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Omega Polynomial in Tubular Nanostructures

Mircea V. Diudea,[a,*] Simona Cigher,[a] Aniela E. Vizitiu,[a] Oleg Ursu,[a] and Peter E. John[b]

[a]*Faculty of Chemistry and Chemical Engineering, Babeş-Bolyai University, 3400 Cluj, Romania*

[b]*Technical University of Ilmenau, Institute of Mathematics, PSF 10 05 65, D-98684 Ilmenau, Germany*

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A new counting polynomial, called the »Omega« Ω(G, *x*) polynomial, was recently proposed by Diudea on the ground of quasi-orthogonal cut »qoc« edge strips in a polycyclic graph. 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_Ω are defined on the newly proposed polynomial and exemplified. Closed analytical formulas for Ω(G, *x*) and *CI* in polyhex tori and tubes are given.

INTRODUCTION

Let G(V, E) be a connected bipartite graph with the vertex set V = V(G) and edge set E = E(G), without loops.

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

$$e \text{ co } e \tag{1}$$

$$e \text{ co } e' \Leftrightarrow e' \text{ co } e \tag{2}$$

$$e \text{ co } e' \;\&\; e' \text{ co } e'' \Rightarrow e \text{ co } e'' \tag{3}$$

though relation (3) is not always valid. A simple counterexample is given in Figure 1.

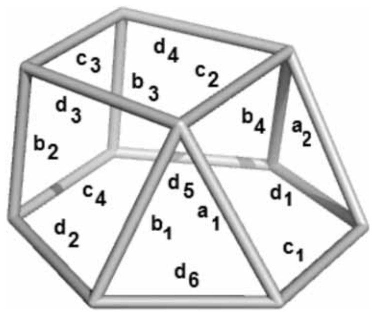

Figure 1. Codistant edges in a graph: {a} and {c} are oc strips; strips {b} and {d} do not have all elements mutually codistant (*e.g.*, b_1&b_4; d_1&d_5), so that {b} and {d} are qoc strips. $\Omega(G, x) = x^4 + 2\cdot x^4 + x^6$; *CI* = 184; *PI* =176.

Let $C(e) = \{ e' \in E(G);\, e' \text{ co } e \}$ denote the set of all edges of G that are codistant to edge e. If all the elements of $C(e)$ satisfy relations (1–3), then $C(e)$ is called an orthogonal cut »oc« of graph G. Graph G is called a co-graph if and only if the edge set E(G) is the union of disjoint orthogonal cuts: $C_1 \cup C_2 \cup \ldots \cup C_k = E$ and $C_i \cap C_j = \varnothing$ for $i \neq j$, $i, j = 1,2,\ldots, k$.

If any two edges of a cut edge sequence are codistant (obeying relations (1) and (2)) and belong to one and the same face of the covering, such a sequence is called

* Author to whom correspondence should be addressed. (E-mail: diudea@chem.ubbcluj.ro)

a quasi-orthogonal cut »qoc« strip. This means that the transitivity relation (3) is not necessarily obeyed.

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). Any oc strip is a qoc strip but the reverse is not always true.

A new index, *CI* (Cluj-Ilmenau), eventually equal to the well-known *PI* index[3–5] in polyhex bipartite graphs embedded in the plane, is calculable, on the ground of the qoc restriction, as:[2]

$$CI(\mathrm{G}) = m^2(\mathrm{G}) - \sum_{\mathrm{Q}\in \mathrm{Q(G)}} c^2(\mathrm{Q}) \tag{4}$$

with m(G) = |E(G)| being the number of edges in the graph, c(Q) = |Q| the cardinality or the length of the quasi-orthogonal cut $\mathrm{Q}(e) = \{e_i, e_j, ..., e_k\}$ and $\underline{\mathrm{Q}} = \underline{\mathrm{Q}}(\mathrm{G})$ the set of all qoc strips in G. Index calculation for the graph in Figure 1 is:

$$CI(\mathrm{G}) = 16^2 - (2^2 + 2\times 4^2 + 6^2) = 184$$

For this graph, *PI* = 176, thus differing from the value of the *CI* index.

COUNTING POLYNOMIALS

A counting polynomial is defined as:

$$\mathrm{C}(\mathrm{G}, x) = \sum\nolimits_k m(\mathrm{G}, k) \cdot x^k \tag{5}$$

In the above relation, m(G,k) is the number of sets, of a topological quantity, of cardinality (*i.e.*, length) k, in graph G and x is simply a parameter. The summation runs up to the maximum k-value in G. A distance-counting polynomial was introduced by Hosoya,[6–8] and similarly the sextet polynomial[9,10] for counting the resonant rings in a benzenoid molecule. The sextet polynomial is important with respect to the Clar aromatic sextets,[11,12] expected to stabilize the aromatic molecules. The reader can find more about polynomials in Ref. 13.

Very recently, Diudea[14] proposed the Omega, Ω(G, x), polynomial for counting the qoc strips in G:

$$\Omega(\mathrm{G}, x) = \sum\nolimits_c m(\mathrm{G}, c) \cdot x^c \tag{6}$$

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

For the graph in Figure 1, the polynomial is: $\Omega(\mathrm{G}, x) = x^4 + 2\cdot x^4 + x^6$.

This counting polynomial is useful in the topological description of benzenoid, bipartite, structures as well as in counting some single number descriptors, *i.e.*, topological indices. The qoc strips could account for the helicity of polyhex nanotubes and tori.

The Omega 1.1 software program includes the qoc strips procedure, as given in the following:

Omega Pseudocode[15]

The polynomial coefficients are stored in the string *coef,* where *coef[i]* is the coefficient of the term X^i. Initially, all the coefficients are zero.

For each non-visited edge *e* execute *detLegUrmX(e, lung).*

lung – length of the qoc strip (at real time) to which edge *e* belongs. At the start of a new qoc strip, *lung* = 1.

At the start, all the edges are considered as non-visited;

Covering (6,3):

```
Procedure detLegUrm6(e,lung)
  Edge e is visited;
  s – left end of edge e
  d – right end of edge e
  For each neighbor x of the point s different from d execute
    For each neighbor xx of the point x different from s execute
      For each neighbor y of the point d different from s execute
        For each neighbor yy of the point y different from d execute
          If xx and yy are the end-points of edge e_xy non-visited
          Then
            Edge e_xy is visited;
            coef[lung+1]=coef[lung+1]+1;
            coef[lung]=coef[lung]-1;
            detLegUrm6(e_xy,lung+1);
          End. If
        End. For
      End. For
    End. For
  End. For
End. Procedure
```

The above *CI* index is derived from Ω(G, x) and its first and second derivatives, in x = 1, as:

$$CI(\mathrm{G}) = (\Omega')^2 - (\Omega' + \Omega'')\,|_{x=1} \tag{7}$$

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

$$I_\Omega(\mathrm{G}) = (1/\Omega'(\mathrm{G}, x)) \cdot \sum\nolimits_d (\Omega^d(\mathrm{G},x))^{1/d}\,|_{x=1} \tag{8}$$

For the graph in Figure 1, I_Ω = 2.513576.

EXAMPLES

In the Schlegel-like representation[16] of a nanotube (Figures 2 and 3), the points lying on the central circle have to be identified to those on the external circle to give the corresponding torus.

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

$$\Omega(\mathrm{G}, x) = \mathrm{R}(\mathrm{G}, x) + \mathrm{C}(\mathrm{G}, x) \tag{9}$$

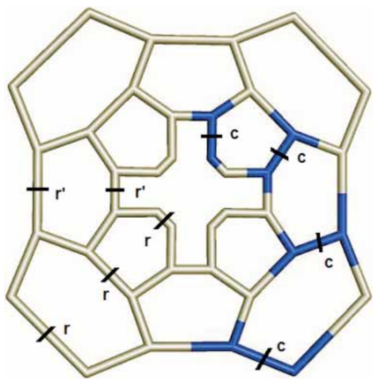

Figure 2. Armchair tube TUV [8,5]; $p = 4$; $q = 5$ and its corresponding torus H [4,8]; $p = 4$; $q = 4$.

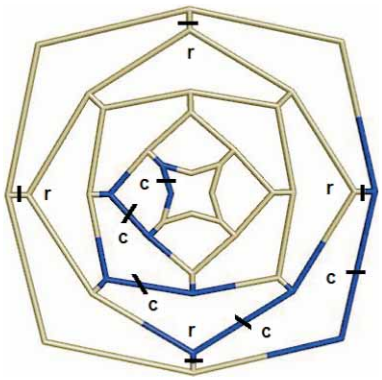

Figure 3. Zig-zag tube TUH [8,5]; $p = 4$; $q = 5$ and the corresponding torus V [4,8]; $p = 4$; $q = 4$.

*Armchair Tubes TUV[*2p,q*] and Tori H[*q,2p*]*

Case of »armchair« tubes, *TUV* [2p,q]. – TUV [2*p*,*q*] or TUV[*c*,*n*] in general, in Diudea's nomenclature,[17,18] with $p = c/2$ and $q = n$, is given in Figure 2.

For all polyhex armchair tubes, the circular term C is the same:

$$\mathrm{C}(\mathrm{G}, x) = 2\,p \cdot x^{q-1} \tag{10}$$

The radial term R varies the function of the tube structure:

q = even:

$$\mathrm{R}(\mathrm{G}, x) = 2\,p \cdot x^{q/2} \tag{11}$$

The corresponding *CI* index is:

$$CI(\mathrm{TUV}[2p,q_e]) = p^2(3q-2)^2 - 2\,p(q-1)^2 - pq^2/2 =$$

$$9p^2q^2 - 12p^2q + 4p^2 - (5/2)pq^2 + 4\,pq - 2p \tag{12}$$

q = odd:

$$\mathrm{R}(G, x) = p \cdot x^{(q+1)/2} + p^{(q-1)/2} \tag{13}$$

$$CI(\mathrm{TUV}[2p,q_o]) = p^2(3q-2)^2 - 2p(q-1)^2 - (p/2)(q^2+1) =$$

$$9\,p^2q^2 - 12\,p^2q + 4p^2 - (5/2)\,pq^2 + 4\,pq - (5/2)\,p \tag{14}$$

For the example in Figure 2: $\Omega(\mathrm{TUV}[8,5], x) = 4 \cdot x^2 + 4 \cdot x^3 + 8 \cdot x^4$; $CI = 2524$; $I_\Omega = 1.404541$.

Case of tori, *H*[q,2p]. – An »armchair« nanotube TUV [2*p*,*q*+1] (Figure 2a, $p = 4$; $q = 4$), transforms into a torus H[*q*,2*p*] as above mentioned, with q (q = even, always in this construction) winding around the tube while p winds around the central hollow of the torus.

The radial term in such tori is the same for all cases:

$$\mathrm{R}(\mathrm{G}, x) = 2\,p \cdot x^{q/2} \tag{15}$$

and the circular term C varies as:

$$\mathrm{C}(\mathrm{G}, x) = k \cdot x^{2\,pq/k} \tag{16}$$

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

The index is calculated as:

$$CI(\mathrm{H}[q,2\,p]) = 9\,p^2q^2 - k\,(2\,pq/k)^2 - 2\,p\,(q/2)^2 =$$

$$(18kp^2q^2 - 8\,p^2q^2 - kpq^2)\,/\,(2k) \tag{17}$$

For the example in Figure 2: $\Omega(\mathrm{H}[4,8], x) = 8 \cdot x^2 + 4 \cdot x^8$; $CI = 2016$; $I_\Omega = 2.247207$.

*Zig-zag Tubes TUH[*2p,q*] and Tori V[*q,2p*]*

Case of zig-zag tubes TUH [2p,q] (*Figure 3*, p = *4*; q = *5*). – The circular and radial terms are as follows:

$$\mathrm{C}(\mathrm{G}, x) = (q-1) \cdot x^{p} \tag{18}$$

$$\mathrm{R}(\mathrm{G}, x) = 2\,p \cdot x^{q} \tag{19}$$

and the corresponding index is:

$$CI(\mathrm{TUH}[2\,p,q]) = p^2\,(3q-1)^2 - (q-1)\,p^2 - 2\,pq^2 =$$

$$9\,p^2\,q^2 - 7\,p^2\,q + 2\,p^2 - 2\,pq^2 \tag{20}$$

For the example in Figure 3: $\Omega(\mathrm{TUH}[8,5], x) = 4 \cdot x^4 + 8 \cdot x^5$; $CI = 2872$; $I_\Omega = 1.578425$.

Case of tori, V[q,2p]. – These tori correspond to »zig-zag« tubes, in a Schlegel-like projection (Figure 2b, p = 4; q = 4). The circular term C is the same for all cases:

$$C(G, x) = q \cdot x^{p} \tag{21}$$

and the radial term R varies as follows:

$$R(G, x) = k \cdot x^{2\,pq/k} \tag{22}$$

with k being as above.

The index is calculable as:

$$CI(V[q, 2p]) = 9\,p^2\,q^2 - k(2\,pq\,/\,k)^2 - p^2\,q =$$

$$(9\,kp^2\,q^2 - 4\,p^2\,q^2 - kp^2\,q)\,/\,k \tag{23}$$

For the example in Figure 3: $\Omega(V[4, 8], x) = 4 \cdot x^4 + 4 \cdot x^8$; CI =1984; I_{Ω} = 2.274070.

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 enables the calculation of two new indices: CI (related to the well-known PI index) and I_{Ω}. These indices can be useful in correlating properties with molecular structures.[19,20]

REFERENCES

1. P. E. John, P. V. Khadikar, and J. Singh, *J. Math. Chem.*, in press.
2. P. E. John, A. E. Vizitiu, S. Cigher, and M. V. Diudea, *MATCH Commun. Math. Comput. Chem.*, in press.
3. P. V. Khadikar, *Nat. Acad. Sci. Letters* **23** (2000) 113–118.
4. P. V. Khadikar, P. P. Kale, N. V. Despande, S. Karmarkar, and V. K. Agrawal, *J. Math. Chem.* **29** (2001) 143–150.
5. P. V. Khadikar, S. Karmarkar, and V. K. Agrawal, *Nat. Acad. Sci. Letters* **23** (2000) 124–128.
6. H. Hosoya, *Discrete Appl. Math*. **19** (1988) 239–257.
7. I. Gutman, S. Klavžar, M. Petkovšek, and P. Žigert, *MATCH Commun. Math. Comput. Chem.* **43** (2001) 49–66.
8. D. Stevanović, *Discrete Math*. **235** (2001) 237–244.
9. N. Ohkami and H. Hosoya, *Theor. Chim. Acta* **64** (1983) 153–170.
10. N. Ohkami, A. Motoyama, T. Yamaguchi, and H. Hosoya, *Tetrahedron* **37** (1981) 1113–1122.
11. E. Clar, *Polycyclic Hydrocarbons*, Academic Press, London, 1964.
12. E. Clar, *The Aromatic Sextet*, Wiley, New York, 1972.
13. M. V. Diudea, I. Gutman, and L. Jäntschi, *Molecular Topology*, Nova, New York, 2002.
14. M. V. Diudea, *Carpath. J. Math*., in press.
15. S. Cigher and M. V. Diudea, Omega 1.1, Babeş-Bolyai University, Cluj, Romania, 2005.
16. V. Schlegel, *Verhandlungen der Kaiserlichen Leopoldinisch-Carolinischen Deutschen Akademie der Naturforscher* **44** (1894) 337–459.
17. M. V. Diudea, *Polyhex tori originating in square tori*, in: M. V. Diudea (Ed.), *Nanostructures-Novel Architecture*, NOVA, New York, 2005, pp. 111.
18. M. Stefu and M. V. Diudea, *MATCH Commun. Math. Comput. Chem.* **50** (2004), 133–144.
19. M. V. Diudea (Ed.), *QSPR/QSAR Studies by Molecular Descriptors*, Nova, New York, 2001.
20. M. V. Diudea, S. Cigher, A. E. Vizitiu, M. S. Florescu, and P. E. John, unpublished paper.

SAŽETAK

Omega polinom u cjevastim nanostrukturama

Mircea V. Diudea, Simona Cigher, Aniela E. Vizitiu, Oleg Ursu i Peter E. John

Diudea je nedavno, na osnovu qoc (*quasi-orthogonal cut*, kvazi-okomiti rez) reznih traka grana u bipartitnim rešetkama, definirao novi prebrojavajući polinom, tzv. omega polinom, $\Omega(G,x)$. Kako unutar qoc-a nisu sve rezne grane nužno okomite, to znači da nisu sve po parovima kodistantne. Dva topološka indeksa, CI (Cluj-Ilmenau) indeks (koji je praktički ekvivalentan PI indeksu) i I_{Ω} indeks, definirani su u ovom radu na omega polinomu i izračunati za više primjera. Dati su također zatvoreni analitički izrazi za omega polinom i CI indeks u poliheksagonalnim torusima i cjevčicama.