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On Certain Aspects of Graph Entropies of Fullerenes

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Abstract

The eccentricity of vertex v is $\varepsilon(v) = \max_{u\in V} d(u,v)$, where $d(u,v)$ is the distance between vertices u and v. In this paper, we study the entropy measures of some classes of fullerene graphs based on eccentricity of vertices.

1 Introduction

Entropies to characterize and quantify the structure networks have been investigated extensively [9-13]. In [10], several types of graph entropies have been discussed and mathematically explored. Therefore, we omit an extensive review on graph entropies here. The main contribution of the paper is to study the entropy of so-called fullerene graphs, e.g., [16,17] by using special eccentricity-based information functionals; a graph class with a long standing history in chemistry and related disciplines.

As graph entropies, we use a special definition thereof due to Dehmer [6-13], see Section 2 for technical details. All graphs considered in this paper are simple, connected and finite. Let x and y be two arbitrary vertices of graph G, the distance between them is the length of the

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shortest path connecting them denoted by $d(x,y)$. The eccentricity of vertex v is defined as $\varepsilon(v) = \max_{u\in V} d(u,v)$, where $d(u,v)$ is the distance between vertices u and v. The minimum and the maximum eccentricity among all vertices of G is called the radius and the diameter of G, respectively denoted by $r(G)$ and $d(G)$. A connected graph G with $d(G) = r(G)$ is called self-centered graph. The eccentric complexity of a graph G, denoted by $C_{ec}(G)$, is defined as the number of different eccentricities of its vertices. It is not difficult to see that a graph G is self-centered if and only if $C_{ec}(G) = 1$. The total eccentricity of a graph G, denoted by $\zeta(G)$, is defined as the sum of eccentricities of its vertices. In other words, $\zeta(G) = \sum_{v\in V} \varepsilon(v)$. The eccentric connectivity index is also defined as $\xi(G) = \sum_{v\in V} d(v)\varepsilon(v)$, where $d(v)$ denotes the degree of vertex v. In the next section, we state necessary definitions and some preliminary results and in Section 3, we determine the entropy of fullerene graphs.

2 Preliminaries

Let Γ be a group acting on the set Ω, namely there is a function φ: $\Gamma \times \Omega \to \Omega$ where $(g,x) \mapsto \varphi(g,x)$ that satisfies in the following two properties (we denote $\varphi(g,x)$ as x^g): $\alpha^e = \alpha$ for all α in Ω and $(\alpha^g)^h = \alpha^{gh}$ for all g, h in Γ. The orbit of an element $\alpha \in \Omega$ is denoted by α^G and it is defined by the set of all α^g, $g \in G$.

A permutation f on the vertices of graph X is called an automorphism of X where $e=uv$ is an edge if and only if $f(e) = f(u)f(v)$ is an edge of E. Denoted by $\mathrm{Aut}(X)$ is the set of all automorphisms of X forming a group under the composition of permutations. This group acts transitively on the set of vertices, if for a pair of vertices such as u and v in $V(X)$, there is an automorphism $g \in \mathrm{Aut}(X)$ such that $g(u) = v$. In this case, we say that X is vertex-transitive. An edge-transitive graph can be defined similarly.

The symbol "log" denotes the logarithm based on the basis 2 in the whole of this paper. The entropy measures based on Shannon's entropy [23] can be defined as follows. Consider a probability vector $p = (p_1, p_2, ..., p_n)$ which satisfies in two conditions $0 \le p_i \le 1$ and $\sum_{i=1}^{n} p_i = 1$. The Shannon's entropy of p is defined as $I(p) = -\sum_{i=1}^{n} p_i \log p_i$.

Dehmer [6-13] introduced the entropy of a graph by using special information functional. In fact, he assigned a probability value to each individual vertex of a graph. This definition of entropy differs from the one based on vertex-orbits, see [10]. Let $G = (V,E)$ be a undirected connected graph. Let $F = \sum_{j=1}^{|V|} f(v_j)$, for a vertex $v_i \in V$, we define

$$p(v_i) := \frac{1}{F} f(v_i),$$

where *f* represents an arbitrary information functional. Observe that $\sum_{j=1}^{|V|} p(v_j) = 1$. Hence, we can interpret the quantities $p(v_i)$ as vertex probabilities. Let *f* be arbitrary information functional. The entropy of *G* is defined by [6-13]:

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

We here use an information functional based on eccentricity. Let $G=(V,E)$, for a vertex $v_i \in V$, we define *f* as $f(v_i) = c_i\varepsilon(v_i)$, where $c_i > 0$ for $1 \le i \le n$. The entropy based on *f* denoted by $If_\varepsilon(G)$ is defined as follows:

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

In addition, if c_i's are equal, then

$$If_\varepsilon(G) = \log\left(\sum_{i=1}^{n} \varepsilon(v_i)\right) - \sum_{i=1}^{n}\frac{\varepsilon(v_i)}{\sum_{j=1}^{n} \varepsilon(v_j)}\log(\varepsilon(v_i)). \quad (2)$$

3 Main results

In [2] it has been proven that if *G* is a vertex-transitive graph, then the eccentricities of any pair of distinct vertices are equal. Hence, it is important to determine the entropy of non-vertex transitive graphs.

Theorem 1 [7]. Let *G* be a vertex-transitive graph on *n* vertices, for all sequences $c_1 \ge c_2 \ge ... \ge c_n$ we have

$$If_\varepsilon(G) = \log(\sum_{i=1}^{n} c_i) - \sum_{i=1}^{n}\frac{c_i}{\sum_{j=1}^{n} c_j}\log(c_i). \quad (3)$$

As a special case, if $c_i = c_j$ for all $i \ne j$ then $If_\varepsilon(G) = \log(n)$.

Similar to the proof of Theorem 1, one can see that if *G* is a self-centered graph, then $If_\varepsilon(G)$ satisfies in Eq. (3). For a given graph *G*, its line graph, denoted by *L*(*G*), is a graph whose vertex set is the edge set of *G* and two vertices are adjacent if and only if their corresponding edges share a common end-vertex in *G*.

Theorem 2. Let *G* be a connected edge-transitive graph on *n* vertices and *m* edges. Then for all sequences $c_1 \ge c_2 \ge ... \ge c_n$, we have

$$If_{\varepsilon}(L(G))=\log(\sum_{i=1}^{m}c_i)-\sum_{i=1}^{m}\frac{c_i}{\sum_{j=1}^{m}c_j}\log(c_i).$$

As a special case, if $c_i = c_j$ for all $i \neq j$ then $If_{\varepsilon}(L(G))=\log(m)$.

Proof. An undirected graph is edge-transitive if and only if its line graph is vertex-transitive. Applying Theorem 1 concludes the proof.

Theorem 3. Suppose G is a graph and $V_1, V_2, ..., V_k$ are all orbits of $\mathrm{Aut}(G)$ under its natural action on $\mathrm{V}(G)$. Then

$$If_{\varepsilon}(G)=\log\left(\sum_{i=1}^{k}\varepsilon(x_i)\sum_{j=1}^{|V_i|}c_j\right)-\sum_{i=1}^{k}\varepsilon(x_i)\sum_{j=1}^{|V_i|}\frac{c_j}{\sum_{t=1}^{k}\varepsilon(x_t)\sum_{l=1}^{|V_i|}c_l}\log\left(c_j\varepsilon(x_j)\right). \tag{4}$$

In addition, if $c_1 = c_2 = \ldots = c_n$, then

$$\log\left(\zeta(G)\right)-\frac{1}{\zeta(G)}\sum_{i=1}^{k}|V_i|\varepsilon(x_i)\log(\varepsilon(x_i)). \tag{5}$$

Proof. For all $x_i, x_j \in V_i$, we have $\varepsilon(x_i)=\varepsilon(x_j)$. By using Theorem 1, This completes the proof of the first claim. In order to continue by utilizing Eq. (4), we infer

$$\begin{aligned} If_{\varepsilon}(G)&=\log\left(\sum_{i=1}^{k}\varepsilon(x_i)\sum_{j=1}^{|V_i|}c_j\right)-\sum_{i=1}^{k}\varepsilon(x_i)\sum_{j=1}^{|V_i|}\frac{c_j}{\sum_{t=1}^{k}\varepsilon(x_t)\sum_{l=1}^{|V_i|}c_l}\log\left(c_j\varepsilon(x_i)\right)\\ &=\log\left(\zeta(G)\right)-\frac{1}{\zeta(G)}\sum_{i=1}^{k}|V_i|\varepsilon(x_i)\log(\varepsilon(x_i)). \end{aligned}$$

Corollary 4. Suppose $\varepsilon(G)=\{\varepsilon(x_1),\ldots,\varepsilon(x_{C_{ec}(G)})\}$ is the set of all distinct eccentricities of graph G, where the multiplicity of $\varepsilon(x_i)$ is n_i, $1 \le i \le C_{ec}(G)$ and $c_1 = c_2 = \ldots = c_n$. Then

$$If_{\varepsilon}(G)\le\log\left(nC_{ec}(G)d(G)\right)-\frac{1}{\zeta(G)}\sum_{i=1}^{k}|V_i|\varepsilon(x_i)\log(\varepsilon(x_i)).$$

Proof. Let $\varepsilon(G)=\{\varepsilon(x_1),\ldots,\varepsilon(x_{C_{ec}(G)})\}$ be the set of all distinct eccentricities of graph G, then

$$\zeta(G)=\sum_{i=1}^{C_{ec}(G)}|V_i|\,\varepsilon(x_i)\le\sum_{i=1}^{C_{ec}(G)}|V_i|\sum_{i=1}^{C_{ec}(G)}\varepsilon(x_i)\le nC_{ec}(G)d(G). \tag{6}$$

By substituting, Eq. (6) in Eq. (5), we obtain the proof.

Theorem 5. Let G be a connected non-partite edge-transitive graph, then

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

Proof. First, we claim that the eccentric complexity of a connected edge-transitive graph is at most 2. To do this, suppose that uv is and edge of $E(G)$. Since G is edge-transitive, for every edge xy in $E(G)$, there is an automorphism $\pi \in Aut(G)$ such that $\pi(u) = x$ and $\pi(v) = y$. We can conclude that

$$\varepsilon(x) = \max_{w \in V} d(x,w) = \max_{w \in V} d(\pi(x), \pi(w)) = \max_{z \in V} d(u,z) = \varepsilon(u).$$

This means that for every vertex w of G, $\varepsilon(w) \in \{\varepsilon(u), \varepsilon(v)\}$ and thus

$$If_{\varepsilon}(G) = \log\left(\varepsilon(u)\sum_{i=1}^{|X|} c_i + \varepsilon(v)\sum_{i=|X|+1}^{n} c_i\right) - \sum_{i=1}^{|X|} \frac{c_i\varepsilon(u)}{\varepsilon(u)\sum_{i=1}^{|X|} c_i + \varepsilon(v)\sum_{i=|X|+1}^{n} c_i} \log\left(c_i\varepsilon(u)\right)$$

$$- \sum_{i=|X|+1}^{|n} \frac{c_i\varepsilon(v)}{\varepsilon(u)\sum_{i=1}^{|X|} c_i + \varepsilon(v)\sum_{i=|X|+1}^{n} c_i} \log\left(c_i\varepsilon(v)\right),$$

where $X = \{x \in V : \varepsilon(x) = \varepsilon(u)\}$ and $Y = \{y \in V : \varepsilon(y) = \varepsilon(v)\}$. It is not difficult to see that $V(G) = X \cup Y$ and $X \cap Y = \Phi$. Since, G is not bipartite for every pair of vertices $a, b \in X$ or Y, $\varepsilon(a) = \varepsilon(b)$ and the eccentric complexity of G is one. This completes the proof.

Theorem 6. Let G be a graph and

$$l = \log\left(\sum_{i=1}^{n} c_i\right) - \frac{1}{\sum_{t=1}^{n} c_j} \sum_{i=1}^{n} c_i \log(c_i).$$

Then $|If_{\varepsilon}(G) - l| \leq 1$. In addition, if $c_1 = c_2 = \ldots = c_n$, then $|If_{\varepsilon}(G) - \log(n)| \leq 1$.

Proof. For every connected graph G, it is not difficult to see that $r(G) \leq d(G) \leq 2r(G)$. This yields that for every vertex v, we have $r(G) \leq \varepsilon(v) \leq d(G)$ and thus

$$If_{\varepsilon}(G) \leq \log\left(\sum_{i=1}^{n} c_i d(G)\right) - \sum_{i=1}^{n} \frac{c_i r(G)}{\sum_{j=1}^{n} c_j r(G)} \log\left(c_i r(G)\right)$$

$$= \log(d(G)) + \log\left(\sum_{i=1}^{n} c_i\right) - \frac{1}{\sum_{j=1}^{n} c_j} \sum_{i=1}^{n} c_i \left[\log\left(r(G)\right) + \log(c_i)\right]$$

$$= \log(d(G)) + \log\left(\sum_{i=1}^{n} c_i\right) - \frac{1}{\sum_{j=1}^{n} c_j} \sum_{i=1}^{n} c_i \log(c_i) - \log\left(r(G)\right)$$

$$= \log\left(\frac{d(G)}{r(G)}\right) + l.$$

On the other hand, by a similar argument we can deduce that

$$If_\varepsilon(G) \geq -\log\left(\frac{d(G)}{r(G)}\right) + l.$$

Hence,

$$| If_\varepsilon(G) - l | \leq \log\left(\frac{d(G)}{r(G)}\right).$$

Since, $d(G) \leq 2r(G)$ we have $| If_\varepsilon(G) - l | \leq \log(2) = 1.$ If $c_1 = c_2 = \ldots = c_n$, then $l = \log(n)$ and the proof is complete.

Lemma 7 [20]. Let G be a nontrivial connected graph of order n. For each vertex v in G, it holds

$$\varepsilon(v) \leq n - d(v).$$

Theorem 8. Let G be a nontrivial connected graph of order n and $c_i = d(v_i)$. Then

$$If_\varepsilon(G) \geq \log(\xi(G)) - \log\left(\prod_{i=1}^{n} d(v_i)(n - d(v_i))\right).$$

Proof. By substituting $c_i = d(v_i)$ in Eq. (1) we have

$$\begin{aligned} If_\varepsilon(G) &= \log\left(\sum_{i=1}^{n} d(v_i)\varepsilon(v_i)\right) - \sum_{i=1}^{n} \frac{d(v_i)\varepsilon(v_i)}{\sum_{j=1}^{n} d(v_j)\varepsilon(v_j)} \log(d(v_i)\varepsilon(v_i)) \\ &= \log(\xi(G)) - \frac{1}{\xi(G)} \sum_{i=1}^{n} d(v_i)\varepsilon(v_i) \log(d(v_i)\varepsilon(v_i)) \\ &\geq \log(\xi(G)) - \frac{1}{\xi(G)} \sum_{i=1}^{n} d(v_i)\varepsilon(v_i) \sum_{i=1}^{n} \log(d(v_i)\varepsilon(v_i)) \\ &= \log(\xi(G)) - \sum_{i=1}^{n} \log(d(v_i)\varepsilon(v_i)). \end{aligned}$$

By using Lemma 7, the proof is complete.

In general, if $\beta(G) = \sum_{i=1}^{n} c_i \varepsilon(v_i)$, by using Lemma 7 and Eq. (2), we have

$$If_\varepsilon(G) \geq \log(\beta(G)) - \log(\prod_{i=1}^{n} c_i\,(n - d(v_i))).$$

4 Entropy of fullerene graphs

A fullerene graph is a planar, 3-regular and 3-connected graph whose faces are pentagons and hexagons. In other words, a fullerene on n vertices has exactly 12 pentagons and $n/2-10$ hexagons, see [16,22]. For more details about the eccentricity of fullerene graphs, see [1-3, 14,15,17-19,21,24]. Here, we introduce three infinite classes of fullerenes with $12n+4$, $18n+10$ and $10n$ vertices, respectively. We denote them by C_{12n+4}, C_{18n+10} and C_{10n}. In the course of this paper, we compute the entropy of these classes of fullerenes. We refer to [4,5] for more details on entropy of graphs.

Theorem 9. If c_i's are equal in Eq. (1), then the entropy of fullerene C_{12n+4}, $n \geq 8$ (Figure 1) is

$$If_{\varepsilon}(C_{12n+4}) = 1 + \log\left(9n^2 + 19n + 8\right) - \frac{2}{9n^2 + 19n + 8}\left((2n+1)\log(2n+1) + 3\sum_{i=1}^{n+1}(n+i)\log(n+i)\right)$$

Proof. From Figure 1, one can see that there are three types of vertices of fullerene graph C_{12n+4}. By using the eccentricity of these vertices as given in Table 1 and using Eq. (2), we have

$$\begin{aligned} If_{\varepsilon}(C_{12n+4}) &= \log\left(4(2n+1) + 12\sum_{i=1}^{n+1}(n+i)\right) \\ &\quad - \frac{1}{4(2n+1) + 12\sum_{i=1}^{n+1}(n+i)}\left(4(2n+1)\log(2n+1) + 12\sum_{i=1}^{n+1}(n+i)\log(n+i)\right) \\ &= 1 + \log\left(9n^2 + 19n + 8\right) \\ &\quad - \frac{2}{9n^2 + 19n + 8}\left((2n+1)\log(2n+1) + 3\sum_{i=1}^{n+1}(n+i)\log(n+i)\right). \end{aligned}$$

Table 1. The eccentricity of vertices of C_{12n+4}, $n \geq 8$.

Vertices	$\varepsilon(x)$	**No.**
The Type 1 Vertices	$2n+1$	4
Other Vertices	$n+i$ $(1 \leq i \leq n+1)$	12

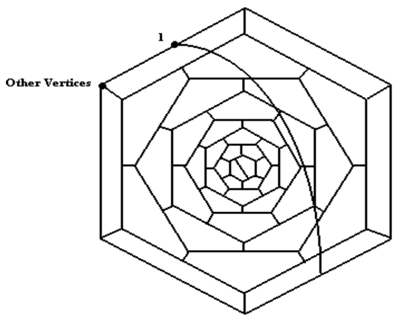

Figure 1. The Molecular Graph of the Fullerene C_{12n+4}.

The exceptional cases are given in Table 2.

Table 2. Some Exceptional Cases of C_{12n+4} Fullerenes.

Fullerene(F)	$If_{\varepsilon}(F)$
C_{28}	4.801607
C_{40}	5.320686
C_{52}	5.696082
C_{64}	5.992826
C_{76}	6.373541
C_{88}	6.438383

Theorem 10. If c_i's are equal in Eq. (1), then the entropy of fullerene C_{18n+10}, $n \geq 14$ (Figure 2) is

$$If_{\varepsilon}(C_{12n+4}) = \log(n) + \log(9n+101) - \frac{1}{9n^2+101n}(7(2n+3)\log(2n+3) + 9(2n+2)\log(2n+2) + 15(2n+1)\log(2n+1) + 30n\log(2n) + 18\sum_{i=2}^{n-1}(n+i)\log(n+i)).$$

Proof. From Figure 2, one can see that there exist three types of vertices of fullerene graph C_{18n+10}. By using the eccentricity of these vertices as given in Table 3 and using Eq. (2), we obtain

$$\begin{aligned} If_{\varepsilon}(C_{12n+4}) &= \log\left(7(2n+3) + 9(2n+2) + 15(2n+1) + 15(2n) + 18\sum_{i=2}^{n-1}(n+i)\right) \\ &- \frac{1}{4(2n+1) + 18\sum_{i=2}^{n-1}(n+i)}(7(2n+3)\log(2n+3) + 9(2n+2)\log(2n+2) \\ &+ 15(2n+1)\log(2n+1) + 30n\log(2n) + 18\sum_{i=2}^{n-1}(n+i)\log(n+i)) \\ &= \log(n) + \log(9n+101) - \frac{1}{9n^2+101n}(7(2n+3)\log(2n+3) + 9(2n+2)\log(2n+2) \\ &+ 15(2n+1)\log(2n+1) + 30n\log(2n) + 18\sum_{i=2}^{n-1}(n+i)\log(n+i)). \end{aligned}$$

The exceptional cases are given in Table 4.

Table 3. The eccentricity of vertices of C_{18n+10}, $n \geq 14$.

Vertices	$\varepsilon(x)$	No.
The Type 1 Vertices	$2n+3$	7
The Type 2 Vertices	$2n+2$	9
The Type 3 Vertices	$2n,2n+1$	15
Other Vertices	$n+i$ $(2\leq i \leq n\text{-}1)$	18

Table 4. Some Exceptional Cases of C_{18n+10} Fullerenes.

Fullerene(F)	$If_{\varepsilon}(F)$	Fullerene(F)	$If_{\varepsilon}(F)$
C_{82}	6.356532937	C_{172}	7.381144182
C_{100}	6.639656114	C_{190}	7.548407362
C_{118}	6.875628442	C_{208}	7.676794255
C_{136}	7.075830676	C_{226}	7.960277124
C_{154}	7.251688191	C_{244}	7.905535260

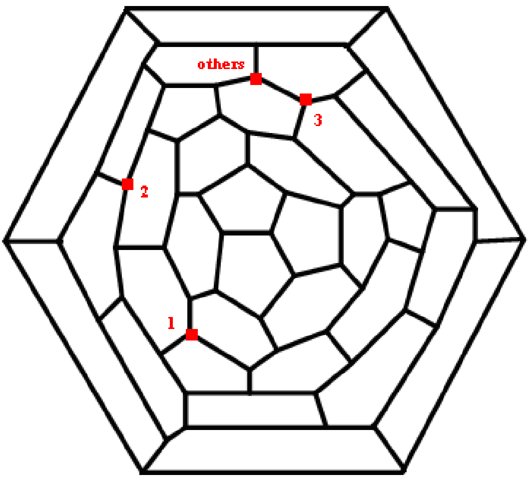

Figure 2. The Molecular Graph of the Fullerene C_{18n+10}.

Theorem 11. If c_i's are equal in Eq. (1), then the entropy of fullerene C_{10n}, $n \geq 8$ (Figure 3) is

$$If_{\varepsilon}(C_{10n}) = \log 5 + \log(n) + \log(3n-1) - \frac{2}{3n^2 - n}\left((2n-1)\log(2n-1) + \sum_{i=2}^{n-1}(2n-i)\log(2n-i)\right).$$

Proof. From Figure 3, one can see that there exist three types of vertices of fullerene graph C_{10n}. By using the eccentricity of these vertices as given in Table 5 and using Eq. (2), we have

$$\begin{aligned}If_{\varepsilon}(C_{10n}) &= \log\left(10(2n-1) + 10\sum_{i=2}^{n-1}(2n-i)\right)\\ &- \frac{1}{10(2n-1)+10\sum_{i=2}^{n-1}(2n-i)}\left(10(2n-1)\log(2n-1) + 10\sum_{i=2}^{n-1}(2n-i)\log(2n-i)\right)\\ &= \log 5 + \log(n) + \log(3n-1)\\ &- \frac{2}{3n^2 - n}\left((2n-1)\log(2n-1) + \sum_{i=2}^{n-1}(2n-i)\log(2n-i)\right).\end{aligned}$$

Table 5. The eccentricity of vertices of C_{10n}, $n \geq 8$.

Vertices	**$\varepsilon(x)$**	**No.**
The Type 1 Vertices	$2n$-1	10
Other Vertices	$2n-i$ ($2 \leq i \leq n$)	10

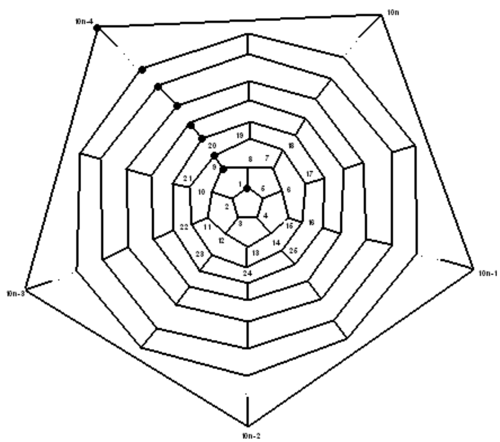

Figure 3. The Molecular Graph of the Fullerene C_{10n}.

The exceptional cases are listed in Table 6.

Table 6. Some Exceptional Cases of C_{10n} Fullerenes.

Fullerene(F)	$If_{\varepsilon}(F)$
C_{20}	6.643856190
C_{30}	7.491853096
C_{40}	5.314542162
C_{50}	5.637271494
C_{60}	5.994935534
C_{70}	6.106497467

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