MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **60** (2008) 935-944

ISSN 0340 - 6253

Omega polynomial in twisted ((4,8)3)R tori

Mircea V. Diudea

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

(Received April 11, 2008)

Abstract. Quasi orthogonal cuts *qoc* with respect to a given edge in a graph $G=G(V,E)$ are defined as the smallest subset of edges closed under taking opposite edges on faces. Omega polynomial $\Omega(G,x)$ counts the qoc strips of all extent in G. The first and second derivatives, in x=1, of this polynomial enables the calculation of the recently proposed *CI* index. Analytical close formulas for calculating $\Omega(G,x)$ in twisted ((4,8)3)R tori are derived.

1. Polynomials in Chemistry

In Quantum Chemistry, the early Hückel theory calculates the levels of π-electron energy of the molecular orbitals, in conjugated hydrocarbons, as roots of the *characteristic polynomial*:[1-4]

$$P(G,x) = \det[x\mathrm{I} - \mathrm{A}(G)] \tag{1}$$

In the above, I is the unit matrix of a pertinent order and A the adjacency matrix of the graph *G*. The characteristic polynomial is involved in the evaluation of topological resonance energy TRE, the topological effect on molecular orbitals TEMO, the aromatic sextet theory, the Kekulé structure count, etc.[4-8]

The coefficients $m(G,k)$ in the polynomial expression:

$$P(G,x) = \sum_k m(G,k)\cdot x^k \tag{2}$$

are calculable from the graph *G* by a method making use of the *Sachs graphs*, which are subgraphs of *G*. Relation (2) was also found by other scientists.[1] Some numeric methods of linear algebra, can eventually be more efficient in large graphs.[9,10]

Relation (1) was generalized by Hosoya[11] and others[12-15] by changing the adjacency matrix with the distance matrix or any other square topological matrix.

Relation (2) is a general expression of a counting polynomial, written as a sequence of numbers, 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, the counting polynomials have first been introduced by Hosoya:[16,17] $Z(G,x)$ counts independent edge sets while $H(G,x)$ (initially called Wiener and later Hosoya)[18,19] counts the distances in G. Further, Hosoya proposed the sextet polynomial[20-23] for counting the resonant rings in a benzenoid molecule.[24,25] Other counting polynomials have later been proposed: *independence*[26-28] *king*, *color*, *star* or *clique polynomials*.[29-33] More about polynomials the reader can find in ref 1.

The aim of this paper is to find close analytical relations for Omega polynomial in some twisted ((4,8)3)R tori .

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 called *codistant* (briefly: $e\ co\ f$) if

$$d(x,v) = d(x,u) + 1 = d(y,v) + 1 = d(y,u) \tag{3}$$

For some edges of a connected graph G there are the following relations satisfied:[34,35]

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

$$e\ co\ f \Leftrightarrow f\ co\ e \tag{5}$$

$$e\ co\ f\ \&\ f\ co\ h \Rightarrow e\ co\ h \tag{6}$$

though the relation (6) is not always valid (Figure 1 and Table 1).

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., $C(e)$ obeys (4) to (6)), 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: $C_1 \cup C_2 \cup ... \cup C_k$ and $Ci \cap Cj = \emptyset$ for $i \neq j,\ i, j = 1,2,..,k$.

Observe *co* is a Θ relation, (*Djoković-Winkler*):[36,37]

$$d(x,u)+d(y,v)\neq d(x,v)+d(y,u) \qquad (7)$$

and Θ *is a co-relation if and only if G is a partial cube,* as Klavžar[38] correctly stated in a recent paper. Relation Θ is reflexive and symmetric but need not be transitive. Klavžar noted by Θ^* the Θ transitive closure, then Θ^* is an equivalence (see also the *co* relation). In this respect, recall some other definitions.

Let $G(V,E)$ be a connected graph and d be its distance function. 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. A *partial cube* is an isometric subgraph of a *hypercube* Q_n; this can be obtained as a Cartesian product $Q_n = \square_{i=1}^{n} K_2$. Examples of partial cubes are even cycles, benzenoid graphs, phenylenes, trees, etc.[39,40]

For any two adjacent vertices $(u,v)\in E(G)$, let denote by W_{uv}, the set of vertices lying closer to u than to b:

$$W_{uv}=\{w\in V \mid d(w,u)<d(w,v)\} \qquad (8)$$

The set W_{uv} and its induced subgraphs $\langle W_{uv}\rangle$ are called *semicubes* of G.[40] A graph G is bipartite if and only if its semicubes W_{uv} and W_{vu} form a partition of V for any $(u,v)\in E(G)$. The semicubes W_{uv} and W_{vu} are called opposite semicubes and they are disjoint. Let $w\in W_{uv}$ for some edge $(u,v)\in E(G)$. Then $d(w,v)=d(w,u)+1$ and consequently $W_{uv}=\{w\in V \mid d(w,v)=d(w,u)+1\}$ (see also (3)). In a partial cube, all semicubes are convex and the relation Θ is an equivalence relation on E. The distinct semicubes are just the Θ-classes and represent the ground for the cut procedure[40] (see below) for the calculation of distance based indices. Note that Cluj polynomial[41] is based on calculation of opposite semicubes (non-equidistant vertices).

In a partial cube, any two opposite edges e and f are in relation Θ. Then an orthogonal cut *oc* with respect to the edge e of G is the smallest subset of edges closed under this operation and C(e) is precisely a Θ-class. Resuming, a *graph G is a co-graph if and only if it is a partial cube.*

A *quasi-orthogonal cut qoc* with respect to a given edge is the smallest subset of edges closed under taking opposite edges on faces. Since the transitivity relation (6) of the *co* relation is not necessarily obeyed, *qoc* represents a new concept within the cut methods. Any *oc* strip is a *qoc* strip but the reverse is not always true.[42,43]

3. Omega Polynomial

Let $m(G,c)$ be the number of *qoc* strips of length c (*i.e.*, the number of cut-off edges); for the sake of simplicity, $m(G,c)$ can be written as m. The Omega polynomial is defined,[44] on the ground of *qoc* strips:

$$\Omega(G,x) = \sum_c m(G,c) \cdot x^c \tag{9}$$

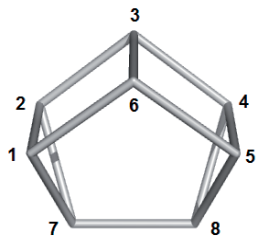
In a counting polynomial, the *first derivative* (in x=1) defines the type of the counted property:

$$\Omega'(G,1) = \sum_c m \cdot c = e = |E(G)| \tag{10}$$

On Omega polynomial, the Cluj-Ilmenau[35] index, $CI=CI(G)$, is calculable as:

$$CI(G) = \{[\Omega'(G,1)]^2 - [\Omega'(G,1) + \Omega''(G,1)]\} \tag{11}$$

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



G_1

Figure 1. Omega polynomial in the graph G_1:

$\Omega(G,x) = 5x + 2x^2 + x^3$; $\Omega'(G,1) = e = 12$; CI = 122

There exist graphs for which the above polynomial and index show degenerate values.

In tree graphs, the Omega polynomial simply counts the non-opposite edges, being included in the term of exponent c=1. The coefficient of the term of exponent c=1 has found utility as a topological index, called n_p, the number of *pentagon*

fusions, appearing in small fullerenes as a destabilizing factor. This index accounts for more than 90 % of the variance in heat of formation HF of fullerenes C_{40} and C_{50}.[45]

4. Omega Polynomial in Twisted ((4,8),3)R Tori

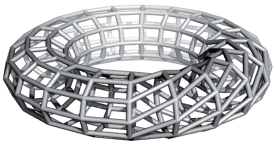
The embedding of the (4,4) net on the torus (Figure 2a) can be made by circulating a *c*-fold cycle, circumscribed to the toroidal tube cross-section, around the large hollow of the torus. The subsequent *n images* of *c*-fold cycle, equally spaced are joined with edges, point by point, to form a polyhedral torus tiled by a tetragonal pattern. In all, $c \times n$ points are generated.[46- 48] The (4,4) covering can also be generated by the Cartesian product $C_c \square C_n$.[39]

The primary (4,4) net can be changed to the "bathroom-floor" ((4,8)3) pattern (Figure 2b) by the Leapfrog Le operation on maps. The reader is invited to consult recent papers[49-54] dealing with operations on maps.

(a) TW(4,4)SH6[1020]; v = 200

(b) Le(TW(4,4)SH6[1020]); v = 800

(a) TW(4,4)SV6[1020]; v = 200



(b) Le(TW(4,4)SV6[1020]); v = 800

Figure 2. Toroidal objects tessellated by (4,4)S (a) and ((4,8)3)R patterns

Observe the (4,4) net can be twisted either horizontally H or vertically V, thus resulting two isomeric embeddings, which are chiral. Accordingly, the leapfrogged lattice will also be twisted and chiral. Since the (4,4) square net is an S-embedding (4,4)S, and the leapfrog operation rotates the original edges by $\pi/4$, the square changes to rhomb and consequently the Le-transform is designated as ((4,8)3)R. The

isomeric ((4,8)3)S network can be designed from the (4,4)R net, which Omega polynomial formulas will be presented in a future paper.

The Omega polynomials were calculated by using our Omega generator software[55] and the results, listed in Table 1, were rationalised in Table 2 in terms of our symbolism for a toroidal network.[46,47]

Table 1. Omega Polynomials in ((4,8)3)R Tiled Tori: Le(Tw(4,4)S(H/V)*t*[*c*,*n*])

(1) H; $c = \text{div } 4$; $n = 2c$; $c = 2^k$		Omega	*CI*
t=div *c*	*t* [16,32]		
	0	$32X^{16}+16X^{32}+32X^{64}$	9281536
	1, 3, 5,15	$16X^{32}+X^{512}+2X^{1024}$	7061504
	2, 6, 10	$16X^{32}+2X^{256}+4X^{512}$	8241152
	4, 12	$16X^{32}+4X^{128}+8X^{256}$	8830976
	8	$16X^{32}+8X^{64}+16X^{128}$	9125888
	16	$96X^{32}$	9338880

(2) H; $c = \text{div } 4$; $n = 2c$; $c \neq 2^k$		Omega	*CI*
t=div *c,n*	*t* [12,24]		
	0	$24X^{12}+12X^{24}+24X^{48}$	2920320
	1,5,7,11	$12X^{24}+X^{288}+2X^{576}$	2232576
	2,10	$12X^{24}+2X^{144}+4X^{288}$	2605824
	3,9	$12X^{24}+3X^{96}+6X^{192}$	2730240
	4	$12X^{24}+20X^{72}$	2875392
	6	$12X^{24}+6X^{48}+12X^{96}$	2854656
	8	$12X^{24}+8X^{36}+8X^{144}$	2802816
	12	$72X^{24}$	2944512

(3) H; $n = 2c$; $c \neq 2^k$; *c*=odd		Omega	*CI*
$n = 2c$; $c \neq 2^k$			
t=div *c,n*	*t* [11,22]		
	0	$22X^{11}+11X^{22}+22X^{44}$	2057726
	1,3,5,7,9	$11X^{22}+5X^{242}$	1810160
	2,4,6,8,10	$11X^{22}+2X^{121}+2X^{484}$	1605186
	11	$66X^{22}$	2076360

(4) H; $n = 2c$; $c \neq 2^k$; c=even t=div c,n	t [10,20]	Omega	*CI*
	0	$20X^{10}+10X^{20}+20X^{40}$	1402000
	1,3,7,9	$10X^{20}+X^{200}+2X^{400}$	1076000
	2,6,	$10X^{20}+10X^{100}$	1336000
	4,8	$10X^{20}+4X^{50}+4X^{200}$	1266000
	5	$10X^{20}+5X^{40}+10X^{80}$	1364000
	10	$60X^{20}$	1416000

(5) H; $c = 0(\mathrm{mod}\,4)$; $n = 3c$ $c = 2^k$ t=div c	t [8,24]	Omega	*CI*
	0	$24X^{8}+8X^{24}+16X^{48}$	1284096
	1,5,7	$8X^{24}+3X^{128}+X^{192}+X^{384}$	1089024
	2	$8X^{24}+6X^{64}+2X^{96}+2X^{192}$	1205760
	3	$8X^{24}+3X^{64}+2X^{384}$	1015296
	4	$8X^{24}+12X^{32}+4X^{48}+4X^{96}$	1264128
	6	$8X^{24}+6X^{32}+4X^{192}$	1168896
	8	$24X^{16}+16X^{24}+8X^{48}$	1293312

(6) V; $n = rc$; $c = 2^k$, $c \neq 2^k$ t=div c	t [20,40]	Omega	*CI*
	0	$40X^{20}+20X^{40}+40X^{80}$	*22736000*
	1,3,7,9,11,13,17,19	$40X^{20}+X^{800}+2X^{1600}$	17264000
	2,6,14,18	$40X^{20}+2X^{400}+4X^{800}$	20144000
	4,8,12	$40X^{20}+4X^{200}+8X^{400}$	21584000
	5,15	$40X^{20}+5X^{160}+10X^{320}$	21872000
	10	$40X^{20}+10X^{80}+20X^{160}$	22448000
	20	$40X^{20}+20X^{40}+40X^{80}$	*22736000*

* not all t provides distinct graphs

In Table 2, the V-twisted isomers behave regularly, within the range of n=kc, according to the only relation, written in the entry (2). For no twisting, t=0 and H=V.

The H-twisted isomers are more complicated in the Omega description, needed being the specification of more narrow cases. As a trend, the general formula (the fist one written for each case) is obeyed for t= *div c* or *div c,n* , i.e., the divisors of the net parameters, and next exceptions are listed. Multiples of these divisors will show the same expression for the polynomial and identical values of *CI* index. It is no mater if the objects generated by the TORUS software are distinct topological objects;

the divisors of the net parameters will always provide distinct polynomials and *CI* index values. The first derivative $\Omega'(G,1) = 6cn$ provides the number of edges in this class of tori.

The dependence by t of the omega polynomial coefficients can be exploited in calculated the helicity of tubular nanostructure. Other cases of the ((4,8)3)R covering embedded in tori will be presented in a future paper.

Table 2. Omega Polynomial in Twisted ((4,8)3)R Tori

(1) H; $n = 2c$ $c = \text{div } 4$; $c = 2^m$ c, n, t, m- integers	$\Omega(G,x) = c \cdot x^n + t \cdot x^{cn/t} + 2t \cdot x^{2cn/t}$	$t = \text{div } c$ except the cases below
	$\Omega(G,x) = 2(c+n) \cdot x^n$	$t = c$
(2) H; $n = 2c$; $c = \text{div } 4$; $c \neq 2^m$ c, n, t, k, m - integers	$\Omega(G,x) = c \cdot x^n + t \cdot x^{cn/t} + 2t \cdot x^{2cn/t}$	$t = \text{div } c, n$ except the cases below
	$\Omega(G,x) = c \cdot x^n + 5t \cdot x^{cn/t}$	$t = 4k; c \leq 5t; k = 1$ $t = 4k; c > 5t; k = 2$ c=div 4
	$\Omega(G,x) = c \cdot x^n + t \cdot x^{cn/t} + t \cdot x^{4cn/t}$	$t = 8; c \leq 5t/2$; div n
	$\Omega(G,x) = 2(c+n) \cdot x^n$	$t = c$
(3) H; $n = 2c$ $c \neq 2^m$; c=odd c,n, t, m - integers	$\Omega(G,x) = c \cdot x^n + 5t \cdot x^{cn/t}$	$t = \text{div } c, n$ $t = 1$
	$\Omega(G,x) = c \cdot x^n + t \cdot x^{cn/t} + t \cdot x^{4cn/t}$	$t = 2$
	$\Omega(G,x) = 2(c+n) \cdot x^n$	$t = c$
(4) H; $n = 2c$ $c \neq 2^m$; c= even c,n, t, m - integers	$\Omega(G,x) = c \cdot x^n + t \cdot x^{cn/t} + 2t \cdot x^{2cn/t}$	$t = \text{div } c, n$ except the cases below
	$\Omega(G,x) = c \cdot x^n + 5t \cdot x^{cn/t}$	t=2 ; c=div2
	$\Omega(G,x) = c \cdot x^n + t \cdot x^{cn/t} + t \cdot x^{4cn/t}$	$t = 4$; div n
	$\Omega(G,x) = 2(c+n) \cdot x^n$	$t = c$
(5) H; $n = rc$; r =3 $c = \text{div } 4$; $c = 2^m$ c, n, t, k, r, m- integers	$\Omega(G,x) = c \cdot x^n + rt \cdot x^{2cn/rt} + t \cdot x^{cn/t} + t \cdot x^{2cn}$	$t = \text{div } c$ except the cases below
	$\Omega(G,x) = c \cdot x^n + t \cdot x^{cn/t} + (2t/r) \cdot x^{2cnr/t}$	$t = 3k$
	$\Omega(G,x) = n \cdot x^{2c} + 2c \cdot x^n + c \cdot x^{2n}$	$t = c$
(6) V; $n = rc$ c, n, t, r, m - integers	$\Omega(G,x) = n \cdot x^c + t \cdot x^{cn/t} + 2t \cdot x^{2cn/t}$	$t = \text{div } c$ $t = 0$; H=V

Conclusions

Omega polynomial is a counting polynomial developed on the *quasi orthogonal cut "qoc"* strips, related to partial cubes. Omega polynomial $\Omega(G,x)$ counts the qoc strips of all extent in *G*. Close formulas for the calculation of the Omega polynomial in toroidal objects tessellated by the ((4,8)3)R pattern in twisted embeddings were derived. The helicity of tubular nanostructures can be evaluated from the coefficients of $\Omega(G,x)$.

Acknowledgements. This work was supported by the Romanian Grant PN-II, ID_506/2007.

References

1. M. V. Diudea, I. Gutman, L. Jäntschi, *Molecular Topology*, NOVA, New York, 2002.
2. F. Harary, *SIAM Rev.*, **1962**, *4*, 202-210.
3. H. Sachs, *Publ. Math. (Debrecen)*, **1964**, *11*, 119-134.
4. N. Trinajstić, *Chemical Graph Theory, IInd Ed.* CRC Press, 1992.
5. I. Gutman, M. Milun, N. Trinajstić, *MATCH Commun. Math. Comput. Chem.*, **1975**, *1*, 171-175.
6. J. Aihara, *J. Am. Chem. Soc.*, **1976**, *98*, 2750-2758.
7. I. Gutman, M. Milun, N. Trinajstić, *J. Am. Chem. Soc.*, **1977**, *99*, 1692-1704.
8. A. Tang, Y. Kiang, G. Yan, S. Tai, *Graph Theoretical Molecular Orbitals*, Science Press, Beijing, 1986.
9. P. S. Dwyes, *Linear Computations*, Wiley, N. Y. 1951.
10. D. K. Fadeev, I. S. Sominskii, *Problems in Higher Algebra*, Freeman, San Francisco, 1965.
11. H. Hosoya, M. Murakami, M. Gotoh, *Natl. Sci. Rept. Ochanomizu Univ.*, **1973**, *24*, 27-34.
12. R. L. Graham, L. Lovasz, *Adv. Math.*, **1978**, *29*, 60-88.
13. M. V. Diudea, O. Ivanciuc, S. Nikolić, N. Trinajstić, *MATCH Commun. Math. Comput. Chem.*, **1997**, *35*, 41-64.
14. O. Ivanciuc, M. V. Diudea, P. V. Khadikar, *Indian J. Chem.*, **1998**, *37A*, 574-585.
15. O. Ivanciuc, T. Ivanciuc, M. V. Diudea, *Roum. Chem. Quart. Rev*. **1999**, *7*, 41-67.
16. H. Hosoya, *Bull. Chem. Soc. Japan*, **1971**, 44, 2332-2339.
17. H. Hosoya, *Discrete Appl. Math.*, **1988**, *19*, 239-257.
18. E. V. Konstantinova and M. V. Diudea, *Croat. Chem. Acta*, **2000**, 73, 383-403.
19. I. Gutman, S. Klavžar, M. Petkovšek, P. Žigert, *MATCH Commun. Math. Comput. Chem.*, **2001**, *43*, 49-66.
20. H. Hosoya, T. Yamaguchi, *Tetrahedron Lett*., **1975**, 4659-4662.
21. N. Ohkami, H. Hosoya, *Theoret. Chim. Acta*, **1983**, *64*, 153-170.

22. N. Ohkami, A. Motoyama, T. Yamaguchi, H. Hosoya, *Tetrahedron*, **1981**, *37*, 1113-1122.
23. H. Hosoya, *Topics Curr. Chem*., **1990**, *153*, 255-272.
24. E. Clar, *Polycyclic Hydrocarbons*, Acad. Press, London, 1964.
25. E. Clar, *The Aromatic Sextet*, Wiley, New York, 1972.
26. I. Gutman, H. Hosoya, *Z. Naturforsch*., **1990**, *45a*, 645-648.
27. I. Gutman, *MATCH Commun. Math. Comput. Chem*., **1992**, *28*, 139-150.
28. D. Stevanović, *Graph Theory Notes New York*, **1998**, *34*, 31-36.
29. A. Motoyama, H. Hosoya, *J. Math. Phys*., **1977**, *18*, 1485-1490.
30. K. Balasubramanian, R. Ramaraj, *J. Comput. Chem*., **1985**, *6*, 447-454
31. E. J. Farrell, *Canad. Math. Bull*., **1978**, *2*, 35-46.
32. E. J. Farrell, C. De Matas, *Ark. Math.*, **1988**, *26*, 185-190.
33. E. J. Farrell, C. De Matas, *Util. Math*., **1988**, *33*, 33-45.
34. P. E. John, P. V. Khadikar, J. Singh, *J. Math. Chem*., **2007**, *42*, 37-45.
35. P. E. John, A. E. Vizitiu, S. Cigher, M. V. Diudea, *MATCH Commun. Math. Comput. Chem.*, **2007**, *57*, 479-484.
36. D. Ž. Djoković, *J. Combin. Theory Ser. B*, **1973**, *14*, 263-267.
37. P. M. Winkler, *Discrete Appl. Math*., **1984**, *8*, 209-212.
38. S. Klavžar, *MATCH Commun. Math. Comput. Chem.*, **2008,** *59***,** 217-222.
39. S. Klavžar, *MATCH Commun. Math. Comput. Chem.*, **2008**, *60*, 255-274.
40. S. Ovchinikov, arXiv: 0704.0010v1 [math CO] 31 Mar 2007.
41. M. V. Diudea, A. E. Vizitiu, D. Janežič, *J. Chem. Inf. Model*., **2007**, *47*, 864-874.
42. M. V. Diudea, S. Cigher, A. E. Vizitiu, O. Ursu, P. E. John, *Croat. Chem. Acta*, **2006**, *79*, 445-448.
43. A. E. Vizitiu, S. Cigher, M. V. Diudea, M. S. Florescu, *MATCH Commun. Math. Comput. Chem.*, **2007**, *57*, 457-462.
44. M. V. Diudea, Omega Polynomial, *Carpath. J. Math*., **2006,** *22*, 43-47.
45. M. V. Diudea, S. Cigher, A. E. Vizitiu, M. S. Florescu, P. E. John, *J. Math. Chem*., **2008**, *44*, 000-000.
46. M. V. Diudea, Cs. L. Nagy, *Periodic nanostructures*, Springer, 2007.
47. M. V. Diudea (Ed.), *Nanostructures, novel architecture*, Nova, N.Y., 2005.
48. M. V. Diudea, *Bull. Chem. Soc. Japan*, **2002**, *75*, 487-492.
49. M. V. Diudea, P. E. John, A. Graovac, M. Primorac, T. Pisanski, *Croat. Chem. Acta*, **2003**, *76*, 153-159.
50. M. V. Diudea, *Forma (Tokyo)*, **2004**, *19*, 131-163.
51. M. V. Diudea, M. Ştefu, P. E. John, A. Graovac, *Croat. Chem. Acta,* **2006,** *79*, 355-362.
52. M. Ştefu, M. V. Diudea, P. E. John, *Studia Univ. "Babes-Bolyai"*, **2005,** *50*, 165-174.
53. M. V. Diudea, *J. Chem. Inf. Model.,* **2005**, *45,* 1002-1009.
54. M. V. Diudea, M. Ştefu, P. E. John, A. Graovac, *Croat. Chem. Acta,* **2006,** *79*, 355-362.
55. S. Cigher, M. V. Diudea, *Omega Polynomial Counter*, "Babes-Bolyai" Univ., **2007.**