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OMEGA POLYNOMIAL IN DIAMOND-LIKE DENDRIMERS

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ABSTRACT. Design of diamond-related molecular structures can be achieved by using some net operations. The repeat unit used in this paper to build a nano-dendrimer is derived from adamantane, the constructive unit of diamond, and proved to be extremely stable, as shown by computed total energy. The dendrimer topology is described in terms of Omega polynomial.

Keywords: *Omega polynomial, dendrimer, diamond*

INTRODUCTION

The beauty (and usefulness) of diamond has kept its leading interest, among the newer "nano" carbon allotropes: fullerenes (zero-dimensional), nanotubes (one dimensional), graphene (two dimensional) or spongy carbon [1,2]. In the "nano-era", the period of the last twenty years which started with the synthesis of fullerenes and nanotubes, theoretical and experimental studies revealed new properties, of interest for new applications. Out of electronic properties, the mechanical characteristics appear of great importance, as the composites can overpass the resistance of steel or other metal alloys. There are well-known the efforts in the production and purification of "synthetic" diamonds, from detonation products [3-9].

In this article, a nano-dendrimer is designed by using a diamond-related repeat unit, derived from the adamantane. The stability and topology of these structures are described in terms of total energy and Omega counting polynomial, respectively.

DENDRIMER BUILDING

The repeat unit used to build the nano-dendrimer here discussed was derived, from the tetrahedron T, by using the map operation [10-14] sequence *Op*(*Trs*(*P*4(T))), as shown in Figure 1: The operation P4 (which transform the initial triangles into quadrilaterals – Figure 1, left) is followed by the selective truncation of the red points, which results in the red triangles (Figure 1, center). Finally, the opening of triangles by Op-operation (which puts one point of valence two on each bond of the red triangles) provides the red hexagons (Figure 1, right). The repeat unit superimposes partly over the

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diamond lattice and plays the role of sp^3 tetrahedral carbon atom. Next, the nano-dendrimer was built up by pair-wise identification of the open faces (i.e., the red hexagons) of the tetrapode. Figure 2 illustrates the dendrimer at the 1st (left) and 2nd (right) generation.

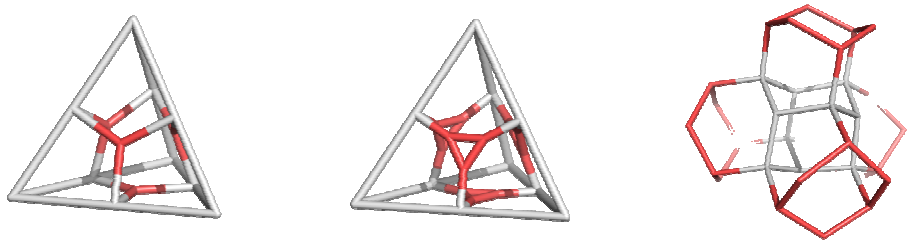

Figure 1. Unit U_34, designed by *Op*(*Trs*(*P*4(T))). The red color is for an easier understanding the map operations used in the design of structures.

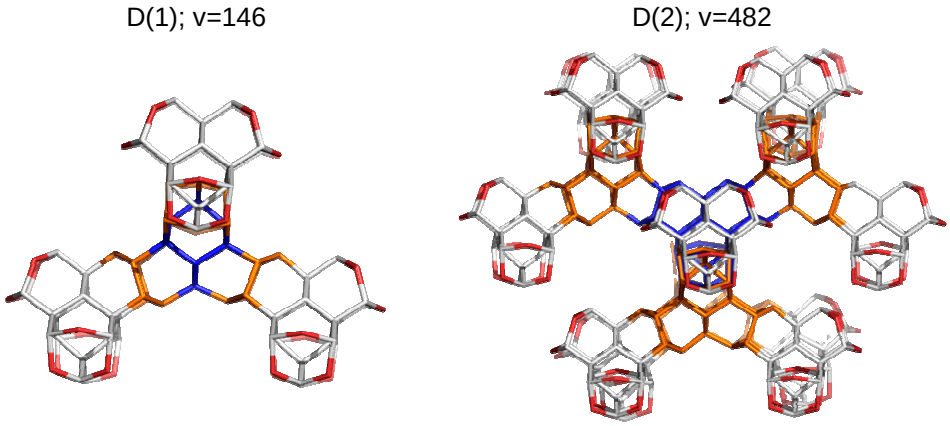

Figure 2. Dendrimers at the 1st (a) and 2nd (b) generation; v is the number of vertices/atoms.

Due to the large number of atoms, we limited here to calculate the total energy at the semi-empirical PM3 level of theory. Table 1 lists data (total energy per heavy atoms and HOMO-LUMO gap) for the new unit, as a hydrogenated sp^3 carbon structure, in comparison to the adamantane and diamantane, units of the diamond network. Data for the reference C_{60} fullerene (an sp^2 carbon structure) are also included. Remark the unit U_34 is closer to the diamond-related structures than to the C_{60} fullerene. The C-C bond length is in the range of 1.53-1.55 Angstroms while C-C-C angles fit between 107 and 110 degrees, as expected for single C-C bond containing compounds.

Table 1. PM3 data for the new diamond-related unit (as hydrogenated molecule) and some reference structures

Molecule	N_heavy	TE(kcal/mol)	TE/N_heavy	HOMO-LUMO Gap (eV)
U_34	34	-107178.99	-3152.32	13.07
Adamantane	10	-33051.90	-3305.19	14.43
Diamantane	14	-45414.05	-3243.86	14.06
C_{60}	60	-163347.18	-2722.45	6.59

OMEGA POLYNOMIAL

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 relation [15]:

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y) \tag{1}$$

which is reflexive, that is, *e co e* holds for any edge *e* of *G*, and 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: $E(G) = C_1 \cup C_2 \cup ... \cup C_k,\ C_i \cap C_j = \emptyset, i \neq j$. Klavžar [16] has shown that relation *co* is a theta Djoković-Winkler relation [17,18].

We say that edges *e* and *f* of a plane graph *G* are in relation *opposite, e 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. Using the relation *op* we can partition the edge set of *G* into *opposite* edge *strips, ops.* An *ops* is a quasi-orthogonal cut *qoc*, since *ops* is not transitive.

Let *G* be a connected graph and $S(G) = s_1, s_2, ..., s_k$ be the *ops* strips of *G*. Then the *ops* strips form a partition of *E(G)*. The length of *ops* is taken as maximum. 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 [19-26]:

$$\Omega(G,x) = \sum_s m(G,s) \cdot x^s \tag{2}$$

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:

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

CALCULATION OF OMEGA POLYNOMIAL IN NANO-DENDRIMER

We used here the topological description by Omega polynomial because this polynomial was created to describe the covering in polyhedral nanostructures and because is the best in describing the constitutive parts of nanostructures, particularly for large structures, with a minimal computational cost. For the monomers/ repeat units, the stability evaluation was shown in Section 2.

Formulas for calculating the Omega polynomial and CI index are written function of the generation number *r* (Table 2); within this paper, the main results refer to F_{max}(6). The number of vertices/atoms *v* and the number of monomers/units *m* are also given. Examples were calculated by our original program called Nano Studio [27].

Table 2. Omega polynomial in *F*[6]*Id* dendrimer.

Unit	Formulas
F[6]*IdD*	$\Omega(F[6]IdD,x) = 4(4\cdot 3^r - 1)\cdot x^3 + \sum_{k=2}^{r} 12k(k-1)\cdot x^{3+4(r-k+1)} + 12\cdot x^{3+4r}$
	$\Omega'(F[6]IdD,1) = 4r^4 + 20r^3 - 4r^2 + 28r + 24 + 48\cdot 3^r$
	$\Omega''(F[6]IdD,1) = (32/5)r^5 + 36r^4 + 64r^3 + 156r^2 +$
	$+ (848/5)r + 48 + 96\cdot 3^r$
	$CI(F[6]IdD) = 16r^8 + 160r^7 + 368r^6 + (288/5)r^5 +$
	$1288r^4 + 652r^3 + 440r^2 + (5732/5)r + 504 +$
	$3^r(384r^4 + 1920r^3 - 384r^2 + 2688^r + 2160 +$
	$2304\cdot 3^r)$
	$v(F[6]Id\mathrm{D}) = 34m - 6(m-1)$
	$m(F[6]Id\mathrm{D}) = 3^{r+1} - 3^r - 1$
Examples	*r*=1; $44x^3+12x^7$; *CI*=45672; *v*=146 ; *e*=216
	r=2; $140x^3+24x^7+12x^{11}$; *CI*=514512; *v*=482 ; *e*=720
	r=3; $428x^3+72x^7+24x^{11}+12x^{15}$; *CI*=4968840; *v*= 1490; *e*=2232

CONCLUSIONS

Design of diamond-like hypothetical structures was performed by using some operations on maps. The computed total energy of the involved repeat unit/monomer indicated stability close to that of adamantane and diamantane, the constructive units of diamond. The topology of the proposed networks was described in terms of Omega polynomial.

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