropies in [6,7] are based on degree distribution [8,9]. As is shown in Figure 1, in a network, vertices with the same degree can be distinguished by measurement on some structural properties of particular vertex such as the number of triangles that a vertex lie on or the shortest path passing through a vertex; see Figure 1.



(**a**) Cuneane (**b**) cube

Figure 1. Illustration of two cubic graphs: (**a**) Cuneane; (**b**) cube.

The molecular graph of cuneane is depicted in Figure 1a. This graph is not vertex-transitive. The 2-D graph of the cube graph Q_3, as depicted in Figure 1b, indicates an example of a vertex-transitive graph. One can easily verify that the vertex partition P = {{1, 8}, {4, 5}, {2, 3, 6, 7}} in the cuneane graph is finer than the degree partition. Furthermore, we can validate that partition P is an orbit decomposition of cuneane.

For most of networks, the orbit-partition of a graph is much finer than the degree partition. The number of automorphism partitions or the number of orbits can interpret the structure of a network. For example, a graph with n vertices has exactly n orbits if and only if it is asymmetric.

3. Fullerene Graphs

In addition to the two popular forms of carbon, namely diamond and graphite, a third form of carbon called fullerene was discovered in 1985; see [18,19]. One of the most well-known members of this class of molecular graphs, the buckminster fullerene C_{60} which contains 60 carbon atoms, 12 pentagons and 20 hexagons, is vertex-transitive.

In general, a fullerene is a cubic three-connected graph on n vertices which has $n/2 - 10$ hexagons and 12 pentagons.

The non-classical fullerenes are formed by a combination of triangles, quadrangles, pentagons, hexagons, etc. There are many problems concerning fullerene graphs, and many properties of them were studied by mathematicians, see [20–64] as well as [65–75]. Fullerenes are individual cases of a larger class of graphs, namely polyhedral graphs. In general, a polyhedral graph is a three-connected simple planar graph and the polyhedral graphs considered in this paper are cubic. In chemistry, a fullerene is a molecule composed of carbon atoms in the form of many shapes such as a hollow sphere, ellipsoid, tube, etc. [51]. The non-classical fullerenes may contain hexagons and other rings.

In [76], a method is described to obtain a fullerene graph from a zig-zag or armchair nanotubes. Here, by continuing that method, we construct some infinite classes of fullerenes. Denoted by $T_Z[m,n]$ means a zig-zag nanotube with m rows and n columns of hexagons, see Figure 2. Combine a nanotube $T_Z[5,n-4]$ with two copies of caps B (Figure 3), to construct a fullerene graph as shown in Figure 4. Two caps have together 40 vertices and thus, the number of vertices of the fullerene graph is $10(n-4)+40=10n$. This is why we did it by A_{10n}.

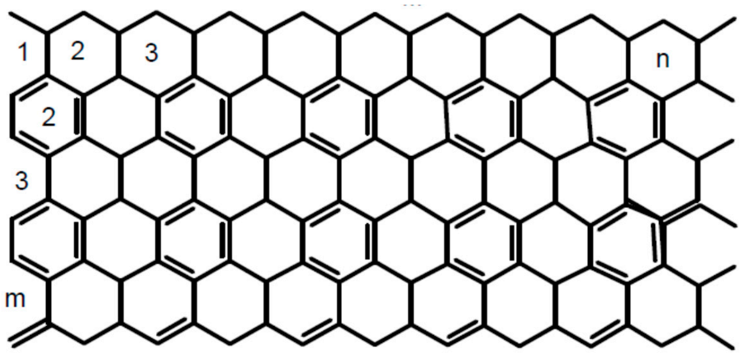


Figure 2. The 2-D graph of zig-zag nanotube $T_Z[5,10]$.

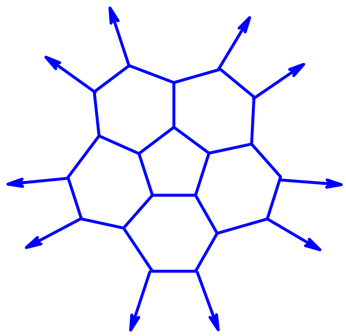


Figure 3. Cap B.

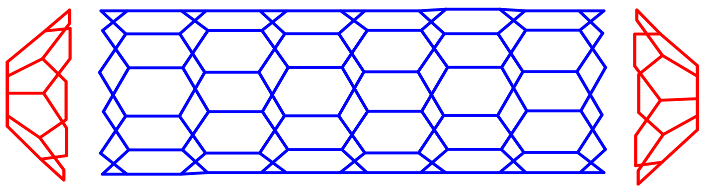


Figure 4. The presentation of fullerene A_{10n} as a combining of two copies of B and the nanotube $T_Z[5,n-4]$.

4. Entropy Measure

The concepts of entropies have been investigated extensively in [77–84] to characterize and quantify the structure of networks. Several types of them are discussed in [1], and mathematically explored. Therefore, we omit an extensive review on graph entropies here. Studying the entropy of dendrimers, a graph class with a long-standing history in chemistry and related disciplines, is done in some references such as [82–84] in which authors considered the individual eccentricity-based information functionals. As graph entropies, we use a specific definition due to Dehmer [85–92] as follows. Consider a probability vector $p = (p_1, \ldots ,p_n)$ that satisfies in two conditions $0 \le p_i \le 1$ and $\sum_{i=1}^{n} p_i = 1$. The Shannon's entropy is $I(p) = -\sum_{i=1}^{n} p_i \log p_i$, where the symbol "log" is the logarithm on the basis 2. Let

$$p_i = \lambda_i / \sum_{j=1}^{n} \lambda_j, \quad (i = 1, 2, \ldots, n),$$

where $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ is a tuple of none-negative integers, $\lambda_i \in \mathbb{N}$, see [90]. The entropy of tuple $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ is given by

$$I(\lambda_1, \lambda_2, \ldots, \lambda_n) = \log\left(\sum_{i=1}^{n} \lambda_i\right) - \sum_{i=1}^{n} (\lambda_i / \sum_{j=1}^{n} \lambda_j) \log \lambda_i.$$

There are many ways to obtain the tuple $(\lambda_1, \lambda_2, \ldots, \lambda_n)$.

For a vertex v_i of graph G, if we put

$$p(v_i) := f(v_i) / \sum_{j=1}^{|V|} f(v_j), \tag{1}$$

Then clearly, $\sum_{j=1}^{|V|} p(v_j) = 1$ and the entropy measure of G based on f is thus

$$I_f(G) = -\sum_{i=1}^{|V|} \frac{f(v_i)}{\sum_{j=1}^{|V|} f(v_j)} \log\left(f(v_i) / \sum_{j=1}^{|V|} f(v_j)\right) = \log\left(\sum_{i=1}^{|V|} f(v_i)\right) - \sum_{i=1}^{|V|} (f(v_i) / \sum_{j=1}^{|V|} f(v_j)) \log f(v_i).$$

In the literature, there are various ways to obtain the tuple $(p_1, \ldots ,p_n)$ like the so-called magnitude-based information measures introduced by Bonchev and Trinajstić [82], or partition—independent graph entropies, introduced by Dehmer based on information functionals; see [91–96] as well as [97–106].

A function $d : G \times G \to \mathbb{R}^+$ in which for any pair of vertices of graph G such as x and y, $d(x,y)$ is defined as the length of shortest path connecting them, indicates the distance between these vertices.

A topological index of graph G is a numerical quantity, which is invariant under its automorphism group. The Wiener index is the first reported distance based topological index, and it defined as half sum of the distances between all the pairs of vertices in a molecular graph; see [107]. In other words,

$$W(G) = \frac{1}{2} \sum_{x,y \in V(G)} d(x, y). \tag{2}$$

The Wiener (or Hosoya) polynomial of a graph [108] is defined as

$$H(G,\ x) = \sum_{uv \in E(G)} x^{d(u,v)}. \tag{3}$$

It is clear that $H(G,1) = W(G)$. For a given vertex v, the function

$$H_v(G, x) = \sum_{u \in V(G), u \neq v} x^{d(u,v)}$$

is called the partial Hosoya polynomial of G at vertex v.

Hence,

$$H(G,x) = \sum_{v \in V(G)} H_v(G,x) \tag{4}$$

Graph entropy measures represent information—theoretic measures for characterizing networks quantitatively. The first concepts in this framework was developed in the 1950s for investigating biological and chemical systems. Seminal work on this problem was done by Rashevsky, Trucco, and Mowshowitz, [100–104,109–112] who studied entropy measures for determining the structural information content of a graph. Graph entropies have been applied to various problems such as biology, computational biology, mathematical chemistry, Web mining, and knowledge engineering.

4.1. Eccentric Entropy Measure

The eccentricity of vertex v is an information functional defined by $\sigma(v) = \max_{u \in V} d(u,v)$, see [113–115]. Now, for a vertex $v_i \in V$ $f(v_i) := c_i \sigma(v_i)$, where $c_i > 0$ for $1 \le i \le n$. Then

$$If_\sigma(G) = \log\left(\sum_{i=1}^{n} c_i \sigma(v_i)\right) - \sum_{i=1}^{n} \frac{c_i \sigma(v_i)}{\sum_{j=1}^{n} c_j \sigma(v_j)} \log(c_i \sigma(v_i)).$$

Moreover, if c_is are equal, then

$$If_\sigma(G) = \log\left(\sum_{i=1}^{n} \sigma(v_i)\right) - \sum_{i=1}^{n} \frac{\sigma(v_i)}{\sum_{j=1}^{n} \sigma(v_j)} \log(\sigma(v_i)).$$

Theorem 1 ([25]). *In a vertex-transitive graph, all vertices have the same eccentricity.*

Theorem 2. *If G is a regular graph on n vertices, then*

$$If_\sigma(G) = \log(\sum_{i=1}^{n} c_i) - \sum_{i=1}^{n} \frac{c_i}{\sum_{j=1}^{n} c_j} \log(c_i). \tag{5}$$

In particular, if $c_i = c_j$ for all, $i \neq j$ then $If_\sigma(G) = \log(n)$.

Proof. By Theorem 1, for all $x, y \in V(G)$, we have $\sigma(x) = \sigma(y)$ which proves the first claim.

If $c_i = c_j$ for all $i \neq j$ then we have

$$If_\sigma(G) = \log(nc_1) - \frac{1}{nc_1} \sum_{i=1}^{n} c_1 \log(c_1) = \log(nc_1) - \log(c_1) = \log(n).$$

□

Theorem 3. *The polyhex nanotori T (Figure 5) is vertex-transitive.*

Figure 5. Three-dimensional graph of zig-zag polyhex nanotori.

Proof. Suppose p and q are even. Consider two vertices u_{ij} and u_{rs} in which both integers i,r are either odd, or even, and suppose σ, π are two permutations that $\sigma(u_{it}) = u_{rt}$, $1 \leq t \leq p$ and $\pi(u_{tj}) = u_{ts}$, $1 \leq t \leq q$. Then, σ and π are automorphisms of T in which πσ maps u_{ij} to u_{rs} and so, they are in the same orbit. Suppose now i is odd and r is even or i is even and r is odd. Then, the permutation θ which maps u_{ij} to $u_{(p+1-i)j}$ is a graph automorphism which implies that u_{ij} and u_{rs} are in the same orbit of Aut(G) and we are done. □

Example 1. *Consider the 2-dimensional graph of zig-zag polyhex nanotori T[p,q], as depicted in Figure 6. It can be easily seen that |V(T[p,q])|=pq. By Theorem 3, T[p,q] is vertex-transitive and if for all i≠j, c_i=c_j then, by Theorem 2, we have* $If_\sigma(T[p,q]) = \log(n) = \log(p) + \log(q)$.

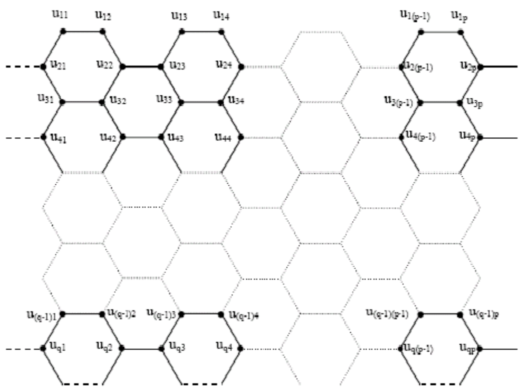


Figure 6. Two-dimensional lattice for *T*[*p*,*q*].

Let *G* be an edge-transitive graph but not vertex-transitive, and *e* = *xy* be an arbitrary edge in *G*. For an arbitrary edge *e* = *uv*, there exists an automorphism σ such that σ(*e*) = *f*. Hence, $\{\sigma(u), \sigma(v)\} = \{\sigma(x), \sigma(y)\}$. Let $\sigma(v_i) = \sigma(x)$ for $1 \leq i \leq r$ and $\sigma(v_j) = \sigma(y)$ for $r + 1 \leq j \leq n$. As a particular case, we consider $c_i = c_j$ for all *i*≠*j*. By some elementary calculations, we obtain

$$If_\sigma(G) = \log(r\sigma(x) + (n-r)\sigma(y)) - \frac{r\sigma(x)\log(\sigma(x)) + (n-r)\sigma(y)\log(\sigma(y))}{r\sigma(x) + (n-r)\sigma(y)}.$$

Hence, we proved the following theorem.

Theorem 4. *Let G be edge-transitive but not vertex-transitive and let $c_i = c_j$ for all i≠j. Then,*

$$If_\sigma(G) = \log(r\sigma(x) + (n-r)\sigma(y)) - \frac{r\sigma(x)\log(\sigma(x)) + (n-r)\sigma(y)\log(\sigma(y))}{r\sigma(x) + (n-r)\sigma(y)}.$$

Example 2. *As usual, suppose that S_n indicates an star graph on n + 1 vertices. Suppose x is the central vertex and denotes the other vertices by $u_1, u_2, \ldots, u_n$. Then $d(x,u_1) = 1$ and $d(u_i,u_j) = 2$ $(1 \leq i,j \leq n)$. If $c_i = c_j$ for all $i \neq j$, then, by using Theorem 4, we infer that*

$$If_\sigma(S_n) = \log(2(n-1)+1) - \frac{2(n-1)\log 2 + \log 1}{2n-1} = \log(2n-1) + \frac{1}{2n-1} - 1.$$

Theorem 5. *Suppose G is a graph and $V_1, \ldots, V_k$ are all orbits of Aut(G) on V(G). Then,*

$$If_\sigma(G) = \log\left(\sum_{i=1}^{k}\sigma(x_i)\sum_{j=1}^{|V_i|}c_j\right) - \sum_{i=1}^{k}\sigma(x_i)\sum_{j=1}^{|V_i|}\frac{c_j}{\sum_{t=1}^{k}\sigma(x_t)\sum_{l=1}^{|V_i|}c_l}\log\Big(c_j\sigma(x_i)\Big).$$

Proof. For all $x_i, x_j \in V_i$, we have $\sigma(x_i) = \sigma(x_j)$ and, the proof is complete. □

Suppose for the vertex v of graph G, $d(v)$ shows the degree of vertex v. If $f(v) \in \left\{\sigma(v), d(v), d(v)\sigma(v), \frac{\sigma(v)}{d(v)}, \frac{d(v)}{\sigma(v)}\right\}$, and we put $f(v)$ in Equation (1), then we achieve four new entropy-based measures as follows:

$$I_{\deg}(G) = \log\left(\sum_{i=1}^{n}d(v_i)\right) - \sum_{i=1}^{n}\frac{d(v_i)}{\sum_{j=1}^{n}d(v_j)}\log\left(\frac{d(v_i)}{\sum_{j=1}^{n}d(v_j)}\right).$$

$$I_\xi(G) = \log\left(\sum_{i=1}^{n}d(v_i)\sigma(v_i)\right) - \sum_{i=1}^{n}\frac{d(v_i)\sigma(v_i)}{\sum_{j=1}^{n}d(v_j)\sigma(v_j)}\log\left(\frac{d(v_i)\sigma(v_i)}{\sum_{j=1}^{n}d(v_j)\sigma(v_j)}\right).$$

$$I_\xi{}^D(G) = \log\left(\sum_{i=1}^{n}\frac{d(v_i)}{\sigma(v_i)}\right) - \sum_{i=1}^{n}\frac{d(v_i)/\sigma(v_i)}{\sum_{j=1}^{n}d(v_j)/\sigma(v_j)}\log\left(\frac{d(v_i)/\sigma(v_i)}{\sum_{j=1}^{n}d(v_j)/\sigma(v_j)}\right).$$

$$I_{\xi_D}(G) = \log\left(\sum_{i=1}^{n}\frac{\sigma(v_i)}{d(v_i)}\right) - \sum_{i=1}^{n}\frac{\sigma(v_i)/d(v_i)}{\sum_{j=1}^{n}\sigma(v_j)/d(v_j)}\log\left(\frac{\sigma(v_i)/d(v_i)}{\sum_{j=1}^{n}\sigma(v_j)/d(v_j)}\right).$$

It is clear that since a fullerene is 3-regular, then $m = 3n/2$ (the number of edges) and

$$\begin{aligned} I_{\deg}(G) &= \log(2m) - \tfrac{1}{2m}\sum_{i=1}^{n}d(v_i)\log(d(v_i)), \\ &= \log(3n) - \tfrac{1}{3n}\sum_{i=1}^{n}d(v_i)\log(d(v_i)). \end{aligned}$$

Moreover, the entropies of graphs based on the eccentricities of vertices are studied in [22–30].

4.2. Ecc-Entropy of Fullerene Graphs

In this section, similarly to the definition of the fullerene A_{10n} in the last section, we present two infinite families of fullerenes namely C_{24n+12} and C_{12n+2} with respectively $24n + 12$ and $12n + 2$ vertices as depicted, respectively, in Figures 7 and 8. For more details about the construction of these classes of fullerenes, see references [25,27].

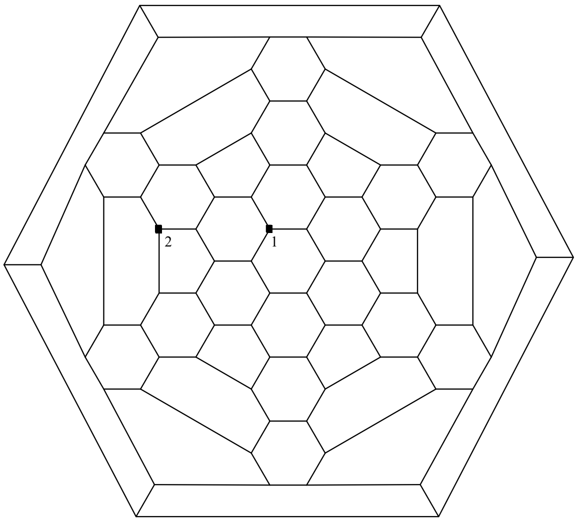


Figure 7. The molecular graph of the fullerene C_{24n+12}, for $n = 3$.

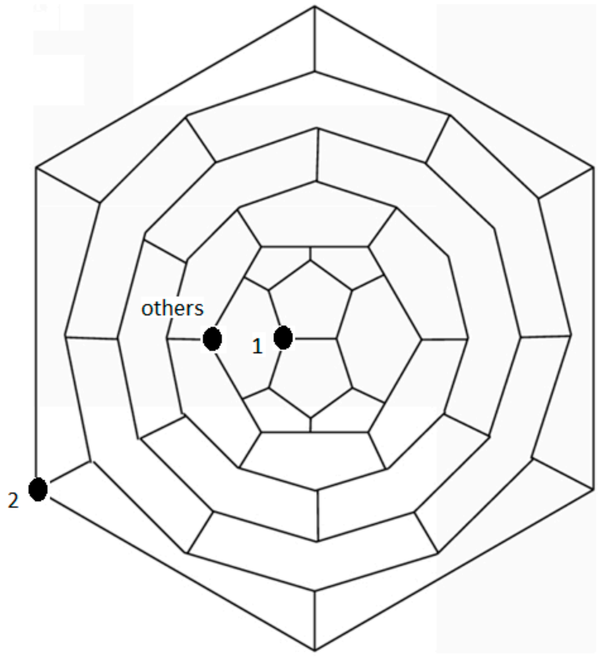


Figure 8. The molecular graph of the fullerene C_{12n+2}.

Theorem 6. *If c_i's are equal, then Equation (5) yields that for $n \geq 7$*

$$\begin{aligned} If_\sigma(C_{24n+12}) &= 2 + \log 3 + \log(3n^2 + 12n + 5) \\ &- \frac{1}{3n^2+12n+5}\left((n+5)\log(n+5) + 2\sum_{i=6}^{n+5}(n+i)\log(n+i)\right). \end{aligned}$$

Proof. Consider the vertices of the central hexagon and other vertices of C_{24n+12} as shown in Figure 7. Consider the eccentric contribution of each vertex as reported in Table 1. As shown in this table, there are two types of vertices. The vertices of the central and outer hexagons and the other vertices. By Equation (2) we have

$$\begin{aligned} If_\sigma(C_{24n+12}) &= \log\left(12(n+5)+24\sum_{i=6}^{n+5}(n+i)\right) \\ &-\frac{1}{12(n+5)+24\sum_{i=6}^{n+5}(n+i)}\left(12(n+5)\log(n+5)+24\sum_{i=6}^{n+5}(n+i)\log(n+i)\right) \\ &= 2+\log 3+\log(3n^2+12n+5) \\ &-\frac{1}{3n^2+12n+5}\left((n+5)\log(n+5)+2\sum_{i=6}^{n+5}(n+i)\log(n+i)\right) \end{aligned}$$

□

Table 1. The eccentricity of vertices of C_{24n+12}, $n \geq 7$.

Vertices	σ (x)	No
Vertices of type 1	$n+5$	12
Vertices of type 2	$n+i$ $(6 \leq i \leq n+5)$	24

The exceptional cases are given in Table 2.

Table 2. Some exceptional cases of C_{24n+12} fullerenes.

Fullerenes	$If_\sigma(F)$
C_{60}	$\log 60$
C_{84}	$\log 84$
C_{108}	$\log 1320-\frac{1008\log 12+312\log 13}{1320}$
C_{132}	$\log 1728-\left(\frac{720\log 12+312\log 13+336\log 14+360\log 15}{1728}\right)$
C_{156}	$\log 2232-\left(\frac{432\log 12+312\log 13+336\log 14+360\log 15+384\log 16+408\log 17}{2232}\right)$

Theorem 7. *If c_i's are equal, then the entropy of fullerene C_{12n+2}, $n \geq 10$ (see Figure 8) is*

$$\begin{aligned} If_\sigma(C_{12n+2}) &= 1+\log(n)+\log(9n+14) \\ &-\frac{1}{n(9n+14)}\left(8n+11n\log(n)+6\sum_{i=1}^{n}(n+i)\log(n+i)\right) \end{aligned}$$

Proof. Similarly, to the proof of Theorem 6 and by using the eccentricity of vertices as reported in Table 3 and by Equation (5), we obtain

$$\begin{aligned} If_\sigma(C_{12n+2}) &= \log\left(22n+12\sum_{i=1}^{n}(n+i)\right) \\ &-\frac{1}{22n+12\sum_{i=1}^{n}(n+i)}\left(16n\log(2n)+6n\log(n)+12\sum_{i=1}^{n}(n+i)\log(n+i)\right) \\ &= 1+\log\left(9n^2+14n\right)-\frac{1}{n(9n+14)}\left(8n+11n\log(n)+6\sum_{i=1}^{n}(n+i)\log(n+i)\right). \end{aligned}$$

□

Table 3. The eccentricity of vertices of C_{12n+2}, $n \geq 10$.

Vertices	$\sigma(x)$	No.
Vertices of type 1	$2n$	8
Vertices of type 2	n	6
Other Vertices	$n + i\ (1 \leq i \leq n)$	12

The exceptional cases are given in Table 4.

Table 4. Some exceptional cases of C_{12n+2} fullerenes.

F	$If_\sigma(F)$
C_{26}	$\log 132 - \frac{120\log 5+12\log 6}{132}$
C_{38}	$\log 266 - \log 7 = \log 38$
C_{50}	$\log 392 - \frac{84\log 7+272\log 8+36\log 9}{392}$
C_{62}	$\log 548 - \frac{192\log 8+216\log 9+140\log 10}{548}$
C_{74}	$\log 720 - \frac{96\log 8+216\log 9+180\log 10+132\log 11+96\log 12}{720}$
C_{86}	$\log 940 - \frac{216\log 9+180\log 10+132\log 11+144\log 12+156\log 13+112\log 14}{940}$
C_{98}	$\log 1088 - \frac{108\log 9+180\log 10+132\log 11+144\log 12+156\log 13+168\log 14+180\log 15+128\log 16}{1088}$
C_{110}	$\log 1500 - \frac{180\log 10+132\log 11+144\log 12+156\log 13+168\log 14+180\log 15+128\log 16+204\log 17+144\log 18}{1088}$

4.3. Eigen—Entropy of Fullerenes

The adjacency matrix $A(G)$ of graph G with vertex set $V(G) = \{v_1, v_2,..., v_n\}$ is the $n \times n$ symmetric matrix $[a_{ij}]$ such that $a_{ij} = 1$ if v_i and v_j are adjacent and 0, otherwise. The characteristic polynomial of graph G is defined as [116]

$$\phi(G,x) = \det(A(G) - xI)$$

The roots of the characteristic polynomial are named the eigenvalues of graph G, which form the spectrum of this graph. If α is an eigenvalue of matrix A, then there exists a vector such as V, in which $A.V = \alpha V$.

Let $\lambda_1,..., \lambda_n$ be the eigenvalues of $A(G)$; then, the energy of G is defined [117,118] as

$$\varepsilon(G) = \sum_{i=1}^{n} |\lambda_i|$$

In theoretical chemistry, the energy is a graph parameter stemming from the Hückel molecular orbital approximation for the total π-electron energy. Thus, the graph energy has some specific chemical interests and has been extensively studied [119,120].

One information functional is based on absolute value of eigenvalues; see [121,122]. The eigen-entropy based on non-zero eigenvalues denoted by $If_\lambda(G)$ is defined as follows:

$$If_\lambda(G) = \log\left(\sum_{i=1}^{n} c_i|\lambda_i|\right) - \sum_{i=1}^{n} \frac{c_i|\lambda_i|}{\sum_{j=1}^{n} c_j|\lambda_j|} \log(c_i|\lambda_i|)$$

where $\lambda_i \neq 0\ (i = 1, \ldots, n-1)$. If c_is are equal, then

$$\begin{aligned} If_\lambda(G) &= \log\left(\sum_{i=1}^{n} |\lambda_i|\right) - \sum_{i=1}^{n} \frac{|\lambda_i|}{\sum_{j=1}^{n} |\lambda_j|} \log(|\lambda_i|) \\ &= \log(\varepsilon(G)) - \frac{1}{\varepsilon(G)} \sum_{i=1}^{n} |\lambda_i| \log(|\lambda_i|). \end{aligned} \tag{6}$$

Theorem 8. *Let G be a connected graph with non-zero eigenvalues*$\lambda_i \neq 0\,(i = 1, \ldots, n-1)$. *Then*

$$\log(2\sqrt{m})) - \frac{2m}{\varepsilon(G)} \leq I_\lambda(G) \leq \log(2m)) - \frac{\alpha^2 s}{\varepsilon(G)},$$

where $\alpha = \min\{|\lambda_i| : i = 1, \ldots, s\}$ and where s is the number of distinct eigenvalues.

Proof. It is a well-known fact that $\varepsilon(G) \leq 2m$. By using Equation (6), we have

$$I_\lambda(G) \leq \log(2m) - \frac{1}{2m}(\sum_{i=1}^{s} |\lambda_i| \log(|\lambda_i|)).$$

Since logarithm is an increasing function, we have $\log|\lambda_i| \leq |\lambda_i|$. On the other hand, $\sum_{i=1}^{s} \lambda_i^2 = 2m$ yields

$$\log(2\sqrt{m})) - \frac{2m}{\varepsilon(G)} \leq I_\lambda(G) \leq \log(2m)) - \frac{\alpha^2 s}{\varepsilon(G)}$$

Now, $2\sqrt{m} \leq \varepsilon(G) \leq 2m$ implies that

$$\log(2\sqrt{m})) - \frac{2m}{\varepsilon(G)} \leq I_\lambda(G) \leq \log(2m)) - \frac{\sum_{i=1}^{s} (\log|\lambda_i|)^2}{\varepsilon(G)} \tag{7}$$

Let $\alpha = \min\{|\lambda_i| : i = 1, \ldots, s\}$. The nullity of G is 1. By reformulating Equation (7), one can see that

$$\log(2\sqrt{m})) - \frac{2m}{\varepsilon(G)} \leq I_\lambda(G) \leq \log(2m)) - \frac{\alpha^2 s}{\varepsilon(G)}.$$

□

Theorem 9. *Let G be a graph whose eigenvalues are in the interval* $[-1, 1]$. *Then*

$$I_\lambda(G) \geq \varepsilon(G)$$

Proof. Clearly, we obtain

$$\begin{aligned} I_\lambda(G) &= \log(\varepsilon(G)) - \tfrac{1}{\varepsilon(G)} \sum_{i=1, \lambda \neq 0}^{n} |\lambda_i| \log|\lambda_i| \\ &= \log(\varepsilon(G)) - \tfrac{1}{\varepsilon(G)} \sum_{i=1, \lambda \neq 0}^{n} \log|\lambda_i|^{|\lambda_i|} \\ &= \log(\varepsilon(G)) - \tfrac{1}{\varepsilon(G)} \log(\Pi|\lambda_i|^{|\lambda_i|}). \end{aligned}$$

On the other hand, $\Pi|\lambda_i|^{|\lambda_i|} \leq \Pi{\lambda_1}^{|\lambda_i|} = {\lambda_1}^{\varepsilon(G)}$. So

$$I_\lambda(G) \geq \log(\varepsilon(G)) - \log(\lambda_1) = \log(\frac{\varepsilon(G)}{\lambda_1}),$$

Since $\lambda_i \in [-1, 1]$, thus $I_\lambda(G) \geq \varepsilon(G)$. □

Theorem 10. *Let G be a graph and* $m_\Delta(G)$ *be the* Δ*-th spectral moment of G. Then*

$$I_\lambda(G) \geq \varepsilon(G) - \frac{m_\Delta(G)}{\varepsilon(G)}.$$

Proof. We have $\sum_{i=1}^{n} |\lambda_i| \log |\lambda_i| \leq \sum_{i=1}^{n} \log |\lambda_i|^{|\lambda_i|} \leq \sum_{i=1}^{n} \log |\lambda_i|^{\Delta} \leq \sum_{i=1}^{n} |\lambda_i|^{\Delta} = m_{\Delta}(G)$.

Thus

$$I_{\lambda}(G) \geq \varepsilon(G) - \frac{m_{\Delta}(G)}{\varepsilon(G)}. \square$$

4.4. The Hosoya Entropy of Fullerenes

Here, we introduce the Hosoya entropy based on the distance between vertices of a graph, see [123–125]. Given a graph G and two vertices u and v, the distance between them is defined as the length of the shortest path connecting them. Let $s_i(u)$ be the number of vertices at distance i from vertex u. Then the sequence $dds(v) = (s_0(v), s_1(v), \ldots, s_d(v))$ is called the distance degree sequence of v.

Two vertices u and v are H-equivalent if $dds(u) = dds(v)$ see [126] and the class of H-equivalent vertices constitutes the H-partitions of a graph.

Suppose G has h H-equivalent classes and the cardinality of ith H-equivalent class is n_i $(1 \leq i \leq h)$. Then, H-entropy of G [127] is

$$H(G) = -\sum_{i=1}^{h} h_i \log(h_i)$$

where $h_i = n_i/|V|$.

Let also $O_1, \ldots, O_l$ be all the orbits of Aut(G) in the set of vertices. If l_i is the cardinality of the i-th orbit for $1 \leq i \leq l$, then the orbit entropy of G [116–119] is given by

$$I_a(G) = -\sum_{i=1}^{l} \mu_i \log(\mu_i)$$

where $\mu_i = |n_i|/|V|$.

The value of $H(G)$ for a graph G with n vertices is between zero and $\log(n)$. The minimum is achieved when all the vertices are H-equivalent; the maximum is reached when a non-pair of vertices are H-equivalent. Complete graphs and cycles have a H-entropy of 0.

Remark 1. *In a vertex-transitive graph, all the vertices are H-equivalent and the H-entropy is zero. The converse of this fact is not true. In other words, there are many examples of non-vertex-transitive graphs with zero H-entropy.*

Theorem 11. *Two vertices in the same orbit are H-equivalent. In addition, the H-entropy of a vertex-transitive graph is zero* [128].

Although two similar vertices are H-equivalent, the converse is not true. For example, in Figure 9, u and v are H-equivalent, and thus $D(u) = D(v)$, while they are in different orbits. Moreover, two vertices u and v in Figure 10 are not H-equivalent but $D(u) = D(v)$.

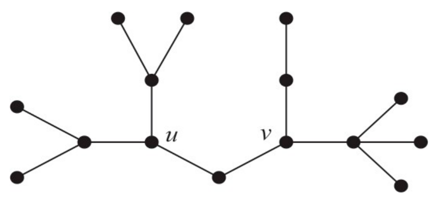


Figure 9. Two vertices with the same total distance which are not H-equivalent.

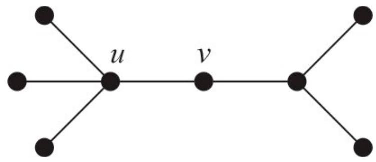


Figure 10. The vertices u and v are not H-equivalent but $D(u) = D(v)$.

Theorem 12 ([128])**.** *If G is a regular graph with diameter* $\rho = 2$*, then* $H(G) = 0$*.*

Theorem 13. *If G is a regular graph with non-zero H-entropy, then its diameter is greater than 2.*

Theorem 14 ([128])**.** *If G is a connected graph on n vertices, then* $H(G) = n$ *if and only if Aut(G) is trivial.*

Theorem 15 ([128])**.** *The H-entropy of a regular graph of degree greater than n/2 is zero.*

Theorem 16 ([128])**.** *The H-entropy of a regular graph of degree greater than or equal with n/2 is zero, if the number of vertices is an even number and G is edge-transitive.*

Theorem 17 ([128])**.** *If G is a graph on at least five vertices which is edge-transitive but not bipartite, and each vertex has odd degree. Then, H-entropy is zero.*

In continuing, we compute the H-entropy of graphs with at most two orbits.

Definition 1. *A graph G is called co-distance, if for each pair of vertices (u,v) their total distances are the same, namely* $D(u) = D(v)$*.*

Each vertex-transitive graph is co-distance, but there are examples of co-distance non-transitive graphs. The graph G in Figure 11 has two orbits $V_1 = \{1, 2, 5, 6, 8, 12\}$ and $V_2 = \{3, 10, 4, 7, 11, 9\}$. It is not difficult to see that $d(G) = 4$ and $D(1) = D(3)$ while the H-entropy is not zero.

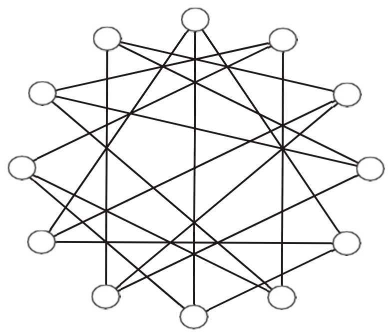


Figure 11. A cubic co-distance graph of diameter 4 with non-zero H-entropy.

Theorem 18 ([128])**.** *Up to isomorphism there are exactly 14 co-distance regular graphs of order at most 14 with two orbits and diameter greater than or equal with 3. Among them, only the graph G depicted in Figure 11 has non-zero H-entropy.*

Theorem 19 ([128])**.** *Suppose the H-entropy of graph G is zero. Then nor G is a tree or a regular graph.*

Theorem 20 ([128])**.** *Suppose G is a graph with two orbits* V_1 *and* V_2 *and non-zero H-entropy. Then* $H(G) = 1$ *if and only if n is even and* $|V_1| = |V_2| = n/2$.

Theorem 21 ([128])**.** *Let G be a regular graph with two orbits and diameter less than four. If G is co-distance, then its H-entropy is zero.*

In the final part of this section, we compute the H-entropy of some infinite classes of fullerene graphs.

Theorem 22. *The fullerene graph A_{12n+4} where $n \geq 4$ satisfies*

$$H(\mathrm{A}_{12n+4}) = \log(12n+4) - \frac{1}{12n+4}((12n+3)\log 3 + 6(2n-4)).$$

Proof. In Figure 12, the vertices of ith (i = 1, 2, 3, 4, 5) layer are in the same orbit. The vertices of the layers 6, 7, . . . , n constitute three orbits labeled by the numbers 1, 2, and 3. Vertices with labels 2, 3 are in the same H-equivalent partition and the other vertices compose the H-equivalent partition. Finally, the vertices of the outer pentagon are H-equivalent. In other words, there are an equivalence class of size 1, nine equivalence classes of size 3, and 2n − 4 equivalence classes of size 6 which yield

$$\begin{aligned} H(A_{12n+4}) &= \tfrac{1}{12n+4}\log(12n+4) + \tfrac{27}{12n+4}\log\left(\tfrac{12n+4}{3}\right) \\ &+ \tfrac{6(2n-4)}{12n+4}\log\left(\tfrac{12n+4}{6}\right) \\ &= \log(12n+4) - \left(\tfrac{27}{12n+4}\log 3 + \tfrac{6(2n-4)}{12n+4}(1+\log 3)\right) \\ &= \log(12n+4) - \tfrac{1}{12n+4}((12n-24) + (12n+3)\log 3). \end{aligned}$$

□

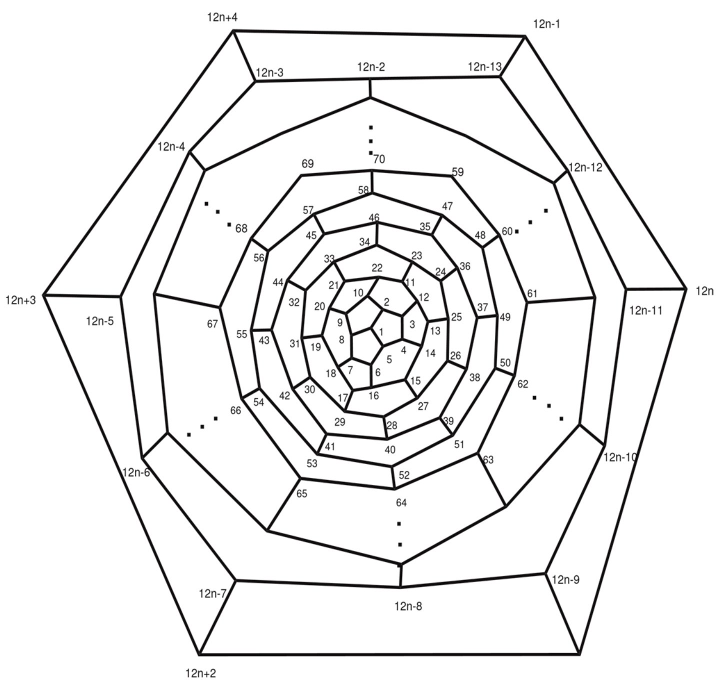


Figure 12. The fullerene A_{12n+4}.

Similarly to the structure of A_{10n} in last section, the fullerene graph A_{12n+4} is composed of a nanotube $Tz[6, n-10]$ together with two caps B_1 and B_2, see Figures 13–16. Thus, the vertices of A_{12n+4} are labeled as given in Figure 17. The H-partitions and the eccentricity of vertices of caps B_1 and B_2 are given in Table 5.

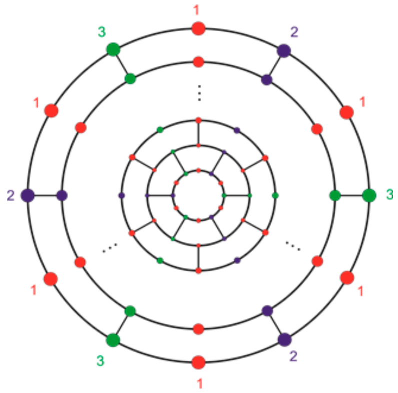


Figure 13. The orbits of the ith layer ($2 \leq i \leq n$)of the fullerene graph A_{12n+4}.

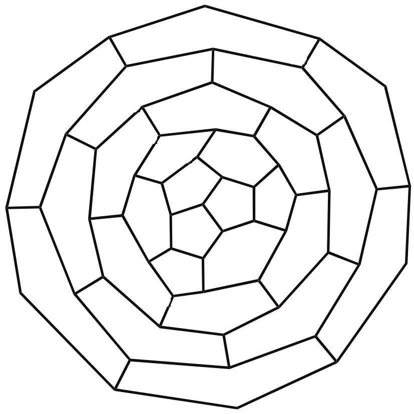


Figure 14. The subgraph B_1.

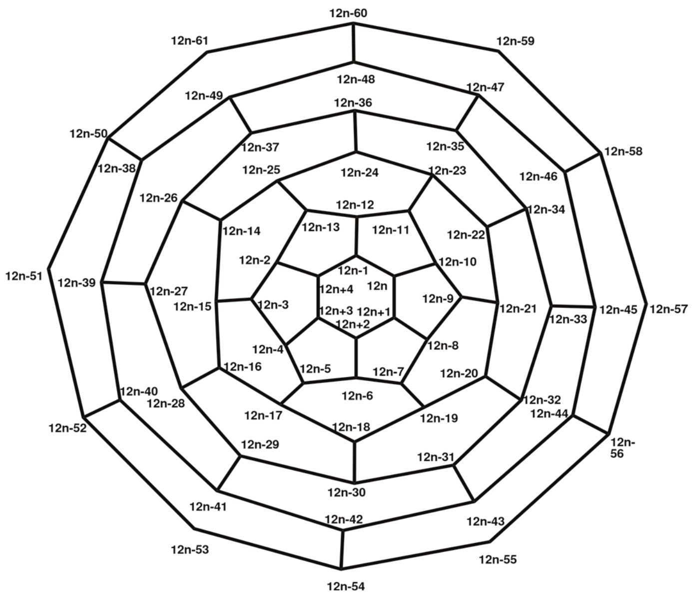


Figure 15. The subgraph B_2.

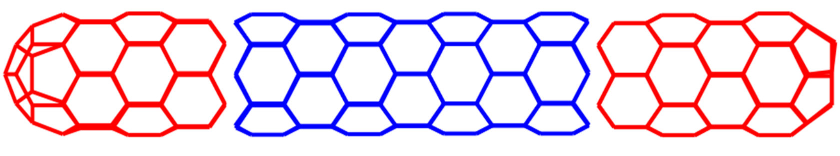


Figure 16. The 3-dimensional structure of fullerene graph A_{12n+4}.

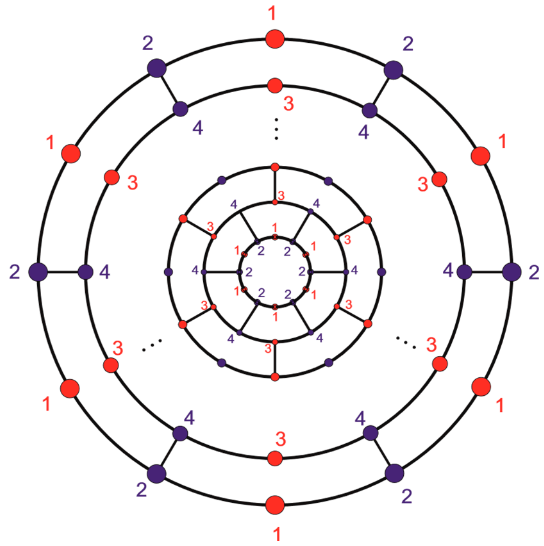


Figure 17. The Hosoya-partitions of $Tz[6,n-10]$.

Table 5. The H-partition and eccentricity of fullerene graph.

Partitions	Elements	ecc
V_1	1	$2n+1$
V_{2n+6}	$12n-1, 12n, 12n+1, 12n+2, 12n+3, 12n+4$	
V_2	2, 5, 8	$2n$
V_{2n+5}	$12n-13, 12n-11, 12n-9, 12n-7, 12n-5, 12n-3$	
V_3	3, 4, 6, 7, 9, 10	$2n-1$
V_{2n+4}	$12n-12, 12n-10, 12n-8, 12n-6, 12n-4, 12n-2$	
V_4	12, 14, 16, 18, 20, 22	$2n-2$
V_{2n+3}	$12n-25, 12n-23, 12n-21, 12n-19, 12n-17, 12n-15$	
V_5	11, 15, 19	$2n-3$
V_6	13, 17, 21	
V_{2n+2}	$12n-24, 12n-22, 12n-20, 12n-18, 12n-16, 12n-14$	
V_7	23, 27, 31	$2n-4$
V_8	25, 29, 33	
V_{2n+1}	$12n-36, 12n-34, 12n-32, 12n-30, 12n-28, 12n-26$	
V_9	24, 26, 28, 30, 32, 34	$2n-5$
V_{2n}	$12n-37, 12n-35, 12n-33, 12n-31, 12n-29, 12n-27$	
V_{10}	36, 38, 40, 42, 44, 46	$2n-6$
V_{2n-1}	$12n-49, 12n-47, 12n-45, 12n-43, 12n-41, 12n-39$	
V_{11}	35, 39, 43	$2n-7$
V_{12}	37, 41, 45	
V_{2n-2}	$12n-48, 12n-46, 12n-44, 12n-42, 12n-40, 12n-38$	
V_{13}	47, 51, 55	$2n-8$
V_{14}	49, 53, 57	
V_{2n-3}	$12n-60, 12n-58, 12n-56, 12n-54, 12n-52, 12n-50$	
V_{15}	48, 50, 52, 54, 56, 58	$2n-9$
V_{2n-4}	$12n-61, 12n-59, 12n-57, 12n-55, 12n-55, 12n-53, 12n-51$	

4.5. Radial Entropy and Orbit Measures

In a network, knowing, for example, the degree of vertices gives us essential information about the number of interconnections of each component. These data provide a narrow understanding of complex networks, because the vertex partition [12] based on degree is coarser than automorphism partition. Hence, it is important to know if we substitute the degree partitions instead of orbit partitions;

then, the study of complex network in the view of symmetry leads us to understand more about the structure of the regarding graph. The orbit entropy is defined as

$$I_a(G) = -\sum_{i=1}^{k} \frac{|O_i|}{|V|} \log(\frac{|O_i|}{|V|})$$

where O_i's ($1 \leq i \leq k$) are orbits of G. Regarding the orbit polynomial, the symmetry index $S(G)$ is defined [127] as follows:

$$S(G) = \log(n) - I_a(G) + \log(|\mathrm{Aut}(G)|).$$

Suppose N_{i_j}, $1 \leq j \leq k$ is the collection of all vertices with eccentricity i_j. Then, the radial entropy is defined by

$$H_{ecc}(G) = -\sum_{i=1}^{k} \frac{|N_i|}{|V|} \log\Big(\frac{|N_i|}{|V|}\Big). \tag{8}$$

Let $p_1,\ldots, p_{n-10}$ be the H-equivalent classes of $Tz[6,n-10]$ which contains the vertices with label i. Then $ecc(p_i) = 2n - i - 9$. Thus, the eccentricity sequence of fullerene graph A_{12n+4} is

$$\Big\{(2n-i)^{12}(1 \leq i \leq n-1), (2n)^9, (2n+1)^7\Big\}. \tag{9}$$

Theorem 23 ([129])**.** *Consider the fullerene graph A_{12n+4}, where $n \geq 4$. If n is even, then*

$$I_a(A_{12n+4}) = \log\,(12n+4) - \frac{1}{12n+4}((12n+3)\log 3 + 6n).$$

If n is odd, then

$$I_a(A_{12n+4}) = \log(12n+4) - \frac{1}{12n+4}((12n+3)\log 3 + 6n + 6).$$

Theorem 24 ([129])**.** *The radial entropy of fullerene A_{12n+4} ($n \geq 4$) is*

$$\begin{aligned} H_{ecc}(A_{12n+4}) \quad &= \log(12n+4) \\ &-\tfrac{1}{12n+4}(24(n-1) + (12n+6)\log 3 + 7\log 7). \end{aligned}$$

Theorem 25 ([129])**.** *If the ci's are equal, the entropy of fullerene A_{12n+4} ($n \geq 11$) is given by*

$$\begin{aligned} If_\sigma(A_{12n+4}) \quad &= \log(18n^2 + 14n + 7) - \tfrac{1}{18n^2+14n+7}((14n+7)\log(2n+1)) \\ &+18n\log\,(2n) + 12A, \end{aligned}$$

where $A = \sum\limits_{i=1}^{n-1} (2n-i)\log(2n-i)$.

Theorem 26 ([129])**.** *The degree-based entropy of fullerene graph A_{12n+4} is*

$$D(A_{12n+4}) = \log(36n+12) - \frac{(36n+12)\log 3}{36n+12} = \log(12n+4).$$

5. Correlation Analysis

The Pearson correlations between all entropies introduced in this paper are given in Equation (1), for fullerene graph A_{12n+4}.

$$\begin{array}{c} \\ If_\sigma \\ H \\ D \\ I_a \\ H_{ecc} \end{array} \begin{array}{c} \begin{array}{ccccc} If_\sigma & H & D & I_a & H_{ecc} \end{array} \\ \left(\begin{array}{cccc} 0.999871662 & 1 & 0.99999826 & 0.999988517 \\ & 0.999872017 & 0.999899809 & 0.999936954 \\ & & 0.999998301 & 0.999988624 \\ & & & 0.999995717 \\ & & & \end{array} \right) \end{array} \quad (10)$$

Moreover, the exact values of energy and five entropies for fullerene graph A_{12n+4} ($11 \le n \le 20$) is reported in Table 6. These results show that the correlation between energy and each entropy measure of A_{12n+4} is greater than 0.99 (see Table 7). It can be found that they release the same structural information about regarding fullerene. In [129], the authors found a similar result for a different class of fullerenes.

Table 6. The graph energy and five types of entropies applied to A_{12n+4}.

n	E	D	If_σ	I_a	H	H_{ecc}
11	212.87	7.08	7.06	5.02	4.72	3.57
12	231.73	7.2	7.18	5.14	4.82	3.68
13	250.59	7.32	7.29	5.25	4.92	3.79
14	269.46	7.42	7.39	5.36	5.01	3.89
15	288.32	7.52	7.49	5.45	5.09	3.98
16	307.19	7.61	7.58	5.54	5.18	4.07
17	326.05	7.7	7.67	5.63	5.25	4.15
18	344.91	7.78	7.75	5.71	5.33	4.23
19	363.78	7.85	7.85	5.78	5.4	4.31
20	382.64	7.93	7.9	5.86	5.46	4.38

Table 7. The correlation between graph energy and entropies applied to A_{12n+4}.

	E,D	E, If_σ	E,I_a	E,H	E,H_{ecc}
Cor	0.9964006	0.9972326	0.99673	0.9975728	0.9974525

Author Contributions: Conceptualization, formal analysis, project administration M.G. and M.D.; methodology, software, F.E.-S. All authors have read and agreed to the published version of the manuscript.

Funding: Modjtaba Ghorbani is partially supported by the Shahid Rajaee Teacher Training University. Also, Matthias Dehmer thanks the Austrian Science Funds for supporting this work (project P30031).

Acknowledgments: This research is partially supported by Shahid Rajaee Teacher Training University. Matthias Dehmer thanks the Austrian Science Fund for supporting this work (P 30031).

Conflicts of Interest: The authors declare no conflict of interest.

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