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Dedicated to Professor Mircea Diudea on the Occasion of His 65th Anniversary

COUNTING POLYNOMIALS IN THE CRYSTAL NETWORK FLU (CMedDu)

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ABSTRACT. The crystal network named *flu*, belonging to the symmetry group *Fm-3m*, can be designed by map operations Medial and Dual, applied subsequently on the Cube. The topology of the network was characterized by Omega, Cluj and related polynomials.

Keywords: *Crystal like network, Omega polynomial, Cluj polynomial, Map operation*

INTRODUCTION

Design of polyhedral units, forming crystal-like lattices, is of interest in crystallography as many metallic oxides or more complex salts have found applications in chemical catalysis. Various applied mathematical studies have been performed, in an effort to give new, more appropriate characterization of the world of crystals. Recent articles in crystallography promoted the idea of topological description and classification of crystal structures. They present data describing real but also hypothetical lattices designed by computer.

Some basic map operations like Leapfrog ***Le***, Quadrupling ***Q*** and Capra ***Ca***, associated or not with the more simple Medial ***Med*** and/or Dual ***Du*** operations, are most often used to transform small polyhedral objects into more complex units. These transforms preserve the symmetry of the parent

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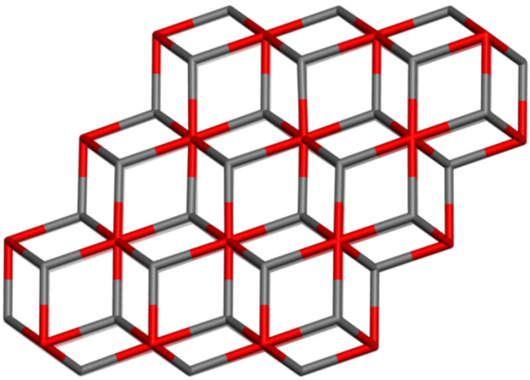
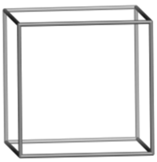
object/net. The article is devoted to the study of a new crystal like network, by using some topological descriptions in terms of Omega, Cluj and related counting polynomials.

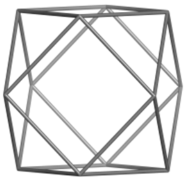
The network in Figure 1 is known as *flu/fluorite; sqc169; CMedDu* (Diudea's name), a 2-nodal net, with the point symbol for net: $(4^{12}.6^{12}.8^{4})(4^{6})2$; 4,8-c net with stoichiometry (4-c)2(8-c) and belonging to the group *Fm*-3*m*. It was drawn by using operations on maps: Medial ***Med*** and Dual ***Du***, applied subsequently on the Cube ***C***.



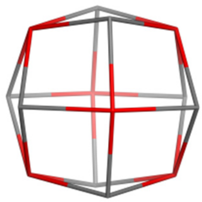
Du(Med(C)_333_174



C_8



Med(C)_12



Du(Med(C))_14

Figure 1. The network flu/CMedDu and its "history" originating in the Cube C

A map *M* is a discretized representation of a (closed) surface. In the following, we denote in a map: *v* – the number of vertices, *e* - the number of edges, *f* – the number of faces and *d* – the vertex degree; a subscript "0" will mark the corresponding parameters in the parent map. The number of vertices and edges in this structure are equal to $v = 3k^3 + 10k^2 + k$ and $e = 8k^3 + 20k^2 - 4k$, respectively.

Dual of a map, *Du*(*M*), is achieved by locating a point in the center of each face,next two such points are joined if their corresponding faces share a common edge. It is the *Dual Du*(*M*). The vertices of *Du*(*M*) represent faces of *M* and vice-versa [1]. The parent and transformed map are related by the parameters: *Du*(*M*); $v = f_0$; $e = e_0$; $f = v_0$**.** Dual of the dual returns the original map: *Du*(*Du*(*M*)) = *M*.

Medial of a map, *Med*(*M*), can be performed if put new vertices in the middle of each of the original edges [1]. Join two vertices if the edges span an angle (and are consecutive within a rotation path around their common vertex in *M*). Medial is a 4-valent graph and *Med*(*M*)=*Med*(*Du*(*M*)). The transformed map parameters are: *Med*(*M*); $v = e_0$; $e = 2e_0$; $f = f_0 + v_0$.

The medial operation rotates parent s-gonal faces by *π*/*s*. Points in the medial transformed map represent 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.

A finite sequence of some graph-theoretical categories/properties, such as the distance degree sequence or the sequence of numbers of k-independent edge sets, can be described by so-called counting polynomials [2]:

$$P(G,x) = \sum_k p(G,k) \cdot x^k \qquad (1)$$

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.

OMEGA POLYNOMIAL

Let *G* be a connected graph with the vertex set *V* =*V* (*G*) and edge set *E*= *E*(*G*), without loops. Two edges *e* = *ab* and *f* = *xy* of *G* are called *co-distant* (briefly: *e co f*) if for *k* = 0,1,2,… there exist the relations: *d*(*a,x*) = *d*(*b,y*) = *k* and *d*(*a,y*) = *d*(*b,x*) = *k*+1 or vice versa. For some edges of a connected graph *G* there are the following relations satisfied:

$$e \ co \ f \qquad (2)$$

$$e \ co \ f \Leftrightarrow f \ co \ e \qquad (3)$$

$$e \ co \ f \ \& \ f \ co \ g \Rightarrow e \ co \ g \qquad (4)$$

though, the relation (4) is not always valid.

Let *C*(*e*):= { *e*'∈ *E*(*G*) ; *e*' *co e* } denote the set of all edges of *G* which are codistant to the edge *e*. If all the elements of *C*(*e*) satisfy the relations (2-4) then *C*(*e*) is called an *orthogonal cut "oc"* of the graph *G*. The graph *G* is called *co-graph* if and only if the edge set *E*(*G*) is the union of disjoint orthogonal cuts: $C_1 \cup C_2 \cup \ldots \cup C_k = E(G)$ and $C_i \cap C_j = \phi$ for $i \neq j$, $i, j = 1,2,\ldots,k$.

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 $S_1, S_2, \ldots, S_k$ 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/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* and define the Omega polynomial as [3-9]:

$$\Omega(G,x) = \sum_{s} m(G,s) \cdot x^{s} \tag{5}$$

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

$$\Omega'(G,1) = \sum_{s} m(G,s) \cdot s = e = |E(G)| \tag{6}$$

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

$$CI(G) = \left\{ [\Omega'(G,1)]^2 - [\Omega'(G,1) + \Omega''(G,1)] \right\} \tag{7}$$

Omega polynomial and Cluj-Ilmenau index of crystal network *flu* with some examples are presented in Table 1.

Table 1. Omega polynomial and CI index in crystal network flu.

Formulas			
	$\Omega(G,x) = \sum_{i=1}^{k-1} 4x^{4k+2+(2k+2)(i-1)} + (2k+2)x^{2k^2+4k}$		
	$CI(G) = \frac{1}{3}(192k^6 + 920k^5 + 832k^4 - 696k^3 + 56k^2 - 8k)$		
	$\lvert R(4) \rvert = 6k^3 + 10k^2 - 5k + 1$		
	Examples		
k	$\Omega(G,x)$	*CI(G)*	|R(4)|
1	$4x^{6}$	432	12
2	$4x^{10}+6x^{16}$	16560	79
3	$4x^{14}+4x^{22}+8x^{30}$	137536	238
4	$4x^{18}+4x^{28}+4x^{38}+10x^{48}$	632608	525
5	$4x^{22}+4x^{34}+4x^{46}+4x^{58}+12x^{70}$	2103120	976

CLUJ POLYNOMIAL

Cluj matrices and indices have been proposed by Diudea on the ground of fragments/subgraphs [10-12] $CJ_{i,j,p}$ that collects vertices *v* lying closer to *i* than to *j*, the endpoints of a path *p(i,j).* Such fragments represent vertex proximities of *i* against any vertex *j*, joined by the path *p*, with the distances measured in the subgraph $D_{(G-p)}$, as shown in relation:

$$CJ_{i,j,p} = \left\{ v \middle| v \in V(G); D_{(G-p)}(i,v) < D_{(G-p)}(j,v) \right\} \tag{8}$$

In graphs containing rings, more than one path could join the pair (*i,j*), thus resulting more than one fragment related to *i* (with respect to *j* and a given path *p*); the entries in the Cluj matrix are taken, by definition, as the maximum cardinality among all such fragments:

$$[\mathbf{UCJ}]_{i,j} = \max_{p} \left| CJ_{i,j,p} \right| \tag{9}$$

Cluj polynomials are developed on the non-symmetric matrices *UCJDI* calculated on path $UCJDI_p$ or on edges $UCJDI_e$.

The general form of Cluj polynomial is [13-16]:

$$CJ(x) = \sum_k m(k) \cdot x^k \tag{10}$$

They count the vertex proximity of the vertex *i* with respect to any vertex *j* in *G*, joined to *i* by an edge (the Cluj-edge polynomials $CJDI_e(x)$) or by a path (the Cluj-path polynomials *CJDIp(x)*). In (10), the coefficients *m(k)* can be calculated from the entries of *UCJDI* matrices by the **TOPOCLUJ** software program [17]. The summation runs over all $k = |\{p\}|$ in *G*.

In bipartite graphs, the coefficients of cluj polynomial can be calculated by an orthogonal edge-cut procedure [18-20]. For this, a theoretical background is needed.

For any edge *e=(u,v)* of a connected graph *G*, let n_{uv} denote the set of vertices lying closer to *u* than to *v*: $n_{uv} = \{ w \in V(G) \mid d(w,u) < d(w,v) \}$. It follows that $n_{uv} = \{ w \in V(G) \mid d(w,v) = d(w,u) + 1 \}$. The sets (and subgraphs) induced by these vertices, n_{uv} and n_{vu}, are called *semicubes* of *G*; the semicubes are called *opposite semicubes* and are disjoint [4,21,22].

A graph *G* is bipartite if and only if, for any edge of *G*, the opposite semicubes define a partition of *G*: $n_{uv} + n_{vu} = v = |V(G)|$. These semicubes are just the vertex proximities (see above) of (the endpoints of) edge *e*=(*u*,*v*), which CJ_e polynomial counts. In partial cubes, the semicubes can be estimated by an orthogonal edge-cutting procedure.

To any orthogonal cut c_k, two numbers are associated: first one represents the *number of edges* e_k intersected (or the cutting cardinality $|c_k|$) while the second is v_k or the number of points lying to the left hand with respect to c_k. Because in bipartite graphs the opposite semicubes define a partition of vertices, it is easily to identify the two semicubes: $n_{uv}= v_k$ and $n_{vu}= v-v_k$ or vice-versa.

By this cutting procedure, four polynomials can be count, they differing only in the mathematical operation used to re-compose the local contributions to the global graph property [19]:

(1) ***Summation;*** the polynomial is called *Cluj-Sum* and is symbolized *CJS* [13-15,23]

$$CJS(x) = \sum_e \left(x^{v_k} + x^{v-v_k} \right) \tag{11}$$

(2) ***Pair-wise summation;*** the polynomial is called PI_v (vertex-Padmakar-Ivan) [24-28]

$$PI_v(x) = \sum_e x^{v_k+(v-v_k)} \tag{12}$$

(3) ***Pair-wise product;*** the polynomial is called *Cluj-Product* (and symbolized *CJP*) [10-12,16,18,19] or also Szeged (and symbolized *SZ*) [26-30]

$$CJP(x) = SZ(x) = \sum_e x^{v_k(v-v_k)} \tag{13}$$

(4) ***Single edge pair-wise product;*** the polynomial is called *Wiener* and symbolized *W* [19]

$$W(x) = \sum_k x^{v_k \cdot (v-v_k)} \tag{14}$$

The first derivative (in x=1) of a counting polynomial provides single numbers, often called topological indices. The coefficients of polynomial terms are calculated (except $W(x)$ as the product of three numbers: sym(G) × freq(c_k) × e_k.

One can see that the first derivative (in x=1) of the first two polynomials gives one and the same value, however, their second derivative is different and the following relations hold in any graph [16,19]

$$CJS'(1) = PI_v'(1)\ ;\ CJS''(1) \neq PI_v''(1) \tag{15}$$

In bipartite graphs, the first derivative (in x=1) of $PI_v(x)$ takes the maximal value:

$$PI_v'(1) = e \cdot v = |E(G)| \cdot |V(G)| \quad (16)$$

Keeping in mind the definition of the corresponding index, one can see that [31]

$$PI_v(G) = PI_v'(1) = \sum_{e=uv} n_{u,v} + n_{v,u} = |V| \cdot |E| - \sum_{e=uv} m_{u,v} \quad (17)$$

where $n_{u,v}$, $n_{v,u}$ count the non-equidistant vertices with respect to the endpoints of the edge e=(u,v) while $m_{u,v}$ is the number of equidistant vertices vs. u and v. However, it is known that, in bipartite graphs, there are no equidistant vertices, so that the last term in (17) is missing. The value of $PI_v(G)$ is thus maximal in bipartite graphs, among all graphs on the same number of vertices; the result of (14) can be used as a criterion for the "bipatity" of a graph [14].

The third polynomial, *CJP*(*x*), uses the pair-wise product; it is precisely the (vertex) Szeged polynomial $SZ_v(x)$, defined by Ashrafi *et al* [26-28]. This comes out from the relations between the basic Cluj (Diudea [11,12]) and Szeged (Gutman [30]) indices:

$$CJP'(1) = CJDI(G) = SZ(G) = SZ_v'(1) \quad (18)$$

All the three above polynomials (and their derived indices) do not count the equidistant vertices, an idea introduced in Chemical Graph Theory by Gutman [30]. We call these: *polynomials of vertex proximity*.

The last polynomial, *W*(*x*), we call Wiener, because it is calculated as Wiener performed the index *W(G)* in tree graphs: multiply the number of vertices lying to the left and to the right of each edge (actually read orthogonal cut c_k):

$$W(G) = W'(1) = \sum\nolimits_k v_k \cdot (v - v_k) \quad (19)$$

where v_k and v-v_k are the disjoint semicubes forming a partition with respect to each edge in c_k taken as a "*single edge*" (as in trees). In partial cubes, the exponents of *W*(*x*) are identical to those in *CJP*(*x*) and *SZ*(*x*) while the coefficients are those in the above polynomials, divided by e_k. When subscript letter is missing, *SZ*(*x*) is $SZ_v(x)$.

Numerical calculation were done by our original software programs **TOPOCLUJ** [17]. In this article all above formulas also examples are presented for flu structure in Tables 2-6.

Table 2. Cluj and related polynomial in crystal network *flu*.

	PI_v , PI_v' and PI_v''
1	$PI_v(G) = (8k^3 + 20k^2 - 4k)\, x^{3k^3+10k^2+k}$
2	$PI_v'(1) = 24k^6 + 140k^5 + 196k^4 - 20k^3 - 4k^2$
3	$PI_v''(1) = 72k^9 + 660k^8 + 2012k^7 + 2016k^6 - 156k^5 - 256k^4 + 16k^3 + 4k^2$

Cluj polynomial

4

$$Cluj(G,x) = \sum_{i=1}^{\left\lfloor \frac{k}{2} \right\rfloor} (8k^2 + 16k)\, x^{(3k^3+7k^2-3k)-(3k^2+7k)(i-1)}$$

$$+ \sum_{i=1}^{\left\lfloor \frac{k}{2} \right\rfloor} (8k^2 + 16k)\, x^{(-6k^2-19k-7)+(3k^2+7k)(i-1)}$$

$$+ \sum_{i=1}^{k-1} \left[(16k+8) + (8k+8)(i-1)\right] x^{(3k^3+10k^2-4k-2)-(8k+5)(i-1)-(3k+3)\frac{(i-1)(i-2}{2}}$$

$$+ \sum_{i=1}^{k-1} \left[(16k+8) + (8k+8)(i-1)\right] x^{(5k+2)+(8k+5)(i-1)+(3k+3)\frac{(i-1)(i-2)}{2}}$$

$$+ \left[(3-(-1)^k)(4k^2 + 8k)\right] x^{\frac{3}{2}k^3+5k^2+\frac{1}{2}k}$$

5 $Cluj'(1) = 24k^6 + 140k^5 + 196k^4 - 20k^3 - 4k^2$

6 $Cluj''(1) = \frac{1}{15}(720k^9 + 6402k^8 + 18786k^7 + 16426k^6 - 6848k^5 - 5082k^4 - 46k^3 - 106k^2 - 12k)$

	Wiener
7	$W(G)=\frac{1}{30}(216k^7+1677k^6+3336k^5+790k^4-76k^3-67k^2+4k)$
	Szeged
8	$CJP(x)=SZ(x)=\sum_{i=1}^{\lfloor \frac{k}{2} \rfloor}(8k^2+16k)\,x^{\left(k^2(3k^2+10k+4-3ki-7i)(-3+3\mathrm{ki}+7\mathrm{i})\right)}$ $+\sum_{i=1}^{k-1}\left[(16k+8)+(8k+8)(i-1)\right]x^{\frac{\left(6k^3+20k^2+2k-7ki-i-3ki^2-3i^2\right)(7k+1+3ki+3i)i}{4}}$ $+\left[(3-(-1)^k)(2k^2+4k)\right]x^{(\frac{3}{2}k^3+5k^2+\frac{1}{2}k)^2}$
9	$Sz(G)=\frac{1}{15}(180k^9+1749k^8+5697k^7+6907k^6+2254k^5+621k^4+143k^3+83k^2+6k)$
	PI_e , $PI_e'(1)$ and $PI_e''(1)$
10	$PI_e(G,x)=\sum_{i=1}^{k-1}\left[(16k+8)+(8k+8)(i-1)\right]x^{(8k^3+20k^2-8k-2)-(2k+2)(i-1)}+(4k^3+12k^2+8k)\,x^{8k^3+18k^2-8k}$
11	$PI_e'(1)=\frac{1}{3}(192k^6+920k^5+832k^4-696k^3+56k^2-8k)$
12	$PI_e''(1)=\frac{1}{3}(1536k^9+10880k^8+22152k^7+2568k^6-20264k^5+4832k^4+240k^3+80k^2+24k)$

Table 3. Examples, PI_v, PI_v', PI_v'' ,number of vertices and edges in crystal network *flu*.

k	PI_v Polynomial	PI_v'	PI_v''	*v*	*e*
1	$24x^{14}$	336	4368	14	24
2	$136x^{66}$	8976	583440	66	136
3	$384x^{174}$	66816	11559168	174	384
4	$816x^{356}$	290496	103126080	356	816
5	$180x^{630}$	932400	586479700	630	1480

Table 4. Cluj and related polynomials in crystal network *flu*.

k	Cluj polynomial	$CJ'(1)$	$CJ''(1)$
1	$48x^{7}$	336	2016
2	$40x^{54} + 64x^{46} + 64x^{33} + 64x^{20} + 40x^{12}$	8976	344144
3	$56x^{157} + 120x^{135} + 88x^{128} + 240x^{87} + 88x^{46} + 120x^{39} + 56x^{17}$	66816	7143792
4	$72x^{334} + 112x^{297} + 192x^{292} + 152x^{245} + 192x^{216} + 192x^{178} + 192x^{140} + 152x^{111} + 192x^{64} + 112x^{59} + 72x^{22}$	290496	65003856
5	$88x^{603} + 136x^{558} + 280x^{535} + 184x^{495} + 280x^{425} + 232x^{414} + 560x^{315} + 232x^{216} + 280x^{205} + 184x^{135} + 280x^{95} + 136x^{72} + 88x^{27}$	932400	373783936

Table 5. Examples; cluj polynomial in crystal network *flu*.

k	Szeged polynomial	Szeged index	Wiener index
1	$24x^{49}$	1176	196
2	$64x^{920}+40x^{648}+32x^{1089}$	119648	8450
3	$120x^{5265}+56x^{2669}+88x^{5888}+120x^{7569}$	2207688	85564
4	$192x^{18688}+192x^{30240}+72x^{7348}+112x^{17523}+152x^{27195}+96x^{31684}$	19061112	467344
5	$280x^{50825}+280x^{87125}+88x^{16281}+136x^{40176}+184x^{66825}+232x^{89424}+280x^{99225}$	106347832	1799524

Table 6. Examples; PI_e, $PI_e^{\prime}(1)$ and $PI_e^{\prime\prime}(1)$ in crystal network flu.

k	PI_e	$PI_e^{\prime}(1)$	$PI_e^{\prime\prime}(1)$
1	$24x^{18}$	432	7344
2	$40x^{126}+96x^{120}$	15560	2000880
3	$536x^{370}+88x^{362}+240x^{354}$	137536	49136576
4	$72x^{798}+112x^{788}+152x^{778}+480x^{768}$	632608	489881696
5	$88x^{1458}+136x^{1446}+184x^{1434}+232x^{1422}+840x^{1410}$	2103120	2986825680

CONCLUSIONS

In this paper we presented the Omega and Cluj polynomials in crystal-like network *flu*. Definitions and relations with other polynomials and topological indices were given. Analytical formulas as well as examples were tabulated.

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