Applied Mathematics and Computation 352 (2019) 88–98

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Hosoya entropy of fullerene graphs

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A R T I C L E I N F O

MSC:
05C70
05C07
05C35
92E10

Keywords:
Graph entropy
Graph automorphism
Fullerene graphs

A B S T R A C T

Entropy-based methods are useful tools for investigating various problems in mathematical chemistry, computational physics and pattern recognition. In this paper we introduce a general framework for applying Shannon entropy to fullerene graphs, and used it to investigate their properties. We show that important physical properties of these molecules can be determined by applying Hosoya entropy to their corresponding graphs.

1. Introduction

Graph entropy measures are applications of information theory designed to characterize networks quantitatively. Such measures were first introduced in the 1950s in the context of biological and chemical systems. Seminal work in this area was done by Rashevsky [25] and Mowshowitz [19–23], who investigated entropy measures for quantifying the so-called structural information content of a graph. To date, numerous graph entropies have been developed and applied to various problems in theoretical and applied disciplines. Examples are biology, computational biology, mathematical chemistry, web mining, and knowledge engineering [4–12] and [19–23].

In this paper, we develop a framework for applying a measure called Hosoya entropy to some fullerene graphs. Section 2 explains the concepts and terminology needed to establish the main results, which are then proven in Section 3.

2. Concepts and terminology

2.1. Graph terminology

All graphs considered in this paper are simple, connected and finite. The terminology used here largely follows that of Harary [16]. The vertex and edge sets of graph G are denoted by $V = V(G)$ and $E = E(G)$, respectively. The graph H is a

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https://doi.org/10.1016/j.amc.2019.01.024
0096-3003/

subgraph of G, if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. Let $G = (V, E)$ be a graph, and let $S \subseteq V$ be any subset of vertices of G. Then the induced subgraph $G[S]$ of G is a subgraph with vertex set S and two vertices in S are adjacent if and only if they are adjacent in G.

The *distance* $d(x, y)$ between two vertices x and y of graph G is the length of shortest path connecting them. The *diameter* of a graph G is the maximum distance between any pair of vertices in G.

A permutation π on the set of vertices of graph G which preserves the adjacency of vertices of G is called an *automorphism*. The set of all automorphisms of G denoted by $Aut(G)$ forms a group under composition of mappings. A graph G is *vertex transitive* if for every $u, v \in V(G)$, there is an automorphism $\beta \in Aut(G)$ such that $\beta(u) = v$, in which case $A = Aut(G)$ has exactly one orbit containing all the vertices of G. In general, we denote the orbit of u by $u^{Aut(G)}$. Vertices u and v satisfying $\beta(u) = v$ are said to be *similar*. The stabilizer of a vertex v under the action of $Aut(G)$ is the set of automorphisms that fix v and is denoted by A_v. A group theory result of special importance to the proofs given in Section 3 is the orbit-stabilizer theorem which states that $|u^A||A_v| = |A|$.

A topological index for a graph G is a numerical quantity invariant under its automorphism group. The Wiener index [28] is a distance based topological index, defined by

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

The Hosoya polynomial (or the Wiener polynomial) of a graph [17] (see also [1,13,26] is defined as

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

The kth coefficient of $H(G, x)$ is the number of pairs of vertices at distance k from each other and

$$H^{'}(G, 1) = W(G).$$

Suppose $d(G)$ is the diameter of graph G and that $d(G, k)$ is the number of pairs of vertices in G at distance k from each other. Then the Hosoya polynomial can be reformulated as

$$H(G, x) := \sum_{k=1}^{d(G)} d(G, k) x^k.$$

The partial Hosoya polynomial with respect to vertex v is given by

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

Using the partial Hosoya polynomial, the Hosoya polynomial can be reformulated as

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

2.2. Entropy applied to graphs

Shannon entropy [27] is defined as $I(p) = -\sum_{i=1}^{n} p_i \log(p_i)$ for a finite probability vector p. Let $\lambda = \sum_{j=1}^{n} \lambda_j$ and $p_i = \lambda_i/\lambda$, $(i = 1, 2, \ldots, n)$. More generally, the entropy of a tuple $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ of real numbers is given by

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

There are many different ways to associate a tuple $(\lambda_1, \lambda_2, \ldots, \lambda_n)$ to a graph G, and each one can be used to define an entropy based measure, see [2–12,15] and [23]. As noted above, methods and measures for quantifying structural properties of networks were developed in the late 1950s and early 1960s, applying information-theoretic measures based on Shannon entropy to structural problems in chemistry and biology, see [27] for a survey. The earliest such measure $I_a(G)$, introduced by Rashevsky [25] and developed further by Mowshowitz and co-workers [19–23], was called the (topological) information content of a graph G. It is defined as follows:

$$I_a(G) = -\sum_{i=1}^{k} \frac{|N_i|}{|V|} \log\left(\frac{|N_i|}{|V|}\right),$$

where N_i $(1 \le i \le k)$ is a set of similar vertices. The collection of k orbits partitions V and thus allows for computing the Shannon entropy of the finite probability scheme with probabilities $|N_i|/|V|$. It is easy to see that every vertex-transitive graph is regular, but it is far from the case that all regular graphs are transitive. It is a well-known fact that $I_a(G)$ reaches its maximum value for networks with the identity automorphism group.

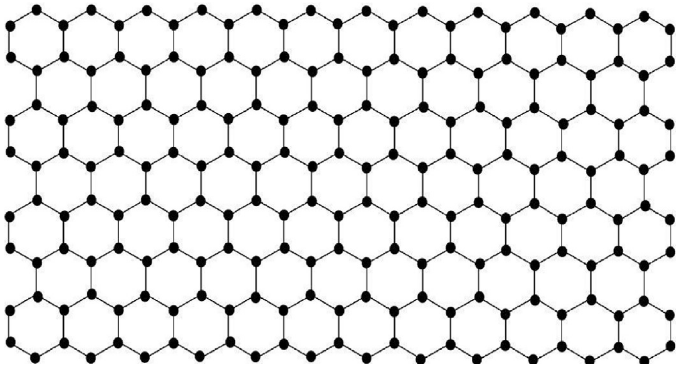

Fig. 1. 2-*D* graph of zig-zag nanotube $T_Z[m,n]$, for $m = 5$, $n = 10$.

In what follows we will apply Hosoya entropy [23], a distance based measure, to a particular class of graphs called *fullerenes*. The analysis involving the Hosoya entropy measure is fully justified by the fact that there is a high correlation between the boiling point of fullerene compounds and the Hosoya entropy of the graphs representing them.

Given a graph G and a vertex $u \in V(G)$, let $\Gamma_i(u)$ be the number of vertices at distance i from the u. Two vertices u and v are said to be *Hosoya-equivalentor H-equivalent* [23] if $\Gamma_i(u) = \Gamma_i(v)$ for $1 \le i \le d(G)$. Clearly, the family of sets of H-equivalent vertices constitutes a partition of the vertices. Let $G = (V, E)$ be a graph, and h the number of sets of H-equivalent vertices in G. If n_i is the cardinality of the *ith* set of H-equivalent vertices for $1 \le i \le h$, the Hosoya entropy (or H-entropy) of G (introduced in [23]) is given by

$$H(G) = -\sum_{i=1}^{h} \lambda_i \log(\lambda_i) \quad and \quad \lambda_i = |n_i|/|V|.$$

Example 1. Let G be a k-regular graph on n vertices in which every two adjacent vertices have λ common neighbors and every two non-adjacent vertices have μ common neighbors. Then the graph G with these parameters is denoted by $srg(n, k, \lambda, \mu)$ and it is called as strongly regular graph. Every strongly regular graph G where $G \neq K_n$ has a path graph P_3 as induced subgraph and so $\mu > 0$. Thus every two vertices that are not adjacent have at least a common neighbor so the diameter of G is 2. Hence, from a result in [23], all of the vertices are H-equivalent which implies that$H(G) = 0$. For example, the Petersen graph P which is an undirected vertex-transitive cubic graph with 10 vertices and 15 edges is a strongly regular graph with $H(P) = 0$.

Example 2. A wheel graph is a graph formed by connecting a single vertex to all vertices of a cycle. Consider the wheel graph W_n on n+1 vertices. It is not a vertex-transitive graph, for $n \geq 3$. By means of group action, the vertices of W_n can be divided in two orbits. The central vertex of degree n is a singleton orbit and all vertices adjacent to the central vertex compose the other orbit of order n. It is clear that the central vertex is not *H-equivalent* with the others. Hence, $\lambda_1 = 1/(n+1)$ and $\lambda_2 = n/(n+1)$. This means that

$$\begin{aligned} H(G) &= -\left(\frac{1}{n+1}\log\left(\frac{1}{n+1}\right) + \frac{n}{n+1}\log\left(\frac{n}{n+1}\right)\right) \\ &= \log(n+1) - \frac{n}{n+1}\log(n). \end{aligned}$$

3. Fullerenes

Diamond and graphite are two well-known forms of carbon. In 1985, a third form of carbon called fullerene was discovered, see [14–18]. Buckminster fullerene C_{60} is the most abundant form of fullerenes. A C_{60} molecule consists of 60 carbon atoms arranged in a spherical structure. Its shape is the same as a soccer ball which contains 12 pentagons and 20 hexagons. In general, a fullerene on n vertices has $n/2-10$ hexagons and 12 pentagons. By this rule, we can construct some classes of fullerene graphs. In [29] a method is described to obtain a fullerene graph from a zig-zag or armchair nanotubes. Using the method of [29], we construct some infinite classes of fullerenes and then determine their Hosoya's entropy. Let $T_Z[m,n]$ denote a zig-zag nanotube with m rows and n columns of hexagons, see Fig. 1. Combine a nanotube $T_Z[5,n]$ with two copies of cap B (Fig. 2) as shown in Fig. 3, the resulting graph is a non IPR fullerene, which has $10n$ vertices and exactly $5n-10$ hexagonal faces, and is denoted by A_{10n}.

We can apply our method to introduce another infinite class of fullerenes. The main goal of this section is to compute the entropy of three infinite classes of fullerenes. With respect to the number of their vertices, we called them as A_{10n}, B_{12n} and C_{12n+2}. First, we determine the entropy of fullerene A_{10n}. The smallest fullerene in this class has fifty vertices. For $n = 5$,

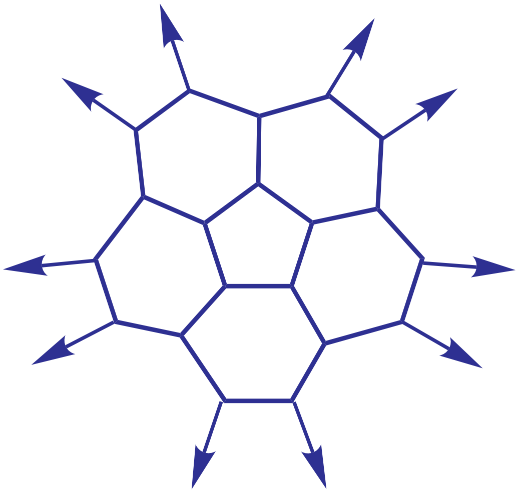

Fig. 2. The cap *B*.

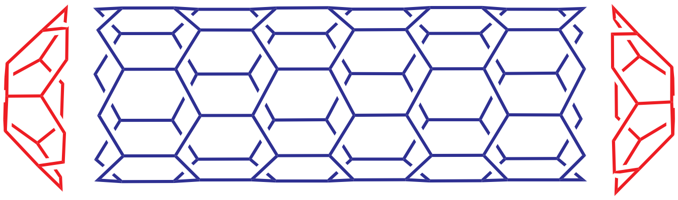

Fig. 3. Fullerene A_{10n} constructed by combining two copies of cap *B* and the zig-zag nanotube $T_Z[5, n]$.

Table 1
The orbits of the automorphism group of A_{10n}, *n* is even.

Orbits	Elements
V_1	$1, 2, 3, 4, 5, 10n-4, 10n-3, 10n-2, 10n-1, 10n$
V_2	$6, 7, 8, 9, 10, 10n-9, 10n-8, 10n-7, 10n-6, 10n-5$
V_3	$11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 10n-19, \ldots, 10n-10$
V_4	$21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 10n-29, \ldots, 10n-20$
$\vdots$	$\vdots$
$V_{n/2+1}$	$5n-9, 5n-8, \ldots, 5n+10$

using a GAP program we find that $H(A_{50}) \approx 1.2094$. For $n = 6$, the fullerene A_{60} is isomorphic with the famous Buckminster fullerene C_{60}. Hence, A_{60} is vertex-transitive and so $H(A_{60}) = 0$.

Theorem 1. *The Hosoya entropy of the fullerene graph* A_{10n}, *with* $n \geq 7$, *is given by*

$$H(A_{10n}) = \begin{cases} \log(n) + \dfrac{2}{n} - 1 & \text{if } n \text{ is even} \\ \log(n) + \dfrac{3}{n} - 1 & \text{if } n \text{ is odd} \end{cases}.$$

Proof. For $n \geq 7$, first suppose *n* is even and consider the graph A_{10n} as depicted in Fig. 4. It is easy to see that the following elements are in the automorphism group of fullerene graph A_{10n}

$$\alpha = (1, 2)(3, 5)\ldots(10n-3, 10n)(10n-2, 10n-1),$$
$$\beta = (1, 10n)(2, 10n-1)\cdots(3, 10n-2)(4, 10n-3)(5, 10n-4),$$
$$\gamma = (1, 2, 3, 4, 5)(6, 7, 8, 9, 10)\ldots(10n-4, 10n-3, 10n-2, 10n-1, 10n).$$

If $\beta\gamma = \rho$, it is clear that $\alpha^2 = \rho^{10} = 1$, $\alpha\rho\alpha = \rho^{-1}$ and thus $\Gamma = \langle \alpha, \rho \rangle \leq A = Aut(A_{10n})$ is isomorphic with dihedral group D_{20} on 20 elements. On the other hand, every symmetry element which fixes 4, must also fixes {9, 10*n*-9, 10*n*-4}. The identity element and the symmetry element α do this. Hence, the orbit-stabilizer property ensures that $|A| = |4^A|.|A_4|$ and thus $|A| = 10 \times 2 = 20$ which implies that $A \cong D_{20}$. The orbits of the automorphism group are given in Table 1. We claim that in fullerene A_{10n} the orbits of the automorphism group and the Hosoya-partitions coincide. For $n = 8$ and 10, by an elementary computation, we see that the Hosoya-partitions are the same as the orbits of its automorphism group. Let $n \geq 12$,

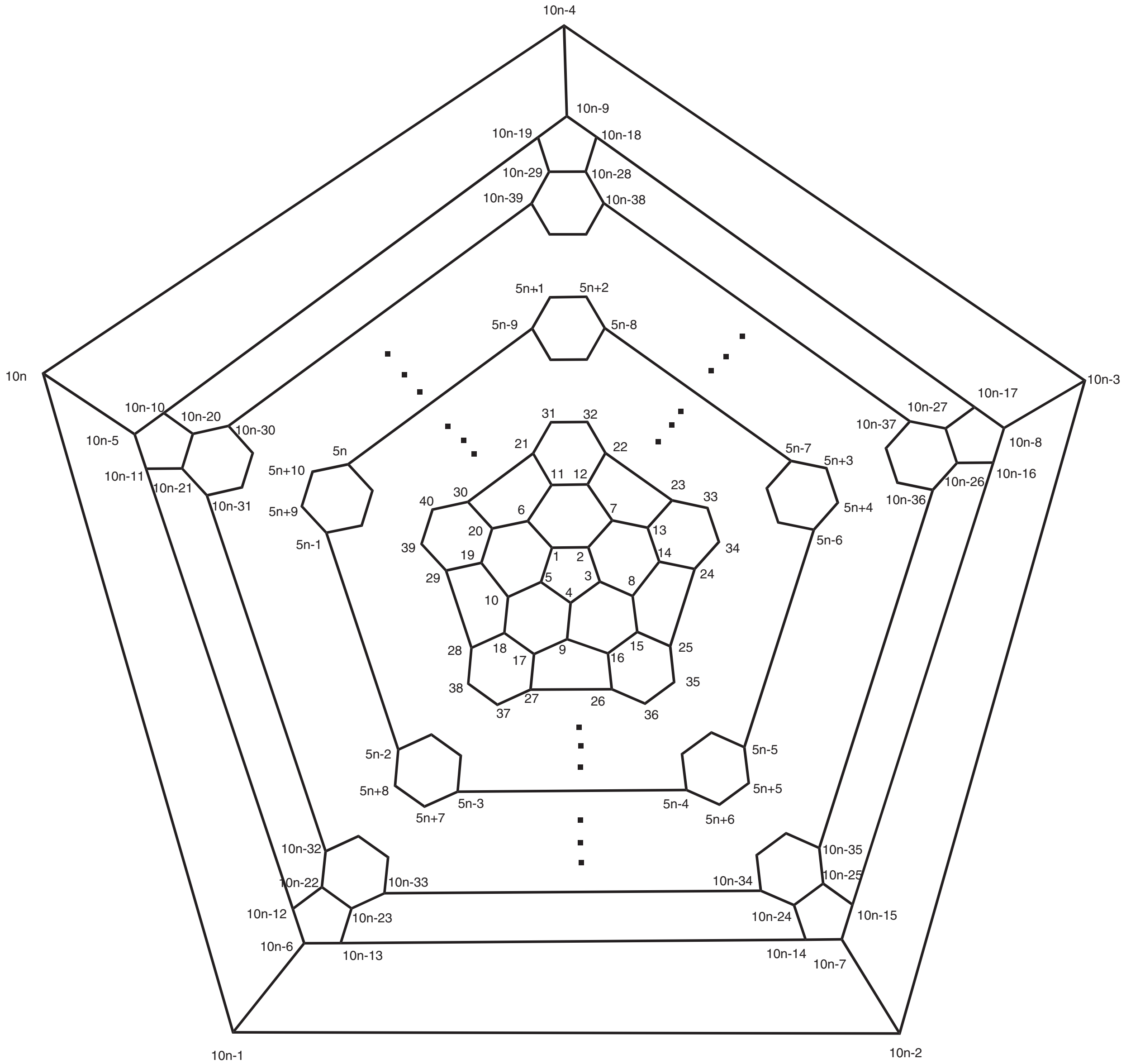

Fig. 4. Labeling the vertices of fullerene graph A_{10n}, n is even.

according to [24], the diameter of this graph is $n + 3$. Also, the vertices of each orbit of size 20 have the eccentricity equal $n+3-i(1 \leq i \leq n/2-1)$. This means that the orbits $V_3, V_4, \ldots, V_{n/2+1}$ are Hosoya-partitions. The vertices of two orbits V_1 and V_2 have the same eccentricity equal with $n+3$. We claim that two orbits V_1 and V_2 are also Hosoya-partitions. To do this, notice that there are ten vertices $\{10n-26, 10n-25, 10n-24, 10n-23, 10n-18, 10n-17, 10n-12, 10n-11, 10n-9, 10n-5\}$ at distance n with vertex 1 while there are eight vertices $\{10n-35, 10n-34, 10n-26, 10n-23, 10n-17, 10n-12, 10n-4, 10n\}$ at distance n with vertex 6. This implies that V_1 and V_2 are Hosoya-partitions. Hence the Hosoya-partitions and the orbits of above action A_{10n} are coincide. This means that there are two equivalence classes of size 10 and $n/2-1$ equivalence classes of size 20. Now, let n is odd and consider the graph A_{10n} depicted in Fig. 5. Similar to the last discussion, one can prove that its automorphism group is isomorphic with dihedral group D_{20}. Again we can prove that the Hosoya-partitions and the set of orbits are coincide which means that the Hosoya-partitions are given in Table 2. By above discussion we found that there are three equivalence classes of size 10 and $(n-3)/2$ equivalence classes of size 20. This completes the proof. □

Theorem 2. *The Hosoya entropy of the fullerene graph* B_{12n} *(shown in Figs. 6 and 7) with* $n \geq 4$ *is given by*

$$H(B_{12n}) = \log(n).$$

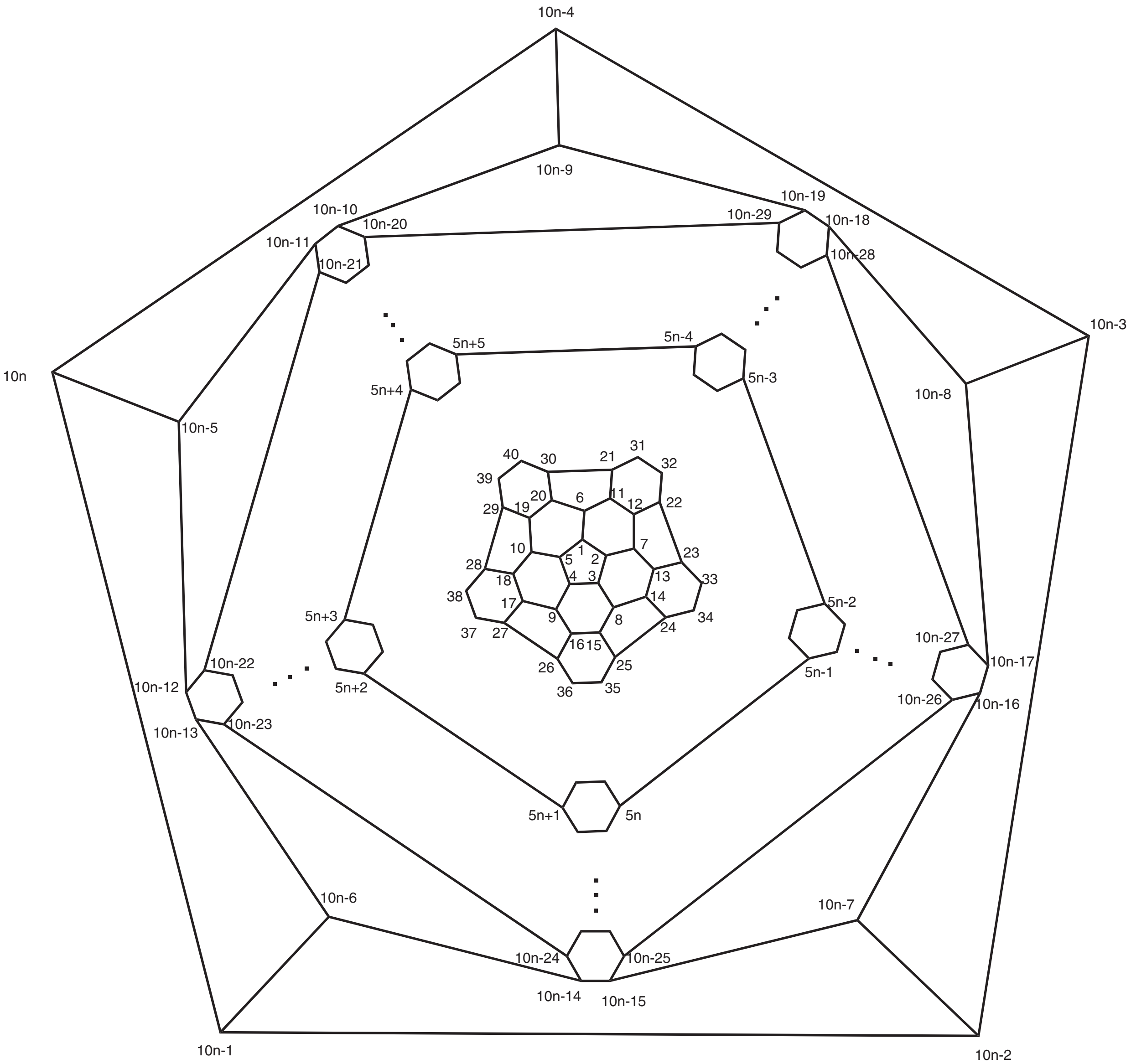

Fig. 5. Labeling the vertices of fullerene graph A_{10n}, n is odd.

Table 2
The Hosoya-partitions of A_{10n}, n is odd.

H-partitions	Elements
V_1	$1, 2, 3, 4, 5, 10n-4, 10n-3, 10n-2, 10n-1, 10n$
V_2	$6, 7, 8, 9, 10, 10n-9, 10n-8, 10n-7, 10n-6, 10n-5$
V_3	$11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 10n-19, \ldots, 10n-10$
V_4	$21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 10n-29, \ldots, 10n-20$
$\vdots$	$\vdots$
$V_{(n+3)/2}$	$5n-4, 5n-3, 5n-2, 5n-1, 5n, 5n+1, \ldots, 5n+5$

Proof. Let n be an even number and consider the fullerene B_{12n} in Fig. 6. Consider two permutations α, β with the following permutation representations:

$$\alpha = (2,6)(3,5)\ldots(12n-5,12n)(12n-4,12n-1)(12n-3,12n-2),$$
$$\beta = (1,12n-2,2,12n-1,3,12n,4,12n-5,5,12n-4,6,12n-3)\ldots$$
$$(6n-5,6n+2,6n-3,6n+4,6n-1,6n+6,6n+1,6n-4,6n+3,6n-2,6n+5,6n).$$

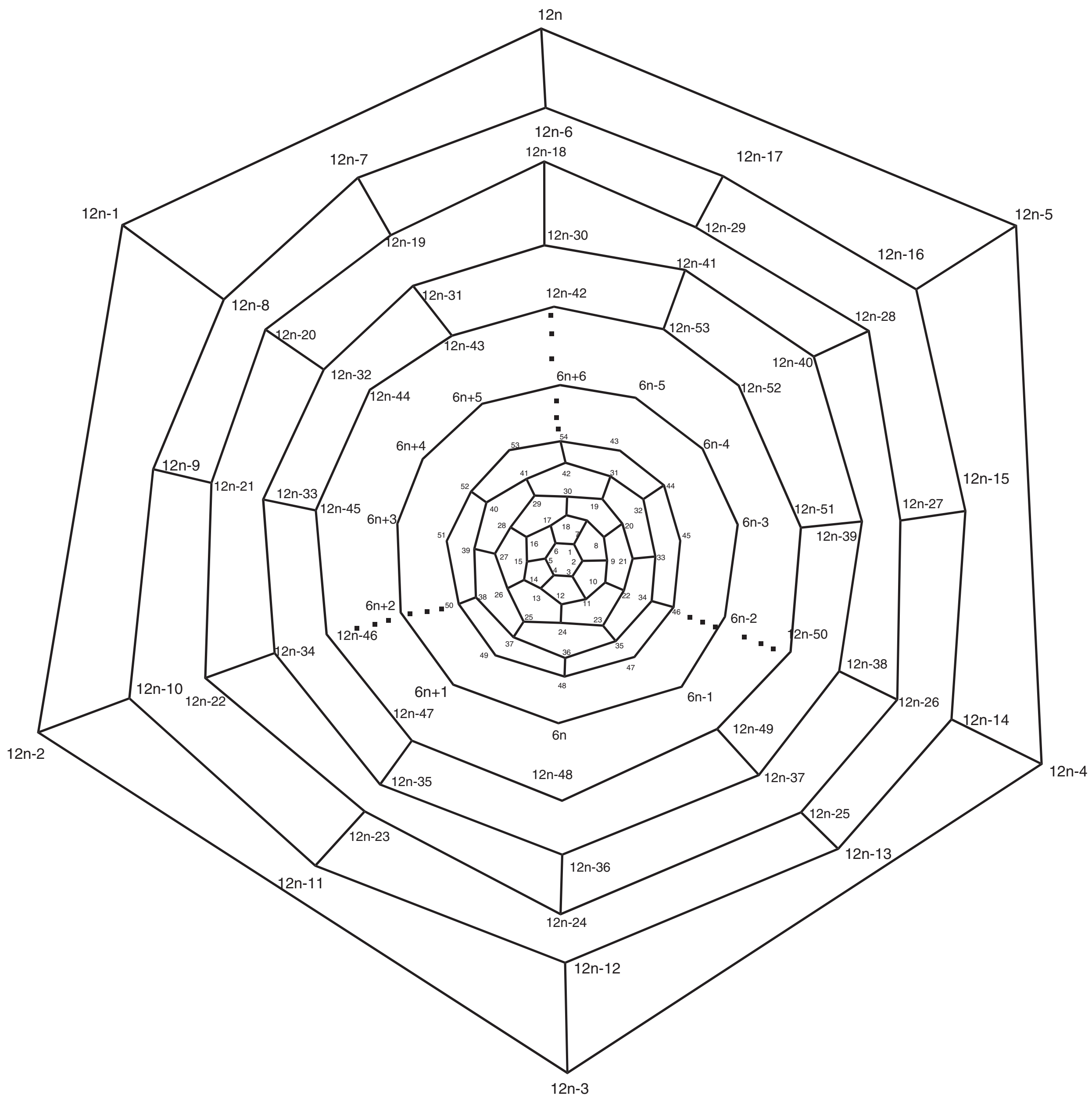

Fig. 6. Labeling of vertices of fullerene graph B_{12n}, n is even.

One can prove that $\alpha^2 = \beta^{12} = 1$, $\alpha\beta\alpha = \beta^{-1}$ and thus $A = Aut(B_{12n}) \geq \langle \alpha, \beta \rangle \cong D_{24}$. On the other hand, the identity element and the symmetry element α fix 1. Hence, the orbit-stabilizer property implies that $|A| = |1^A|.|A_1|$ and thus $|A| = 12 \times 2$ and thus $A \cong D_{24}$.

Similar to the proof of Theorem 1, all orbits of the action of automorphism group of the set of vertices are the same as the Hosoya-partitions. They are reported in Table 3. This means that the vertices of this graph are partitioned to n equivalence classes of size 12 and its entropy is

$$H(B_{12n}) = n\left(\frac{12}{12n}\log\left(\frac{12n}{12}\right)\right) = \log(n).$$

Now, suppose n is an odd number, see Fig. 7. Again, similar to the proof of Theorem 1, we can prove that for $n \geq 5$ the set of orbits and equivalence classes coincide and the Hosoya-partitions are as given in Table 4. The exceptional cases are given in Table 5.

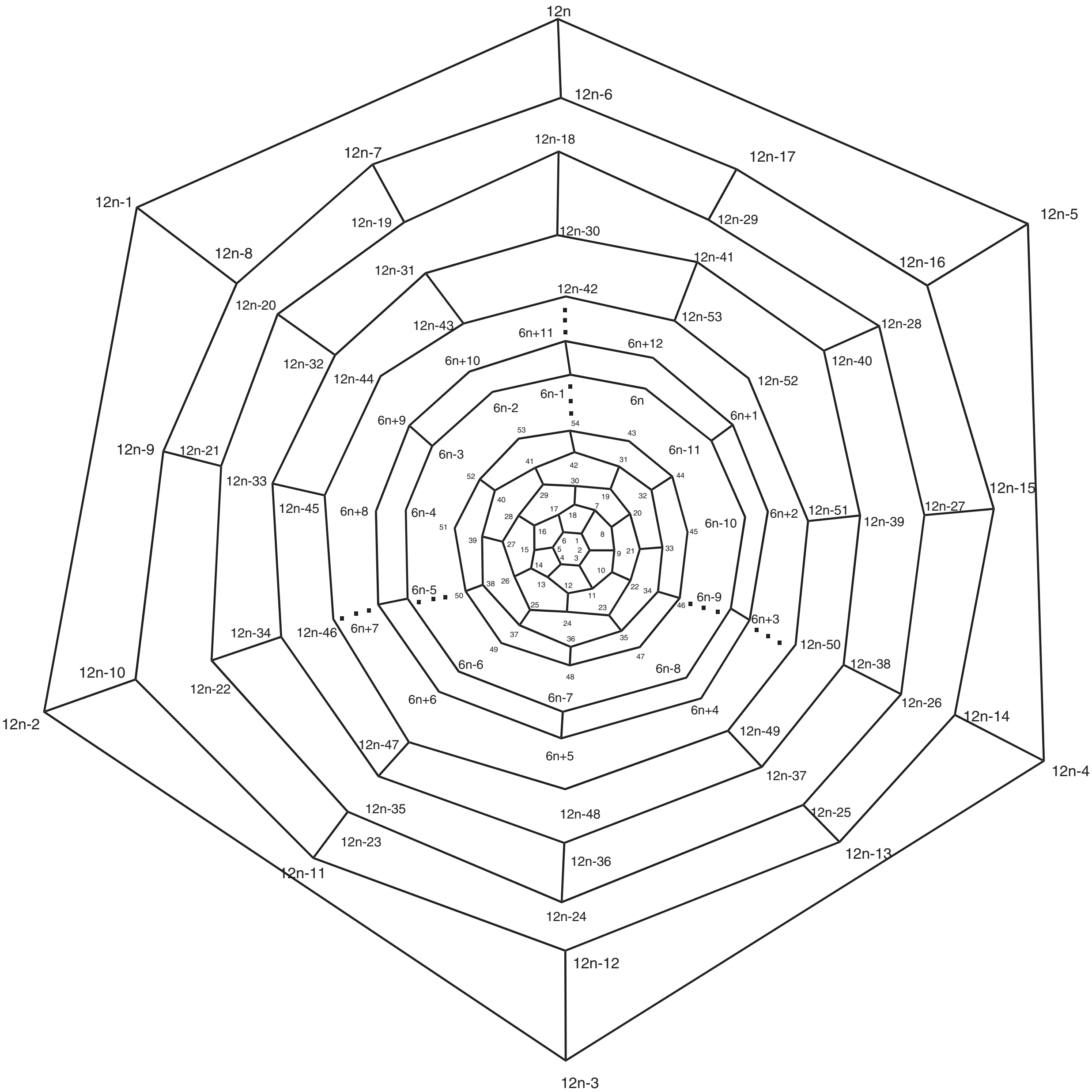

Fig. 7. Labeling of vertices of fullerene graph B_{12n}, n is odd.

As a result of Theorem 2, one can see that there is a correlation between entropy and the boiling point of fullerene B_{12n}. In other words, the boiling points of 7 members of fullerene graph B_{12n} are given in Table 6. By comparing these values with the Hosoya entropy of these fullerenes computed directly from Theorem 2, one can easily determine the correlation $R = 0.998$ between them. It should be noted that, this is the first attempt to estimate the boiling point of fullerene graphs with respect to Hosoya entropy. We can apply our method for other classes of fullerenes introduced in this paper. □

Theorem 3. *The Hosoya entropy of the fullerene graph* C_{12n+2}, *with* $n \geq 7$, *is given by*

$$H(C_{12n+2}) = \log(12n+2) - \frac{1}{12n+2}(12n+26+(12n-36)\log 3).$$

Proof. For $n \geq 7$, consider the graph shown in Fig. 8. If

$$\alpha = (1,5)(2,4)(6,8)\ldots(12n-3,12n-1)(12n+2,12n),$$
$$\beta = (2,8)(3,7)(4,6)\ldots(12n-3,12n+2)(12n-2,12n+1)(12n-1,12n).$$

Table 3
The Hosoya-partitions of fullerene graph B_{12n}, n is even.

H-partitions	Elements
V_1	$1, 2, 3, 4, 5, 6, 12n-5, \ldots, 12n$
V_2	$7, 9, 11, 13, 15, 17, 12n-16, \ldots, 12n-6$
V_3	$8, 10, 12, 14, 16, 18, 12n-17, 12n-15, \ldots, 12n-7$
V_4	$19, 21, 23, 25, 27, 29, 12n-28, 12n-26, 12n-24,$ $12n-22, 12n-20, 12n-18$
V_5	$20, 22, 24, 26, 28, 30, 12n-29, 12n-27, 12n-25,$ $12n-23, 12n-21, 12n-19$
V_6	$31, 33, 35, 37, 39, 41, 12n-40, 12n-38, 12n-36,$ $12n-34, 12n-32, 12n-30$
V_7	$32, 34, 36, 38, 40, 42, 12n-41, 12n-39, 12n-37,$ $12n-35, 12n-33, 12n-31$
V_8	$43, 45, 47, 49, 51, 53, 12n-52, 12n-50, 12n-48,$ $12n-46, 12n-44, 12n-42$
V_9	$44, 46, 48, 50, 52, 54, 12n-53, 12n-51, 12n-49,$ $12n-47, 12n-45, 12n-43$
$\vdots$	$\vdots$
V_n	$6n-5, 6n-4, 6n-3, 6n-2, 6n-1, 6n, 6n+1, 6n+2,$ $6n+3, 6n+4, 6n+5, 6n+6$

Table 4
The Hosoya-partitions of fullerene graph B_{12n}, n is odd.

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

Table 5
The exceptional cases of the entropy of fullerene B_{12n}.

Fullerene	entropy
B_{24}	$H(B_{24}) = \log 2$
B_{36}	$H(B_{36}) = -\frac{1}{3}\log 3 + \frac{2}{3}$

Table 6
Compairing the entropy with boiling point of fullerene B_{12n}.

Fullerenes	entropy	BP (Centigrade degree)
B_{24}	$H(B_{24}) = \log 2$	443.5
B_{36}	$H(B_{36}) = -(\log 3)/3 + 2/3$	601.7
B_{48}	$H(B_{48}) = \log 4$	733.6
B_{60}	$H(B_{60}) = \log 5$	849
B_{72}	$H(B_{72}) = \log 6$	953
B_{84}	$H(B_{84}) = \log 7$	1048
B_{96}	$H(B_{96}) = \log 8$	1136

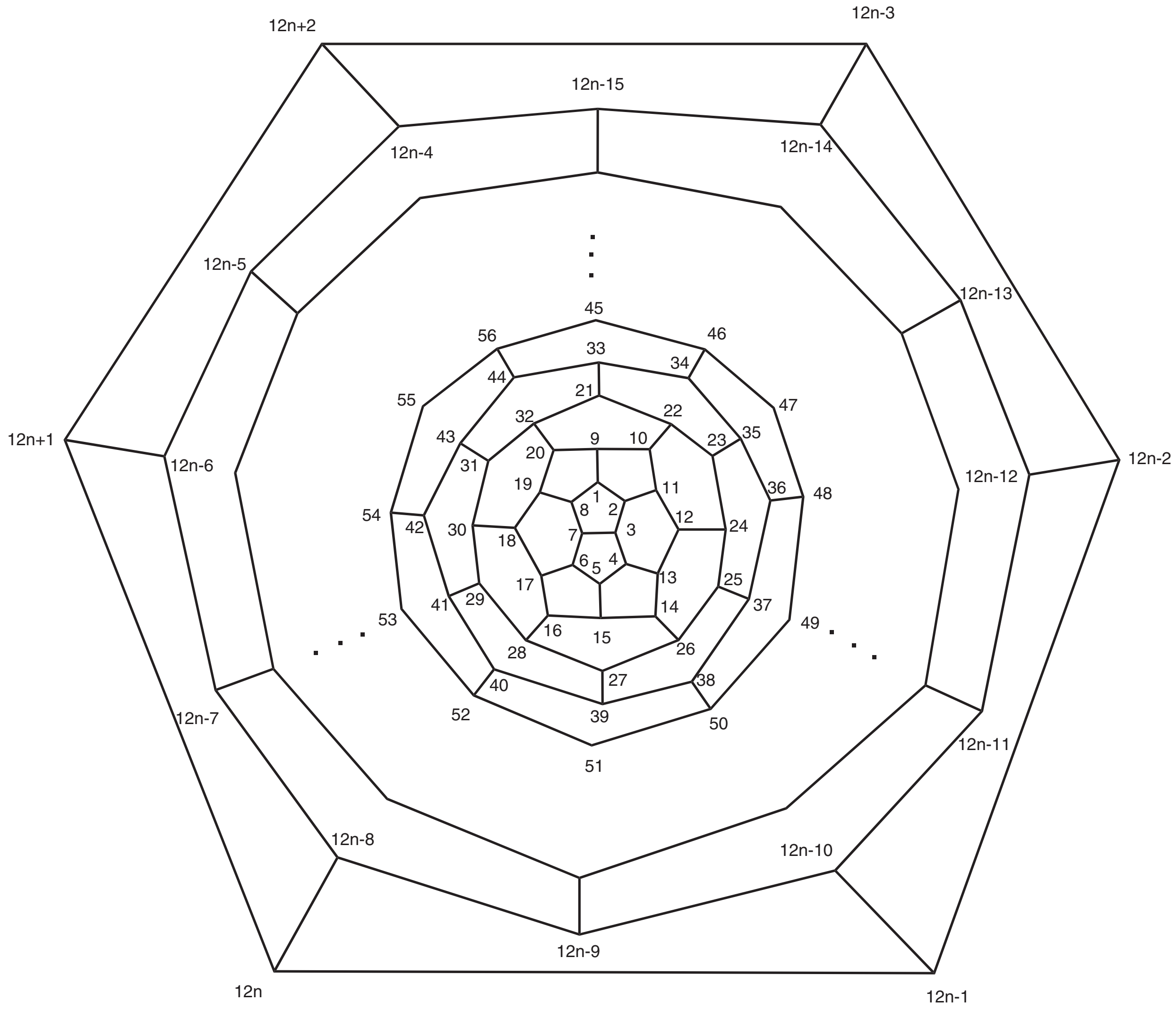

Fig. 8. Labeling the vertices of fullerene graph C_{12n+2}.

Table 7
Some exceptional cases of fullerene C_{12n+2}.

Fullerenes	entropy
C_{26}	$H(C_{26}) = \log 13 - \frac{21}{13}\log 3$
C_{38}	$H(C_{38}) = \log 19 - \frac{6}{19}\log 3 - \frac{14}{19}$
C_{50}	$H(C_{50}) = \log 25 - \frac{3}{25}\log 3 - \frac{18}{25}$
C_{62}	$H(C_{62}) = \log 31 - \frac{12}{31}\log 3 - \frac{18}{31}$
C_{74}	$H(C_{74}) = \log 37 - \frac{15}{37}\log 3 - \frac{20}{37}$

then $\Gamma = \langle\alpha, \beta\rangle \leq A = Aut(C_{12n+2})$ and the orbit-stabilizer property implies that $|A| = |1^A|.|A_1|$ and thus one can see that $A \cong Z_2 \times Z_2$. By a method similar to that used in the proof of Theorem 1, we can show that the Hosoya-partitions are

$$\{1,5\}, \{2,4,6,8\}, \{3,7\}, \{9,15\}, \{10,14,16,20\}, \{11,13,17,19\},$$
$$\{21,27\}, \{22,26,28,32\}, \{23,25,29,31\}, \{24,30\}, \{33,39\},$$
$$\{34,36,38,40,42,44\}, \{35,37,41,43\}, \{45,47,49,51,53,55\},$$

$$\{12, 18\}, \{46, 48, 50, 52, 54, 56\}, \ldots,$$
$$\{12n-15, 12n-13, 12n-11, 12n-9, 12n-7, 12n-5\},$$
$$\{12n-14, 12n-12, 12n-10, 12n-8, 12n-6, 12n-4\},$$
$$\{12n-3, 12n-2, 12n-1, 12n, 12n+1, 12n+2\}.$$

In other words, there are seven equivalence classes of size 2, six equivalence classes of size 4 and $2n-6$ equivalence classes of size 6. The exceptional cases are given in Table 7 and this completes the proof. □

4. Summary and conclusion

In this paper we have applied the concept of Hosoya entropy, introduced in [23], to study properties of a class of graphs representing chemical molecules known as fullerenes. We have shown that important physical properties of these molecules can be determined by applying Hosoya entropy to their corresponding graphs. Hosoya entropy is a very specialized measure, and of course other entropy measures might capture other different properties of these molecules. Future work in this area is needed to identify the particular physical properties of fullerenes captured by different entropy based graph measures.

Acknowledgments

Matthias Dehmer thanks the Austrian Science Fund for supporting this work (project P 30031).

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