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Omega and Sadhana Polynomials of Dendrimers Designed from Tetrapodal Graphitic Junctions

Katalin Nagy,* Csaba L. Nagy and Mircea V. Diudea

Babeş-Bolyai University, Faculty of Chemistry and Chemical Engineering
Arany Janos str 11, 400028, Cluj-Napoca, ROMANIA
* E-mail: knagy@chem.ubbcluj.ro

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Abstract

Dendrimers are hyper-branched structures with rigorously tailored architecture. If the tetrahedral carbon atoms are substituted, *in silico*, by tetrapodal graphitic junctions, as those possibly appearing at the intersection (and annealing) of nanotubes, the resulting nano-dendrimers will show a polyhedral tubular structure. The construction of tetrapodal junctions is given in terms of both map operations and fullerene spanning. The topology of such dendrimers can be described by the aid of some counting polynomials, such as the recently proposed Omega and Sadhana polynomials. Analytical formulas for counting the above polynomials, and derived indices, in nano-dendrimers, are given in terms of the number of monomeric repeat units.

Introduction

Junctions of carbon nanotubes can appear by "nano-welding" of crossing tubes in an electron beam.[1] Tetrapodal junctions[2,3] are open structures of genus g=2 and negative Gaussian curvature [4] which can be designed by introduction of polygonal faces larger than hexagons in the graphite honeycomb. Such tetrapodal units are entirely built of sp^2 carbon atoms. The structures considered within this paper are junctions of (3,3) armchair carbon nanotubes.

Dendrimers are hyper-branched structures with rigorously tailored architecture. If the tetrahedral carbon atoms are substituted, *in silico*, by tetrapodal graphitic junctions, as introduced above, the resulting nano-dendrimers will show a polyhedral tubular structure. The construction of tetrapodal junctions will be detailed in the next section.

Visiting the associate graph of such a dendrimer is equivalent to the counting of monomeric units and their consisting substructures. In Chemical Graph Theory, several counting polynomials have been defined and used for characterizing the topology of molecules.

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 in relation "*co*" (i. e., *codistant*): *e co f*) if

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

If "*co*" is an equivalence relation, the set of edges $C(e) := \{f \in E(G); f\ co\ e\}$ 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 $i \neq j, i, j = 1,2,..,k$.

A set of opposite or topologically parallel edges within the same face/ring eventually forming a strip of adjacent faces, is called a *quasi-orthogonal cut qoc* or *ops.*(opposite edge strip). Relation *qoc/ops* does not necessarily asks for the transitivity of "*co*".

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 as: [5]

$$\Omega(G,x) = \sum_c m(G,c) \cdot x^c \tag{1}$$

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

$$\Omega'(G,1) = \sum_c m \cdot c = e = |E(G)| \tag{2}$$

A topological index, called Cluj-Ilmenau,[6] CI=$CI(G)$, was defined on Omega polynomial:

$$CI(G) = \{[\Omega'(G,1)]^2 - [\Omega'(G,1) + \Omega''(G,1)]\} \tag{3}$$

The Sadhana polynomial can also be defined on the ground of *qoc* strips:[7, 8]

$$Sd(G,x) = \sum_c m(G,c) \cdot x^{e-c} \tag{4}$$

with e being the cardinality of the edge set $e = |E(G)|$. This polynomial is based on a recently introduced 'Sadhana index', Khadikar *et al.*[9, 10]

$$Sd(G) = \sum_c m(G,c) \cdot (|E(G)| - c) \tag{5}$$

From the definition of Omega polynomial,[6, 11-13] one can obtain the Sadhana polynomial by replacing x^c with $x^{|E|-c}$. Then the Sadhana index will be the first derivative of $Sd'(G,x)$ evaluated at x=1. In fact, the first derivative (in x=1) is a multiple of $e(G)$:[14]

$$\begin{aligned} Sd'(G,1) &= \sum_c m(G,c) \cdot (e-c) = \sum_c m(G,c)e - \sum_c m(G,c)c = \\ &= e\sum_c m(G,c) - e = e\left(\sum_c m(G,c) - 1\right) = e\left(Sd(G,1) - 1\right) \end{aligned} \tag{6}$$

The relation of Sadhana index with Omega polynomial, out of the basic definition, is:

$$Sd(G) = Sd'(G,1) = \Omega'(G,1)\left((\Omega(G,1) - 1\right) \tag{7}$$

The way for calculating the above two counting polynomials in nano-dendrimers will be presented below.

Construction of tetrapodal junctions

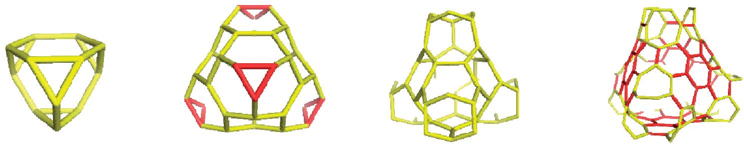
There are at least two ways to design a tetrapodal junction:

1. Tetrapodal junctions by map operations. Large structures with high symmetry can be obtained by the aid of map operations [5, 15] (*e.g.*, *leapfrog*, *chamfering*, *capra* and *opening*) starting from smaller objects (basically, the Platonic solids). These transformations preserve the symmetry of the parent map, therefore tetrapodal junctions, of T_d or T symmetry can be obtained from the tetrahedron.

Leapfrog [16-18] (tripling) *Le* is a composite operation that involves triangulation P_3, dualization *Du* and/or truncation *Tr*:

$$Le(M) = Du(P_3(M)) = Tr(Du(M))$$

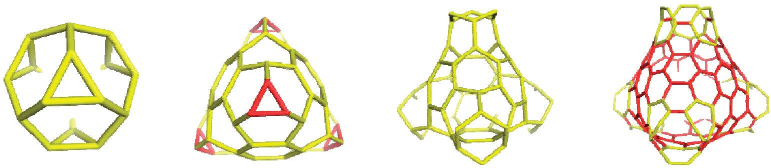
This operation rotates the parent s-gonal faces by π / s. Figure 1 provides a molecular realization of *Le*.



$Le(T)$ $Le(Le(T))$ $Op(Le(Le(T)))$ $Le(Op(Le(Le(T))))$

Figure 1. Design of a tetrapodal junction by leapfrog *Le* map operation

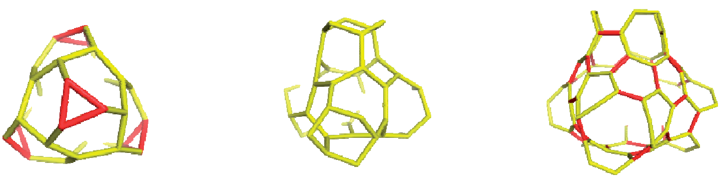
Chamfering (quadrupling) Q is another composite operation, which can be achieved by the sequence: $Q(M) = RE(Tr_{P_3}(P_3(M)))$ where RE denotes the (old) edge deletion in the truncation Tr_{P_3} of each central vertex of the P_3 capping. Figure 2 gives an example of such a transformation.



$Q(T)$ $Le(Q(T))$ $Op(Le(Q(T)))$ $Le(Op(Le(Q(T))))$

Figure 2. Tetrapodal junction designed by *Chamfering Q* operation

A third composite operation on maps is called *Capra Ca* [19] (or *septupling* operation) and it was developed by TOPO GROUP Cluj. It can be written as a sequence of simple operations: $S_1(M) = Tr_{P_5}(P_5(M))$, with Tr_{P_5} being the truncation of the face centered vertex introduced by P_5 pentangulation. Figure 3 illustrates this last operation.

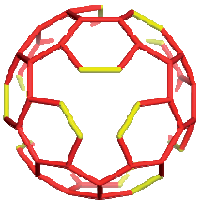


$Ca(T)$ $Op(Ca(T))$ $Le(Op(Ca(T)))$

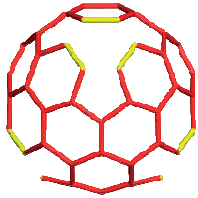
Figure 3. Tetrapodal junction designed by *Capra Ca* operation

2. Tetrapodal junctions by fullerene spanning

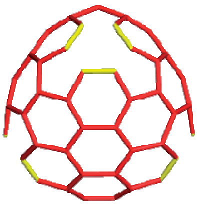
Four small fullerene cages C_{60}-I_h, C_{76}- T_d, C_{84}-20-T_d, and C_{120}-T were here chosen as the core of tetrapodal junctions [16]. The basic structural motif of the selected cages is the sumanene, a benzene ring surrounded by alternating pentagons and hexagons [6:(5,6)$_3$]. Figure 4 illustrates the studied opened fullerenes.



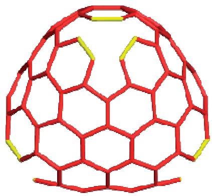
Op(C_{60})



Op(C_{76})



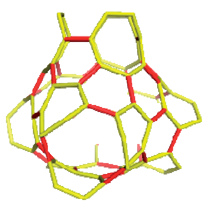
Op(C_{84})



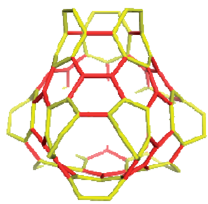
Op(C_{120})

Figure 4. Opened *Op* fullerenes

A tetrapodal junction can be designed by opening a fullerene graph and next attaching four nanotube arms.[20] By inserting two divalent vertices on the bonds shared by a pentagon and the core hexagon in the sumanene unit, a heptagon is created and the fullerene polyhedron is thus opened. Figure 5 illustrates these junctions.



C_{60}-junction



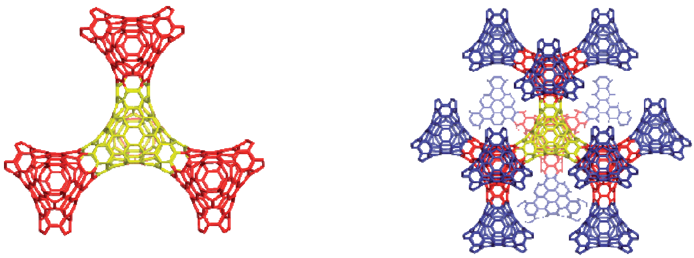
C_{76}-junction

C_{84}-junction C_{120}-junction

Figure 5. Tetrapodal Junctions

In all cases, the (3,3) armchair tube is the fitted tube.

Tetrapodal junctions were next connected by identification (a procedure implemented in our software Nano Studio [21]) to build dendritic molecules. Nano-dendrimers, at the first and second-generation stages, respectively, are illustrated in Figure 6.



First dendrimer level Second dendrimer level

Figure 6. Dendrimer of C_{84}-junction ($Le(Op(Le(Le(T))))$)

Omega and Sadhana polynomials in tetrapodal junctions

As above mentioned, a set of opposite or topologically parallel edges within the same face/ring eventually forming a strip of adjacent faces, is called a *qoc* or an *ops*. The number of *ops* of length c is given by the polynomial coefficients of terms at exponent c; the number of distinct c exponents equals the number of equivalence classes of opposite edges in G. Figure 7 illustrates an *ops* of c=7 in a dimmer structure.

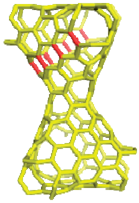


Figure 7. A *qoc*/*ops* of length *c*=7, in a tetrapodal junction dimmer [1, 5]

Analytical formulas of the Omega [6] and Sadhana[7] polynomial in tetrapodal junctions were derived; in every formula, *m* represents the number of monomers. Examples of Omega, Sadhana polynomials and derived indices, in the case of dendrimers built up from tetrapodal junctions are presented in the tables below.

Table 1. Omega and Sadhana polynomials of C_{60}-T_d-junction.

C_{60}-T_d-junction $Le(Op(Ca(T)))$ TU(3.3.0); $v = 84, f_6 = 16, f_7 = 12, e = 114$
$\Omega(G,x) = 12(2m+1)X^1 + 12mX^2 + 18mX^3$ $\Omega(G,1) = 54m+12$ $\Omega'(G,1) = 102m+12$
$CI = 102^2 \cdot m^2 + 2214m + 132$; Example: $m = 2; CI = 46176$
$Sd(G,x) = 12(2m+1)^{102m+11} + 12mX^{102m+10} + 18mX^{102m+9}$ $Sd'(G,1) = 5508m^2 + 1770m + 132$

Table 2. Omega and Sadhana polynomials of C_{76}-T_d-junction.

C_{76}-T_d-junction TU(3.3.0); $v = 100, f_6 = 24\ f_7 = 12, e = 138$
$\Omega(G,x) = 12(2m+1)X^1 + 12mX^2 + 6mX^3 + 12mX^5$ $\Omega(G,1) = Sd(G,1) = 54m+12$ $\Omega'(G,1) = 126m+12$
$CI = 126^2 \cdot m^2 + 2598m + 132$; Example $m = 2; CI = 68832$
$Sd(G,x) = 12(2m+1)X^{126m+11} + 12mX^{126m+10} + 6mX^{126m+9} + 12mX^{126m+7}$ $Sd'(G,1) = 6804m^2 + 2034m + 132$

Table 3. Omega and Sadhana polynomials of C_{84}-T_d-junction.

C_{84}-T_d-junction $Le(Op(Le(Le(T))))$ TU(3.3.0); $v = 108$, $f_6 = 28, f_7 = 12, e = 150$
$\Omega(G,x) = 12(2m+1)X^1 + 24mX^3 + 6mX^7$ $\Omega(G,1) = Sd(G,1) = 54m+12$ $\Omega'(G,1) = 138m+12$

$CI = 138^2 \cdot m^2 + 2778m + 132$; Example: $m = 3; CI = 179862$
$Sd(G,x) = 12(2m+1)X^{138m+11} + 24mX^{138m+9} + 6mX^{138m+5}$ $Sd'(G,1) = 7452m^2 + 2166m + 132$

Table 4. Omega and Sadhana polynomials of C_{120}-T_d-junction.

C_{120}-T-junction $Le(Op(Le(Q(T))))$ TU(3.3.0); $v = 144, f_6 = 46, f_7 = 12, e = 204$
$\Omega(G,x) = 12(2m+1)X^1 + 12mX^3 + 6mX^4 + 12mX^6 + 3mX^{12}$ $\Omega(G,1) = Sd(G,1) = 57m + 12$ $\Omega'(G,1) = 192m + 12$
$CI = 192^2 \cdot m^2 + 3516m + 132$; Example: $m = 2; CI = 154620$
$Sd(G,x) = 12(2m+1)X^{192m+11} + 12mX^{192m+9} + 6mX^{192m+8} + 12mX^{192m+6} + 3mX^{192m}$ $Sd'(G,1) = 10944m^2 + 2796m + 132$

The first derivative of Omega polynomial [22, 23] gives the number of the edges in G. The first derivative of Sadhana polynomials in x=1 is a multiple of the number of the edges, as shown above. The Cluj-Ilmenau CI index [24] is a topological index, useful in correlating properties with molecular structures.

By construction, the "negative" polygon is 7 (an odd ring, with no opposite edges), so that the strip remains at the level of a single monomer unit and the polynomials are additive in their coefficients. In the above, "negative" refers to polygons inducing the negative curvature at the junction of tetrapodal units. The terms at c=1 (in Omega polynomial) account for the non-opposite edges or the odd rings.

Remark, in these tables, the simplicity, at exponents, of Omega *vs* Sadhana polynomials; the polynomial order increases as the size of fullerenes increases. The first derivative is 1st and 2nd order in m, for Omega and Sadhana, respectively. The value in x=1 is the same for both polynomials and accounts for the total number of strips. For the first three units, the same value $\Omega(G,1); Sd(G,1)$ are obtained, telling about their structural relatedness.

Conclusions

Omega $\Omega(G,x)$ and Sadhana polynomials count the opposite edge strips ops of all extent in G. Analytical formulas for the calculation of the two polynomials in nano-dendrimers build up from four tetrapodal junctions were given in terms of the number of monomer units m. The Omega polynomial is remarkably simpler than Sadhana one and enables direct interpretation of the exponents. Even the number of generations of such (yet hypothetical dendrimers) is rather limited, the established formulas are of diagnostic value, as composition rules of a global (topological) property by local contributions of the monomeric repeat units.

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