CARPATHIAN J. MATH.
**22** (2006), No. 1 - 2, 43 - 47

# Omega Polynomial

MIRCEA V. DIUDEA

ABSTRACT. A new counting polynomial, called the "Omega" $\Omega(G,x)$ polynomial, is proposed on the ground of quasi-orthogonal cut "*qoc*" edge strips in a bipartite lattice. Within a *qoc* not all cut edges are necessarily orthogonal, meaning not all are pairwise codistant. Two topological indices: $CI$ (Cluj-Ilmenau), eventually equal to the well-known $PI$ index, in planar, bipartite graphs and $I_\Omega$ are defined on the newly proposed polynomial and exemplified. Closed analytical formulas for $\Omega(G,x)$ in polyhex tori are given.

## 1. INTRODUCTION

A graph may be represented by a matrix, a sequence of numbers, a single number (i.e., a topological index) or by a polynomial. Various graph-theoretical polynomials are applied to many different areas of chemistry. The spectrum (i.te., the non-increasing sequence of all eigenvalues) of the characteristic polynomial of graphs was studied in connection to the Hűckel molecular orbitals [8]. The acyclic [2] (also called the reference [1]) polynomial was proposed to evaluate the aromatic character (the topological resonance energy TRE) of polycyclic hydrocarbons.

Further, Farrell introduced the matching polynomial [5] related to the Kekulé structure count. The rotational polynomial [9] was used for analysis of the entropy of chain hydrocarbon molecules. More about polynomials the reader can find in [2].

A distance-counting polynomial was introduced by Hosoya (1988) [10] as:

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

with $d(G,0) = N$ and $d(G,1) = e$. In the above relations, $N$ is the number of vertices in the graph $G$, $e$ is the number of edges and $d(G,k)$ is the number of pair vertices lying at distance k to each other. Summation runs up to $d(G)$,the topological diameter (*i.e.*, the longest topological distance in $G$). The polynomial was called Wiener, by its author but Hosoya, in the more recent literature [7], [19].

The **sextet polynomial** of a benzenoid system $B(G,x)$, proposed by Hosoya et al. [15], [16] is then defined as:

$$B(G,x) = \sum_k r(G,k) \cdot x^k \tag{1.2}$$

Received: 29.11.2005; In revised form: 02.04.2006; Accepted: 01.11.2006
2000 *Mathematics Subject Classification:* 92E10.
Key words and phrases: *Counting polynomial, opposite cuts, topological index.*
Dedicated to Professor Haruo Hosoya, Ochanomizu Univ., Tokyo, for his bright contribution to the Chemical Graph Theory.

where, the resonant sextet number, is the number of ways in which $k$ mutually resonant rings can be selected in the benzenoid molecule $G$. Summation runs up to m, the largest number of mutually resonant rings in $G$. By definition, $r(G,0) = 1$, in any $G$. The number of the sextet patterns is then equal to $B(G,x)|_{x=1}$. The sextet polynomial is important in connection to the Clar aromatic sextets, expected to stabilize the aromatic molecules. The above $H(G,x)$ and $B(G,x)$ are both counting polynomials.

## 2. OMEGA POLYNOMIAL

Let $G(V,E)$ be a connected graph with the vertex set $V = V(G)$ and edge set $E = E(G)$.

Two edges $e = (1,2)$ and $e' = (1',2')$ of $G$ are called codistant (briefly: e co e') if for $k = 0,1,2,\ldots$ there exist the relations: $d(1,1') = d(2,2') = k$ and $d(1,2') = d(2,1') = k+1$ or vice versa. For some edges of a connected graph $G$ there are the following relations satisfied [3]:

(2.3) $e \; co \; e$

(2.4) $e \; co \; e' \Longleftrightarrow e' \; co \; e$

(2.5) $e \; co \; e' \& e' \; co \; e'' \Longleftrightarrow e \; co \; e''$

though the relation (2.5) is not always valid.

Let $C(e) := \{e' \in E(G); e' \; co \; e\}$ denote the set of all edges of $G$ which are codistant to the edge $e$. If all the elements of $C(e)$ satisfy the relations (2.3) - (2.5) then $C(e)$ is called an orthogonal cut "oc" of the graph $G$. The graph $G$ is called co-graph if and only if the edge set $E(G)$ is the union of disjoint orthogonal cuts: $C_1 \cup C_2 \cup ... \cup C_k = E$ and $C_i \cap C_j = \phi$ for $i \neq j$, $i,j = 1,2,...,k$.

If any two consecutive edges of a cut edge sequence are codistant (obeying the relations (2.3) and (2.4)) and belong to one and the same face of the covering, such a sequence is called a quasi-orthogonal cut "*qoc*" strip. This means that the transitivity relation (2.5) is not necessarily obeyed. Any *oc* strip is a qoc one but the reverse is not always true [3].

A *qoc* strip starts and ends either out of $G$ (at an edge with endpoints of degree lower than 3, if $G$ is an open lattice) or in the same starting polygon (if $G$ is a closed lattice).

The Omega $\Omega(G,x)$ polynomial of the qoc counting is defined as:

(2.6) $$\Omega(G,x) = \sum_c m(G,c) \cdot x^c$$

with $m(G,c)$ being the number of *qocs* of length $c$. The summation runs up to the maximum length of *qocs* in $G$.

This counting polynomial is useful in topological description of benzenoid structures as well as in counting some single number descriptors, also called topological indices. The qoc strips could account for the helicity of nanotubes and nanotori.

An index, called $CI$ (Cluj-Ilmenau), is derived from and its first and second derivatives, in $x = 1$, as [3]:

(2.7) $$CI(G) = (\Omega')^2 - (\Omega' + \Omega'')|_{x=1}.$$

$CI$ is eventually equal to the well-known $PI$ index [11], [13], in polycyclic graphs embedded in the plane.

Another single number descriptor is calculable from the $\Omega(G,x)$ derivatives $d$, in $x=1$, and normalized to the first polynomial derivative, i. e. the number of edges in $G$:

$$I_\Omega(G) = (1/\Omega'(G,x)) \sum_d (\Omega^d(G,x))^{1/d}|_{x=1}. \tag{2.8}$$

Examples:

Two simple molecular graphs are considered for the first examples: anthracene (Figure 1a) and phenanthrene (Figure 1b).

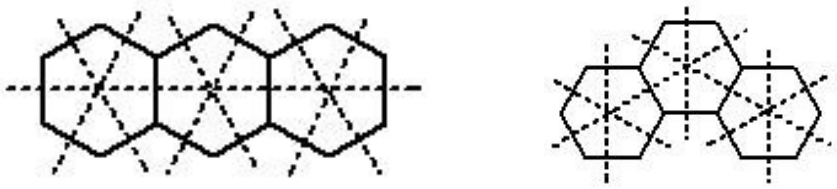

**Figure 1.** Anthracene (a) and Phenanthrene (b) molecular graphs.

Anthracene:

$$\Omega(G) = 6x^2 + x^4;\ I_\Omega(G) = 1.6248;\ CI = PI = 216.$$

Phenanthrene:

$$\Omega(G) = 5x^2 + 2x^3;\ I_\Omega(G) = 1.4362;\ CI = PI = 218.$$

## 3. Toroidal structures

Polyhex toroidal structures [14] can be represented as in Figure 2: phenacenic $H[q,2p]$ (2a) and acenic $V[q,2p]$ tori (2b), corresponding to the "armchair" and "zig-zag" tubes resulted by cutting edges around the central hollow of the torus. In the Schlegel-like representation the points lying on the central circle have to be identified to those on the external circle. The objects in Figure 2 have only three hexagons around the tube, corresponding to $q=6$ and $q=3$, respectively [17].

Two types of cuts appear in polyhex, untwisted tori: one radial (denoted $R$) and another circular (denoted $C$), as shown in the corresponding polynomial:

$$\Omega(G,x) = R(G,x) + C(G,x). \tag{3.9}$$

In the following, only non-chiral (i.e. non-twisted) tori are considered.

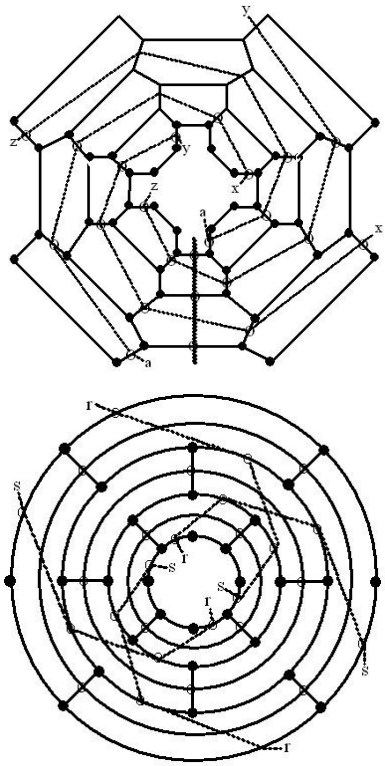

**Figure 2.** (a) $H[6,8]$; $q=6$; $p=4$; "armchair"; (b) $V[3,8]$; $q=3$; $p=4$; "zig-zag" in the Schlegel-like projection; the white circles denote the cut edges while the letters indicate the way of continuing the cut edge set.

**(a) Torus** $H[q,2p]$ (corresponding to "armchair" tube, in the Schlegel-like projection).

In this case, $q$ is always even; $q$-winding around the tube while $p$ around the central hallow of the torus.

The radial term $R$ is the same for all the cases:

$$R(G,x) = 2p \cdot x^{q/2} \tag{3.10}$$

The circular term $C$ vary as follows:

$$C(G,x) = k \cdot x^{2pq/k} \tag{3.11}$$

with $k$ being the greatest common divisor of $q$ and $2p$.

For the case in Figure 2a, $H[6,8]$; $q=6$; $p=4$: $\Omega(G,x) = 8x^3 + 2x^{24}$; $I_\Omega = 7.123765$, $CI = 3960$.

**(b) Torus** $V[q,2p]$ (corresponding to "zig-zag" tube, in the Schlegel-like projection)

The circular term $C$ is the same for all the cases:

$$C(G,x) = q \cdot x^{p}. \tag{3.12}$$

The radial term R vary as follows:

(3.13) $R(G,x) = k \cdot x^{2pq/k}$

with $k$ being as above.

For the case in Figure 2b, $V[3,8]$; $q = 3$; $p = 4$: $\Omega(G,x) = 3x^4 + 2x^{12}$; $I_\Omega = 4.106674$, $CI = 960$.

## 4. Conclusions

A new counting polynomial was proposed to account for the opposite cuts in a bipartite lattice. The polynomial is an elegant form of topological description of lattice graphs. It is related to the well-known $PI$ index and enables the calculation of two new indices: $CI$ and $I_\Omega$. These indices can be useful in correlating properties with molecular structures [18].

## References


[1] Aihara, J., *A new definition of Dewar-type resonance energy*, J. Am. Chem. Soc., **98** (1976) 2750-2758

[2] Diudea, M. V., Gutman, I. and Jäntschi, L., *Molecular Topology*, NOVA, New York, 2002

[3] Diudea, M. V., *Hydrocarbons Using Orthogonal Cuts*, J. Math. Chem., (in print)

[4] Diudea, M. V., *QSPR/QSAR Studies by Molecular Descriptors*, NOVA, New York, 2001.

[5] Farrell, E.J., *An introduction to matching polinomials*, J. Combin. Theory Ser.B, **27** (1979), 60-86

[6] Gutman, I., Milun, M., Trinajstić, N., *Non-parametric resonance energies of arbitrary conjugated systems*, J. Am. Chem. Soc. **99** (1977), 1692-1704

[7] Gutman, I., Klavžar, S., Petkovšek, M. and Žigert, P., *On Hosoya polynomials of benzenoid graphs*, MATCH Commun. Math. Comput. Chem., **43** (2001), 49-66

[8] Hosoya, H., *Graphical enumeration of the coefficients of the secular polynomials of the Hückel molecular orbitals*, Theor. Chim. Acta (Berlin), **25** (1972), 215-222

[9] Hosoya, H., Kisu, Y., Marumi, H., *Rotational polynomial*, Proceedings of the Symposium on Molecular Structure, Sapporo,1977

[10] Hosoya, H., *On some counting polynomials in chemistry*, Discrete Appl. Math., **19** (1988), 239-257

[11] John, P. E., Vizitiu, A. E., Cigher, S., Diudea, M. V., *CI index in tubular nanostructures*, MATCH Commun. Math. Comput. Chem. (in print)

[12] Khadikar, P. V., *On a novel structural descriptor PI*, Nat. Acad. Sci. Letters, **23** (2000), 113-118

[13] Khadikar, P. V., Kale, P. P., Despande, N. V., Karmarkar, S. and Agrawal, V. K., *Novel PI Indices of Hexagonal Chains*, J. Math. Chem, **29** (2001), 143-150

[14] Khadikar, P. V., Karmarkar, S. and Agrawal, V. K., *PI Indices of Polyacenes and Its Use in Developing QSAR*, Nat. Acad. Sci. Letters, **23** (2000), 124-128

[15] 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

[16] Ohkami, N., Motoyama, A., Yamaguchi, T. and Hosoya, H., *Mathematical properties of the set of the Kekule patterns and the sextet polynomial for polycyclic aromatic hydrocarbons*, Tetrahedron, **37** (1981), 1113-1122

[17] Schlegel, V., *Verhandlungen der Kaiserlichen Leopoldinisch-Carolinischen Deutshen Akademie der Naturforscher*, **44** (1893), 337-459

[18] Stefu, M. and Diudea, M. V., *Wiener index of C4C8 nanotubes*, MATCH Commun. Math. Comput. Chem., **50** (2004), 133-144

[19] Stevanović, D., *Hosoya polynomial of composite graphs*, Discrete Math., **235** (2001), 237-244



Faculty of Chemistry and Chemical Engineering
"Babeş-Bolyai" University
400028 Cluj-Napoca, Romania
*E-mail address*: diudea@chem.ubbcluj.ro