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Dedicated to the memory of Prof. dr. Ioan Silaghi-Dumitrescu marking 60 years from his birth

TOPOLOGY OF A NEW LATTICE CONTAINING PENTAGON TRIPLES

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ABSTRACT. A new crystal-like network is designed by using some net operations. The topology of this hypothetical lattice is characterized by Omega polynomial and Cluj-Ilmenau CI index.

Keywords: *map operations, Omega polynomial, Cluj-Ilmenau index*

INTRODUCTION

In the nano-era, several new carbon structures: fullerenes (zero-dimensional), nanotubes (one dimensional), graphene (two dimensional), spongy carbon (three dimensional) and nano-diamond (three dimensional) [1,2] have been discovered. Inorganic clusters, like zeolites, also attracted the attention of scientists.

Zeolites are natural or synthetic aluminosilicates with an open three-dimensional crystal structure. Zeolites are members of the family of microporous solids known as "molecular sieves." This term refers to the property of these materials to selectively sort molecules based primarily on a size exclusion process. This is due to a regular structure of pores, of molecular dimensions, forming channels. The maximum size of the molecular or ionic species that can enter the pores of a zeolite is controlled by the dimensions of the channels [3-7].

Recent articles in crystallography promoted the idea of topological description and classification of crystal structures [8-13].

The present study presents a hypothetical crystal-like nano-carbon structure, with the topological description in terms of Omega counting polynomial.

OPERATIONS ON MAPS

Several operations on maps are known and used for various purposes.

Dualization *Du* of a map is achieved as follows: locate a point in the center of each face. Join two such points if their corresponding faces share

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a common edge. The transformed map is called the (Poincaré) *dual Du*(*M*). The vertices of *Du*(*M*) represent the faces of *M* and *vice-versa* [14]. Thus the following relations exist between the parent map parameters (denoted by subscript zero) and those of the transformed map:

$$Du(M):\ v=f_0\ ;\ e=e_0\ ;\ f=v_0 \tag{1}$$

Dual of the dual recovers the original map: *Du*(*Du*(*M*)) = *M*. Tetrahedron is self dual while the other Platonic polyhedra form pairs: *Du*(Cube) = Octahedron; *Du*(Dodecahedron) = Icosahedron (see Figure 1 for symbols hereafter used). It is also known the Petrie dual.

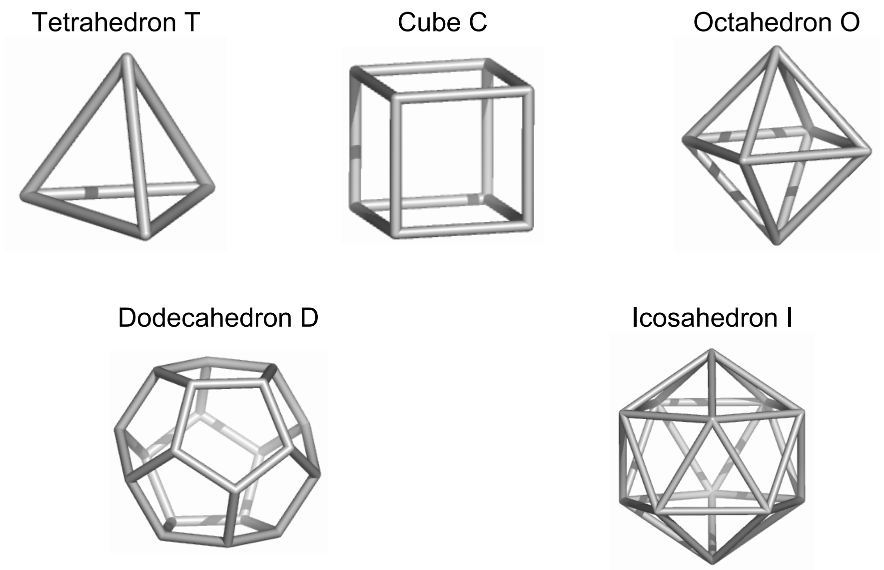


Figure 1. The five Platonic polyhedra.

Medial *Med* is another important operation on maps [15-17]. It is constructed as follows: put the new vertices as the midpoints of the original edges. Join two vertices if and only if the original edges span an angle (more exactly, the two edges must be incident and consecutive within a rotation path around their common vertex in the original map).

The medial graph is a subgraph of the line-graph [18]. In the line-graph each original vertex gives rise to a complete graph while in the medial graph only a cycle C_d (*i.e.*, a *d*-fold cycle, *d* being the vertex degree/ valence) is formed.

The medial of a map is a 4-valent graph and *Med*(*M*) = *Med*(*Du*(*M*)). The transformed parameters are:

$$Me(M)\text{: } v=e_0\,;\ e=2e_0\,;\ f=f_0+v_0 \tag{2}$$

The medial operation rotates parent *s*-gonal faces by *π/s*. Points in the medial represent original edges, thus this property can be used for topological analysis of edges in the parent polyhedron. Similarly, the points in dual give information on the topology of parent faces.

Cuboctahedron = *Med*(*C*)

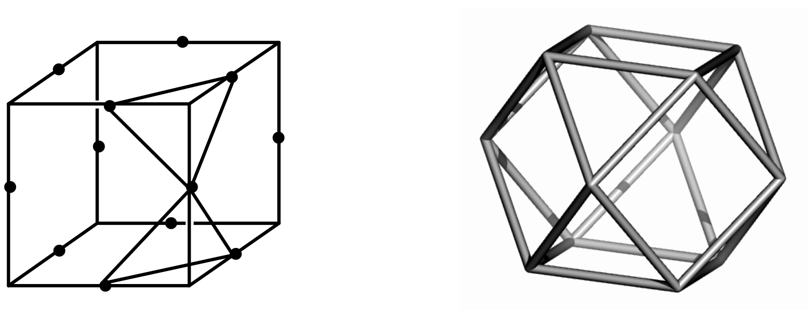
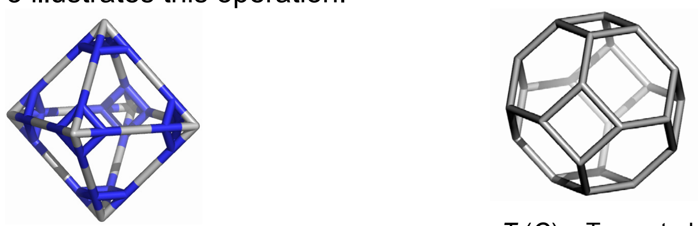


Figure 2. Medial operation; construction (left) and realization (right).

Truncation *Tr* is achieved by cutting of the neighborhood of each vertex by a plane close to the vertex, such that it intersects each edge incident to the vertex. Truncation is similar to the medial, with the main difference that each old edge will generate three new edges in the truncated map. The transformed parameters are:

$$Tr(M)\text{: } v=2e_0=d_0v_0\,;\ e=3e_0\,;\ f=f_0+v_0 \tag{3}$$

This was the main operation used by Archimedes in building his well-known 13 solids [3]. Note that truncation always provides a trivalent net. Figure 3 illustrates this operation.



Tr(*O*) = Truncated Octahedron

Figure 3. Truncation; construction (left) and realization (right).

Leapfrog *Le* is a composite operation [16,17-24] that can be written as:

Le(M): Tr(Du(M))=Du (4)

This operation rotates parent *s*-gonal faces by *π/s*. Note that the vertex degree in *Le*(*M*) is *always* 3. Leapfrog operation is illustrated, for a tetragonal face, in Figure 4.

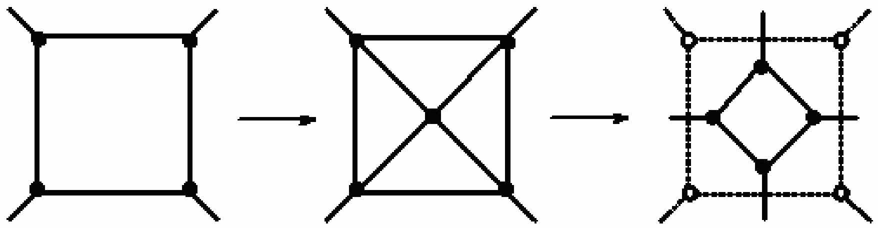


Figure 4. Leapfrogging a tetragonal face of a trivalent map; the white circles are the new vertices of *Le*(*M*).

A bounding polygon, of size $2d_0$, is formed around each original vertex. In the most frequent cases of 4- and 3-valent maps, the bounding polygon is an octagon and a hexagon, respectively (Figure 5).

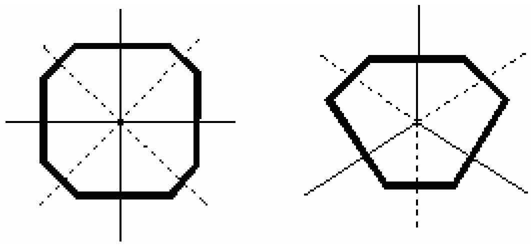


Figure 5. The bounding polygon around a 4-degree (left) and 3-degree (right) vertex.

In trivalent maps, *Le*(*M*) is the *tripling* operation. The complete transformed parameters are:

Le(*M*): $v = s_0 f_0 = d_0 v_0$; $e = 3e_0$; $f = v_0 + f_0$ (5)

being the same as for *Tr*(*M*), eq 3.

A nice example of *Le* operation realization is: *Le*(D) = Fullerene C_{60} (Figure 6). The leapfrog operation can be used to insulate the parent faces by surrounding bounding polygons (see above).

Dodecahedron *Le* (Dodecahedron)= C_{60}

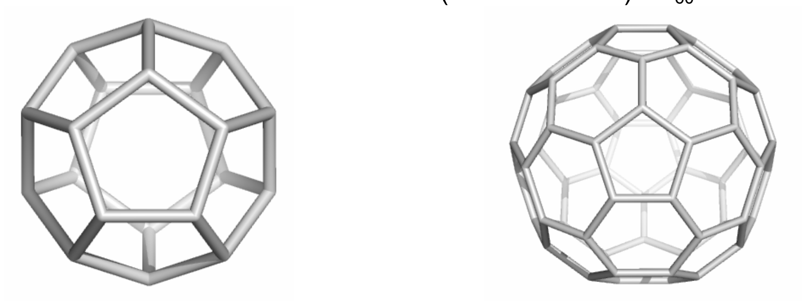


Figure 6. Leapfrog operation – molecular realization.

LATTICE BUILDING

The lattice under study (Figure 7), named S_2CL, was designed by the sequence: *Trs*(*Du*(*Med*(*Le*(Oct)))) and is a triple periodic network. In the above sequence, *Trs* means the truncation of some selected vertices. This sequence of operations introduces pentagon triples in a polygonal covering, which apparently violate the IPR (Isolated Pentagon Rule) condition in fullerene stability [25,26].

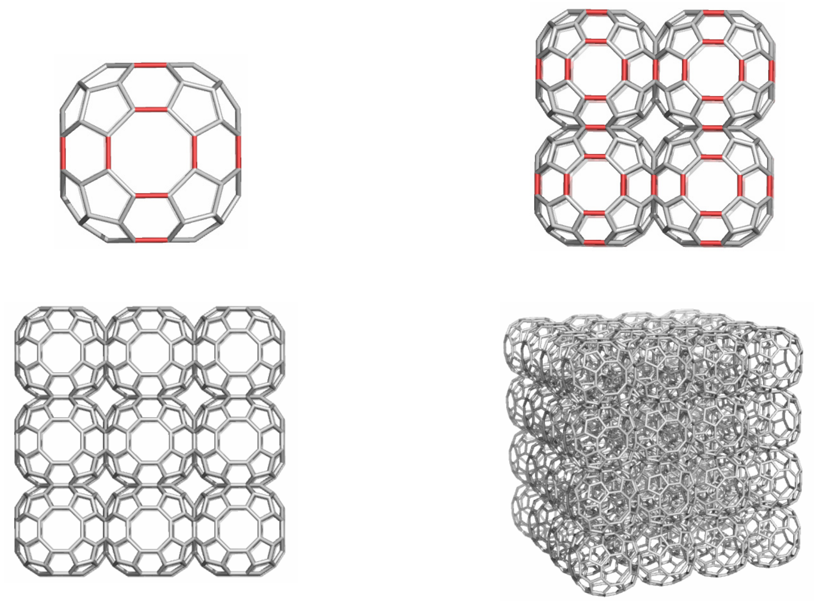


Figure 7. Lattice S_2CL; unit designed by *Trs*(*Du*(*Med*(*Le*(Oct)))); the red bonds mark the octagonal faces to be identified in construction of the network.

However, fullerenes which tessellation included pentagon triples have been obtained as real molecules. Calculation of stability of cages bearing pentagon triples [27] makes the subject of another article.

Network was performed by identifying the octagons in two neighbor units (Figure 7, left top corner). In this way, ordered channels appear, like those in zeolites.

For the topological characterization, cubic domains were constructed (Figure 7, right, bottom, corner). Formulas for Omega polynomial and examples are given in the next section.

OMEGA POLYNOMIAL IN CRYSTAL LATTCE

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*. Then *e co f* holds by assuming the faces are isometric. Note that relation *co* involves distances in the whole graph while *op* is defined only locally (it relates face-opposite edges).

Using the relation *op* we can partition the edge set of *G* into *opposite* edge *strips, ops*: any two subsequent edges of an *ops* are in *op* relation and any three subsequent edges of such a strip belong to adjacent faces.

Note that John *et al*. [28,29] implicitly used the "*op*" relation in defining the Cluj-Ilmenau index *CI*.

Denote by *m*(*s*) or simply *m* the number of *ops* of length $s=|s_k|$ and define the Omega polynomial as [30-32]:

$$\Omega(x) = \sum_{s} m(s) \cdot x^{s} \tag{6}$$

The exponent counts just the *ops* of length *s*; the coefficients *m* are easily counted from the symmetry of *G*. The first derivative (in *x*=1) provides the number of edges in *G*:

$$\Omega'(1) = \sum_{s} m \cdot s = e = |E(G)| \tag{7}$$

On Omega polynomial, the Cluj-Ilmenau index [33], *CI*=*CI*(*G*), was defined:

$$CI(G) = \left\{ [\Omega'(1)]^2 - [\Omega'(1) + \Omega''(1)] \right\} \tag{8}$$

We used here the topological description by Omega polynomial because this polynomial was created to describe the covering in polyhedral nanostructures and because it is the best in describing the constitutive parts of nanostructures, particularly for large structures, with a minimal computational cost [34].

Formulas for Omega polynomial in S_2CL network and examples are given in Table 1.

Table 1. Omega polynomial in S_2CL; R_{max}[8].

Formulas		
$\Omega(S2CL,x)=24a^3\cdot x^1+6a(a^2+9a-4)\cdot x^2+12a(a-1)^2\cdot x^4+3a\cdot x^{a(8+4(a-1))}$		
$\Omega'(S2CL,1)=24a^2(4a+1)$		
$\Omega''(S2CL,1)=48a(a^4+2a^3+4a^2-4a+2)$		
$CI(S2CL)=24a(384a^5+190a^4+20a^3-12a^2+7a-4)$		
Examples		
Net	Omega	*CI*
111	$24x+36x^2+3x^8$	14040
222	$192x+216x^2+24x^4+6x^{24}$	741600
333	$648x+576x^2+144x^4+9x^{48}$	7858872
777	$8232x+4536x^2+3024x^4+21x^{224}$	1161954360
888	$12288+6336x^2+4704x^4+24x^{288}$	2567169792

Data were calculated by the original software Nano-Studio, developed at TOPO Group Cluj, Romania.

CONCLUSIONS

Design of S_2CL hypothetical crystal structure was performed by using some operations on maps. This network is aimed to simulate the ordered channels existing in some zeolites. The topology of the proposed network was described in terms of Omega polynomial.

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