MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **65** (2011) 131-142

ISSN 0340 - 6253

Omega and Related Polynomials in Crystal-like Structures

Mircea V. Diudea,[a*] Aniela E. Vizitiu,[a] and Simona Cigher[a]

Faculty of Chemistry and Chemical Engineering,
"Babes-Bolyai" University, 400028 Cluj, Romania

(Received July 10, 2009)

Abstract

Counting polynomials are those polynomials having at exponent the extent of a property partition and as coefficients the number of the corresponding partition. In the present paper four related counting polynomials are discussed: Omega Ω, Pi Π, Theta Θ and Sadhana Sd. Analytical close formulas for the calculation of these polynomials in some hypothetical crystal-like lattices are derived.

1. Introduction

A graph can be described by a connection table, a sequence of numbers, a matrix, a polynomial or by a single number (often called a topological index). A counting polynomial can be written as:

$$P(G,x) = \sum_k m(G,k) \cdot X^k \tag{1}$$

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.

Counting polynomials have been introduced, in the Mathematical Chemistry literature, by Hosoya:[1,2] $Z(G,X)$ counts independent edge sets while $H(G,X)$ (initially

This paper is dedicated to Prof. Ante Graovac, Rudjer Bošković Institute, Zagreb, and Faculty of Science, University of Split, Croatia, for his bright activity to the development of Chemical Graph Theory.

called Wiener and later Hosoya)[3,4] counts the distances in the graph. Hosoya also proposed the sextet polynomial[5-8] for counting the resonant rings in a benzenoid molecule. More about polynomials the reader can find in ref 9.

Some distance-related properties can be expressed in polynomial form, with coefficients calculable from the layer and shell matrices.[10-13] These matrices are built up according to the vertex distance partitions of a graph, as provided by the TOPOCLUJ software package.[14] The most important, in this respect, is the evaluation of the coefficients of Hosoya $H(G,X)$ polynomial from 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 $e = (u,v)$ and $f = (x,y)$ of G are called *codistant*: $e\ co\ f$ if

$$d(v,x) = d(v,y)+1 = d(u,x)+1 = d(u,y) \tag{2}$$

If *co* is an equivalence relation:[15,16]

$$e\ co\ e \tag{3}$$

$$e\ co\ f \Leftrightarrow f\ co\ e \tag{4}$$

$$e\ co\ f\ \&\ f\ co\ h \Rightarrow e\ co\ h \tag{5}$$

Then, $C(e) := \{f \in E(G);\ f\ co\ e\}$ is the set of edges in G, codistant to the edge $e \in E(G)$ and G is called a *co-graph*. Consequently, $C(e)$ is called an *orthogonal cut* set *ocs* of G and $E(G)$ is the union of disjoint orthogonal cuts: $C_1 \cup C_2 \cup ... \cup C_k$ and $Ci \cap Cj = \text{Ø}$ for $i \neq j$ and $i, j = 1,2,..,k$.

Observe *co* is a θ relation, (*Djoković-Winkler* relation)[17,18] and *G is a co-graph if and only if it is a partial cube,* a result due to Klavžar.[19] In a plane bipartite graph, an edge e is in relation θ with any opposite edge f if the faces of the plane graph are isometric (which is the case of the most chemical graphs). Then an orthogonal cut *oc* with respect to a given edge is the smallest subset of edges closed under this operation and $C(e)$ is precisely a θ-class of G.

Concluding, a *graph G is a co-graph if and only if it is a partial cube.* A partial cube is always a bipartite graph, but the reciprocal is not true (see Figure 1 and Table 1).

A set of opposite edges $S(e) := \{f \in E(G);\ f\ op\ e\}$ within the same face/ring eventually forming a strip of adjacent faces/rings of a covering/tiling, is called an "opposite edge strip" *ops*. Under *ops* relation, $E(G)$ is the union of disjoint *ops*: $S_1 \cup S_2 \cup ... \cup S_k$ and $S_i \cap S_j = \text{Ø}$

for $i \neq j$ and $i, j = 1, 2, .., k$. The relation *ops* is *not necessarily transitive*. Observe *ops* is an *ocs* only in partial cubes.

Figure 1. Bipartite, non-partial (a) and partial (b) Cubes

Table 1. Polynomials of cubic structures in Figure 1.

	Cubic Cage (Figure 1a)		Cubic Net (Figure 1b)	
Name	Polynomial	Index	Polynomial	Index
$\Omega(G,x)$	$6X^{8}$	$CI(G) = 1920$	$6X^{9}$	$CI(G) = 2430$
$Sd(G,x)$	$6X^{40}$	$Sd(G) = 240$	$6X^{45}$	$Sd(G) = 270$
$\Theta(G,x)$	$24X^{8}+24X^{10}$	$\Theta(G) = 432$	$54X^{9}$	$\Theta(G) = 486$
$\Pi(G,x)$	$24X^{38}+24X^{40}$	$\Pi(G) = 1872$	$54X^{45}$	$\Pi(G) = 2430$

Omega polynomial[20] is defined on *ops* as:

$$\Omega(G,X) = \sum_{s} m(G,s) \cdot X^{s} \tag{6}$$

where $m(G,s)$ is the number of opposite edge strips of length s.

If *ops* is an *ocs*, as in partial cubes, we can write the following counting polynomials:

$$\Omega(G,X) = \sum_{k} m \cdot X^{k} \tag{7}$$

$$Sd(G,X) = \sum_{k} m \cdot X^{e-k} \tag{8}$$

$$\Theta(G,X) = \sum_{k} m \cdot k \cdot X^{k} \tag{9}$$

$$\Pi(G,X) = \sum_{k} m \cdot k \cdot X^{e-k} \tag{10}$$

$\Omega(G,X)$ and $\Theta(G,X)$ count *equidistant edges* in G while $Sd(G,X)$ and $\Pi(G,X)$, count non-equidistant edges. The first two polynomials are counted once for a strip while the last two are counted for each edge, so that the coefficients are multiplied with k.

In a counting polynomial, the *first derivative* (in X=1) defines the type of property which is counted. For the above polynomials they are:

$$\Omega'(G,1) = \sum_{k} m \cdot k = e = |E(G)| \tag{11}$$

$$Sd'(G,1)=\sum_k m\cdot(e-k)=Sd(G) \tag{12}$$

$$\Theta'(G,1)=\sum_k m\cdot k^2=\theta(G) \tag{13}$$

$$\Pi'(G,1)=\sum_k m\cdot k\cdot(e-k)=\Pi(G) \tag{14}$$

An index, called Cluj-Ilmenau *CI*(*G*), is defined on $\Omega(G,X)$:

$$CI(G)=\left\{[\Omega'(G,1)]^2-[\Omega'(G,1)+\Omega''(G,1)]\right\} \tag{15}$$

3. Properties of counting polynomials

In general, *k* is different for the two pairs $\{\Omega(G,X);Sd(G,X)\}$ and $\{\Theta(G,X);\Pi(G,X)\}$.

Proposition: In partial cubes *k* takes the same value in the all above polynomials, meaning the *opposite edge sets superimpose to the equidistant edge ones* and *ops* is an *ocs.*

Consequence: In partial cubes $CI(G)=\Pi(G)$. Applying definition (15), *CI* is calculated as:

$$CI(G)=\left(\sum_c m\cdot c\right)^2-\left[\sum_c m\cdot c+\sum_c m\cdot c\cdot(c-1)\right]=e^2-\sum_c m\cdot c^2=\Pi(G) \tag{16}$$

This is the case of cubic lattice (Figure 1b), of planar bipartite graphs, like those of acene or phenacene benzenoids,[21] and also of some bipartite 3D structures, as that in Figure 2. However, in the bipartite cage in Figure 1a, *ops* is not an *ocs*, the two opposite red edges at the top and bottom, respectively, being not equidistant (see also Table 1).

One can reformulate (14) function of (11) and (13) to write:

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

Figure 2. Bipartite, partial cubes: (a) five fold and (b) two fold symmetry, of the cage designed by sequence *Du*(*Med*(D)): *v*=32; *e*=60; f_4=30; $\Omega(G,x)=6X^{10}$; $\Pi(G,X)=60X^{50}$; $CI(G)=\Pi(G)=3000$

The first part of relation (17) and the last part of (16) as well, is just the formula proposed by John *et al.*[15] to calculate the Khadikar's *PI*=*PI*(*G*) topological index[22] (which counts the non-equidistant edges in *G*). Note that our $\Pi(G,X)$ equals *PI*(*G*) only in partial cubes, in part because the *edge equidistance* relation includes, besides parallel edges condition (*op* relation, (2)), a condition for perpendicular edges (tetrahedron condition):

$$d(u,x)=d(u,y)=d(v,x)=d(v,y) \qquad (18)$$

It is noteworthy that Ashrafi *et al.*[23] was first who proposed a polynomial PI(*G*,*X*), of which first derivative (in *X*=1) eventually gives the Khadikar's *PI* index. Differences in version of *PI* index calculation appeared also because of the *min*-condition put in evaluating the edge equidistance.[24]

An interesting degeneracy of $CI(G)$ and $\Pi(G)$ may appear: the coefficients in the pair $\{\Theta(G,X);\Pi(G,X)\}$ correspond to the product *m.k* (as in $\Omega(G,X)$, see relation (10)) but the exponents are such that $\Pi(G)=CI(G)$. Examples are given for two bipartite tori, in Table 2.

Table 2. Polynomials of two bipartite tori showing degenerate $CI(G)$ and $\Pi(G)$ values

T(6,3)H[8,12]; *v*=96; *e*=144		T((4,8),3)H[20,8]; *v*=160; *e*=144	
Polynomial	Index	Polynomial	Index
$\Omega=12X^4+4X^{24}$	$CI(G)=18240$	$\Omega=10X^8+8X^{10}+2X^{40}$	$CI(G)=52960$
$Sd=4X^{120}+12X^{140}$	$Sd(G)=2160$	$Sd=2X^{200}+8X^{230}+10X^{232}$	$Sd(G)=4560$
$\Theta=48X^8+96X^{22}$	$\Theta(G)=2496$	$\Theta=80X^{16}+80X^{20}+80X^{22}$	$\Theta(G)=4640$
$\Pi=96X^{122}+48X^{136}$	$\Pi(G)=18240$	$\Pi=80X^{218}+80X^{220}+80X^{224}$	$\Pi(G)=52960$

It is easily seen that, for a single *ops*, called Hamiltonian strip, by analogy to the path visiting once all the vertices of the graph, one calculates the polynomial:

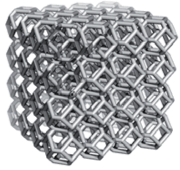
$\Omega(G,X)=1\times X^s$ and the index $CI(G)=s^2-(s+s(s-1))=s^2-s^2=0$.

In tree graphs, the Omega polynomial is either not defined or it simply counts the non-opposite edges, being included in the term of exponent *s*=1, thus: $\Omega(G,X)=m\times X^1$; $\Omega'(G,1)=m\times 1=e(G)$; $CI(G)=m(m-1)=e(e-1)=\Pi(G)$, *m* being the number of edges in that tree graph. Also, $PI(G)=(v-1)(v-2)$, a result known from Khadikar[13] and *e*=*v*-1, the tree graphs being partial cubes. In such graphs, Omega and Theta polynomials show the same expression (compare (9) and (10)).

4. Counting polynomials in crystal-like lattices

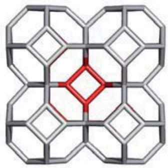
Omega polynomial was thought to describe the covering of polyhedral nano-structures or the tiling of crystal-like lattices. In this section we present four infinite, periodic, networks designed by using some operations on maps/nets.[25-29] The first three nets are obtained by map operations applied on the Cube C, while the last one on the Icosahedron I.

(a)
*Le*4(C(1,1,1)); v=24
$\Omega(C,X)=6X^6$; *CI*=1080



(b)
*Le*4(C(4,4,4)); v=960

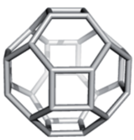
(c)
*Le*4(C(2,2,2)); v=144



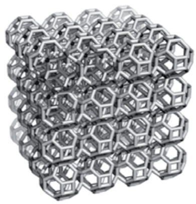
(d)
*Le*4(C(2,2,2)); v=144; ortho view

Figure 3. Triple periodic lattice designed by *Le*(C) and identifying f_4 faces.

By applying the leapfrog *Le* and Chamfering *Q* on the Cube, results in the repeat units illustrated in Figures 3a to 5a. Next, by iteratively identifying, faces of size (4,4) or (4,6) it results in various networks, even the starting object is one and the same (see the cases of *Q*-transformed objects).



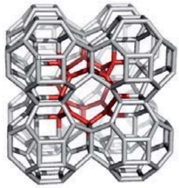
(a)



(b)

*Q*4(C(1,1,1)); v=32
$\Omega(C,X)=4X^6+3X^8$; *CI*=1968

(b) *Q*4(C(4,4,4)); v=1472



(c)

(d)

$Q4$(C(2,2,2)); v=208 $Q4$(C(2,2,2)); v=208; ortho view

Figure 4. Triple periodic lattice designed by Q(C) and identifying f_4 faces.

Observe, the networks in Figures 3 to 5 are defined by eight units, to express their periodicity: the first two structures $Le4$(C(2,2,2)) and $Q4$(C(2,2,2)) are triple-periodic while the third, $Q4,6$(C(2,2,2)) is only double-periodic. The analytical formulas were developed for either incomplete (a,b,c), $a \geq b \geq c$ or complete (a,a,a) cube lattice (see below).

***G=Le*4(C(*a,b,c*));** $a \geq b \geq c$ **:**

$$\Omega(G,X) = 4\sum_{i=1}^{c-1} X^{4ai+2i} + 2(b-c+1)X^{(4a+2)c} +$$
$$4\sum_{i=1}^{c-1} X^{4bi+2i} + 2(a-c+1)X^{(4b+2)c} +$$
$$4\sum_{i=1}^{b-1} X^{4ci+2i} + 2(a-b+1)X^{(4c+2)b}$$

***G=Le*4(C(*a,a,a*)):**

$$\Omega(G,X) = 12\sum_{i=1}^{a-1} X^{2i(2a+1)} + 6X^{2a(2a+1)}$$
$$\Omega'(G,1) = 12a^2(2a+1)$$

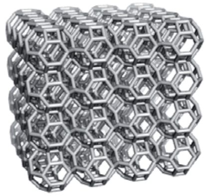
***G=Q*4(C(*a,b,c*));** $a \geq b \geq c$ **:**

$$\Omega(G,X) = 4abcX^6 + aX^{4bc+2b+2c} + bX^{4ac+2a+2c} + cX^{4ab+2a+2b}$$

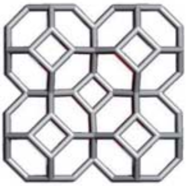
***G=Q*4(C(*a,a,a*)):**

$$\Omega(G,X) = 4a^3X^6 + 3aX^{4a(a+1)}$$
$$\Omega'(G,1) = 12a^2(3a+1)$$

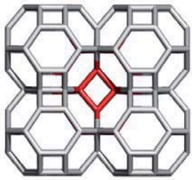
Q4,6(C(1,1,1)); v=32
$\Omega(C,X) = 4X^6+3X^8$; CI=1968



Q4,6(C(4,4,4)); v=1280



Q4,6(C(2,2,2)); v=192; (a)



Q4,6(C(2,2,2)); v=192; (b,c)

Figure 5. Double periodic lattice designed by Q(C(a,b,c)) and identifying f_4 & f_6 faces.

***G*=*Q*4,6(C(*a*,*b*,*c*));** $a \geq b \geq c$ **:**

$$\Omega(G,X) = 4\sum_{i=1}^{b-1} X^{2(3c+1)i} + 2(a-b+1)X^{2(3c+1)b} +$$
$$4\sum_{i=1}^{c-1} X^{2(2a+1)i} + 2(b-c+1)X^{2(2a+1)c} +$$
$$4\sum_{i=1}^{c-1} X^{2(2b+1)i} + 2(a-c+1)X^{2(2b+1)c} + cX^{4ab+2a+2b}$$

***G*=*Q*4,6(C(*a*,*a*,*a*)):**

$$\Omega(G,X) = 4\sum_{i=1}^{a-1} X^{2i(3a+1)} + 8\sum_{i=1}^{a-1} X^{2i(2a+1)} + 2X^{2a(3a+1)} + 4X^{2a(2a+1)} + aX^{4a(a+1)}$$
$$\Omega'(G,1) = 16a^2(2a+1)$$

Examples are given for each discussed lattice, both for polynomials and indices, in the tables below.

Table 3. Examples for *Le*4(C(*a,b,c*)) lattice

*Le*4(C(*a,b,c*))_atoms	Omega polynomial	*CI*_Index
111_24	$6X^{6}$	1080
222_144	$12X^{10}+6X^{20}$	54000
422_272	$4X^{10}+4X^{14}+4X^{18}+6X^{20}+6X^{28}+2X^{36}+2X^{44}$	363408
442_512	$4X^{14}+8X^{18}+4X^{28}+12X^{36}+4X^{42}+2X^{56}+2X^{80}$	1353664
444_960	$12X^{18}+12X^{36}+12X^{54}+6X^{72}$	2900448
	Sadhana polynomial	*Sd*_Index
111_24	$6X^{30}$	180
222_144	$6X^{220}+12X^{230}$	4080
422_272	$2X^{572}+2X^{580}+6X^{588}+6X^{596}+4X^{598}+4X^{602}+4X^{606}$	16632
442_512	$2X^{1104}+2X^{1128}+4X^{1142}+12X^{1148}+4X^{1156}+8X^{1166}+4X^{1170}$	41440
444_960	$6X^{1656}+12X^{1674}+12X^{1692}+12X^{1710}$	70848

Table 4. Examples for *Q*4(C(*a,b,c*)) lattice

*Q*4(C(*a,b,c*))_atoms	Omega polynomial	*CI*_Index
111_32	$4X^{6}+3X^{8}$	1968
222_208	$32X^{6}+6X^{24}$	108288
331_240	$36X^{6}+6X^{20}+1X^{48}$	141456
332_444	$72X^{6}+6X^{34}+2X^{48}$	521688
333_648	$108X^{6}+9X^{48}$	1141776
444_1472	$256X^{6}+12X^{80}$	6144000
	Sadhana polynomial	*Sd*_Index
111_32	$3X^{40}+4X^{42}$	288
222_208	$6X^{312}+32X^{330}$	12432
331_240	$X^{336}+6X^{364}+36X^{378}$	16128
332_444	$2X^{684}+6X^{698}+72X^{726}$	57828
333_648	$9X^{1032}+108X^{1074}$	125280
444_1472	$12X^{2416}+256X^{2490}$	666432

The last lattice (Figure 6) is constructed by identifying parts of the *Med*(*Med*(IP)), designed by applying twice the Medial *Med* operation on the centered Icosahedron IP, so that the structure be periodic on the X-coordinate.

Table 5. Examples for *Q*4,6(C(*a,b,c*)) lattice

*Q*4,6(C(*a,b,c*))_atoms	Omega polynomial	*CI*_Index
222_192	$8X^{10}+4X^{14}+4X^{20}+2X^{24}+2X^{28}$	96496
422_360	$4X^{10}+4X^{14}+4X^{18}+6X^{20}+6X^{28}+2X^{36}+2X^{44}$	363408
442_672	$4X^{14}+8X^{18}+4X^{28}+12X^{36}+4X^{42}+2X^{56}+2X^{80}$	1353664
444_1280	$8X^{18}+4X^{26}+8X^{36}+4X^{52}+8X^{54}+4X^{72}+4X^{78}+4X^{80}+2X^{104}$	5166304
	Sadhana polynomial	*Sd*_Index
222_192	$2X^{292}+2X^{296}+4X^{300}+4X^{306}+8X^{310}$	6080
422_360	$2X^{572}+2X^{580}+6X^{588}+6X^{596}+4X^{598}+4X^{602}+4X^{606}$	16632
442_672	$2X^{1104}+2X^{1128}+4X^{1142}+12X^{1148}+4X^{1156}+8X^{1166}+4X^{1170}$	41440
444_1280	$2X^{2200}+4X^{2224}+4X^{2226}+4X^{2232}+8X^{2250}+4X^{2252}+8X^{2268}+4X^{2278}+8X^{2286}$	103680

Formulas for Omega polynomial are given function of the number of polytopes n consisting the periodic structure. The reader is invited to consult, in this respect, a recent paper of our group.[30] Table 6 provides examples of polynomial and index calculations.

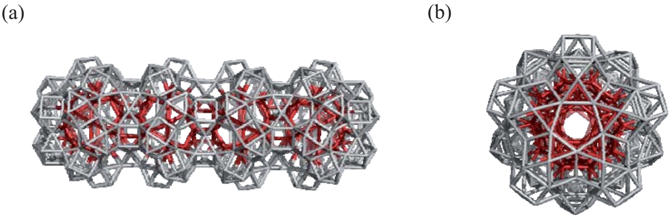


Figure 6. *Med*(*Med*(IP)); n (number of polytopes) =4

G = ***Med*(*Med*(IP)):**

$$\Omega(G,X,R<6)=\left[120+90(n-1)\right]X^2+10(n+2)X^3+5(n-1)X^4+\left[12+11(n-1)\right]X^5$$

$$\Omega'(G,1)=105+285n;\ \Omega''(G,1)=140+520n$$

$$CI(G)=10780+59045n+81225n^2$$

$\Omega(G,X,R\geq 6)=1X^{390n-105(n-1)}$; *CI*=0; Hamiltonian *ops*

$$v=150+105(n-1)$$

Note the difference in Omega polynomial function of the maximum ring size, in case of *Med*(*Med*(IP)) lattice: when ring R≥6, a unique strip is obtained, called here *Hamiltonian ops*, because it visited once all the edges in the graph. Of course, in such a case, *CI*=0.

Table 6. Examples for *Med*(*Med*(IP)) lattice

n	Omega polynomial	*CI*_Index
1	$120X^2+30X^3+12X^5$	151050
2	$210X^2+40X^3+5X^4+23X^5$	453770
4	$390X^2+60X^3+15X^4+45X^5$	1546560
5	$480X^2+70X^3+20X^4+56X^5$	2336630
7	$660X^2+90X^3+30X^4+78X^5$	4404120
	Sadhana polynomial	*Sd*_Index
1	$120X^{388}+30X^{387}+12X^{385}$	62790
2	$210X^{673}+40X^{672}+5X^{671}+23X^{670}$	186975
4	$390X^{1243}+60X^{1242}+15X^{1241}+45X^{1240}$	633705
5	$480X^{1528}+70X^{1527}+20X^{1526}+56X^{1525}$	956250
7	$660X^{2098}+90X^{2097}+30X^{2096}+78X^{2095}$	1799700

Sadhana polynomial is immediately derived, keeping in mind its definition (relation 8) and that the first derivative of Omega polynomial in X=1 is just the number of edges in G. The other two polynomials $\Theta(G,X)$ and $\Pi(G,X)$ show, in general, more terms than the pair $\Omega(G,X)$ and $Sd(G,X)$ while the interpretation of relation polynomial-graph structure is rather laborious.

Calculation of polynomials and corresponding indices were performed on our original software Omega counter[31] and Nano_Studio.[32]

5. Conclusions

Omega and three related counting polynomials were investigated in view of establishing mutual inter-relations. All these polynomials count sets of edges related to edge-cut procedures used for calculating some topological indices, such as Szeged and PI indices.

It was shown that the indices $CI(G)$ and $\Pi(G)$ show identical values in graphs embeddable in the hypercube. Examples of graphs showing $CI(G)=\Pi(G)$ and $CI(G)\neq\Pi(G)$, respectively, were presented.

Extension from faces to rings (namely *strong rings*, which are not the sum of other smaller rings) enabled calculation of $\Omega(G,X)$ in 3D networks. Analytical close formulas for Omega polynomial in some crystal-like lattices were derived.

Acknowledgements. This work was supported by the Romanian Grant Id_506.

References

1. H. Hosoya, *Bull. Chem. Soc. Japan*, **1971**, *44*, 2332-2339.
2. H. Hosoya, *Discrete Appl. Math.*, **1988**, *19*, 239-257.
3. E. V. Konstantinova and M. V. Diudea, *Croat. Chem. Acta,* **2000**,*73*, 383-403.
4. I. Gutman, S. Klavžar, M. Petkovšek, and P. Žigert, *MATCH Commun. Math. Chem.*, **2001**, *43*, 49-66.
5. H. Hosoya and T. Yamaguchi, *Tetrahedron Lett.*, **1975**, 4659-4662.
6. N. Ohkami and H. Hosoya, *Theoret. Chim. Acta*, **1983**, *64*, 153-170.
7. N. Ohkami, A. Motoyama, T. Yamaguchi, and H. Hosoya, *Tetrahedron*, **1981**, *37*, 1113-1122.
8. H. Hosoya, *Topics Curr. Chem.*, **1990**, *153*, 255-272.

9. M. V. Diudea, I. Gutman, and L. Jäntschi, *Molecular Topology*, Nova, N. Y. 2002.
10. M. V. Diudea, *J. Chem. Inf. Comput. Sci.*, **1994**, *34*, 1064-1071.
11. M. V. Diudea, *MATCH Commun. Math. Comput. Chem.*, **2002**, *45*, 109-122.
12. M. V. Diudea and O. Ursu, *Indian J. Chem.*, 42*A*, **2003**, 1283-1294.
13. M. V. Diudea, M. S. Florescu and P. V. Khadikar, *Molecular Topology and Its Applications*, EFICON, Bucharest, 2006.
14. O. Ursu and M. V. Diudea, *TOPOCLUJ*, Babes-Bolyai University, Cluj, 2005.
15. P. E. John, P. V. Khadikar, J. Singh, *J. Math. Chem.*, 2007, 42, 37-45.
16. P. E. John, A. E. Vizitiu, S. Cigher, and M. V. Diudea, *MATCH Commun. Math. Comput. Chem.*, **2007**, *57*, 479-484.
17. D. Ž. Djoković, *J. Combin. Theory Ser. B*, **1973**, 14, 263–267.
18. P. M. Winkler, *Discrete Appl. Math.*,**1984**, 8, 209–212.
19. S. Klavžar, *MATCH Commun. Math. Comput. Chem.*, **2008,** *59***,** 217-222.
20. M. V. Diudea, Omega Polynomial, *Carpath. J. Math.*, **2006,** *22*, 43-47.
21. M. V. Diudea, S. Cigher and P. E. John, *MATCH Commun. Math. Comput. Chem.*, **2008**, *60*, 237-250.
22. P. V. Khadikar, *Nat. Acad. Sci. Letters,* **2000**, *23*, 113-118.
23. A. R. Ashrafi, M. Manoochehrian and H. Yousefi Azari, *Util. Math.*, **2006**, *71*, 97-108.
24. A. R. Ashrafi, M. Jalali, M. Ghorbani and M. V. Diudea, *MATCH Commun. Math. Comput. Chem.*, **2008**, *60*, 905-916.
25. M. V. Diudea, P. E. John, A. Graovac, M. Primorac, and T. Pisanski, *Croat. Chem. Acta*, **2003**, *76*, 153-159.
26. M. V. Diudea, *Forma (Tokyo)*, **2004**, *19*, 131-163.
27. M. V. Diudea, M. Ştefu, P. E. John, and A. Graovac, *Croat. Chem. Acta*, **2006**, *79*, 355-362.
28. M. Ştefu, M. V. Diudea, and P. E. John, *Studia Univ. "Babes-Bolyai"*, **2005**, *50*, 165-174.
29. M. V. Diudea, *J. Chem. Inf. Model.,* **2005**, *45,* 1002-1009.
30. M. V. Diudea and Cs. L. Nagy, *MATCH Commun. Math. Comput. Chem.*, **2008**, *60*, 835-844.
31. S. Cigher and M. V. Diudea, *Omega Polynomial Counter*, "Babes-Bolyai" Univ., **2007**.
32. Cs. L. Nagy, and M. V. Diudea, *Nano_Studio*, "Babes-Bolyai" Univ., **2009**.