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OMEGA AND RELATED POLYNOMIALS IN NANOSTRUCTURES

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Abstract. Omega polynomial was proposed by Diudea (Omega Polynomial, *Carpath. J. Math.*, **2006**, *22*, 43-47) to count opposite, topologically parallel, edges in graphs, particularly to describe the polyhedral nanostructures.

Basic definitions are given and clear relations with other three related polynomials are discussed. These relations are supported by close formulas and appropriate examples.

Close formulas for the calculation of Omega and its relative polynomials and derived single numbers, in several classes of nanostructures are given.

1. INTRODUCTION

A counting polynomial can be written as $P(x) = \sum_k m(k) \cdot x^k$, with the exponents showing the extent of partitions $p(G)$, $\cup p(G) = P(G)$ of a graph property $P(G)$ while the coefficients $m(k)$ are related to the number of partitions of extent k.

Hosoya [1, 2] was the first who introduced the counting polynomials in the Mathematical Chemistry literature: the Z-polynomial (counting the sets of independent edge) and Wiener polynomial (latter called Hosoya polynomial[3,4] which counts the distances in the graph). This author also proposed the sextet polynomial [5, 6] to count the resonant rings in a benzenoid molecule. Other counting polynomials are the independence polynomial [7-9], domino [10] star [11] , and clique [12] polynomials. More about polynomials the reader can find in [13].

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Some distance-related properties can be expressed in the polynomial form, with coefficients calculable from the layer and shell matrices.[14-17] These matrices are built up according to the vertex distance partitions of a graph, as provided by the TOPOCLUJ software package [18].The most important, in this approach, is the evaluation of the Hosoya $H(x)$ polynomial coefficients from the layer of counting LC matrix. The aim of this paper is to give a unified approach to these polynomials and derived invariants.

2. DEFINITIONS

Let $G=(V(G),E(G))$ be a connected graph, with the vertex set $V(G)$ and edge set $E(G)$. Two edges $e=(u,v)$ and $f=(x,y)$ of G are called *codistant* (briefly: *e co f*) if the notation can be selected such that [19]

$$d(v,x)=d(v,y)+1=d(u,x)+1=d(u,y)\,, \qquad (1)$$

where d is the usual shortest-path distance function. The above relation *co* is reflexive (*e co e*) and symmetric (*e co f*) for any edge e of G but in general is not transitive.

A graph is called a *co-graph* if the relation *co* is also transitive and thus an equivalence relation.

Let $C(e):=\{f \in E(G);\, f\ co\ e\}$ be the set of edges in G that are codistant to $e \in E(G)$. The set $C(e)$ can be obtained by an orthogonal edge-cutting procedure: take a straight line segment, orthogonal to the edge e, and intersect it and all other edges (of a polygonal plane graph) parallel to e. The set of these intersections is called an *orthogonal cut* (*oc* for short) of G, with respect to e.

If G is a *co-graph* then its orthogonal cuts $C_1, C_2, ..., C_k$ form a partition of $E(G)$: $E(G)=C_1 \cup C_2 \cup ... \cup C_k$, $C_i \cap C_j = \varnothing, i \neq j$.

A subgraph $H \subseteq G$ is called *isometric*, if $d_H(u,v)=d_G(u,v)$, for any $(u,v)\in H$; it is *convex* if any shortest path in G between vertices of H belongs to H. The n-cube Q_n is the graph whose vertices are all binary strings of length n, two strings being adjacent if they differ in exactly one position.[20] The distance function in the n-cube is the Hamming distance: the distance between two vertices of Q_n is equal to the number of positions in which they differ. A hypercube can also be expressed as the Cartesian product: $Q_n = \Pi_{i=1}^{n} K_2$.

For any edge $e=(u,v)$ of a connected graph G let n_{uv} denote the set of vertices lying closer to u than to v: $n_{uv}=\{w \in V(G) \mid d(w,u)<d(w,v)\}$. It

follows that $n_{uv} = \{w \in V(G) \mid d(w,v) = d(w,u)+1\}$. The sets (and subgraphs) induced by these vertices, n_{uv} and n_{vu}, are called *semicubes* of *G*; the semicubes are *opposite* and disjoint ones. [21,22]

A graph *G* is bipartite if and only if, for any edge of *G*, the opposite semicubes define a partition of *G*: $n_{uv} + n_{vu} = v = |V(G)|$.

The relation *co* is related to ~ (Djoković[23]) and Θ (Winkler[24]) relations: [25] in a connected bipartite graph, $co = \sim = \Theta$. For two edges *e*=(*u*,*v*) and *f*=(*x*,y) of *G* the theta relation is defined as: $e \Theta f$ if $d(u,x)+d(v,y) \neq d(u,y)+d(v,x)$.

A connected graph *G* is a *co-graph* if and only if it is a *partial cube*, and all its semicubes are convex; relation co / Θ is then transitive [22].

Two edges *e* and *f* of a plane graph *G* are in relation *opposite, e op f,* if they are opposite edges of an inner face of *G*. Then *e co f* holds by the assumption that faces are isometric. The relation *co* is defined in the whole graph while *op* is defined only in faces/rings (see below), thus being included in relation *co*. Note that John *et al*.[19, 26] implicitly used the "*op*" relation in defining the Cluj-Ilmenau index *CI*.

Relation *op* will partition the edges set of *G* into *opposite* edge *strips ops*, as follows. (i) Any two subsequent edges of an *ops* are in *op* relation; (ii) Any three subsequent edges of such a strip belong to adjacent faces; (iii) In a plane graph, the inner dual of an *ops* is a path, an open or a closed one (however, in 3D networks, the ring/face interchanging will provide *ops* which are no more paths); (iv) The *ops* is taken as maximum possible, irrespective of the starting edge. The choice about the maximum size of face/ring, and the face/ring mode counting, will decide the length of the strip.

The Ω-polynomial [27] is defined on the ground of opposite edge strips $S_1, S_2, ..., S_k$ in the graph:

$$\Omega(x) = \sum_k x^{|S_k|} \qquad (2)$$

Similarly, a Θ -polynomial [21] can be defined on the co-distant edge sets C_k:

$$\Theta(x) = \sum_k x^{|C_k|} \qquad (3)$$

If the graph is a co-graph or a partial cube, the edge equidistance (see below) will be accounted for by only relation (1), regarding the parallel edges. In such graphs, the following is true

Proposition 1: *In a co-graph/partial cube, the sets of co-distant edges superimpose over the opposite edge strips and the equality* $|C_k| = |S_k|$ *holds for any integer k.*

Denoting by $m(s)$, or simply m, the number of opposite edge strips of cardinality/length $s=|S|$, then we can write [21], [22], [29-30]:

$$\Omega(x)=\sum_s m\cdot x^s \quad (4)$$

$$\Theta(x)=\sum_s ms\cdot x^s \quad (5)$$

$$\Pi(x)=\sum_s ms\cdot x^{e-s} \quad (6)$$

$$Sd(x)=\sum_s m\cdot x^{e-s} \quad (7)$$

In the above relations, $\Omega(x)$ and $\Theta(x)$ count *equidistant edges* in G while $\Pi(x)$ and $Sd(x)$ count non-equidistant edges. The Omega and Sadhana polynomials count each edge once while the other two count the corresponding sets for each edge, so that the polynomial coefficients are multiplied by s.

The first derivative (in x=1) can be taken as a graph invariant or topological index:

$$\Omega'(1)=\sum_s m\cdot s=e=\left|E(G)\right| \quad (8)$$

$$\Theta'(1)=\sum_s m\cdot s^2=\theta(G) \quad (9)$$

$$\Pi'(1)=\sum_s ms\cdot(e-s)=\Pi(G) \quad (10)$$

$$Sd'(1)=\sum_s m\cdot(e-s)=Sd(G) \quad (11)$$

An index, called Cluj-Ilmenau [19] $CI(G)$, was defined on $\Omega(x)$:

$$CI(G)=\left\{[\Omega'(1)]^2-[\Omega'(1)+\Omega''(1)]\right\} \quad (12)$$

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

(a) The equidistance of (topologically) parallel edges, as defined by eq (1); since *co* is a particular case of *eqd* relation, a relation to account for the perpendicular edges in G, is to be added (Diudea [21, 28]) to the relation (1):

$$d(u,x)=d(u,y)=d(v,x)=d(v,y) \quad (13)$$

(b) The distance from a vertex z to an edge $e=(u,v)$ is taken as the minimum distance (Ashrafi [28]) between the given point and the two endpoints of e:

$$d(z,e)=\min\{d(z,u),d(z,v)\} \quad (14)$$

Then, the edge $e=(u,v)$ and $f=(x,y)$ are in relation *e eqd f* if:

$$d(x,e)=d(y,e) \text{ and } d(u,f)=d(v,f) \quad (15)$$

Relations (1)&(13) are stronger than relations (14)&(15): in bipartite graphs they superimpose to each other but not in general graphs (see below).

The problem of equidistance of vertices was firstly put by Gutman when defined the Szeged index [31] *SZ*(*G*) of which calculation leaves out the equidistant vertices. Similarly, the Khadikar's *PI*(*G*) (Padmakar-Ivan) index [32] does not count the equidistant edges. According to Ashrafi's notations [33], *PI*(*G*) can be written as:

$$PI_e(G) = PI_e'(1) = \sum_{e \in E(G)} \left[n(e,u) + n(e,v) \right] - m(u,v) \qquad (16)$$

where $n(e,u)$ is the number of edges lying closer to the vertex u than to the vertex and $m(u,v)$ is the number of equidistant edges from u and v. This index can be calculated as the first derivative, in x=1, of the polynomial defined by Ashrafi [33] as:

$$PI_e(x) = \sum_{e \in E(G)} x^{n(e,u)+n(e,v)} \qquad (17)$$

3. PROPERTIES OF COUNTING POLYNOMIALS AND DERIVED INDICES

As stated in Proposition 1, in co-graphs/partial cubes, the sets of co-distant edges superimpose over the opposite edge strips and the equality $|C_k| = |S_k|$ holds for any integer k. It follows that in co-graphs s takes the same value in Omega and its related polynomials (relations (4) to (7)).

Proposition 2. *In co-graphs/partial cubes, the equality* $CI(G) = \Pi(G)$ *holds.*

This can be demonstrated by expanding definition (12), *CI* calculation leading to $\Pi(G)$ [21, 22]:

$$CI(G) = \left(\sum_s m \cdot s\right)^2 - \left[\sum_s m \cdot s + \sum_s m \cdot s \cdot (s-1)\right] = e^2 - \sum_s m \cdot s^2 = \Pi(G) \qquad (18)$$

Relation (25/18) is valid only in the hypothesis $|C_k| = |S_k|$, which provides the same value for the exponent s and this is achieved only in co-graphs/partial cubes.

A graph, of which $\Theta(x)$ can be written exactly in the terms of $\Omega(x)$, according to the pair of relations {(4)&(5)}, will precisely show the equality $CI(G) = \Pi(G)$ according to (25). This equality can, however, appear even the pair relations {(4)&(5)} are not related. The relatedness of the two polynomials (and identity $CI(G) = \Pi(G)$) is provided rather by the equality of cardinalities $|S_k| = |C_k|$ than by the corresponding sets superposition $\{S_k\} \equiv \{C_k\}$, the condition {(4)&(5)} being thus necessary but not sufficient in order a graph to be declared *co*-graph/partial cube. Finally, the transitivity of *ops*/*ocs* must be proven.

A question about a simple and rapid criterion/condition to be used in order to decide if a given bipartite graph is a *co*-graph (or a partial cube) can be raised. Unfortunately, no such a condition is known and, in fact, such a condition would be a big breakthrough in the area of metric graph theory. In the papers [34, 35], two algorithms of the complexity O(*mn*) for recognizing co-graphs have been developed, where *n* is the order and *m* the size of a given graph. (Note that in a co-graph, *m*=O(*n* log *n*).) Recently Eppstein [36], using some sophisticated computational tricks, reduced the complexity to $O(n^2)$. In some special cases the complexity can be further reduced, see [37], but in general a (close to) linear criterion does not seem realistic.

In graphs, other than co-graphs or partial cubes, however $|S_i| \neq |C_k|$ and the pair relations ((4)&(5)) are no more related. As a consequence, in general graphs, $CI(G) \neq \Pi(G)$. This appears because the *edge equidistance eqd* relation includes both the *parallel* (*co* and *op* relations) and *perpendicular* (tetrahedron's) edges conditions.

In bipartite graphs, the only equality that holds is: $\Pi(G) = PI_e(G)$, which, however, does not hold in general graphs. Since any partial cube is also a bipartite graph, then we can expand the previous double equality to the triple one

$$CI(G) = \Pi(G) = PI_e(G) \tag{19}$$

a relation which is true only in partial cubes/co-graphs. In the opposite, in general graphs, the following inequality holds

$$CI(G) \neq \Pi(G) \neq PI_e(G) \tag{20}$$

Now let us reformulate relation (10) function of (8) and (9) to write:

$$\Pi'(1) = e^2 - \sum_s m \cdot s^2 = \{[\Omega'(1)]^2 - \Theta'(1)\} = \Pi(G) = PI(G) \tag{21}$$

The first part of relation (21) and the last part of (18) as well, represent the formula proposed by John *et al*. [26] to calculate the Khadikar's Padmakar-Ivan *PI*(*G*) topological index [32] (which counts the non-equidistant edges) in bipartite graphs. This index equals *CI*(*G*) index only in co-graphs/partial cubes (see (19)).

Returning to the main definitions (relations (4) to (7) and (8) to (11)), we can find the relatedness of the discussed descriptors:

$$\Theta'(1) + \Pi'(1) = (\Omega'(1))^2 = e^2 \tag{22}$$

$$\Theta(1) = \Pi(1) = \Omega'(1) = e \tag{23}$$

$$Sd'(1) = \Omega'(1)\big(\Omega(1)-1\big) = e\big(\Omega(1)-1\big) \tag{24}$$

From (24), it appears that the first derivative (in x=1) of Sadhana polynomial is the product of the number of edges e=|E(G)| and the number of strips $\Omega(1)$ less one.

By definition, an *ops* starts/ends in either one even face/ring or two edges of odd-fold faces/rings; in the first case the ops is a cycle while in the second it is a path. In a planar bipartite graph, representing a polyhedron, all *ops* strips are cycles. [38]

There are graphs with a single *ops*, of length $s = e = |E(G)|$, which is precisely a *cycle* (called a Hamiltonian *ops* in ref. [38]). At the opposite side, there are graphs with s=1, namely graphs with either odd rings or with no rings, *i.e.*, tree graphs. For such graphs, minimal and maximal value, respectively, of *CI* is calculated:

$$\Omega(x)_{CI_{\min}} = 1 \cdot x^e \,;\; CI_{\min} = e^2 - (e + e(e-1)) = 0 \tag{25}$$

$$\Omega(x)_{CI_{\max}} = e \cdot x^1 \,;\; CI_{\max} = e^2 - (e+0) = e(e-1) \tag{26}$$

Among the graphs on v vertices, $CI_{\min}$ is provided by the complete bipartite graphs $K_{2,v\text{-}2}$ (with e=2(v-2)) while $CI_{\max}$ is given by the complete graphs K_v, (with e=v(v-1)/2)):

$$CI_{\min} = CI(K_{2,v-2}) = 0 \tag{27}$$

$$CI_{\max} = CI(K_v) = (1/4)v(v-1)(v^2 - v - 2) \tag{28}$$

4. EXAMPLES

The examples below will present the most interesting structures, from the point of view of the studied descriptors, considered here to bring complementary information on the graph topology, thus often all these descriptors are calculated.

4.1. *Degeneracy of $CI(G)$ and $\Pi(G)$.*

There exist plane bipartite graphs, which are *co*-graphs and for which $CI(G) = \Pi(G)$. This is the case of acenes and phenacenes, which are polyhex molecular structures. For these classes of structures and others, like phenylenes, spiranes, pyrenes and coronenes, analytical formulas, for calculating Omega and related polynomials, were presented in references [21], [39].

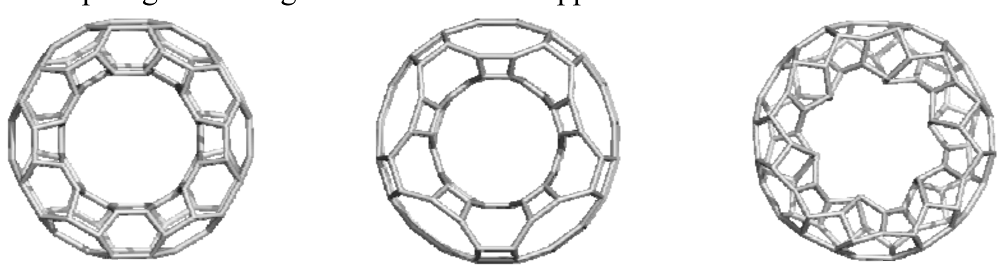
In tree graphs, Omega polynomial is either not defined or it simply counts the non-equidistant edges as self-equidistant ones, being included in the term of exponent s=1. In such graphs, $CI(G) = \Pi(G) = (v-1)(v-2)$ (a result known from Khadikar [40] – see also (26)) and the Omega and Theta polynomials show the same expression; the tree graphs behave as partial cubes.

There are distinct bipartite graphs, such as (4,4) tori in Table 1, with degenerate both $\Omega(x)$ polynomial and index *CI*(*G*) (rows 1 and 2, in italics), for which $\Pi(x)$ and $\Theta(x)$ are distinct. Next, there are bipartite graphs which shows degenerate $\{\Pi(G) \& \Theta(G)\}$ index values but distinct $\{\Pi(x) \& \Theta(x)\}$ polynomials (as the tori in Table 1, rows 1 and 3). Finally, there are non-bipartite graphs which show the equality $CI(G) = \Pi(G)$, as the true co-graphs (*e.g*., the torus in the forth row of Table 1.

Table 1. Polynomials in (4,4) tori: bipartite graphs for which $CI(G) \neq \Pi(G)$ (rows 1 to 3) and a non-bipartite graph showing $CI(G) = \Pi(G)$ (row 4).

	Torus	$\Omega(x)$		$\Pi(x)$		$\Theta(x)$	
	(4,4)		$CI(G)$		$\Pi(G)$		$\Theta(G)$
1	TWH2D[6,10]	***$6x^{10}+2x^{30}$***	***12000***	$60x^{96}+60x^{102}$	***11880***	$60x^{18}+60x^{24}$	***2520***
2	TWH6D[6,10]	***$6x^{10}+2x^{30}$***	***12000***	$60x^{92}+60x^{94}$	11160	$60x^{26}+60x^{28}$	3240
3	TWV2D[6,10]	$10x^{6}+2x^{30}$	12240	$60x^{94}+60x^{104}$	***11880***	$60x^{16}+60x^{26}$	***2520***
4	**TWV3D[6,10]**	**$10x^{6}+3x^{20}$**	**12840**	**$60x^{100}+60x^{114}$**	**12840**	**$60x^{6}+60x^{20}$**	**1560**

There are cases for which the equality $CI(G) = \Pi(G)$ is true despite the pair relations ((4)&(5)) are not related. Indeed, the coefficients in the pair $\{\Theta(x); \Pi(x)\}$ correspond to the product *m.s* (as in $\Omega(x)$), but the exponents differ from those in $\Omega(x)$, however the above equality holds. We consider this case as an accidental equality or a degeneracy of index values. The first two examples given in Figure 1 and Table 2 support the above statements.



T(6,3)H[8,12] T((4,8),3)V[8,20] T((5,7),3)H[8,12]

v=96; e=144 v=160; e=144 v=96; e=144

Figure 1. Tori calculated in Table 1

Table 2. Polynomials in bipartite and non-bipartite tori

T(6,3)H[8,12]; v=96; e=144; bipartite	
Polynomial	Index
$\Omega(x)=12x^4+4x^{24}$	$CI(G)=18240$
$Sd(x)=4x^{120}+12x^{140}$	$Sd(G)=2160$
$\Theta(x)=48x^8+96x^{22}$	$\Theta(G)=2496$
$\Pi(x)=96x^{122}+48x^{136}$	$\Pi(G)=18240$
$PI_e(x)=96x^{122}+48x^{136}$	$PI_e'(1)=18240$
T((4,8),3)V[8,20]; v=160; e=144; bipartite	
Polynomial	Index
$\Omega(x)=10x^8+8x^{10}+2x^{40}$	$CI(G)=52960$
$Sd(x)=2x^{200}+8x^{230}+10x^{232}$	Sd(G) = 4560
$\Theta(x)=80x^{16}+80x^{20}+80x^{22}$	$\Theta(G)=4640$
$\Pi(x)=80x^{218}+80x^{220}+80x^{224}$	$\Pi(G)=52960$
$PI_e(x)=80x^{218}+80x^{220}+80x^{224}$	$PI_e'(1)=52960$
T((5,7),3)H[8,12]; v=96; e=144; non-bipartite	
Polynomial	Index
$\Omega(x)=144x^1$	$CI(G)=20592$
$Sd(x)=144x^{143}$	$Sd(G)=20592=CI(G)$
$\Theta(x)=48x^6+36x^8+36x^{10}+24x^{11}$	$\Theta(G)=1200$
$\Pi(x)=24x^{133}+36x^{134}+36x^{136}+48x^{138}$	$\Pi(G)=19536$
$PI_e(x)=24x^{75}+12x^{102}+24x^{103}+12x^{108}+12x^{130}+36x^{132}+24x^{134}$	$PI_e'(1)=16320$

A third example in Figure 1 and Table 2 is a non-bipartite torus, covered by odd faces, in a ((5,7)3) tessellation. It is included here to illustrate the triple inequality $CI(G)\neq\Pi(G)\neq PI_e(G)$ and an extreme case of $\Omega(x)$, with a single term, of exponent 1 (see relation (26)).

4.2. *Planar 3D bipartite, non co-graphs.*

There are bipartite 3D graphs for which $CI(G)\neq\Pi(G)$. This is the case of the cage in Figure 3b which is bipartite but represents a *non-isometric subgraph* of a partial cube, which is the cubic lattice in Figure 2a: the red edges are not *co*-distant to each other, despite they both belong to the same *ops,* thus $CI(G)\neq\Pi(G)$. Conversely, Figure 2a represents precisely a partial cube (in our terms, *a co-graph*) and their *ops* represent orthogonal cuts *oc*; as a consequence $CI(G)=\Pi(G)$.

To the list of 3D bipartite graphs which are non *co*-graphs and obey the inequality $CI(G)\neq\Pi(G)$ we add the toroidal lattices of even faces. Only exceptional tori show $CI(G)=\Pi(G)$ values (Tables 1 and 2).

(a) (b)

(a)

$\Omega(x)=6x^9;\Omega(1)=54$; $CI=2430$; (R[4])

$\Theta(x)=54x^9$; $\Theta'(1)=486$

$\Pi(x)=54x^{45}$; $\Pi'(1)=2430$

$Sd(x)=6x^{54-9}=6x^{45}$; $Sd'(1)=270$

$PI_e(x)=54x^{45}$; $PI_e(1)=2430$

(b)

$\Omega(x)=6x^8;\Omega'(1)=48;\ CI=1920\ (f_4)$

$\Theta(x)=24x^8+24x^{10}$; $\Theta'(1)=432$

$\Pi(x)=24x^{38}+24x^{40}$; $\Pi'(1)=1872$

$Sd(x)=6x^{48-8}=6x^{40}$; $Sd'(1)=240$

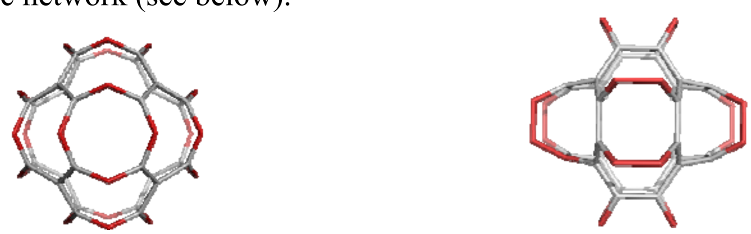
$PI_e(x)=24x^{38}+24x^{40}$; $PI_e{}'(1)=1872$

non-isometric subgraph (see edges in red)

Figure 2. 3D Bipartite graphs which are (left) or are not (right) co-graphs/partial cubes

4.3. *Non-partial cubes showing* $CI(G)=\Pi(G)$

The structures in Figure 3 behave as co-graphs/partial cubes, namely the equality $CI(G)=\Pi(G)$ holds. The units designed by the sequence of map operations [41-45] $Op_x(Q(C))$ are representations of the celebrate Dyck graph [46], built up on only octagonal faces/rings. The networks [47, 48]constructed by these units show no more co-graph/partial cube behavior, in the opposite to the *pcu* cubic network (see below).



***Op*(*Q*(C)_56; R[8]=18;**

$\Omega(x)=4x^6+6x^8;\Omega'(1)=e=72;CI=4656$

***Op*$_{2a}$(*Q*(C))_56; R[8]=18;**

$\Omega(x)=9x^8;\Omega'(1)=e=72;CI=4608$

$\Pi(x) = 24x^{66} + 48x^{64}; \Pi'(1) = 4656$
$\Theta(x) = 24x^{6} + 48x^{8}; \Theta'(1) = 528$
$Sd(x) = 4x^{66} + 6x^{64}; Sd'(1) = 648$
$PI_e(x) = 24x^{66} + 48x^{64}; PI_e{}'(1) = 4656$

$\Pi(x) = 72x^{64}; \Pi'(1) = 4608$
$\Theta(x) = 72x^{8}; \Theta'(1) = 576$
$Sd(x) = 9x^{64}; Sd'(1) = 576$
$PI_e(x) = 72x^{64}; PI_e{}'(1) = 4608$

Figure 3. Non-cubes which are co-graphs

4.4. Formulas for counting polynomials in pcu cubic lattice

Formulas for the evaluation of the discussed counting polynomials in the *pcu* cubic lattice, of dimensions *(a,b,c)* are presented in Table 3. Examples of application of these formulas are also included.

Table 3. Formulas for edge counting polynomials in pcu cubic C(a,b,c) network[21]

	Type	Polynomial (edge counting)
1	ops	$\Omega(\mathrm{C}(a,b,c),x) = a \cdot x^{(b+1)(c+1)} + b \cdot x^{(a+1)(c+1)} + c \cdot x^{(a+1)(b+1)}$ $\Omega(\mathrm{C}(a,a,c),x) = 2a \cdot x^{(a+1)(c+1)} + c \cdot x^{(a+1)^2}$ $\Omega(\mathrm{C}(a,a,a),x) = 3a \cdot x^{(a+1)^2}$ $\Omega'(C(a),1) = e = 3a(a+1)^2$ $\Omega''(C(a),1) = 3a^2(a+1)^2(a+2)$ $CI(C(a)) = 3a(3a-1)(a+1)^4$ $v(C(a)) = (a+1)^3$; $s(C(a)) = (a+1)^2$
2	non-ops	$Sd(C(a),x) = m \cdot x^{e-s} = 3a \cdot x^{(a+1)^2(3a-1)}$ $Sd'(C(a),1) / \Omega'(C(a),1) = (3a-1)$ $Sd'(C(a),1) / \Omega'(C(a),1) = m(e-s)/ms = (e/s)-1$ $e/s = 3a$
3	non-equi-distance	$\Pi(C(a)) = PI_e(C(a),x) = ms \cdot x^{e-s} = 3a(a+1)^2 \cdot x^{(a+1)^2(3a-1)}$ $\Pi'(C(a),1) = PI_e{}'(C(a),1) = e(e-s) = 3a(3a-1)(a+1)^4 = CI(C(a))$
4	equi-distance	$\Theta(C(k),x) = ms \cdot x^{s} = 3a(a+1)^2 \cdot x^{(a+1)^2}$ $\Theta'(C(a),1) = 3a(a+1)^4$ $\Pi'(C(a),1) / \Theta(C(a),1) = (3a-1)$

5		$v=\|V(G)\|=(a+1)^3$; $e=\|E(G)\|=3a(a+1)^2$
6	Examples	
	a=4	$\Omega(x)=12x^{25}; \Omega'(1)=300; CI=82500$ $Sd(x)=12x^{275}; Sd'(1)=3300$ $\Pi(x)=300x^{275}; \Pi'(1)=82500$ $\Theta(x)=300x^{25}; \Theta'(1)=7500$
	a=5	$\Omega(x)=15x^{36}; \Omega'(1)=540; CI=272160$ $Sd(x)=15x^{504}; Sd'(1)=7560$ $\Pi(x)=540x^{504}; \Pi'(1)=272160$ $\Theta(x)=540x^{36}; \Theta'(1)=19440$

Note that, in [39] $\Pi(x)$ was denoted by $N\Omega(x)$. The polynomial calculations were done by the software programs developed at TOPO Group Cluj: Omega Counter [49] and Nano Studio [50].

Omega polynomial found applications in the topological description of complex nanostructures with polyhedral covering [51-56]. In tubular/toroidal structures this polynomial accounts for the spirality and ring distribution. The coefficient at exponent s=1 has found to have good ability in predicting the heat of formation and strain energy in small fullerenes or the resonance energy in planar benzenoids [39], [57], [58].

CONCLUSIONS

Omega polynomial was designed to count the opposite topologically parallel edges in graphs, particularly to describe the polyhedral nanostructures. In three years, (2006-2009) 35 papers have been published or sent for publication by TOPO Group Cluj and other papers by abroad scientists, Omega polynomial already getting a scientific success. In this paper, its behavior and relatedness with other counting polynomials, in partial cubes and other graphs, is described. Appropriate examples were given.

References

1. Hosoya H., **Topological index. A newly proposed quantity characterizing the topological nautre of structural isomers of saturated hydrocarbons**, Bull. Chem. Soc. Japan, **44** (1971), 2332–2339.
2. Hosoya, H., **On some counting polynomials in chemistry**, Discrete Appl. Math., **19** (1988), 239–257.

3. Konstantinova, E. V., Diudea, M. V., **The Wiener polynomial derivatives and other topological indices in chemical research**, Croat. Chem. Acta, **73** (2000), 383–403.
4. Gutman, I., Klavžar, S., Petkovšek, M., Žigert, P., **On Hosoya polynomials of benzenoid graphs**, MATCH Commun. Math. Chem. **43** (2001), 49–66.
5. Hosoya, H., Yamaguchi, T., **Sextet polynomial: A new enumeration and proof technique for the resonance theory applied to the aromatic hydrocarbons,** Tetrahedron Lett., **52** (1975), 4659–4662.
6. Hosoya, H., **Clar's aromatic sextet and sextet polynomial**, Topics Curr. Chem., **153** (1990), 255–272.
7. Gutman, I., Hosoya, H., **Molecular graphs with equal Z-counting and Independence polynomials**, Z. Naturforsch., **45a** (1990), 645-648.
8. Gutman, I., **Topological properties of benzenoid systems. Merrifield-Simmons indices and Independence polynomials of unbranched catafusenes**, Rev. Roum. Chim., **36** (1991), 379-388.
9. Stevanović, D., **Graphs with palindromic Independence polynomial**, Graph Theory Notes New York, **34** (1998), 31-36.
10. Motoyama, A., Hosoya, H. King., **Domino polynomials for polyomino graphs**, J. Math. Phys., **18** (1977), 1485-1490.
11. Farrell, E. J., De Matas, C., **On Star polynomials, graphical partitions and reconstruction**, Int. J. Math. Math. Sci., **11**, (1988), 87-94.
12. Hoede, C., Li, X. L., **Clique polynomials and Independent Set polynomials of graphs**, Discr. Math., **125** (1994), 219-228.
13. Diudea, M. V., Gutman, I., Jäntschi, L., **Molecular topology**, NOVA, New York, 2002.
14. Diudea, M. V., **Layer matrices in molecular graphs**, J. Chem. Inf. Comput. Sci., **34** (1994), 1064-1071.
15. Diudea, M. V., Ursu, O., **Layer Matrices and distance property descriptors**, Indian J. Chem., **42A** (2003), 1283-1294.
16. Diudea, M. V., **Hosoya polynomial in tori**, MATCH Commun. Math. Comput. Chem., **45** (2002), 109-122.
17. Stefu, M., Diudea, M. V., **Distance counting in tubes and tori: Wiener index and Hosoya polynomial**, in: Diudea, M. V. (Ed.), *Nanostructures, Novel Architecture*, Nova, New York, (2005), 127-165.

18. Ursu, O., Diudea, M. V., **TOPOCLUJ software program**, Babes-Bolyai University, Cluj, 2005; Available, on line at http://chem.ubbcluj.ro/~diudea
19. John, P. E., Vizitiu, A. E., Cigher, S., Diudea, M. V., **CI index in tubular nanostructures**, MATCH Commun. Math. Comput. Chem., **57** (2007), 479-484.
20. Harary, F., **Graph theory**, Addison-Wesley, Reading, MA, (1969).
21. Diudea, M. V., Cigher, S., John, P. E., **Omega and related counting polynomials**, MATCH Commun. Math. Comput. Chem., **60** (2008), 237-250.
22. M. V. Diudea and S. Klavžar, **Omega polynomial revisited**, Carpath. J. Math., (2009), accepted.
23. Djoković, D. Ž., **Distance preserving subgraphs of hypercubes**, J. Combin. Theory Ser. B, **14** (1973), 263-267.
24. Winkler, P.M., **Isometric embedding in products of complete graphs**, Discrete Appl. Math., **8** (1984), 209-212.
25. Klavžar, S., **Some comments on co graphs and CI index**, MATCH Commun. Math. Comput. Chem., **59** (2008), 217-222.
26. John, P. E., Khadikar, P. V., Singh, J., **A method of computing the PI index of benzenoid hydrocarbons using orthogonal cuts**, J. Math. Chem., **42** (2007), 37-45.
27. Diudea, M. V., **Omega polynomial**, Carpath. J. Math., **22** (2006), 43-47.
28. Ashrafi, A. R., Jalali, M., Ghorbani, M., Diudea, M. V., **Computing PI and Omega polynomials of an infinite family of fullerenes**, MATCH Commun. Math. Comput. Chem., **60** (2008), 905-916.
29. Ashrafi, A. R., Ghorbani, M., Jalali, M., **Computing Sadhana polynomial of V-phenylenic nanotubes and nanotori**, Indian J. Chem., **47A** (2008), 535–537.
30. Diudea, M. V., Vizitiu, A. E., Mirzargar, M., Ashrafi, A. R., **Sadhana polynomial in nano-dendrimers**, Carpath. J. Math. (2009), accepted.
31. Gutman, I., **A formula for the Wiener number of trees and its extension to graphs containing cycles**, Graph Theory Notes of New York, **27** (1994), 9-15.
32. Khadikar, P. V., **On a Novel Structural Descriptor PI**, Nat. Acad. Sci. Lett., **23** (2000), 113-118.
33. Ashrafi, A. R., Manoochehrian, B., Yousefi-Azari, H., **On the PI polynomial of a graph**, Util. Math., **71** (2006), 97-108.

34. Aurenhammer, F., Hagauer, J., **Recognizing binary Hamming graphs in O(n^2logn) time**, Math. Systems Theory, **28** (1995), 387-396.
35. Imrich W., Klavžar S., **A simple O(mn) algorithm for recognizing Hamming graphs**, Bull. Inst. Comb. Appl., **9** (1993), 45-56.
36. Eppstein, D., **Recognizing partial cubes in quadratic time**, 19th ACM-SIAM Symp. Discrete Algorithms, San Francisco, (2008), 1258-1266.
37. Brešar B.; Imrich W.; Klavžar S., **Fast recognition algorithms for classes of partial cubes**, Discrete Appl. Math., **131** (2003), 51-61.
38. Diudea, M. V.; Ilić, **A. Note on Omega polynomial**, Carpath. J. Math. **25** (2) (2009), 177-185.
39. Diudea, M. V.; Vizitiu A. E.; Janežič, D., **Cluj and related polynomials applied in correlating studies**, J. Chem. Inf. Model., **47** (2007), 864-874
40. Diudea, M. V.; Florescu, M. S.; Khadikar, P. V., **Molecular topology and its applications**, EFICON, Bucharest, (2006).
41. Diudea, M. V.; John, P. E.; Graovac, A.; Primorac, M.; Pisanski, T., **Leapfrog and related operations on toroidal fullerenes**, Croat. Chem. Acta, **2003**, *76*, 153-159.
42. Diudea, M. V., **Covering forms in nanostructures**, Forma (Tokyo), **19** (2004), 131-163.
43. Diudea, M. V.; Ştefu, M.; John, P. E.; Graovac, **A. Generalized operations on maps**, Croat. Chem. Acta, **79** (2006), 355-362.
44. Ştefu, M.; Diudea, M. V.; John, P. E., **Composite operations on maps**, Studia Univ. "Babes-Bolyai", **50** (2005), 165-174.
45. Diudea, M. V., **Nanoporous carbon allotropes by septupling map operations**, J. Chem. Inf. Model., **45** (2005), 1002-1009.
46. Dyck, W., **Ueber Aufstellung und Untersuchung von Gruppe und Irrationalität regulärer Riemann'sher Flächen**, Mathematische Annalen, **17** (1880), 473-509.
47. Diudea, M. V., **Omega polynomial in all_R[8] lattices**, Iranian J. Math., (2009) , accepted.
48. Diudea, M. V.; Ilić, A., **Omega polynomial in crystal-like single-type face/ring networks**, Int. J. Chem. Model., (2009**),** accepted.
49. Cigher, S., Diudea, M. V., **Omega polynomial counter**, "Babes-Bolyai" Univ., 2007.
50. Cs. L. Nagy and M. V. Diudea, **Nano-Studio software**, *"Babes-Bolyai"* Univ., 2009.

51. Diudea, M. V.; Cigher, S.; Vizitiu, A. E.; Ursu, O.; John, P. E., **Omega polynomial in tubular nanostructures**, Croat. Chem. Acta, **79** (2006), 445-448.
52. Vizitiu, A. E.; Cigher, S.; Diudea, M. V.; Florescu, M. S., **Omega polynomial in ((4,8)3) tubular nanostructures**, MATCH Commun. Math. Comput. Chem., **57** (2007), 457-462.
53. Vizitiu, A. E.; Diudea, M. V., **Omega and Theta polynomials in conical nanostructures**, MATCH Commun. Math. Comput. Chem., **60** (2008), 927-933.
54. Diudea, M. V., **Omega polynomial in twisted/chiral polyhex tori**, J. Math. Chem., **45** (2009), 309-315.
55. Diudea, M. V.; Vizitiu, A. E.; Gholaminezhad, F.; Ashrafi, A. R. **Omega polynomial in twisted (4,4) tori**, MATCH Commun. Math. Comput. Chem., **60** (2008), 945-953.
56. Diudea, M. V., **Omega polynomial in twisted ((4,8)3)R tori**, MATCH Commun. Math. Comput. Chem., **60** (2008), 935-944.
57. Diudea, M. V.; Cigher, S.; Vizitiu, A. E.; Florescu, M. S.; John, P. E., **Omega polynomial and its use in nanostructures description**, J. Math. Chem., **45** (2009), 316-329.
58. Diudea, M. V.; Nagy, Cs. L., **Periodic nanostructures**, Springer, (2007).

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