CARPATHIAN J. MATH.
20 (2009), No. 1, 177 - 185

Online version available at http://carpathian.ubm.ro
Print Edition: ISSN 1584 - 2851 Online Edition: ISSN 1843 - 4401

Note on Omega Polynomial

M. V. DIUDEA AND A. ILIĆ

ABSTRACT.
Omega polynomial, counting opposite edge strips *ops*, was proposed by Diudea to describe cycle-containing molecular structures, particularly those associated with nanostructures. In this paper, some theoretical aspects are evidenced and particular cases are illustrated.

1. INTRODUCTION

A counting polynomial can be written as:

$$P(G,x) = \sum_k m(G,k) \cdot x^k \tag{1.1}$$

with the exponents showing the extent of partitions $p(G)$, $\cup p(G) = P(G)$ of a graph property $P(G)$, while the coefficients $m(G,k)$ are related to the number of partitions of extent k.

In the Mathematical Chemistry literature, counting polynomials have been introduced by Hosoya in [15] and [16]: $Z(G,x)$ counts independent edge sets while $H(G,x)$ (initially called Wiener and later Hosoya [21] and [14]) counts the distances in the graph. Hosoya next proposed the sextet polynomial [18]–[17] for counting the resonant rings in a benzenoid molecule. More about polynomials the reader can find in [7].

Some distance-related properties can be expressed in polynomial form, with coefficients calculable from the layer and shell matrices [2]–[9]. These matrices are built up according to the vertex distance partitions of a graph, as provided by the TOPOCLUJ software package [26]. Nice results have been obtained in the evaluation of the coefficients of Hosoya $H(G,x)$ polynomial by using the layer of counting LC matrix.

2. DEFINITIONS

Let $G(V,E)$ be a connected bipartite graph, with the vertex set $V(G)$ and edge set $E(G)$. Two edges $e=(x,y)$ and $f=(u,v)$ of G are *codistant* e *co* f if they obey the relation [1], [19] :

$$d(v,x) = d(v,y)+1 = d(u,x)+1 = d(u,y) \tag{2.2}$$

If ″*co*″ is an equivalence relation in G, then the set of edges $C(G) = \{f \in E(G) \| f \text{ co } e\}$ is called an *orthogonal cut oc* of G and $E(G)$ is the union of disjoint orthogonal cuts: $E(G) = C_1 \cup C_2 \cup \ldots \cup C_k$, $C_i \cap C_j = \emptyset$ for $i \neq j$.

It is easily seen that ″*co*″ is a Θ relation, (Djoković-Winkler relation [13], [27]) and G is a *co-graph if and only if it is a partial cube*, a result due to Klavžar [20]. In a plane bipartite graph, an edge e is in the relation Θ with any opposite edge f if the faces of the plane graph are isometric. Then an orthogonal cut oc with respect to a given edge is the smallest subset of edges closed under this relation and $C(e)$ is precisely a Θ-class of G. A partial cube is always a bipartite graph, but the reciprocal is not true.

A set of opposite or topologically parallel edges within the same face/ring eventually forming a strip of adjacent faces, is called an *opposite edge strip ops*, which is a quasi-ortogonal cut *qoc* (i.e., the transitivity relation is not necessarily obeyed) [5].

By definition, an *ops* starts/ends in either (1) one even face/ring or (2) two edges of odd-fold faces/rings; in case (1), the ops is a cycle while in case (2) it is a path. In case of open structures, the open (or infinite) faces are equivalent to the odd faces [5].

Proposition 2.1. *Let G be a planar graph that represents a polyhedron with exactly k odd faces f_{odd}, insulated from each other. The family of ops strips contains a number of ops paths which is exactly half of the number of odd face edges $e_{odd}/2$.*

Proof. Consider an even face f_{even}. If an edge e belongs to an *ops*, then the opposite edge e' must also be in the same *ops*. Since the number of faces is finite, the *ops* ends, that means either a cycle is closed, or arrived at an odd face edge e_{odd}. Therefore, every ops path must have the ends in two edges belonging to either different odd faces (most often) or to the same odd face. Finally, by a simple counting argument, the number of *ops* paths is $np = e_{odd}/2$. The number e_{odd} is even, because the sum of all face sizes equals twice the number of edges. □

Corollary 2.1. *In a planar bipartite graph, representing a polyhedron, all ops strips are cycles.*

Received: 13.07.2009; In revised form: 04.09.2009; Accepted: 27.08.2009
2000 *Mathematics Subject Classification.* 05C10, 92E10, 05C12.
Key words and phrases. *Counting polynomial, opposite cuts, CI index, map operations.*

Let $m(G,s)$ be the number of *ops* of length s (i.e., the number of cut-off edges); for the sake of simplicity, $m(G,s)$ can be written as m. The Omega polynomial is defined as [5]:

$$\Omega(G,x) = \sum_s m(G,s) \cdot x^s. \tag{2.3}$$

The first derivative (in $x=1$) equals the number of edges in the graph:

$$\Omega'(G,x) = \sum_s m \cdot s = e = |E(G)|. \tag{2.4}$$

A topological index, called Cluj-Ilmenau [19] $CI = CI(G)$, was defined on Omega polynomial:

$$CI(G) = \Omega'(G,1)^2 - (\Omega'(G,1) - \Omega''(G,1)). \tag{2.5}$$

3. Number of ops paths

In general, the odd faces can be non-insulated, with two extremes:

(1) The graph consists of all joined odd faces, like the Platonic solids (Tetrahedron T, Octahedron Oct, Icosahedron Ico and Dodecahedron Do, excepting Cube C); its *ops* are all paths of length 1, and $\Omega(G,x) = ex^1$, $np = e$, $CI = e(e-1)$, e being here the number of edges in G. It is also the case of a tree graph.

(2) A bipartite cycle-containing graph has a single *ops*; it is precisely a cycle (a Hamiltonian *ops*); $np = 1$, $\Omega(G,X) = 1 \cdot X^s$, $CI(G) = s^2 - (s + s(s-1)) = 0$. Examples will be given below.

(3) Most often, mixed cases appear; to evaluate *np*, according to the above proposition, some additional symbols are needed.
Denote the number of odd/even face edges by e_{odd} and e_{even} respectively. Next, the number of odd face edges lying inside the contour of joined odd faces is denoted by e_{odd_in} while that of the contour by e_{odd_ex}. The "in"-type edges are counted like in Case 1 (i.e., all joined odd faces) while the "ex"-type edges will give account for the number of *ops* paths (as presented in the above proposition): $np_{ex} = e_{odd\_ex}/2$. Thus, the total number of *ops* paths is as follows:

$$np(G) = e_{odd\_in} + e_{odd\_ex}/2. \tag{3.6}$$

The remaining Omega terms (if any) represent *ops* cycles, with the extreme case as in Case 2.

4. Examples

In this section, the above statements are illustrated.
Figure 1 presents a bipartite cycle-containing graph, showing a single *ops*, that is precisely a cycle *ops*.

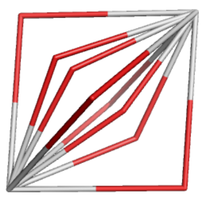


FIGURE 1. *A bipartite complete graph $K_{2,8}$; $\Omega(G,X) = 1X^{16}$; $CI(G) = 0$; Hamiltonian ops.*

Platonic objects show all odd faces, except the Cube. Table 1 presents the Omega polynomial, which shows a single term, at exponent unity, meaning all the path *ops* are internal (see above). The ring polynomial $R(G,X)$ is also given in tables, and CI index, as well.

TABLE 1. Omega and Ring polynomials in Platonics

	Structure	Ring	Omega	CI
1	T	$4X^3$	$6X^1$	30
2	Oct	$8X^3$	$12X^1$	132
3	Do	$12X^5$	$30X^1$	870
4	Ico	$20X^3$	$30X^1$	870
5	C	$6X^4$	$3X^4$	96

Some of the map operations [11]–[3], particularly the *Leapfrog* Le and *Capra* Ca, preserve the number of paths of the patterns in their transforms; the only change is in the exponent (i.e., the length of *ops*), which is multiplied by 3 and 7, in case of Le and Ca, respectively (Table 2).

TABLE 2. Map operations' transforms and Omega polynomial in Platonics

	Graph	Omega	CI
1	Ca(T)	$6X^7$	1470
2	Ca(Oct)	$12X^7$	6468
3	Ca(Do,Ico)	$30X^7$	42630
4	Le(T)	$6X^3$	270
5	Ca(Le(T))	$6X^{21}$	13230
6	Q(T)	$6X^2 + 3X^4$	504
7	Ca(Q(T))	$6X^{14} + 3X^{28}$	24696

When Le is iterated n-times (Figure 2a), the number of terms in Omega polynomial increases, but the first term preserves the original number of *ops* paths in the Platonic parent. If Ca is the second type operation (Figure 2b), it multiplies the exponents by 7. Table 3 gives examples, while here we give formulas for Omega polynomial in iterated $Le_n(T)$.

$$\Omega(Le_n(T), X) = a_1 \cdot X^{e_1} + a_2 \cdot X^{e_2}$$

$$a_1 = 6 \qquad a_2 = 3 \cdot \left(3^{\lfloor n/2 \rfloor} - 1\right) = \begin{cases} 3 \cdot (3^{n/2} - 1) & \text{if } n \text{ is even} \\ 3 \cdot (3^{(n-1)/2} - 1) & \text{if } n \text{ is odd} \end{cases}$$

$$e_2 = 2e_1 \qquad e_1 = 3^{\lfloor (n+1)/2 \rfloor} = \begin{cases} 3^{n/2} & \text{if } n \text{ is even} \\ 3^{(n+1)/2} & \text{if } n \text{ is odd} \end{cases}$$

The number of edges in $Le_n(T)$ is $\Omega'(Le_n(T), 1) = 2 \cdot 3^{n+1}$. Here, $\lfloor x \rfloor$ denotes the integer part of a real number x.

(a) $Le_3(T); v = 108$ (b) $Ca(Le_3(T)); v = 756$

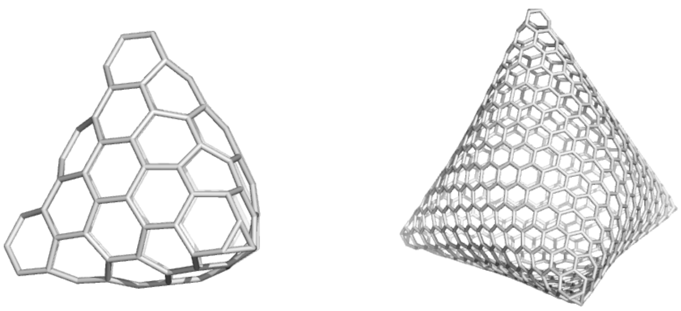


FIGURE 2. Non-chiral (a) and chiral (b) tetrahedral structures designed by iterated Le_n and (Le_n & Ca) map operations

The next examples refer to cages having all joint f_5-tuples, with only insulated even-fold faces (Table 4; Figure 3, column a); in such cases, no pure even face edges e_{even} exist and the number of all *ops* paths is larger than the number of all edges in G: $np > e/2$.

Finally, cages showing disjoint f_5-tuples are considered (Table 6 and Figure 3, column b); they consist in all types of edges, so the number of *ops* paths approaches that predicted for the insulated odd-fold edges: $np = e/2$. However, there is one case (Table 5, entry 2) that shows also *ops* cycle, and this result is clearly recognized by the proposed formula (3.6).

It is the place to remind that the number "internal" ops paths, of length/exponent 1, can be used as a true topological index. In a previous paper [10], we denoted by n_p (number of fused pentagon), the coefficients of the term at exponent 1 in Omega polynomial and correlated it with the strain energy in small fullerenes, in monovariate regression, with excellent results.

TABLE 3. Examples for Omega and Ring polynomials in iterated $Le_n(T)$ ended by Ca

Graph	**Omega**	**CI**	**Ring**
$Le_n(T)$			
1	$6X^3$	270	$4X^3 + 4X^6$
2	$6X^3 + 6X^6$	2646	$4X^3 + 16X^6$
3	$6X^9 + 6X^{18}$	23814	$4X^3 + 52X^6$
4	$6X^9 + 24X^{18}$	227934	$4X^3 + 160X^6$
5	$6X^{27} + 24X^{54}$	2051406	$4X^3 + 484X^6$
6	$6X^{27} + 78X^{54}$	18900054	$4X^3 + 1456X^6$
$Ca(Le_n(T))$			
1	$6X^{21}$	13230	-
2	$6X^{21} + 6X^{42}$	129654	-
3	$6X^{63} + 6X^{126}$	1166886	-
4	$6X^{63} + 24X^{126}$	11168766	-
5	$6X^{189} + 24X^{378}$	100518894	-
6	$6X^{189} + 78X^{378}$	926102646	-

TABLE 4. Graphs* with joint f_5-tuples; no e_{exen}; insulated f_{even}; all *ops*=paths

	Graph	Omega	CI	Ring	e	e_{odd_ex}	np_{ex}	np
1	$S_2(T)$	$18X^1 + 12X^2$	1698	$12X^5 + 4X^6$	42	24	12	30
2	$S_2(Oct)$	$36X^1 + 24X^2$	6924	$24X^5 + 8X^6$	84	48	24	60
3	$S_2(Ico)$	$90X^1 + 60X^2$	43770	$60X^5 + 20X^6$	210	120	60	150
4	$S_2(C)$	$36X^1 + 24X^2$	6924	$24X^5 + 6X^8$	84	48	24	60
5	$S_2(Do)$	$90X^1 + 60X^2$	43770	$60X^5 + 12X^{10}$	210	120	60	150
6	$Corazene$	$60X^1 + 42X^2$	20508	$24X^5 + 14X^6 + 12X^7$	144	84	42	102

* cages at entries 1 to 5 designed by S_2 while 6 by $Trs(S_{1f}(Q(T)))$

TABLE 5. Graphs* with disjoint f_5-tuples

	Graph	Omega	CI	Ring	e	e_{even}	e_{odd_ex}	np_{ex}	np
1	$Trs(Du(Med(Le(T))))$	$12X^1 + 12X^2 + 6X^4$	3444	$12X^5 + 10X^6$	60	12	36	18	30
2	$Trs(Du(Med(Le(Oct))))$**	$24X^1 + 36X^2 + 3X^8$	14208	$24X^5 + 12X^6 + 6X^8$	120	24	72	36	60**
3	$Trs(Du(Med(Le(Ico))))$	$60X^1 + 60X^2 + 30X^4$	89220	$60X^5 + 30X^6 + 12X^{10}$	300	60	180	90	150
4	$Trs(Du(Med(Le(C))))$	$24X^1 + 24X^2 + 12X^4$	14088	$24X^5 + 20X^6$	120	24	72	36	60
5	$Trs(Du(Med(Le(Do))))$	$60X^1 + 60X^2 + 30X^4$	89220	$60X^5 + 50X^6$	300	60	180	90	150

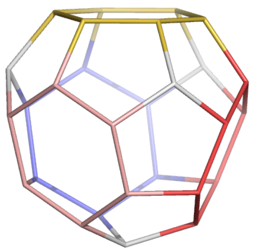
* cages designed by the sequence of map operations indicated in their name-second column
** the reminder of the *ops_path* (entry 2), represents *ops_cycles*

Numerical computations have been done by our new software Nano-Studio [22].

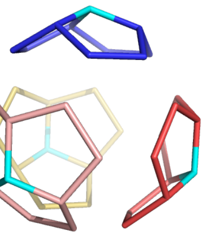
5. Further remarks

It is obvious that setting a larger maximum face size, some open faces will became normal faces and, if even, the *ops* counting can continue, sometimes, up to all opposite edges in the graph will form a unique *ops* (case 2, above).

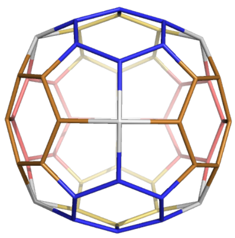
(a) $S_2(T); v = 21$



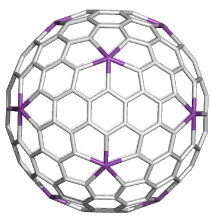
(b) $Trs(Du(Med(Le(T)))); v = 40$



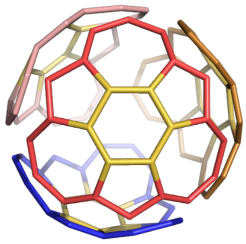
(a) $S_2(Oct); v = 54$



(b) $Trs(Du(Med(Le(Do)))); v = 192$



(a) Corazene; $v = 96$



(b) $Trs(Du(Med(Le(Oct)))); v = 80$

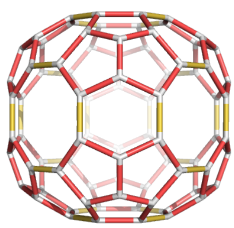


FIGURE 3. *Cages with (a) joint f_5-tuples and insulated f_{even} (Table 4) and (b) disjoint f_5-tuples (Table 5); the cage in the right bottom corner shows 3 ops cycles (Table 5, entry 2).*

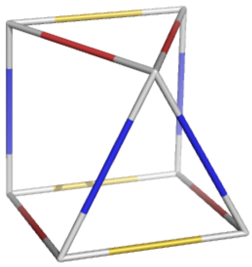
A special case is that of paths ending in two odd edges of one and the same face; this could be called a *pseudo ops* cycle, because e_0 and e_n are not topologically parallel. Figure 4 illustrates two such cases: case (a), of which *np* count uses odd-infinite faces and case (b) which gives different results if faces or rings are counted. For covering study, the face-version is to be used while for network study the ring-version is needed. It is noteworthy to mention that the ring-version of Omega counting polynomial is associated, in cyclic graphs, to the detour counting, as the maximal length of ops is searched. Details of the ring-version polynomial will be presented in a future paper.

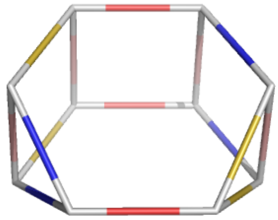
6. Conclusions

Omega polynomial was proposed by Diudea to describe polyhedral molecular structures, particularly those associated with nanostructures. In this paper, some theoretical aspects, related to the type (and counting) of the opposite edge strips, path or cycle, and particular cases were illustrated.

Acknowledgement. This paper is dedicated to Prof. Ivan Gutman, Faculty of Science, Kragujevac, Serbia, for his bright contribution to the development of Mathematical Chemistry.

The second author (A. I.) is grateful to European Society of Mathematical Chemistry ESMC, for support in traveling and working at TOPO GROUP Cluj, Romania.





$\Omega(G, X) = 1X^3 + 3X^4; CI = 168$
$R(G, X) = 2X^3 + 3X^4 + 2X^6$
$e_{ex} = 6 + 2e_{in} = 8; np = 8/2 = 4$

$\Omega(G, X) = 2X^2 + 2X^3 + 2X^4; CI = 266$ (face)
$\Omega(G, X) = 2X^1 + 4X^4; CI = 258$ (ring)
$R(G, X) = 4X^3 + 7X^4; e_{ex} = 12; np = 12/2 = 6$

FIGURE 4. *Ops paths ending in two edges of the same odd face, to form a pseudo ops cycle*

REFERENCES

[1] Ashrafi, A. R., Jalali, M., Ghorbani, M. and Diudea, M. V., *Computing PI and Omega Polynomials of an Infinite Family of Fullerenes*, MATCH, Commun. Math. Comput. Chem. **60** (2008), 905–916
[2] Diudea, M. V., *Layer matrices in molecular graphs*, J. Chem. Inf. Comput. Sci. **34** (1994), 1064–1071
[3] Diudea, M. V., *Nanoporous carbon allotropes by septupling map operations*, J. Chem. Inf. Model. **45** (2005), 1002–1009
[4] Diudea, M. V., *Hosoya polynomial in tori*, MATCH Commun. Math. Chem. **45** (2002), 109–122
[5] Diudea, M. V., *Omega polynomial*, Carpath. J. Math **22** (2006), 43–47
[6] Diudea, M. V., *Covering forms in nanostructures*, Forma (Tokyo) **19** (2004), 131–163
[7] Diudea, M. V., Gutman, I. and Jäntschi, L., *Molecular topology*, Huntington, NY: Nova Science Publishers, 2002
[8] Diudea, M. V. and Ursu, O., *Layer matrices and distance property descriptors*, Indian J. Chem **42A** (2003), 1283–1294
[9] Diudea, M. V., Florescu, M. S. and Khadikar, P. V., *Molecular topology and its applications*, EFICON, Bucharest, 2006
[10] Diudea, M. V., Cigher, S., Vizitiu, A. E., Florescu, M. S. and John, P. E., *Omega polynomial and its use in nanostructure description*, J. Math. Chem. **45** (2009), 316–329
[11] Diudea, M. V., John, P. E., Graovac, A., Primorac, M. and Pisanski, T., *Leapfrog and Related Operations on Toroidal Fullerenes*, Croat. Chem. Acta **76** (2003), 153–159
[12] Diudea, M. V., Stefu, M., John, P. E. and Graovac, A., *Generalized Operations on Maps*, Croat. Chem. Acta **79** (2006), 355–362
[13] Djoković, D. Ž., *Distance-preserving subgraphs of hypercubes*, J. Combin. Theory Ser. B **14** (1973), 263–267
[14] Gutman, I., Klavžar, S., Petkovšek, M. and Žigert, P., *On Hosoya polynomials of benzenoid graphs*, MATCH Commun. Math. Chem. **43** (2001), 49–66
[15] 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
[16] Hosoya, H., *On some counting polynomials in chemistry*, Discrete Appl. Math., **19** (1988), 239–257
[17] Hosoya, H., *Clar's aromatic sextet and sextet polynomial*, Topics Curr. Chem. **153** (1990), 255–272
[18] Hosoya, H. and 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
[19] John, P. E., Vizitiu, A. E., Cigher, S. and Diudea, M. V., *CI index in tubular nanostructures*, MATCH, Commun. Math. Comput. Chem. **57** (2007), 479–484
[20] Klavžar, S., *Some comments on co graphs and CI index*, MATCH, Commun. Math. Comput. Chem. **59** (2008), 217–222
[21] Konstantinova, E. V. and Diudea, M. V. *The Wiener polynomial derivatives and other topological indices in chemical research*, Croat. Chem. Acta **73** (2000), 383–403
[22] Nagy, Cs. L. and Diudea, M. V., *Nano Studio*, Babes-Bolyai University, Cluj, 2009
[23] Ohkami, N. and Hosoya, H., *Topological dependency of the aromatic sextets in polycyclic benzenoid hydrocarbons: Recursive relations of the sextet polynomial*, Theoret. Chim. Acta **64** (1983) 153–170
[24] Ohkami, N., Motoyama, A., Yamaguchi, T., Hosoya, H. and Gutman, I., *Graph-theoretical analysis of the Clar's aromatic sextet*, Tetrahedron **37** (1981), 1113–1122
[25] Stefu, M., Diudea, M. V. and John, P. E., *Composite operations on maps*, Studia Univ. "Babes-Bolyai" **50** (2005), 165–174
[26] Ursu O., Diudea, M. V., *TOPOCLUJ*, Babes-Bolyai University, Cluj, 2005
[27] Winkler, P. M., *Isometric embedding in products of complete graphs*, Discrete Appl. Math. **7** (1984), 221–225

BABEŞ BOLYAI UNIVERSITY
FACULTY OF CHEMISTRY AND CHEMICAL ENGINEERING
400028 CLUJ NAPOCA, ROMANIA
E-mail address: diudea@chem.ubbcluj.ro

UNIVERSITY OF NIŠ
FACULTY OF SCIENCES AND MATHEMATICS
VIŠEGRADSKA 33, 18000 NIŠ, SERBIA
E-mail address: aleksandari@gmail.com