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Symmetry and PI Polynomials of C_{50+10n} Fullerenes

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Abstract

A counting polynomial is a sequence description of a topological property such that the exponents are the extent of its partitions while the coefficients are related to the occurrence of these partitions. In this paper, the symmetry and then PI polynomials of an infinite family of fullerenes with 50 + 10n carbon atoms with D_{5h} point group symmetry are computed. As a consequence the PI index of this class of fullerenes is computed.

1. Introduction

Throughout this paper, all graphs considered are assumed to be finite, simple and connected. A ***molecular graph*** is the graph in which the degree of each vertex is at most four. In such a graph vertices are atoms and edges are chemical bonds of a chemical compound.

A graph can be algebraically described by a matrix or a polynomial. In the latter case, we speak of a ***counting polynomial***. Suppose P is a graph theoretical property. The polynomial $P(G,k) = \Sigma_k P(G,k) \,.\, x^k$, where $P(G,k)$ is the frequency of occurrence of the property partitions of G is called the counting polynomial of P. The first two reported counting polynomial in the mathematical chemistry literature are the Z–counting polynomial,

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to consider the number of k–matchings into account, and distance degree polynomials initially called the ***Wiener*** and later ***Hosoya polynomial*** [1,2]. The roots and coefficients of these polynomials are used for the characterization of topological nature of hydrocarbons. More about polynomials the reader can find in [3].

Sagan et al. [4], presented a treatment apparently independent of Hosoya's. Perhaps the most interesting property of $H(G,x)$ is the first derivative, evaluated at $x = 1$, which equals the Wiener index: $H'(G,1) = W(G)$. One of us (ARA) continued the line of the mentioned paper of Sagan *et al*. to introduce the notion of **PI polynomial** of a molecular graph G as:

$$PI(G,x) = \sum_{(u,v)=e\in E(G)} x^{N(u,v)} \tag{1}$$

where $N(u,v) = n_u(e) + n_v(e)$ and $n_u(e)$ is the number of edges lying closer to u than v while the number of edges **parallel** to the edge $e = uv \in E(G)$ is given by $N(e) = |E(G)| - N(u,v)$ [5]. In the mentioned paper it is shown that this new polynomial has the same basic properties as the Wiener polynomial. Thus, its first derivative gives the PI index, which can also be calculated by subtracting the total number of equidistant edges in G from the square of the edge set cardinality:

$$PI(G) = PI'(G,1) = \left(|E|\right)^2 - \sum_e N(e) \tag{2}$$

relation also found in [6] to calculate the PI index. We encourage the interested reader to consult [7–11] for more information on this topic.

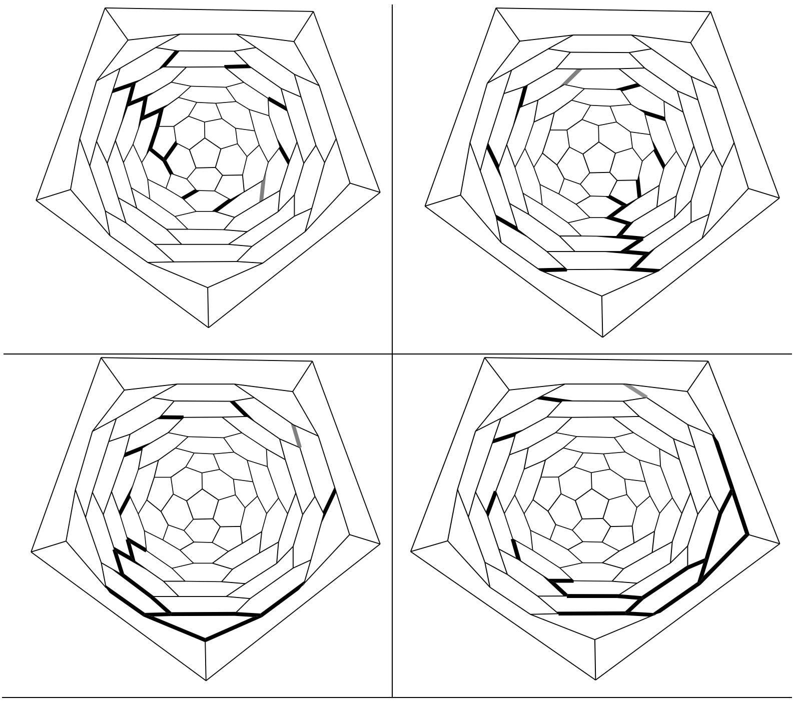
There are four important packages for such calculations. These are TopoCluj [12], Omega 1.1 [13], HyperChem [4] and GAP [15]. Calculations given this paper are done by using a combination of these packages. Our programs are accessible from the authors upon request. All notations are standard and taken from [16,17].

2. Symmetry of C_{50+10n} Fullerenes

The fullerenes are an allotropic form of the carbon, for the first time evidenced in 1985 by Kroto et al. [18]. These are cage molecules in which a large number of carbon atoms are bonded in a nearly spherical shape configuration. Assuming that F is a fullerene and p, h, n and m are the number of pentagons, hexagons, carbon atoms and bonds between them. Since each atom lies in exactly 3 faces and each edge lies in 2 faces, the number of atoms is n = (5p+6h)/3, the number of edges is m = (5p + 6h)/2 = 3/2n and the number of faces is f = p + h. By the Euler's formula n − m + f = 2 and we can deduce that (5p + 6h)/3 – (5p + 6h)/2 + p + h = 2. Thus, p = 12, v = 2h + 20 and e = 3h + 30. This implies that such molecules made up entirely of n carbon atoms will have 12 pentagonal and (n/2 – 10) hexagonal faces, where n ≠ 22 is a natural number equal or greater than 20, see [19,20] for details.

An automorphism of a graph is a permutation of its vertices preserves their adjacency. A permutation of the vertices of a graph belongs to its automorphism group if it satisfies $P^tAP = A$, where P^t is the transpose of permutation matrix P and A is the adjacency matrix of the graph under consideration. In this paper symmetry means topological symmetry which is word equivalent to automorphism. Symmetry of fullerenes is a classical problem in chemistry. There are too many algorithms for computing symmetry of fullerenes. We encourage the interested readers to consult the famous book of Fowler and Manolopoulos [19].

Consider a $C_{50 + 10n}$ fullerene depicted in Figure 1. Suppose *G* is the symmetry group of this fullerene. We consider the action of this group on the set of vertices. Then the number of orbits of this action is $[n/2] + 4$ and each orbit has length 10 or 20. The number of orbits of length 10 is equal 2, if n is odd; and 3, otherwise. The orbits of length 10 are {1, …, 5, 46+10n, …, 50+10n} and {6,…,10, 41 + 10n,…,45 + 10n}. If n is even then we have an additional orbit {5n + 21, …, 5n + 30} of length 10.



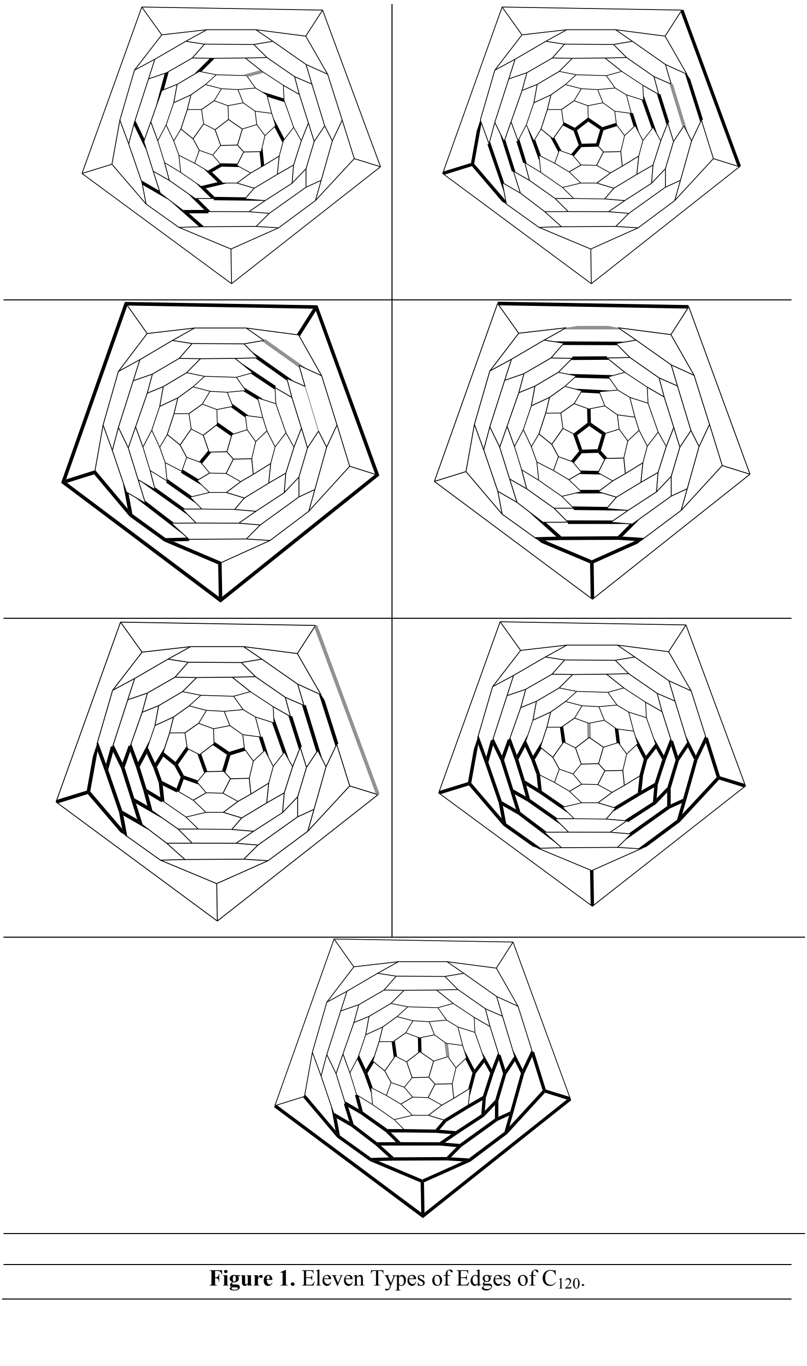


Figure 1. Eleven Types of Edges of C_{120}.

On the other hands, the orbits of length 20 in general are as follows:

{11, …, 20, 31 + 10n, …,40 + 10n},

{21, …, 30, 21 + 10n, …, 30 + 10n},

{31, …, 40, 11 + 10n, …, 20 + 10n},

{41, …, 50, 1 + 10n, …, 10 + 10n}.

⋮

In the next section, we apply these information to compute PI polynomial of this class of fullerenes.

3. PI Polynomial of C_{50+10n} Fullerenes

In this section, we apply our calculations given the previous section to compute the PI polynomial and then PI index of these fullerenes. Let us describe our algorithm for computing PI polynomials and then PI index of fullerenes C_{50+10n}. To do this, we first draw the fullerene molecule F = C_{50+10n} by HyperChem for some different values of *n*. Then compute the distance matrix of the molecular graph of F by TopoCluj. Finally, we prepare a GAP pseudocode for computing the PI index and PI polynomial of these fullerenes. This program is accessible from the authors upon request.

In Tables 1 – 9, the type of edges, the number of parallel edges for each type and the number of types for nine exceptional classes of together with their PI indices are given.

Table 1: n = 2 & PI = 8900.

Types of Edge	1	2	3	4	5	6	7
Number of Parallel Edges	13	15	18	20	21	22	25
Frequency	5	10	20	20	10	20	20

Table 2: n = 3 & PI = 11640.

Types of Edge	1	2	3	4	5	6	7
Number of Parallel Edges	16	18	20	21	22	26	32
Frequency	10	30	10	20	10	10	30

Table 3: n = 4 & PI = 15060.

Types of Edge	1	2	3	4	5	6	7	8	9
Number of Parallel Edges	13	16	17	19	21	23	27	36	37
Frequency	10	20	10	20	20	5	20	20	10

Table 4: n = 5 & PI = 18680.

Types of edge	1	2	3	4	5	6	7	8	9	10	11
Number of parallel edges	16	17	18	19	20	21	22	24	32	44	46
Frequency	10	20	10	20	10	20	10	10	10	10	20

Table 5: n = 6 & PI = 22980.

Types of Edge	1	2	3	4	5	6	7	8	9	10
Number of Parallel Edges	13	15	17	19	21	25	29	33	49	50
Frequency	5	10	40	30	20	10	10	10	10	20

Table 6: n = 8 & PI = 32660.

Types of Edge	1	2	3	4	5	6	7	8	9	10
Number of Parallel Edges	15	17	18	19	21	27	31	39	61	64
Frequency	10	50	20	20	30	15	10	10	10	20

Table 7: n = 10 & PI = 44100.

Types of Edge	1	2	3	4	5	6	7	8	9	10
Number of Parallel Edges	17	18	19	21	23	29	33	45	73	78
Frequency	55	40	30	20	10	20	10	10	10	20

Table 8: n =12 & PI = 57300.

Types of Edge	1	2	3	4	5	6	7	8	9	10
Number of Parallel Edges	17	18	19	21	25	31	35	51	85	92
Frequency	40	60	40	30	10	25	10	10	10	20

Table 9: n =14 & PI = 72260.

Types of Edge	1	2	3	4	5	6	7	8	9	10	11
Number of Parallel Edges	17	18	19	21	23	27	33	37	57	97	106
Frequency	40	80	20	45	10	10	30	10	10	10	20

From Tables 1 – 9, one can calculate the PI polynomials of these fullerenes. We record these polynomials in Table 10.

Table 10: The PI Polynomials of C_{70}, C_{80}, C_{90}, C_{110}, C_{130}, C_{150}, C_{170} and C_{190}.

n	
2	$5x^{92} + 10x^{90} + 20x^{87} + 20x^{85} + 10x^{84} + 20x^{83} + 20x^{80}$
3	$10x^{104} + 30x^{102} + 10x^{100} + 20x^{99} + 10x^{98} + 10x^{94} + 30x^{88}$
4	$10x^{122} + 20x^{119} + 10x^{118} + 20x^{116} + 20x^{114} + 5x^{112} + 20x^{108} + 20x^{99} + 10x^{98}$
6	$5x^{152} + 10x^{150} + 40x^{148} + 30x^{146} + 20x^{144} + 10x^{140} + 10x^{136} + 10x^{132} + 10x^{116} + 20x^{115}$
8	$10x^{180} + 50x^{178} + 20x^{177} + 20x^{176} + 30x^{174} + 15x^{168} + 10x^{164} + 10x^{156} + 10x^{134} + 20x^{131}$
10	$55x^{208} + 40x^{207} + 30x^{206} + 20x^{204} + 10x^{202} + 20x^{196} + 10x^{192} + 10x^{180} + 10x^{152} + 20x^{147}$
12	$40x^{238} + 60x^{237} + 40x^{236} + 30x^{234} + 10x^{230} + 25x^{224} + 10x^{220} + 10x^{204} + 10x^{170} + 20x^{163}$
14	$40x^{268} + 80x^{267} + 20x^{266} + 45x^{264} + 10x^{262} + 10x^{258} + 30x^{252} + 10x^{248} + 10x^{228} + 10x^{188} + 20x^{179}$

We now apply our calculations given the Tables 11 and 12 to prove the following theorem:

Table 11: F_{50+10n}, n is even, n>14

Types of edge	1	2	3	4	5	6	7	8	9	10	11	12
Number of parallel edges	17	18	19	21	n+7	n+9	n+13	n+19	n+23	3n+15	6n+13	7n+8
Number of Types	40	10n-60	20	20	2.5n-10	10	10	2.5n-5	10	10	10	20

Table 12: F_{50+10n}, n is odd, n> 5

Types of edge	1	2	3	4	5	6	7	8	9	10	11
Number of parallel edges	17	18	19	21	n+13	n+15	n+17	n+19	3n+17	6n+14	7n+11
Number of Types	40	10n-60	20	20	5n-15	10	10	10	10	10	10

Theorem: The PI polynomial of C_{50+10n} fullerene can be computed by the following formulas:

1. If $n > 3$ is odd then $PI(C_{50+10n}, x) = 40x^{15n+58} + (10n-60)x^{15n+57} + 20x^{15n+56} + 20x^{15n+54} + (5n-15)x^{14n+62} + 10x^{14n+60} + 10x^{14n+58} + 10x^{14n+56} + 10x^{12n+58} + 10x^{9n+61} + 20x^{8n+64}$.
2. If $n > 14$ is even then $PI(C_{50+10n}, x) = 40x^{15n+58} + (10n-60)x^{15n+57} + 20x^{15n+56} + 20x^{15n+54} + ((5/2)n-10)x^{14n+68} + 10x^{14n+66} + 10x^{14n+62} + ((5/2)n-5)x^{14n+56} + 10x^{14n+52} + 10x^{12n+60} + 10x^{9n+62} + 20x^{8n+67}$.

In particular, the PI index of these fullerenes can be computed by the following formula:

$$PI(C_{50+10n}) = \begin{cases} 220n^2 + 1760n + 4380 & 2 \nmid n \\ 220n^2 + 1760n + 4500 & 2 \mid n \end{cases}.$$

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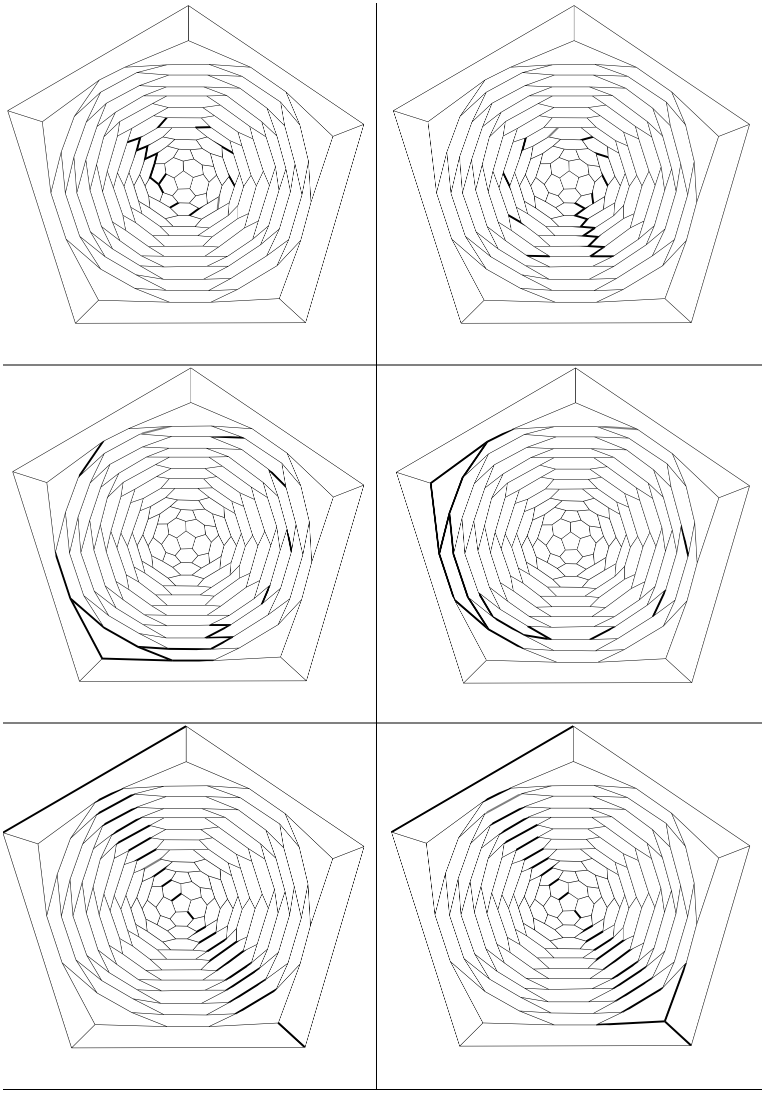

Figure 2. Twelve Types of Edges of C_{210}.

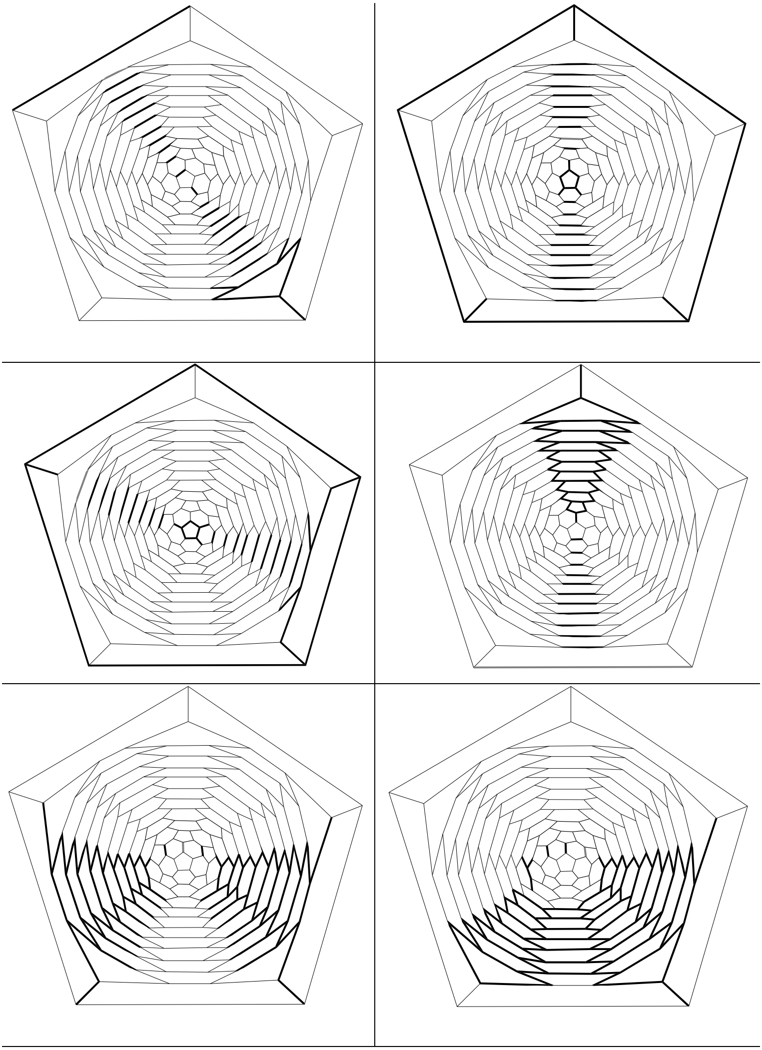

Figure 2. (Continued).