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Omega Polynomial in All R[8] Lattices•

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ABSTRACT

Omega polynomial $\Omega(G,X)$ is defined on opposite edge strips ops in a graph G = G(V,E). The first and second derivatives, in X = 1, of Omega polynomial provide the Cluj-Ilmenau CI index. Close formulas for calculating these topological descriptors in an infinite lattice consisting of all R[8] faces, related to the famous Dyck graph, is given.

Keywords: Omega polynomial; Dyck graph; lattice, map operations.

1. INTRODUCTION

The rigorous and often aesthetically appealing architecture of crystal lattices, attracted the interest of scientists in a broad area, from crystallographers, to chemists and mathematicians [1–9]. The studies on classification have been followed by studies on the usefulness, in chemical reactions or in physical devices, and more recently by applied mathematical studies, in an effort to give new, more appropriate characterization of the world of crystals. Thus, recent articles in crystallography promoted the idea of topological description and classification of crystal structures [1–6]. They present data on real but also hypothetical lattices designed by computer.

Dendrimers are hyper-branched macromolecules [10–15] with the size in the nanometer scale. The endgroups (i.e., the groups reaching the outer periphery) can be functionalized, thus modifying their physico-chemical or biological properties. Vertices in a dendrimer, except the external endpoints, are called branching points. A regular dendrimer has all the branching points of the same degree, otherwise it is irregular. A dendrimer is

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called homogeneous if all its branches have the same length. The growth of a dendrimer follows a mathematical progression.

Dendrimers have gained a wide range of applications in supra-molecular chemistry, particularly in host-guest reactions and self-assembly processes or as gene transfer vectors [16,17].

The present work describes the design and topology (in terms of Omega polynomial) of two all R[8] lattices. The article is organized as follows: The second section presents the construction of the repeat units as well as that of a nano-dendrimer and studied lattices. The third section provides the definition of Omega polynomial and CI index, while the forth section gives the main results. Conclusions and references will close the article.

2. DESIGN OF NANO-STRUCTURES

The units in building the lattices under study in this paper are built up by using some map operations, namely the Quadrupling (or Chamfering) *Q*, Capra, *Ca* and Opening *Op* operations. For the smallest unit, the sequence $Op_{2a}(Q(C))$ is used (Figure 1). Op_{2a} says the opening is achieved by putting two points on alternating edges in the parent structure (in our case, the quadrupling transform of the Cube C).

More about map operations, the reader is kindly addressed to consult the refs. [18–22].

(a) $56\_Op_{2a}(Q(C))$ (b) $56\_Op_{2a}(Q(C))$, optimized; R[8] = 12

Figure 1. R[8_2] lattice: unit (1,1,1) generation (a) and (1,1,1) optimized form (b)

We name this unit R[8_2]_(1,1,1), meaning two octagons emerge from the contour of each open face, all-together 2×6=12 octagons, in the unit (1,1,1) cube of the lattice. The open faces are also R[8] and their number is 6; its genus [23] (*i.e.*, the number of simple tori consisting a structure) of this unit is g = 3.

The unit R[8_2] can be assembled in a dendrimer (Figure 2). The growth of such a dendrimer goes up to the first generation (with the number of vertices v= 344). At a second generation, the endings of the units are no more free, they fit to each other and thus forming the lattice symbolized R[8_2] (see below).

The number of units in the k^{th} orbit (*i.e.*, that located at distance k from the center) of a regular dendrimer can be expressed as a function vertex degree d

$$u_k = d(d-1)^{k-1} \tag{1}$$

By using the progressive degree p=d-1, relation (1) becomes

$$u_k = (p+1)p^{k-1} \tag{2}$$

The total number of units u(D) in dendrimer is obtained by summing the populations on all orbits (up to the radius/generation r) and the core

$$u(\mathrm{D}) = 1 + (p+1)\sum_{k=1}^{r} p^{k-1} \tag{3}$$

By developing the sum in (3) one obtains [10]

$$u(\mathrm{D}) = \frac{2(p^{r+1}-1)}{p-1} - p^r \tag{4}$$

For the case in Figure 2, one obtains: p=5; r=1; u(D) = 7.

v=344, top view 3D view

Figure 2. A dendrimer built up from the R[8_2] unit (1,1,1); u(D) = 7

The second unit was designed by the sequence $Op_{2a}(Ca(C))$, as shown in Figure 3. The number of octagonal faces emerging from the contour of open faces in this unit is four, thus we named this R[8_4]_(1,1,1,) unit. The total number of octagonal faces is 24; the open faces are R[12] and their number is 6 while g = 3.

The unit R[8_4] cannot be assembled in a dendrimer because: (i) it is chiral (the Capra *Ca* operation is prochiral) and (ii) already at the first generation the units for the lattice, named here R[8_4]. The units fit only right/left *R/L* to form an alternating, non-chiral, *mezzo*-net (Figure 3).

The two lattices R[8_2] and R[8_4] coexist: any lattice has its co-lattice (a complementary one). In fact is only one lattice R[8_2]&R[8_4] (Figure 4) but the boundary structure is different. Accordingly, the topology and polynomial description of the two lattice will also differ.

3. OMEGA POLYNOMIAL DEFINITION

Let G(V,E) be a connected graph, 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 following relation:

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y) \qquad (5)$$

Relation *co* is reflexive, that is, *e co e* holds for any edge *e* of *G*; it is also symmetric, if *e co f* then *f co e*. In general, relation *co* is not transitive, an example showing this fact is the complete bipartite graph $K_{2,n}$. If "*co*" is also transitive, thus an equivalence relation, then *G* is called a *co-graph* and the set of edges $C(e) := \{f \in E(G);\ f\ co\ e\}$ is called an *orthogonal cut oc* of *G* , *E*(*G*) being the union of disjoint orthogonal cuts: $E(G) = C_1 \cup C_2 \cup ... \cup C_k,\ C_i \cap C_j = \varnothing, i \neq j$. Klavžar [29] has shown that relation *co* is a theta Djoković-Winkler relation [30,31].

Let *e* = *uv* and *f* = *xy* be two edges of *G* which are *opposite* or topologically parallel and denote this relation by *e op f*. A set of opposite edges, within the same face/ring, eventually forming a strip of adjacent faces/rings, is called an *opposite* edge *strip ops*, which is a quasi-ortogonal cut *qoc* (*i.e*., the transitivity relation is not necessarily obeyed). Note that *co* relation is defined in the whole graph while *op* is defined only in a face/ring.

The *ops* relation has the properties: (i) any two subsequent edges of such a strip are in *op* relation; (ii) any three subsequent edges belong to adjacent (edge sharing) faces/ rings; (iii) the inner dual of an *ops* is a path or a cycle, thus neither revisiting nor branching is allowed.

An *ops* starts/ends in either one even face/ring or in two odd faces/rings; in the first case, the *ops* is a cycle while in the second one it is a path. In case of open structures, the open (or infinite) faces are equivalent to the odd faces. There are cases in which the two odd faces/rings superimpose and *ops* is a *pseudo* cycle, because the *op* relation in the first/last odd face/ring is not obeyed.

Let *m*(*G*,*s*) be the number of *ops* strips of length *s*. The Omega polynomial is defined as [32].

$$\Omega(G,X) = \sum_s m(G,s) \cdot x^s \qquad (6)$$

The first derivative (in *x*=1) equals the number of edges in the graph

$$\Omega'(G,1) = \sum_s m(G,s) \cdot s = e = |E(G)| \qquad (7)$$

A topological index, called Cluj-Ilmenau,[22] *CI*=*CI*(*G*), was defined on Omega polynomial

$$CI(G) = \{[\Omega'(G,1)]^2 - [\Omega'(G,1) + \Omega''(G,1)]\} \qquad (8)$$

It is easily seen that, for a single *ops*, one calculates the polynomial $\Omega(G,X) = 1 \times X^s$ and the index $CI(G) = s^2 - (s + s(s-1)) = s^2 - s^2 = 0$.

The coefficient of the term at exponent s=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} [33].

4. OMEGA POLYNOMIAL IN R[8_2]& R[8_4] LATTICE

Omega polynomial is given here in terms of the lattice dimension a = number of repeat units on a given direction of the 3D coordinates; the formulas are derived for a cube (a,a,a)-lattice. The polynomial is calculated in the *ring-version*, on two maximal rings $R_{max}[8]$ and $R_{max}[12]$, according to the lattice structure.

In case of lattice R[8_2], the polynomial, calculated at $R_{max}[8]$, consists of two terms (see Table 1). The first term refers to the "oblique" *ops* while the second one to the "orthogonal" *ops.*

Table 1. Omega polynomial in R[8_2] lattice, designed by $Op_{2a}(Q(C))$ operations.

	Formulas; (lattice (a,a,a); $R_{max}[8]$)
1	$\Omega(\mathrm{R}[8\_2],X) = c_1 X^{e_1} + c_2 X^{e_2}$
2	$v(\mathrm{R}[8\_2]) = 24a^2 + 32a^3$
3	$R[8] = 18a^3 - 3(a-1)a^2 = 3a^2(5a+1)$; $R[12] = 6a(2a^2 - a + 1)$
4	$\Omega(\mathrm{R}[8\_2],X) = 6a^2 \cdot X^{6a+2} + 3a \cdot X^{4a(a+1)}$
	$\Omega'(\mathrm{R}[8\_2],1) = 24a^2 + 48a^3$
5	$\Omega''(\mathrm{R}[8\_2],1) = 144a^3 + 312a^4 + 48a^5$
	$CI(G) = -24a^2 - 192a^3 + 264a^4 + 2256a^5 + 2304a^6$
	Examples
6	*CI*: (a=1)=4608; (a=2)=222240; (a=3)=2243808; (a=8)=678885888.
7	$v(G)$: (a=1)=56; (a=2)=352; (a=3)=1080; (a=8)=17920.
8	R[8]: (a=1)=18; (a=2)=132; (a=3)=432; (a=8)=7872.
9	R[12]: (a=1)=12; (a=2)=84; (a=3)=288; (a=8)=5808.

Table 2. Omega polynomial in R[8_2] lattice; $R_{max}[12]$.

	Formulas; (lattice (*a*,*a*,*a*); $a \geq 2$; $R_{max}[12]$)
1	$\Omega(\text{R}[8\_2], X) = X^{e}$
2	$\Omega(\text{R}[8\_2], X) = X^{24a^2(2a+1)}$
	$\Omega'(\text{R}[8\_2],1) = 24a^2(2a+1) = 24a^2 + 48a^3$
3	$\Omega''(\text{R}[8\_2],1) = 24a^2(2a+1)(48a^3 + 24a^2 - 1)$
	$CI(G) = [(24a^2(2a+1)]^2 - [24a^2(2a+1) + 24a^2(2a+1)(48a^3 + 24a^2 - 1)] = 0$

Observe in formulas for the number of vertices (Table 1, entry 2) and edges (Ω' , Table 1, entry 5), the maximal terms remind of the parameters of Duck graph. At $R_{max}[12]$, the polynomial has only one term (Table 2), and because there is only one *ops*, *CI*=0 (see text).

In case of lattice R[8_4], the polynomial, calculated at $R_{max}[8]$, shows five terms (Table 3). The maximal term in calculating CI, in both lattices is the same: $2304a^6$, also supporting the fact of a single lattice with two different boundaries. At $R_{max}[12]$, the polynomial has only two terms (Table 4). Observe Ω' has the same form as in case of $R_{max}[8]$, its meaning being the number of edges in the graph.

Table 3. Omega polynomial in R[8_4] lattice, designed by $Op_{2a}(Ca(C))$ operations.

	Formulas; (lattice (*a*,*a*,*a*); $R_{max}[8]$)
1	$\Omega(\text{R}[8\_4], X) = \sum_{i=1}^{5} c_i X^{e_i}$
2	$v(\text{G}) = 8a^2(13 + 4(a-1))$
3	$R[8](\text{G}) = 24a^3 - 3a(a(3a-2)-1) = 3a(5a^2 + 2a + 1)$
4	$\Omega(\text{R}[8\_4], X) = 36a \cdot X^3 + 6(3a^2 + 2a - 4) \cdot X^4 + 12(a-1)^2 \cdot X^6 + 6(a-1)^2 \cdot X^{6a+4} + 3(a-1) \cdot X^{4a^2}$
	$\Omega'(\text{R}[8\_4],1) = 84a^2 + 48a^3$
5	$\Omega''(\text{R}[8\_4],1) = 144 - 252a + 372a^2 - 192a^3 + 168a^4 + 48a^5$
	$CI(G) = -144 + 252a - 456a^2 + 144a^3 + 6888a^4 + 8016a^5 + 2304a^6$
	Examples
6	*CI*: (*a*=1)=17004; (*a*=2)=513864; (*a*=3)=4185828; (*a*=8)=894907728.
7	*v*(*G*): (*a*=1)=104; (*a*=2)=544; (*a*=3)=1512; (*a*=8)=20992.
8	R[8]: (*a*=1)=24; (*a*=2)=150; (*a*=3)=468; (*a*=8)=8088.

Table 4. Omega polynomial in R[8_4] lattice; R_{max}[12].

	Formulas; (lattice (*a*,*a*,*a*); $a \geq 2$; R_{max}[12])
1	$\Omega(\mathrm{R}[8\_4], X) = c_1 X^4 + X^{e_2}$
4	$\Omega(\mathrm{R}[8\_4], X) = 6a^2 X^4 + X^{12a^2[4(a-2)+13]}$
	$\Omega'(\mathrm{R}[8\_4],1) = 84a^2 + 48a^3$
5	$\Omega''(\mathrm{R}[8\_4],1) = 12a^2(1 - 4a + 300a^2 + 480a^3 + 192a^4)$
	$CI(G) = 96a^2(36a^2 + 24a^3 - 1)$
	Examples
6	*CI*: (*a*=2)=128640; (*a*=3)=838944; (*a*=8)=89647104.

Formulas for *CI*, number of atoms *v*, and rings *R* are also given in Table. Numerical evaluation of Omega polynomial was made by our software program Nano Studio [34].

5. CONCLUSIONS

Complex lattices can be designed by using sequences of map operations. Omega polynomial $\Omega(G,x)$ provided a good characterization of the lattice topology along with other lattice characteristics. Formulas for calculating $\Omega(G,x)$ in R[8_2] and R[8_4] lattices, at two maximal ring values (8 and 12, respectively) according to their topology, were derived. Counting formulas for the number of atoms, and rings were also given.

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