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Computing PI and Omega Polynomials of an Infinite Family of Fullerenes

A. R. Ashrafi,[1] M. Jalali,[1] M. Ghorbani[1] and M. V. Diudea[2]

[1]*Institute of Nanoscience and Nanotechnology, University of Kashan, Kashan 87317-51167, I R Iran*
[2]*Faculty of Chemistry and Chemical Engineering, Babes-Bolyai University, Arany Janos 11, 400028 Cluj, Romania*

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Counting of non-equidistant edges in a graph can be achieved in the formalism of *PI*-type polynomials. At least three ways of evaluating the equidistance of edges are discussed and the corresponding conditions established. Two versions of polynomials counting non-equidistant edges (*PI*-type polynomials) and two polynomials counting equidistant edges (Theta and Omega polynomials) are discussed and analytical formulas for an infinite series of tubulenes/fullerenes, derived from the dodecahedron C_{20}, are developed.

1. Introduction

Fullerenes are molecules in the form of cage-like polyhedra, consisting solely of carbon atoms. Fullerenes C_n can be drawn for $n = 20$ and for all even $n \geq 24$. They have n carbon atoms, $3n/2$ bonds, 12 pentagonal and $n/2$-10 hexagonal faces. The most important member of the family of fullerenes is C_{60}.[1,2]

Let $G = (V,E)$ be a connected bipartite graph with the vertex set $V = V(G)$ and the edge set $E = E(G)$, without loops and multiple edges. In 1988, Hosoya[3] introduced what he termed the Wiener (and latter called Hosoya) polynomial of a graph as $H(G,x) = \sum_{1<k<l} m(G,k) \cdot x^k$, where m(G,k) is the number of pairs of vertices in G that are distance k apart, and l is the maximum value of k or the diameter of G. Sagan, Yeh and Zhang[4] produced 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: $H'(G,1) = W(G)$. Ashrafi, Manoochehrian and

Yousefi-Azari[5,6] 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 $N(u,v) = n_{eu}(e \mid G) + n_{ev}(e \mid G)$ and $n_{eu}(e \mid G)$ is the number of edges lying closer to u than v (*i.e*., the *non-equidistant* edges) while the number of edges *equidistant* to the edge $e = (u,v) \in E(G)$ is given by: $N(e) = |E(G)| - N(u,v)$

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

which is just the formula proposed by John *et al*.[8] to calculate the *PI* index.

Two edges $e = (u,v)$ and $f = (x,y)$ of a graph *G* are called *equidistant* if the two ends of one edge show the same distance to the other edge. However, the distance between edges can be defined in several modes, as presented below.

(a) The distance from a vertex z to an edge $e = (u,v)$ is taken as the minimum distance between the given point and the two endpoints of that edge:[5]

$$d(z,e) = \min\{d(z,u), d(z,v)\} \tag{3}$$

Then, the edge $e = (u,v)$ is equidistant to $f = (x,y)$ if:

$$d(x,e) = d(y,e) \tag{4}$$

Or the edges $e = (u,v)$ and $f = (x,y)$ are equidistant if:

$$d(x,e) = d(y,e) \text{ and } d(u,f) = d(v,f) \tag{4`}$$

(b) A second definition for equidistant edges joins the conditions for (topologically) parallel and perpendicular edges:[9]

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y), \text{ for } \| \text{ edges} \tag{5}$$

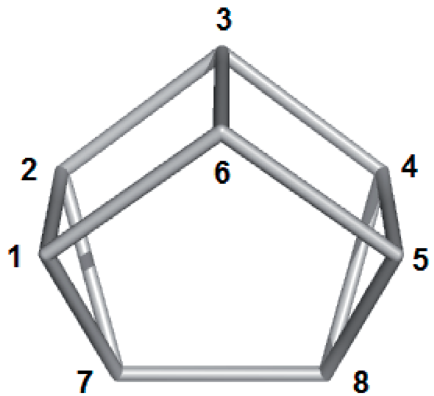
$$d(u,x) = d(u,y) = d(v,x) = d(v,y), \text{ for } \perp \text{ edges} \tag{6}$$

Clearly, the two polynomials $PI(G,x)$ (counted cf. version (a) - patterned by Ashrafi's group) and $\Pi(G,x)$ (provided by version (b) - patterned by Diudea's group) are different and their first derivatives in x=1 will give different *PI*-type indices.

Keeping in mind relation (2) and accounting that condition (4) is less strong than conditions (5) and (6) it is easily seen that:

$$PI'(G,1) \le \Pi'(G,1) \tag{7}$$

The above results are exemplified for the graph G_1 (Figure 1) in Table 1 (for each edge, the corresponding non-equidistant edges are listed).



***G*₁**

Figure 1. Cuneane graph and its numbering

Table 1. Counting polynomials for the structure ***G*₁**

	Version	c	Polynomial/index
1	$PI(G,x)$: non-equidistant edges (Ashrafi)		(comments)
	1-2 7-8 5-6 3-4 2-7 2-3 1-7 1-6	7	$PI(G,x)\overset{7}{=}2x^7+x^8+8x^9+x^{10}$
	1-6 7-8 5-8 5-6 4-5 3-6 3-4 2-7 1-7 1-2	9	$PI'(G,1)$ =104
	1-7 7-8 5-8 5-6 4-8 3-6 2-7 2-3 1-2 1-6	9	
	2-3 7-8 5-6 4-8 4-5 3-6 3-4 2-7 1-2 1-7	9	
	2-7 7-8 5-8 4-8 3-6 3-4 1-2 1-6 1-7 2-3	9	
	3-4 7-8 5-8 4-8 4-5 3-6 1-2 1-6 2-3 2-7	9	Edge 2-7 is equidistant to
	3-6 5-8 5-6 4-8 1-6 1-7 2-3 2-7 3-4	8	5-6 and 4-5, cf. (4)
	4-5 7-8 5-8 5-6 4-8 1-6 2-3 3-4	7	*e.g.,* 7
	4-8 7-8 5-8 5-6 1-7 2-3 2-7 3-4 3-6 4-5	9	$\begin{cases} d[(6,5),2]=d[(6,5)7]=2 \\ d[5,(2,7)]=d(6,(2,7)]=2 \end{cases}$
	5-6 7-8 5-8 1-2 1-6 1-7 2-3 3-6 4-5 4-8	9	
	5-8 7-8 1-6 1-7 2-7 3-4 3-6 4-5 4-8 5-6	9	
	7-8 1-2 1-6 1-7 2-3 2-7 3-4 4-5 4-8 5-6 5-8	10	

2	$\Pi(G,x)$: non-equidistant edges (Diudea)		
	1-2 7-8 5-8 5-6 4-8 3-4 2-7 2-3 1-7 1-6	9	$\Pi(G,x) = x^8 + 2x^9 + 5x^{10} + 4x^{11}$
	1-6 7-8 5-8 5-6 4-8 4-5 3-6 3-4 2-7 1-7 1-2	10	$\Pi'(G,1) = 120$
	1-7 7-8 5-8 5-6 4-8 4-5 3-6 3-4 2-7 2-3 1-2 1-6	11	
	2-3 7-8 5-8 5-6 4-8 4-5 3-6 3-4 2-7 1-2 1-7	10	
	2-7 7-8 5-8 5-6 4-8 4-5 3-6 3-4 1-2 1-6 1-7 2-3	**11**	Edge 2-7 is equidistant to no any edge
	3-4 7-8 5-8 4-8 4-5 3-6 1-2 1-6 1-7 2-3 2-7	10	cf. (5) and (6)
	3-6 5-8 5-6 4-8 1-6 1-7 2-3 2-7 3-4	8	
	4-5 7-8 5-8 5-6 4-8 1-6 1-7 2-3 2-7 3-4	9	9
	4-8 7-8 5-8 5-6 1-2 1-6 1-7 2-3 2-7 3-4 3-6 4-5	11	
	5-6 7-8 5-8 1-2 1-6 1-7 2-3 2-7 3-6 4-5 4-8	10	
	5-8 7-8 1-2 1-6 1-7 2-3 2-7 3-4 3-6 4-5 4-8 5-6	11	
	7-8 1-2 1-6 1-7 2-3 2-7 3-4 4-5 4-8 5-6 5-8	10	
3	$\Theta(G,x)$: equidistant edges		
	1-2 4-5 3-6	3	$\Theta(G,x) = 4x + 5x^2 + 2x^3 + x^4$
	1-6 2-3	2	Θ' =24
	1-7	1	
	2-3 1-6	2	Edge 2-7 is equidistant to no any edge
	2-7	1	cf. (5) and (6)
	3-4 5-6	2	Edge 3-6 is $\parallel$ to (1-2) and (4-5)
	3-6 1-2 4-5 **7-8**	4	and $\perp$ to 7-8
	4-5 1-2 3-6	3	which, cf. (5) and (6), are equidistant
	4-8	1	
	5-6 3-4	2	
	5-8	1	Edge 7-8 is equidistant to 3-6
	7-8 3-6	2	
4	$\Omega(G,x)$: strips		
	1-2 3-6 4-5	3	$\Omega(G,x) = 5x + 2x^2 + x^3$
	1-6 2-3	2	CI=122
	1-7	1	
	2-7	1	
	3-4 5-6	2	
	4-8	1	
	5-8	1	
	7-8	1	

2. Omega Polynomial

Two edges $e = (u,v)$ and $f = (x,y)$ of G are called *codistant* (briefly: $e\ co\ f$) if they obey the *topologically parallel edges* relation (5).

For some edges of a connected graph G there are the following relations satisfied:[8,10]

$$e\ co\ e \tag{8}$$

$$e\ co\ f \Leftrightarrow f\ co\ e \tag{9}$$

$$e\ co\ f\ \&\ f\ co\ h \Rightarrow e\ co\ h \tag{10}$$

though the relation (10) is not always valid.

Let $C(e) := \{f \in E(G);\ f\ co\ e\}$ denote the set of edges in G, codistant to the edge $e \in E(G)$. If relation *co* is an equivalence relation (*i.e.*, all the elements of $C(e)$ satisfy the relations (8) to (10), then G is called a *co-graph*. Consequently, $C(e)$ is called an *orthogonal cut oc* of G and $E(G)$ is the union of disjoint orthogonal cuts: $E(G) = C_1 \cup C_2 \cup ... \cup C_k$ and $Ci \cap Cj = \emptyset$ for $i \neq j,\ i, j = 1,2,..,k$.

Observe *co* is a Θ relation, (*Djoković-Winkler* relation[11-13]) and G *is a co-graph if and only if it is a partial cube,* as Klavžar correctly stated in a recent paper.[14]

If any two consecutive edges of an edge-cut sequence are *topologically parallel* within the same face of the covering, such a sequence is called a *quasi-orthogonal cut qoc* strip. This means the transitivity relation (10) of the *co* relation is not necessarily obeyed. Any *oc* strip is a *qoc* strip but the reverse is not always true.[15,16]

Let $m(G,c)$ be the number of *qoc* strips of length c (*i.e.*, the number of cut-off edges) in the graph G; for the sake of simplicity, $m(G,c)$ will hereafter be written as m. Three counting polynomials have been defined[9] on the ground of *qoc* strips:

$$\Omega(G,x) = \sum\nolimits_c m \cdot x^c \tag{11}$$

$$\Theta(G,x) = \sum\nolimits_c m \cdot c \cdot x^c \tag{12}$$

$$\Pi(G,x) = \sum\nolimits_c m \cdot c \cdot x^{e-c} \tag{13}$$

$\Omega(G,x)$ and $\Theta(G,x)$ polynomials count equidistant edges in G while $\Pi(G,x)$, non-equidistant edges (Table 1).

In a counting polynomial, the first derivative (in x=1) defines the type of property which is counted; for the three polynomials, they are:

$$\Omega'(G,1)=\sum_c m\cdot c=e=|E(G)| \tag{14}$$

$$\Theta'(G,1)=\sum_c m\cdot c^2 \tag{15}$$

$$\Pi'(G,1)=\sum_c m\cdot c\cdot(e-c) \tag{16}$$

Reformulating (16) taking into account (2) and (11) to (13), we can write:

$$\Pi'(G,1)=e^2-\sum_c m\cdot c^2=\{[\Omega'(G,x)]^2-\Theta'(G,x)\} \tag{17}$$

Comparing (17) with (2) one can observe that $\sum_e N(e)$ and $\sum_c m\cdot c^2$ both evaluate equidistant edges in G.

On the other hand, the Cluj-Ilmenau[10] index, $CI=CI(G)$, is calculable from Omega[17] polynomial as:

$$CI(G)=\{[\Omega'(G,1)]^2-[\Omega'(G,1)+\Omega''(G,1)]\} \tag{18}$$

It is easily seen that, for a single *qoc*, one calculates the polynomial: $\Omega(G,x)=x^c$ and $CI(G)=c^2-(c+c(c-1))=0$.

There exist graphs for which *CI* equals *PI* (or its $\Pi'(G,1)$ analogue). Applying definition (18), *CI* is calculated as:

$$CI(G)=\left(\sum_c m\cdot c\right)^2-\left[\sum_c m\cdot c+\sum_c m\cdot c\cdot(c-1)\right]=e^2-\sum_c m\cdot c^2=PI(G) \tag{19}$$

The two indices *CI* and *PI* will show identical values if the edge equidistance evaluation in the graph involves only the locally parallel edges, condition (5); this is obeyed in partial cubes. Next, *PI* will be equal to $\Pi'(G,1)$ if only the relations (5) and (6) are involved. Planar polyhex graphs such as acenes A_n and phenacenes Ph_n (Table 2) show identical values for the three indices derived from the Omega and *PI*-type polynomials. Analytical formulas for the Omega and related polynomials, in these two classes of polyhex molecular graphs were given eswhere.[9]

Table 2. Counting polynomials in acenes A_n, and phenacenes Ph_n

	Omega	CI	$\Pi(G,x) = PI(G,x)$	$\Pi'(G,1) = PI$
A3	$6x^2 + x^4$	**216**	$4x^{12} + 12x^{14}$	**216**
A4	$8x^2 + x^5$	**384**	$5x^{16} + 16x^{19}$	**384**
A5	$10x^2 + x^6$	**600**	$6x^{20} + 20x^{24}$	**600**
Ph3	$5x^2 + 2x^3$	**218**	$6x^{13} + 10x^{14}$	**218**
Ph4	$6x^2 + 3x^3$	**390**	$9x^{18} + 12x^{19}$	**390**
Ph5	$7x^2 + 4x^3$	**612**	$12x^{23} + 14x^{24}$	**612**

Other examples are given on square (4,4) tori (Table 3).The torus in the first row is bipartite (but not a partial cube), so that only the *PI*-type indices show identical values. Conversely, the object in row 7 is non-bipartite but shows all the three indices of the same value. Concerning the relation $\Pi'(G,1)$: *PI*, the majority objects in Table 3 show identical values but, rows 3 and 5 give examples of objects showing different values; note that inequality (7) is here obeyed.

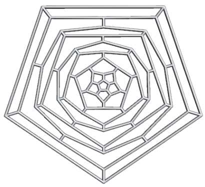
Table 3. Polynomials in square tiled (4,4) tori

	Torus	$\Omega(G,x)$		$\Pi'(G,x)$		$PI(G,x)$	
	(4,4)		CI		$\Pi'(G,1)$		PI
1	T[6,10]	$10x^6+6x^{10}$	13440	$60x^{100}+60x^{108}$	12480	$60x^{100}+60x^{108}$	12480
2	TWH2D[6,10]	$6x^{10}+2x^{30}$	12000	$60x^{96}+60x^{102}$	11880	$60x^{96}+60x^{102}$	11880
3	**TWH3D[6,10]**	$6x^{10}+x^{60}$	10200	$\mathbf{120x^{110}}$	**13200**	$\mathbf{60x^{108}+60x^{110}}$	**13080**
4	TWH6D[6,10]	$6x^{10}+2x^{30}$	12000	$60x^{92}+60x^{94}$	11160	$60x^{92}+60x^{94}$	11160
5	**TWV1D[6,10]**	$10x^6+x^{60}$	10440	$\mathbf{60x^{102}+60x^{114}}$	**12960**	$\mathbf{60x^{100}+60x^{114}}$	**12840**
6	TWV2D[6,10]	$10x^6+2x^{30}$	12240	$60x^{94}+60x^{104}$	11880	$60x^{94}+60x^{104}$	11880
7	**TWV3D[6,10]**	$\mathbf{10x^6+3x^{20}}$	***12840***	$\mathbf{60x^{100}+60x^{114}}$	***12840***	$\mathbf{60x^{100}+60x^{114}}$	***12840***

Another example is the pcu cubic lattice,[9] which is precisely a partial cube (in our terms, a co-graph) and the strips represent orthogonal cuts oc; it means that all the three relations (8) to (10) are valid. In such a lattice, all the three indices show the same value and the results appear to imply relations (5) and (6).

3. Main Results

The aim of this section is to compute the counting polynomials of equidistant (Omega and Theta polynomials) and non-equidistant (*PI*-type polynomials) edges of an infinite family F_n of fullerenes with $10n$ carbon atoms and $15n$ bonds (the graph G_2, Figure 2 is n=8).



G_2

Figure 2. The graph of fullerene F_n , n=8

By Figure 3, there are six distinct cases of qoc strips:

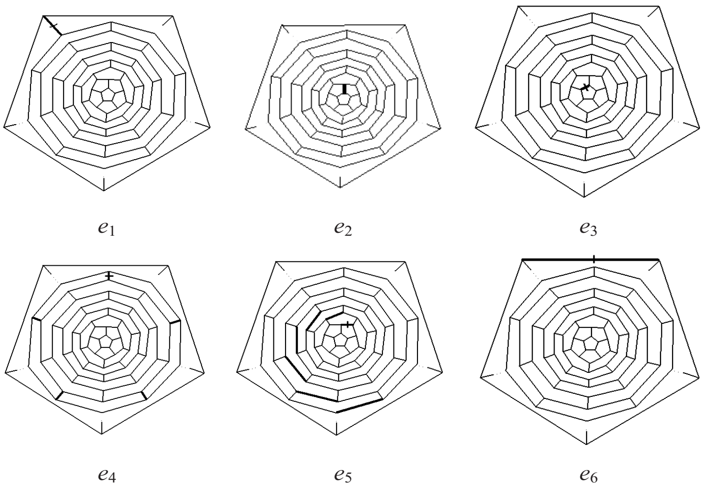


Figure 3. The **qoc** strips of edges e_1, e_2, …, e_6 in G_2

We denote the corresponding edges by e_1, e_2, …, e_6. One can see that $|C(e_1)| = |C(e_2)| = |C(e_3)| = |C(e_6)| = 1$, $|C(e_4)| = 5$ and $|C(e_5)| = n - 1$. On the other hand there are five similar edges for each of edges e_1, e_2, e_3 and e_6. There are n–2 edges similar to e_4 and 10 edges similar to e_5. Therefore,

$$\Omega(F_n, x) = 20 \cdot x + (n-2) \cdot x^5 + 10 \cdot x^{(n-1)} \quad (20)$$

By Figure 4, for $n \geq 10$, there are ten separate edges f_1, f_2, …., f_{10} that the number of equidistant edges are different. By this figure, one can see that $N(f_1) = N(f_2) = N(f_9) = 16$, $N(f_3) = N(f_4) = 15n - 40$, $N(f_5) = 5$, $N(f_6) = 13$, $N(f_7) = 14$, $N(f_8) = 15$ and $N(f_{10}) = 18$.

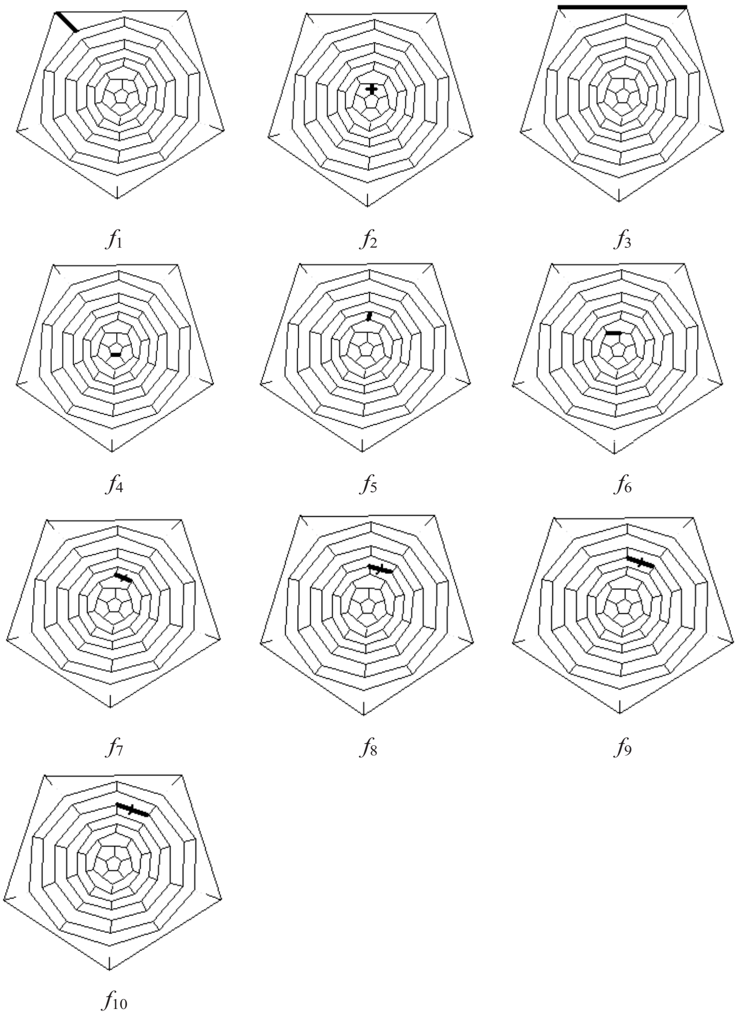


Figure 4. The equidistant edges $f_1, f_2, \ldots, f_{10}$ in G_2

There are five similar edges for each of edges f_1, f_2, f_3 and f_4. There are also $5(n-2)$ edges similar to f_5, 20 edges similar to f_6, f_7, f_8, f_9, and $10(n-9)$ edges similar to f_{10}. Therefore, for $n \geq 10$ we have (see also relation (4)):

$$PI(F_n, x) = 5(n-2) \cdot x^{15n-5} + 20 \cdot x^{15n-13} + 20 \cdot x^{15n-14} + 20 \cdot x^{15n-15} + 30 \cdot x^{15n-16} + 10(n-9) \cdot x^{15n-18} + 10 \cdot x^{40}$$

$$= \cdot \; - + \cdot \; - + \cdot \; - + \cdot \; - + \cdot \; - + \cdot \; - + \; - \cdot \; -$$

(21')

In version of relations (5) and (6) (Diudea) the polynomial is:

$$\Pi(F_n, x) = 10 \cdot x^{15n-1} + 5(n-2) \cdot x^{15n-5} + 10 \cdot x^{15n-6} + 20 \cdot x^{15n-10} + 20 \cdot x^{15n-12} + 20 \cdot x^{15n-14} + 20 \cdot x^{15n-16} + 10(n-9) \cdot x^{15n-18} \tag{22}$$

Correspondingly, the equidistant edges are counted by the Theta polynomial as:

$$\Theta(A_n, x) = 10 \cdot x^1 + 5(n-2) \cdot x^5 + 10 \cdot x^6 + 20 \cdot x^{10} + 20 \cdot x^{12} + 20 \cdot x^{14} + 20 \cdot x^{16} + 10(n-9) \cdot x^{18} \tag{23}$$

Table 4 lists the *PI* polynomial of F_n for $n \leq 9$.

Table 4. Counting polynomials and indices of eight sporadic cases.

F_n	*PI* Polynomial	*PI*
	PI Polynomial (eq 4)	
C_{20}	$30x^{22}$	660
C_{30}	$5x^{40}+20x^{36}+20x^{32}$	1560
C_{40}	$10x^{55}+30x^{50}+10x^{44}+10x^{36}$	2850
C_{50}	$15x^{70}+40x^{64}+10x^{59}10x^{40}$	4600
C_{60}	$20x^{85}+30x^{78}+20x^{77}+10x^{74}+10x^{40}$	6720
C_{70}	$25x^{100}+40x^{92}+20x^{91}+10x^{89}+10x^{40}$	9290
C_{80}	$30x^{115}+20x^{107}+30x^{106}+20x^{105}+10x^{104}+10x^{40}$	12310
C_{90}	$35x^{130}+30x^{119}+20x^{122}+20x^{121}+20x^{120}+10x^{40}$	15780
	PI Polynomial (eq 4`)	and
C_{20}	$30X^{24}$	720
C_{30}	$30X^{38}+10X^{39}+5X^{40}$	1730
C_{40}	$10X^{50}+20X^{51}+10X^{52}+10X^{54}+10X^{55}$	3130
C_{50}	$50X^{65}+25X^{70}$	5000
C_{60}	$30X^{78}+20X^{79}+10X^{80}+30X^{85}$	7270
C_{70}	$40X^{92}+20X^{93}+10X^{95}+35X^{100}$	9990
C_{80}	$20X^{105}+10X^{106}+20X^{107}+20X^{108}+10X^{110}+40X^{115}$	13160
C_{90}	$20X^{119}+20X^{120}+20X^{122}+20X^{123}+10X^{125}+45X^{130}$	16780

	Π Polynomial (eqs (5) and (6))	$\Pi'(G,1)$
C_{20}	$30X^{28}$	840
C_{30}	$5X^{40}+20X^{41}+10X^{43}+10X^{44}$	1890
C_{40}	$30X^{54}+10X^{55}+10X^{56}+10X^{59}$	3320
C_{50}	$40X^{67}+10X^{69}+15X^{70}+10X^{74}$	5160
C_{60}	$50X^{80}+10X^{84}+20X^{85}+10X^{89}$	7430
C_{70}	$40X^{93}+20X^{95}+10X^{99}+25X^{100}+10X^{104}$	10150
C_{80}	$30X^{106}+20X^{108}+20X^{110}+10X^{114}+30X^{115}+10X^{119}$	13320
C_{90}	$20X^{119}+20X^{121}+20X^{123}+20X^{125}+10X^{129}+35X^{130}+10X^{134}$	16940
	Θ polynomial	
C_{20}	$30X^{2}$	60
C_{30}	$10X^{1}+10X^{2}+20X^{4}+5X^{5}$	135
C_{40}	$10X^{1}+10X^{4}+10X^{5}+30X^{6}$	280
C_{50}	$10X^{1}+15X^{5}+10X^{6}+40X^{8}$	465
C_{60}	$10X^{1}+20X^{5}+10X^{6}+50X^{10}$	670
C_{70}	$10X^{1}+25X^{5}+10X^{6}+20X^{10}+40X^{12}$	875
C_{80}	$10X^{1}+30X^{5}+10X^{6}+20X^{10}+20X^{12}+30X^{14}$	1080
C_{90}	$10X^{1}+35X^{5}+10X^{6}+20X^{10}+20X^{12}+20X^{14}+20X^{16}$	1285
	Ω polynomial	
C_{20}	$30X^{1}$	870
C_{30}	$20X^{1}+1X^{5}+10X^{2}$	1940
C_{40}	$20X^{1}+2X^{5}+10X^{3}$	3440
C_{50}	$20X^{1}+3X^{5}+10X^{4}$	5370
C_{60}	$20X^{1}+4X^{5}+10X^{5}$	7730
C_{70}	$20X^{1}+5X^{5}+10X^{6}$	10520
C_{80}	$20X^{1}+6X^{5}+10X^{7}$	13740
C_{90}	$20X^{1}+7X^{5}+10X^{8}$	17390

Conclusions

Counting equidistant edges is not a trivial task. At least two ways of evaluating the equidistance of edges were discussed and the corresponding conditions established. Thus, three versions of polynomials counting non-equidistant edges (*PI*-type polynomials) and two polynomials counting equidistant edges (Theta and Omega polynomials) were calculated for an infinite series of tubulenes/fullerenes derived from the dodecahedron C_{20}. The analytical formulas for these polynomials in the considered family of fullerenes were presented.

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References

1. Kroto H. W., Heath J. R., O'Brien S. C., Curl R. F., Smalley R.E. *Nature* **1985***, 318***,** 162.
2. Kroto H. W., Fichier J. E., Cox D. E, *The Fulerene*, Pergamon Press, New York, **1993**.
3. H. Hosoya, *Disc. Appl. Math*. **1988**, *19*, 239.
4. B. E. Sagan, Y. -N. Yeh, P. Zhang, *Int. J. Quantum Chem.*, **1996**, *60*, 959.
5. A. R. Ashrafi, B. Manoochehrian, H. Yousefi-Azari, *Util. Math*., **2006**, *71*, 97.
6. B. Manoochehrian, H. Yousefi-Azari, A. R. Ashrafi, *MATCH Commun. Math. Comput. Chem.,* **2007**, *57*, 653.
7. P. V. Khadikar, *Nat. Acad. Sci. Letters,* **2000**, *23*, 113.
8. P. E. John, P. V. Khadikar, J. Singh, *J. Math. Chem*., **2007**,*42*, 37.
9. M. V. Diudea, S. Cigher, P. E. John, *MATCH Commun. Math. Comput. Chem.*, **2008**, *60*, 237.
10. P. E. John, A. E. Vizitiu, S. Cigher, M. V. Diudea, *MATCH Commun. Math. Comput. Chem.*, **2007**, *57*, 479.
11. D. Ž. Djoković, *J. Combin. Theory Ser. B*, **1973**, *14*, 263.
12. P. M. Winkler, *Discrete Appl. Math*.,**1984**, *8*, 209.
13. S. Ovchinikov, arXiv: 0704.0010v1 [math CO] 31 Mar 2007.
14. S. Klavžar, *MATCH Commun. Math. Comput. Chem.*, **2008**, *59*, 217.
15. M. V. Diudea, S. Cigher, A. E. Vizitiu, O. Ursu, P. E. John, *Croat. Chem. Acta*, **2006**, *79*, 445.
16. A. E. Vizitiu, S. Cigher, M. V. Diudea, M. S. Florescu, *MATCH Commun. Math. Comput. Chem.*, **2007**, *57*, 457.
17. M. V. Diudea, *Carpath. J. Math*., **2006,** *22*, 43.