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OMEGA POLYNOMIAL IN OCT-P_4TRS NETWORK

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ABSTRACT. Design of a hypothetical crystal network, by using *Trs*(P_4(M)) sequence of map operations, is presented. It is shown that the octahedral monomer is the most stable, among the similar structures designed from the Platonic solids, as hydrogenated species, and all these have a moderate stability, between adamantane and C_{60} fullerene, as calculated at the PM3 level of theory. The topology of the network is described in terms of Omega polynomial, function of the net parameters. Close formulas for this polynomial and examples are tabulated.

Keywords*: Omega polynomial; crystal-like network.*

INTRODUCTION

In the last two decades, several new carbon allotropes have been discovered and studied for applications in nano-technology. Among the carbon structures, fullerenes (zero-dimensional), nanotubes (one dimensional), graphene (two dimensional) and spongy nanostructures (three dimensional) were the most studied [1,2]. Inorganic compounds also attracted the attention of scientists. Recent articles in crystallography promoted the idea of topological description and classification of crystal structures [3-7].

The present study deals with a hypothetical crystal-like nano-carbon structure, designed by a sequence of map operations [8-11], of which topology is described in terms of Omega polynomial.

OMEGA POLYNOMIAL

Let $G(V,E)$ be a graph, with $V(G)$ and $E(G)$ being the sets of vertices/ atoms and edges/bonds, respectively. Two 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*. Relation *op* will partition the edges set of *G* into *opposite* edge *strips ops*, as follows. (i) Any two subsequent edges of an *ops* are in *op* relation; (ii) Any three subsequent edges of such a strip belong to adjacent faces; (iii) In a plane graph, the inner dual of an *ops* is a path, an open or a closed one (however,

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in 3D networks, the ring/face interchanging will provide *ops* which are no more paths); (iv) The *ops* is taken as maximum possible, irrespective of the starting edge [12-18].

The Ω-polynomial [12] is defined on the ground of opposite edge strips *ops* $S(G) = S_1, S_2, ..., S_k$ in the graph. Denoting by *m* the number of *ops* of length *s*=|*S*|, then we can write

$$\Omega(x) = \sum_s m \cdot x^s \quad (1)$$

The first derivative (in *x*=1) can be taken as a graph invariant or a topological index; in this case, it equals the number of edges in the graph.

$$\Omega'(1) = \sum_s m \cdot s = e = |E(G)| \quad (2)$$

On Omega polynomial, the Cluj-Ilmenau index [13], *CI*=*CI*(*G*), was defined:

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

The first derivative (in *x*=1) can be taken as a graph invariant or a topological index:

$$\Omega'(1) = \sum_s m \cdot s = |E(G)| \quad (4)$$

In tree graphs, the Omega polynomial simply counts the non-opposite edges, being included in the term of exponent *c*=1.

LATTICE BUILDING AND MONOMER STABILITY

The lattice was constructed by using the unit designed with the net operation sequence *Trs*(P_4(M)), where M=Oct (Octahedron). More about map/net operations, the reader can find in refs. [8-11].

The net (Figure 1) was built up by identifying the identical (quadrilateral) faces of the unit structure The crystal-like structure shows oriented hollows, as those encountered in zeolites, natural alumino-silicates widely used in synthetic chemistry as catalysts.

The unit involved in these constructions, namely *Trs*(P_4(M)), M=Oct, as a hydrogenated structure, shows moderate stability as given by their heat of formation HF, total energy TE and HOMO-LUMO Gap HLGAP, calculated at the PM3 level of theory (Table 1).

Figure 1: Network *Trs*(P_4(M)); [2,2,2]; M=Octahedron, in two different views.

For example, the total energy per heavy atoms of the structures in Table 1 are between the values of adamantane (-3305.19 kcal/mol), which is the most related small structure (see Figure 2, left, in red) and C_{60} (-2722.45

kcal/mol), the standard molecule in nanostructures. The same is true about the HOMO-LUMO gap. Calculations by using a density functional-based tight binding method combined with the self-consistent charge technique (SCC-DFTB) on hydrogenated units of diamond and a diamond-like network[19] have shown the same ordering of stability as given by PM3 approach; thus, our results reported here can be considered as pertinent ones.

Table 1. Quantum Chemistry PM3 data for some units designed by *Trs*(P_4(M)): Heat of Formation HF, Total energy TE and HOMO-LUMO Gap HLGAP

M	N-heavy atoms	HF (kcal/mol)	HF/N heavy	TE (kcal/mol)	TE/N heavy	HLGAP (eV)	Sym.
Ico	110	1216.81	11.06	-328026	-2982.05	11.79	I_h
Oct	44	448.67	10.19	-131248	-2982.92	12.17	o_h
T	22	308.48	14.022	-65540	-2979.09	11.99	T_d

OMEGA POLYNOMIAL IN *Trs*(P_4(M)) Network

The Omega polynomial (calculated at R_{max}[4]) for the investigated network is as follows:

$$\Omega(G,x) = 24a(a+1)x + 12(a(a+1)+(a-2))x^2 + 24(a(a-2)+1)x^3 + 4(a-1)^3 x^6 + 3(a-1)x^{(2a)^2} \quad (5)$$

$$\Omega'(G,1) = |E(G)| = 36a^2(a+1) \quad (6)$$

$$CI(G) = 1296a^6 + 2544a^5 + 1344a^4 - 144a^3 + 144a^2 - 120a + 24 \quad (7)$$

The above formulas can be verified with the examples listed in Table 2. Calculations were performed by our Nano Studio[20] software program.

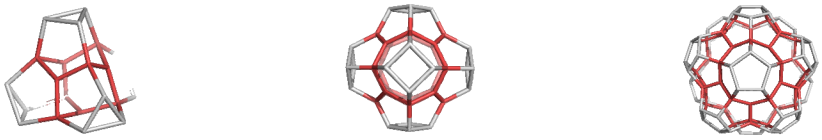

Figure 2. Platonic structures transformed by *Trs*(P_4(M)) sequence of map operations: M=Tetrahedron T (left); M=Octahedron Oct (central) and M=Icosahedron Ico (right). The red color is only to show the related substructures.

Table 2. Examples of Omega polynomial and CI calculation

a	Omega polynomial	CI
1	$48x+12x^2$	5088
2	$144x+72x^2+24x^3+4x^6+3x^{16}$	185064
3	$288x+156x^2+96x^3+32x^6+6x^{36}$	1668912
4	$480x+264x^2+216x^3+108x^6+9x^{64}$	8250168
5	$720x+396x^2+384x^3+256x^6+12x^{100}$	29025024
6	$1008x+552x^2+600x^3+500x^6+15x^{144}$	81963528

CONCLUSIONS

A hypothetical crystal network was built up by using a repeat unit designed by *Trs*(P_4(M)) sequence of map operations. It was shown that the octahedral monomer (i.e., the repeat unit of this network) is the most stable (as hydrogenated species), among the similar structures derived from the Platonic solids, and all these have a moderate stability, between adamantane and C_{60} fullerene, as calculated at the PM3 level of theory. The topology of the network was described in terms of Omega polynomial, function of the net parameters. Close formulas for this polynomial and examples were tabulated. Omega polynomial description proved to be a simple and efficient method in topological characterization of new designed nano-structures.

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