

Omega and PI_v Polynomial in Dyck Graph-like Z(8)-Unit Networks

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Abstract:

Design of crystal-like lattices can be achieved by using some net operations. Hypothetical networks, thus obtained, can be characterized in their topology by various counting polynomials and topological indices derived from them. The networks herein presented are related to the Dyck graph and described in terms of Omega polynomial and PI_v polynomials.

Keywords: Dyck Graphs, Omega Polynomial, PI_v Polynomial, Net Operation

1. INTRODUCTION

Novel carbon allotropes have been discovered and studied for applications in nano-technology, in the last twenty years. Among the carbon structures, fullerenes (zero-dimensional), nanotubes (one dimensional), graphene (two dimensional) and spongy carbon (three dimensional) were the most challenging materials [1, 2]. Inorganic clusters, like zeolites, also attracted the attention of scientists. Recent articles in crystallography promoted the idea of topological description and classification of crystal structures [3-8].

This study presents two hypothetical crystal-like nano-carbon structures, with the topological description in terms of Omega and PI_v counting polynomials.

2. LATTICE BUILDING

The networks making - the subject of our discussion - were built up by the unit designed by the net operation sequence $Op(Q(C))$, performed on the Cube C.

Recall, the Quadrupling Q (also called Chamfering) is a composite operation, which truncates the triangulation on the old faces of a polyhedral object and finally deletes the original edges. The Q operation leaves unchanged the orientation of the polygonal faces. The *opening* operation Op is achieved by adding one point of degree two on each of the boundary edges of the parent faces that become the *open* faces. In Op_{2a} version (see below), two points are alternatively added on the boundary edges of the parent faces. More about map/net operations, the reader can find in refs. [9-13].

This unit is the zig-zag isomer (Figure 1, left) and, together with its “armchair” isomer (Figure 1,

right), were designed by the sequence $Op_{2a}(Q(C))$, and proposed by Diudea as representations of the celebrated Dyck graph [14]; this graph is built up on 32 vertices of valence 3, it has 48 edges, 12 octagons, girth 6, diameter 5, and the chromatic number 2; it is non-planar and has the minimal genus $g = 1$ (i.e., there exists an embedding of the graph on the torus). Cycle counting on the finite representation revealed 12 octagons and 16 hexagons. As units of infinite lattices, the units show 12 octagons and their genus [15] (i.e., the number of simple tori consisting a structure) is $g=3$.

There are two ways to design networks using a repeating unit: (i) *junction* J_n by an edge of the vertices/atoms of degree 2 (Figure 2a) and (ii) *identification* I_d of some identical features (Figure 2,b and c), in two close units. In our case, the atoms

of degree 2 were identified, thus resulting in four-connected atoms (and rings); by this reason we call this a “spiro” lattice.

The J_n net is triple periodic (Figure 3) while the I_d net is only double periodic ((b,c,c), in Figure 2) as also shown in the corner representation of a cubic domain of the lattice (Figure 4, left).

These structures show large hollows, as those encountered in zeolites, natural alumino-silicates widely used in synthetic chemistry as catalysts.

3. DEFINITIONS

In a connected graph $G(V,E)$, with the vertex set $V(G)$ and edge set $E(G)$, two edges $e = uv$ and $f = xy$ of G are called *codistant e co f* if they obey the

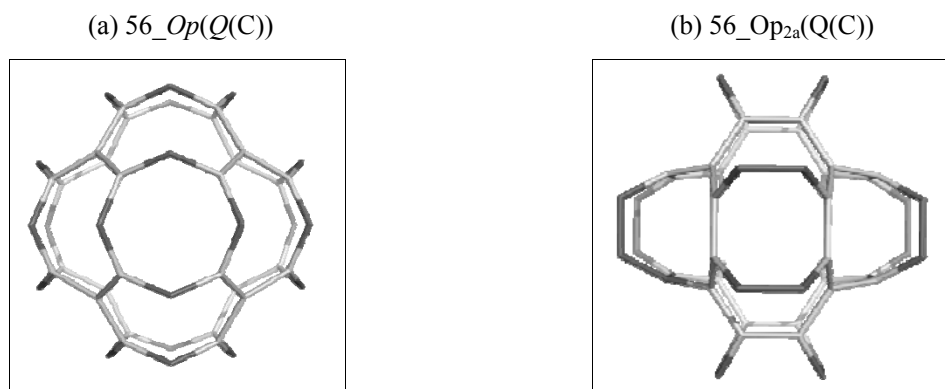


Figure 1: Dyck graph-like units with $R[8]=12$: the zig-zag “Z” unit (left) and the armchair unit “A” (right)

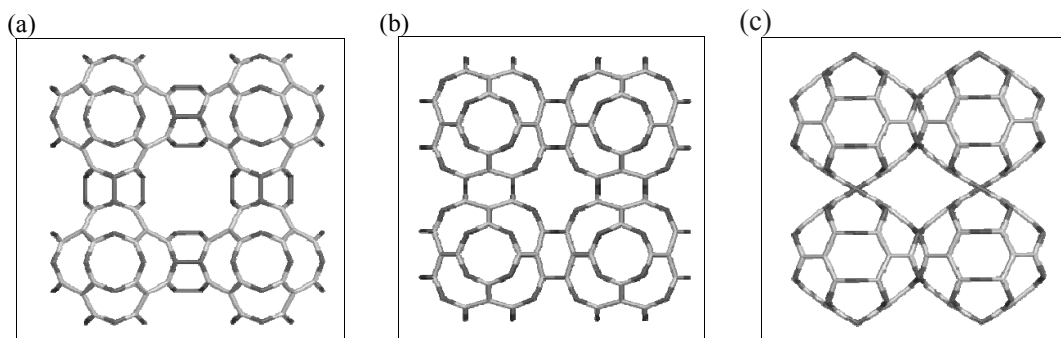


Figure 2: The unit $56_Op(Q(C))$ in lattice building by junction (a) and identification (b and c).

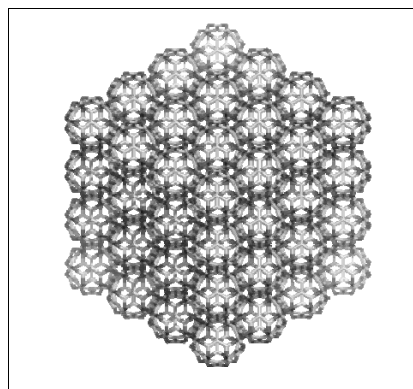
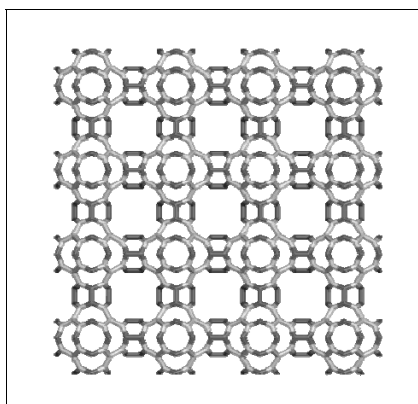


Figure 3: Unit (designed by $Op(Q(C))$) in a “Jn” ($R[6],R[8]$) network; the cubic domain (left) in its corner representation (right).

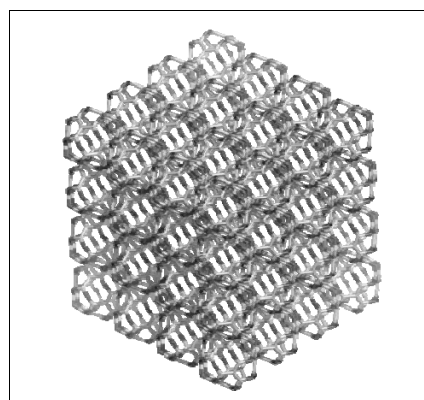
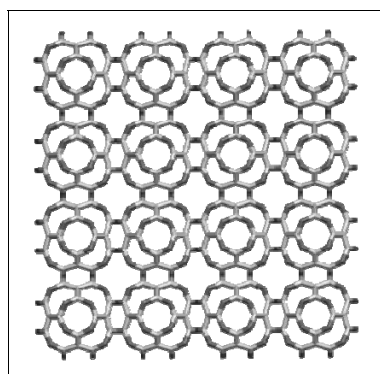


Figure 4: Unit (designed by $Op(Q(C))$) in an “Id” ($R[4],R[8]$) network; the cubic domain (left) in its corner representation (right - only two pair edges of the domain are the same while the third pair is distinct, the net being double periodic).

relation [16]:

$$d(v, x) = d(v, y) + 1 = d(u, x) + 1 = d(u, y) \quad (1)$$

Which is reflexive, that is, $e \text{ co } e$ holds for any edge e of G , and symmetric, *i.e.*, if $e \text{ co } f$ then $f \text{ co } e$ but, in general, relation co is not transitive. If “ co ” is also transitive, thus an equivalence relation, then G is called a *co-graph* and the set of edges $c(e) := \{f \in E(G); f \text{ co } e\}$ is called an *orthogonal cut oc* of G , $E(G)$ being the union of disjoint orthogonal cuts: $E(G) = c_1 \cup c_2 \cup \dots \cup c_k$, $c_i \cap c_j = \emptyset, i \neq j$. Klavžar [17] has shown that relation co is a theta Djoković-Winkler relation [18, 19].

Two edges e and f of a plane graph G are in relation

opposite, $e \text{ op } f$, if they are opposite edges of an inner face of G . Note that the relation co is defined in the whole graph while op is defined only in faces/rings. Using the relation op the edge set of G can be partitioned into *opposite edge strips*, *ops*. An *ops* is a quasi-orthogonal cut *qoc*, since op is, in general, not transitive. In *co-graphs*, the two strips superimpose to each other, then $\{c_k\} = \{s_k\}$, for any integer k .

A graph G is a *partial cube* if it is embeddable in the n -cube Q_n , which is the regular graph whose vertices are all binary strings of length n , two strings being adjacent if they differ in exactly one position [15]. The distance function in the n -cube is the Hamming distance. A hypercube can also be expressed as the Cartesian product: $Q_n = \prod_{i=1}^n K_2$

For any edge $e=(u,v)$ of a connected graph G let n_{uv} denote the set of vertices lying closer to u than to v : $n_{uv} = \{w \in V(G) \mid d(w,u) < d(w,v)\}$. It follows that $n_{vu} = \{w \in V(G) \mid d(w,v) = d(w,u) + 1\}$. The sets (and subgraphs) induced by these vertices, n_{uv} and n_{vu} , are called *semicubes* of G ; the *semicubes* n_{uv} and n_{vu} are *opposite semicubes* and disjoint (to each other) [20,21]. A graph G is bipartite if and only if, for any edge of G , the opposite semicubes define a partition of $V(G)$: $n_{uv} + n_{vu} = v = |V(G)|$.

The semicubes W_{ab} and W_{ba} are opposite semicubes

Let G be a connected graph and $S(G)=\{S_1, S_2, \dots, S_k\}$ be the *ops* strips of G . Then the *ops* strips form a partition of $E(G)$. The length of *ops* is taken as maximum (among all possible *ops*). It depends on the size of the maximum fold face/ring F_{\max}/R_{\max} considered, so that any result on Omega polynomial will have this specification.

Denote by $m(G,s)$ the number of *ops* of length $s=|S_k|$ and define the Omega polynomial as [22-30]:

$$\Omega(G,x) = \sum_s m(G,s) \cdot x^s \quad (2)$$

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

$$\Omega'(G,1) = \sum_s m(G,s) \cdot s = e = |E(G)| \quad (3)$$

On Omega polynomial, the Cluj-Ilmenau [15] index, $CI=CI(G)$, was defined:

$$CI(G) = \{[\Omega'(G,1)]^2 - [\Omega'(G,1) + \Omega''(G,1)]\} \quad (4)$$

The opposite semicubes of a partial cubes represent (in general graphs) the vertex proximities of (the endpoints of) edge $e=(u,v)$, which the PI_v (Ashrafi *et al.* [31-34]) and Cluj CJ_e (Diudea [35-39]) polynomials count. The $PI_v(x)$ is defined as:

$$PI_v(x) = \sum_e x^{n_{uv} + n_{vu}} \quad (5)$$

Relation (5) holds in any graph. The first derivative (in $x=1$) of $PI_v(x)$ gives the topological index $PI_v(G)$, which takes the maximal value in bipartite

graphs:

$$PI_v'(1) = e \cdot v = |E(G)| \cdot |V(G)| \quad (6)$$

In general graphs, this index can be written according to Ilić [40]:

$$PI_v(G) = PI_v'(1) = \sum_{e=uv} n_{u,v} + n_{v,u} = |V| \cdot |E| - \sum_{e=uv} m_{u,v} \quad (7)$$

where $n_{u,v}$, $n_{v,u}$ count the non-equidistant vertices with respect to the endpoints of the edge $e=(u,v)$ while $m(u,v)$ is the number of equidistant vertices vs. u and v . However, in bipartite graphs, there are no equidistant vertices so that the last term in (7) will be missing. The value of $PI_v(G)$ is thus maximal in bipartite graphs, among all graphs on the same order; the result of (7) can be used as a criterion for checking the “bipativity” of a graph.

4. POLYNOMIALS IN CRYSTAL-LIKE NETWORKS

Formulas for calculating the two above polynomials, in the two networks here designed, are given in the following tables, along with some examples. The formulas were derived by inspecting the networks included in a cubic domain (a,a,a) . The indices were calculated by the Topo Cluj original program called Nano Studio [41] and a home-made program (supplied by A. Ilić), respectively.

5. CONCLUSIONS

Two new hypothetical crystal-like networks were designed, starting from the Z-isomer of a Dyck graph representation, by using some net operations. Their topology is described in terms of Omega and PI_v polynomials. Close formulas for calculating this polynomial and the derived indices were given.

The polynomial description was proved to be useful in discriminating among structures built up from the same constructive repeat unit but following

Table 1: Omega and PIv polynomials in “Jn” (R[6],R[8]) net (unit designed by Op(Q(C)))

Unit	Formulas
$Jn_{a_{even}}$	$\Omega(Jn_{a_{even}}, x) = 3a^2(a-1)x^4 + 4a^3x^6 + 8x^{6a^3}$ $\Omega'(Jn_{a_{even}}, 1) = 12a^2(7a-1)$ $\Omega''(Jn_{a_{even}}, 1) = 288a^6 + 108a^3 - 36a^2$ $CI(Jn_{a_{even}}) = 48a^2(141a^4 - 42a^3 + 3a^2 - 4a + 1)$
$Jn_{a_{odd}}$	$\Omega(Jn_{a_{odd}}, x) = 3a^2(a-1)x^4 + 4a^3x^6 + 2x^{6a(a^2-1)} + 6x^{6(6a^2+2)}$ $\Omega'(Jn_{a_{odd}}, 1) = 12a^2(7a-1)$ $\Omega''(Jn_{a_{odd}}, 1) = 288a^6 + 108a^3 + 60a^2$ $CI(Jn_{a_{odd}}) = 48a^2(141a^4 - 42a^3 + 3a^2 - 4a - 1)$
Jn	$v(Jn) = 56a^3$ $PI_v(Jn, x) = e \cdot x^v = 12a^2(7a-1) \cdot x^{56a^3}$ $PI'_v(Jn, 1) = e \cdot v = 672a^5(7a-1)$

Table 2: Examples to the formulas in Table 1.

a_{even}	Omega (R _{max} [8])	v	e	CI	PI_v
2	$12x^4 + 32x^6 + 8x^{48}$	448	624	369600	279552
4	$144x^4 + 256x^6 + 8x^{384}$	3584	5184	25682688	18579456
6	$540x^4 + 864x^6 + 8x^{1296}$	12096	17712	300238272	214244352
a_{odd}					
3	$54x^4 + 108x^6 + 2x^{144} + 6x^{168}$	1512	2160	4450032	3265920
5	$300x^4 + 500x^6 + 2x^{720} + 6x^{760}$	7000	10200	99514800	71400000
7	$882x^4 + 1372x^6 + 2x^{2016} + 6x^{2072}$	19208	28224	762643056	542126592

Table 3: Omega polynomial in Id, spiro (R[4],R[8]) net (unit designed by Op(Q(C)))

$\Omega(Id, spiro, x) = 2a^2 \cdot x^{12a} + 2a^2 \cdot x^{16a} + a \cdot x^{16a^2}$ $\Omega'(Id, spiro, 1) = 72a^3$ $\Omega''(Id, spiro, 1) = 8a^3(32a^2 + 100a - 9)$ $CI(Id, spiro) = 32a^4(162a^2 - 8a - 25)$ $v(ID, spiro) = a^2(104 + 48(a - 2)) = 8a^2(6a + 1)$ $PI_v(Id, spiro, x) = e \cdot x^v = 72a^3 \cdot x^{8a^2(6a+1)}$ $PI'_v(Id, spiro, 1) = e \cdot v = 576a^5(6a + 1)$

Table 4: Examples of the formula in Table 3.

<i>a</i>	Omega (R_{\max} [8])	<i>v</i>	<i>e</i>	<i>CI</i>	PI_v
3	$18x^{36}+18x^{48}+3x^{144}$	1368	1944	3652128	2659392
4	$32x^{48}+32x^{64}+4x^{256}$	3200	4608	20766720	14745600
5	$50x^{60}+50x^{80}+5x^{400}$	6200	9000	79700000	55800000

different schemes of assembling, e.g. joining “Jn” or identifying “Id” ones. Formulas for the structure parameters as: the number of atoms/vertices and bonds/edges were also derived and examples of calculations were given.

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