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OMEGA POLYNOMIAL IN TWO APPEARANCESOF THE CRYSTAL NETWORK *DIU15*, SPACE GROUP *IM-3M*

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ABSTRACT. Omega polynomialΩ(G,x) is defined on opposite edge strips ops in a graph. The first and second derivatives, in X = 1, of Omega polynomial provide the Cluj-Ilmenau CI index. Design of a new crystal network, called diu15, by means of the Medial map operation is presented. The topology of this network, in two different appearances, is described in terms of Omega polynomial, function of the net parameters. Close formulas for the polynomial are given and examples tabulated.

Keywords: *Omega polynomial**,** CI index, map operation, diu15 crystal network*

INTRODUCTION

Mathematical calculations are absolutely necessary to explore important concepts in Chemistry. Mathematical Chemistry is a branch of Theoretical Chemistry developed for discussion and prediction of molecular structures using mathematical methods without necessarily referring to quantum mechanics. Chemical Graph Theory is an important tool for studying molecular structures. This theory had an important effect on the development of the chemical sciences.

Numbers reflecting certain structural features of organic molecules, obtained from their associate molecular graphs are usually called graph invariants or more commonly topological indices. The oldest and most

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thoroughly examined topological index in Chemistry was proposed and used by Wiener [1] in the study of paraffin thermodynamic properties and this topological index was called the Wiener index.

A finite sequence of some graph-theoretical categories/properties, such as the distance degree sequence or the sequence of the number of k-independent edge sets, can be described by so-called counting polynomials:

$$P(\mathrm{G},x)=\sum_{k} p(G,k)\cdot x^{k} \tag{1}$$

where*p(G,k)*is the frequency of occurrence of the property partitions of G, of length k, and x is simply a parameter to hold k.

Counting polynomials were introduced, in the Mathematical Chemistry literature, by Hosoya with his Z-counting (independent edgesets) and the distance degree polynomials, initially called Wiener and later Hosoya polynomial [2]. Their coefficients are used for the characterization of the topological nature of hydrocarbons.

The present work describes the design and topology (in terms of Omegapolynomial) of two appearances of Diudea'sdiu15 3-periodic lattice.

LATTICE BUILDING

The repeating unit of diu15 network is designed by using a map operation, named medial Med (or subdivision). This operation is achieved by putting new vertices in the middle of the original edges of a map M (i.e. a discretized closed surface)); next join two such vertices if the corresponding edges span an angle (and are consecutive within a rotation path around their common vertex in M). The transform Med(M) is a 4-valent graph and Med(M)=Med(Du(M)). The transformed map parameters are: $v=e_0$; $e=2e_0$; $f=f_0+v_0$.(the subscript zero denoted the original map parameters). The medial of Cube and Octahedron is the Cuboctahedron CO (Figure 1).The medial operation rotates parent s-gonal faces by π/s. Points in the medial map represent the original edges; this property can be used in topological analysis of edges in the parent polyhedron. Similarly, the points in the dual map give information on the topology of parent faces.

Figure 1. The Cuboctahedron CO=Med(C)

The unit **CO@(CO$_8$)_60** (Figure 2, top left) is composed of eight CO disposed around an empty hollow having also the geometry of CO; it can be obtained as***Med*(Oct@Oct$_8$_18)**by applying the Med operation on**Oct@Oct$_8$_18** (Figure 2, top right) that is a hyperstructure of the Octahedron Oct. Note, the last number in the above object names is the number of points/atoms.

The lattice diu15 is built by translating the unit **CO@(CO$_8$)_60**, with the identification of the superposed hyper-faces; this results in two appearances diu15X (Figure 2, bottom left) and diu15 (Figure 2, bottom right). This is a new 2-nodal network (by TOPOS database), belonging to the space group ***Im-3m***and having the point symbol for net: (33.46.56)2(34.410.512.62)6,8-c net with stoichiometry (6-c)2(8-c).

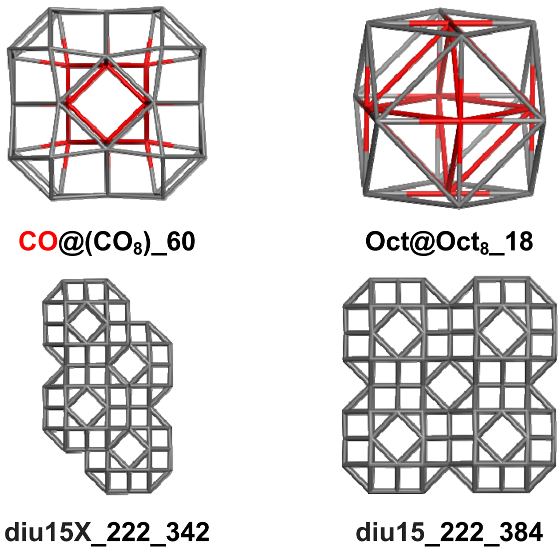

Figure 2. Top row: a spongy unit **CO@(CO$_8$)_60** consisting of cuboctahedra CO, designed by Medial (i.e., Subdivision) map operation applied on**Oct@Oct$_8$_18**; Bottom row: two apearances of the crystal network**diu15**, space group ***Im-3m***.

OMEGA POLYNOMIAL

The Omega polynomial is a counting polynomial introduced by Diudea. In the recent years, several papers on methods for computing Omega polynomial in molecular graphs and nanostructures have been published [11 – 17].

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 [3]:

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y) \tag{2}$$

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 it is 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 [4] has shown that relation co is a theta Djoković-Winkler relation[5,6].

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 infaces. 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 $S_1, S_2, \ldots, S_k$ 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/ringF_{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 and define the Omega polynomial as[7-9]:

$$\Omega(G,x) = \sum\nolimits_s m(G,s) \cdot x^s \tag{3}$$

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

$$\Omega'(G,1) = \sum\nolimits_s m(G,s) \cdot s = e = |E(G)| \tag{4}$$

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

$$CI(G) = \{[\Omega'(G,1)]^2 - [\Omega'(G,1) + \Omega''(G,1)]\} \tag{5}$$

MAIN RESULTS

Within this paper, the Omega polynomial and derived Cluj-Ilmenau CI index refer toF_{max}(4).Data were calculated by software program Nano Studio [10], developed at the TOPO Group Cluj. Formulas for the infinite networks of the two series were derived by numerical analysis, function of k that is the number of repeating units in a row of a cubic domain (k,k,k), and are listed in Tables 1 and 2; examples are given at the bottom of these tables.

Table1. Omega polynomials in **diu15X** Network

Formulas
$\Omega(G,x) = 2\left(4k^2+9k-1\right)x^2 + 2\left(14k^2-5k-3\right)x^3 + 2\left(3k^3+3k^2+5k-2\right)x^4 + 2\left(8k^2-13k+5\right)x^5 + 2\left(3k^3-4k^2+k\right)x^6$
$\lvert V(G)\rvert = 18k^3+58k^2-18k+2$
$\lvert E(G)\rvert = 60k^3+156k^2-72k+12$
$CI(G) = 3600k^6+18720k^5+15696k^4-21336k^3+8436k^2-1292k+20$

k	Omega polynomial: examples	*V(G)*	*E*(*G*)	*CI*(*G*)
1	$24x^2+12x^3+18x^4$	60	156	23844
2	$66x^2+86x^3+88x^4+22x^5+20x^6$	342	972	941068
3	$124x^2+216x^3+242x^4+76x^5+96x^6$	956	2820	7940732
4	$198x^2+402x^3+516x^4+162x^5+264x^6$	2010	6060	36697380
5	$288x^2+644x^3+946x^4+280x^5+560x^6$	3612	11052	122097460
6	$394x^2+942x^3+1513x^4+430x^5+1020x^6$	5870	18156	329557724
7	$516x^2+1296x^3+2418x^4+612x^5+1680x^6$	8892	27732	768935628

Table 2.

Omega polynomials in **diu15** Network

Formulas
$\Omega(G,x)=24k\,x^2+12k\,(4k-3)\,x^3+6k\,(2k^2+1)\,x^4+6k\,(2k^2-3k+1)\,x^6$
$\lvert V(G)\rvert=12k^2(3k+2)$
$\lvert E(G)\rvert=120k^3+36k^2$
$CI(G)=14400k^6+8640k^5+12966k^4-624k^3+216k^2-84k$

k	Omega polynomial: examples	*V(G)*	*E*(*G*)	*CI*(*G*)
1	$24x^2+12x^3+18x^4$	60	156	23844
2	$48x^2+120x^3+108x^4+36x^6$	384	1104	1214520
3	$72x^2+324x^3+342x^4+180x^6$	1188	3564	12686940
4	$96x^2+624x^3+792x^4+504x^6$	2688	8256	68124720
5	$120x^2+1020x^3+1530x^4+1080x^6$	5100	15900	252736980
6	$144x^2+1512x^3+2628x^4+1980x^6$	8640	27216	740583144
7	$168x^2+2100x^3+4158x^4+3276x^6$	13524	42924	1842265740

CONCLUSION

Omega polynomial description proved to be a simple and efficient method in topological characterization of some new designed nano-structures.

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