STUDIA UBB CHEMIA, LXI, 3, Tom II, 2016 (p. 485-493)
(RECOMMENDED CITATION)

Dedicated to Professor Emil Cordoș on the occasion of his 80th anniversary

CLUJ AND RELATED POLYNOMIALS IN BIPARTITE HYPERCUBE HYPERTUBES

MAHBOUBEH SAHELI[a], AMIR LOGHMAN[a], MIRCEA V. DIUDEA[b*]

ABSTRACT. A novel class of counting polynomials, called Cluj polynomials was proposed on the ground of Cluj matrices. The polynomial coefficients are calculated from the above matrices or by means of orthogonal edge-cuts. In this paper Cluj polynomial in bipartite hypercube hypertubes is presented. Definitions and relations with other polynomials and topological indices are derived.

Keywords: *Cluj polynomial, vertex-Padmakar-Ivan index, Wiener index.*

INTRODUCTION

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*:

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

where *p(G,k)* is the frequency of occurrence of the property partitions of *G*, $\cup p(G) = P(G)$, of length *k*, and *x* is simply a parameter to hold *k*. In the Mathematical Chemistry literature, the counting polynomials have first been introduced by Hosoya [1]. Cluj indices and polynomial have been introduced by Diudea [2-6]. In bipartite graphs, the coefficients of *CJ* polynomial can be calculated by an orthogonal edge-cut procedure [7-9]. For this, a theoretical background is needed.

[a] *Department of Mathematics, Payame Noor Universtiy, PO BOX 19395-3697 Tehran, Iran.*
[b] *Department of Chemistry, Faculty of Chemistry and Chemical Engineering, "Babes-Bolyai" University, 400028 Cluj, Romania.*
[*] *Corresponding author: diudea@chem.ubbcluj.ro*

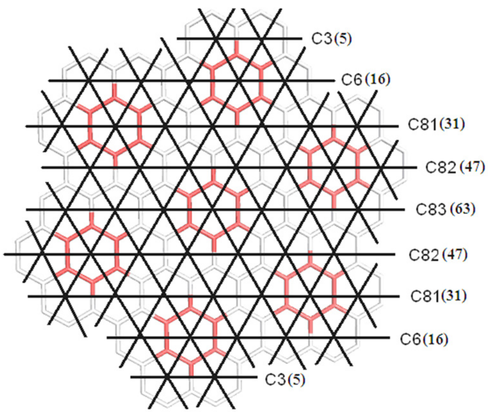
A graph *G* is a *partial cube* if it is embeddable in the *n*-cube Q_n, which is the regular graph whose vertices are all binary strings of length *n*, two strings being adjacent if they differ in exactly one position. The distance function in the *n*-cube is the Hamming distance. A hypercube can also be expressed as the Cartesian product: $Q_n = \prod_{i=1}^{n} K_2$.

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 [2,10].

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* polynomial counts. In partial cubes, the semicubes can be estimated by an orthogonal edge-cutting procedure. The orthogonal cuts form a partition of the edges in *G*:

$$E(G) = c_1 \cup c_2 \cup ... \cup c_k,\ \ c_i \cap c_j = \varnothing, i \neq j\ .$$

To perform an orthogonal edge-cut, take a straight line segment, orthogonal to the edge *e*, and intersect *e* and all its parallel edges (in a plane graph). The set of these intersections is called an *orthogonal cut* $c_k(e)$, $k=1,2,..,k_{max}$. An example is given in Figure 1.



$CJS(x) =$
$3·2·3(x^{5}+x^{121})+3·2·6(x^{16}+x^{110})+$
$3·2·8(x^{31}+x^{95})+3·2·8(x^{47}+x^{79})+$
$3·1·8(x^{63}+x^{63})$
$CJS'(1)=21924$
$PI_v(x) =$
$3·2·3(x^{5}+{}^{121})+$
$3·2·6(x^{16}+{}^{110})+3·2·8(x^{31}+{}^{95})+$
$3·2·8(x^{47}+{}^{79})+3·1·8(x^{63}+{}^{63})$
$PI_v'(1)=21924$
$CJP(x) =$
$3·2·3(x^{5·121})+ 3·2·6(x^{16·110})+$
$3·2·8(x^{31·95})+ 3·2·8(x^{47·79})+$
$3·1·8(x^{63·63})$
$CJP'(1)=489090=CJP(G)=SZ_v'(1)$

Figure 1. Cutting procedure in the calculation of several topological descriptors

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, three cases have to be considered, as summarized in Table 1.

Table 1: Mathematical operations and defined three polynomials

	Operation	Polynomial name	Formula
1	Summation	Cluj-Sum	$CJS(x) = \sum_e \left(x^{v_k} + x^{v-v_k} \right)$
2	Pairwise summation	vertex-Padmakar-Ivan	$PI_v(x) = \sum_e x^{v_k + (v-v_k)}$
3	Pairwise product	Cluj-Product	$SZ(x) = \sum_e x^{v_k (v-v_k)}$

The first derivative, for x=1, of a counting polynomial provides single numbers, often called topological indices. It is easily seen that the first derivative (in x=1) of the first two polynomials gives one and the same value, but their second derivative is different and the following relations hold in any graph [11-13]

$$CJS'(1) = PI_v'(1)\,; \tag{2}$$

$$CJS''(1) \neq PI_v''(1) \tag{3}$$

In bipartite graphs, $PI_v'(1)$ takes the maximal value, among all the graphs on the same number of vertices:

$$PI_v'(1) = e \cdot v = |E(G)| \cdot |V(G)| \tag{4}$$

This result can be used as a criterion for the “bipartivity” of a graph [7,8].

The third polynomial, $CJP(x)$, uses the pairwise product; it is precisely the (vertex) Szeged polynomial $SZ_v(x)$, defined by Ashrafi *et al* [12-14]. This comes out from the relations between the basic Cluj (Diudea [2,5]) and Szeged (Gutman [15]) indices:

$$CJP'(1) = CJDI(G) = SZ(G) = SZ_v'(1) \tag{5}$$

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

LATTICE BUILDING

In some recent papers [16,17], Diudea *et al*. proposed the embedding of *n*-Cube in surfaces other than the sphere. In case of open tubes, some examples are given in Figure 2.

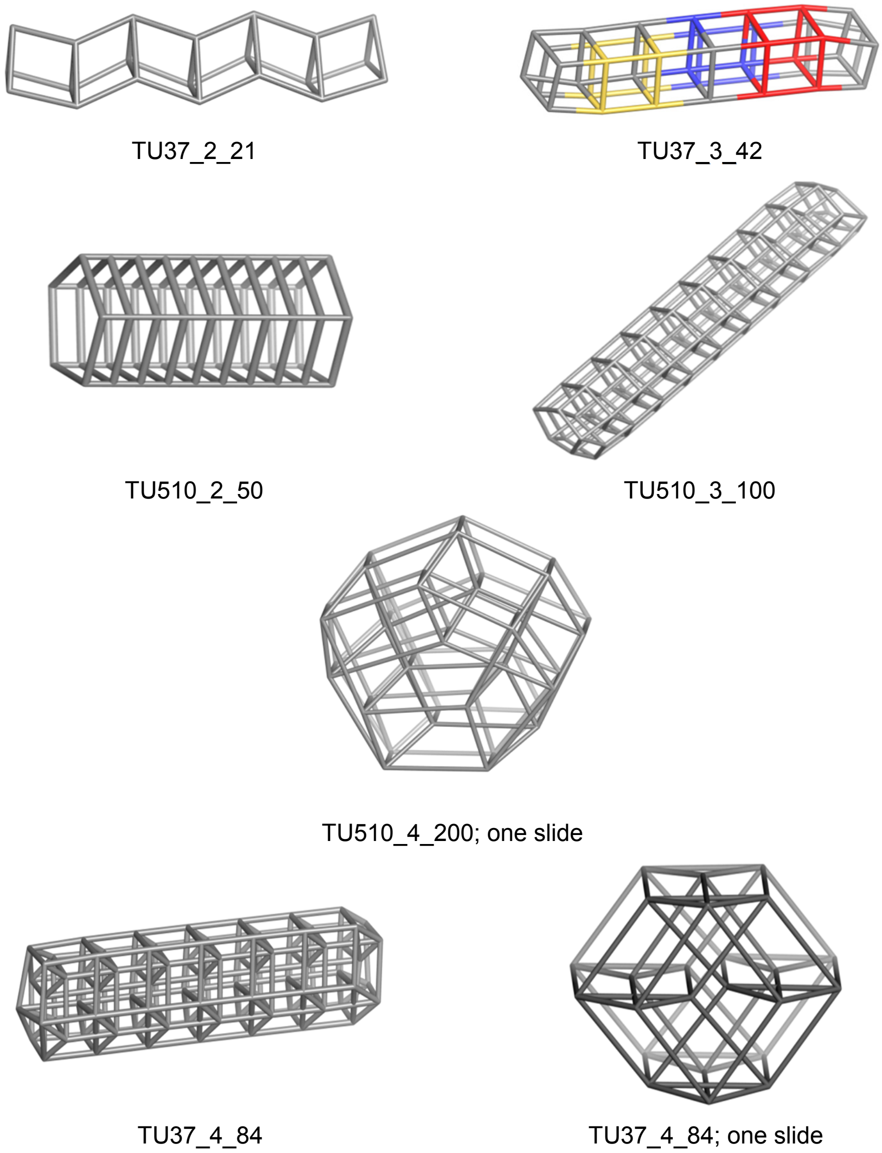


Figure 2. Examples of hypercube embedded in the (nano)tubes

RESULTS AND DISCUSSION

All the three polynomials listed in Table 1 are exemplified, for some bipartite hypercube hypertubes TU*rs* in Tables 2 to 9. The analytical formulas were derived by numerical analysis. Numerical calculations have been done by TOPOCLUJ software [18].

Table 2: Cluj and related polynomials in **TU4*s***

Number of vertices and edges	
1	$\lvert V(TU4s)\rvert = 2^{n-1}s \quad \lvert E(TU4s)\rvert = 2^{n-2}(sn+s-2)$
***PI$_v$*; *PI$_v$*\` and *PI$_v$*\`\`**	
2	$PI_v(TU4s,x) = 2^{n-2}(sn+s-2)x^{2^{n-1}s}$
3	$PI_v'(1) = 2^{2n-3}s(sn+s-2)$
4	$PI_v''(1) = 4^{n-2}s\,(2^n s-2)(sn+s-2)$
Cluj polynomial and its derivatives	
5	$CJS(TU4s,x) = \sum_{i=1}^{\lfloor \frac{s-1}{2} \rfloor} 2^n\left[x^{2^{n-1}i} + x^{2^{n-1}(s-i)}\right] + \left[2^{n-1}\left(sn-s+1+(-1)^s\right)\right]x^{2^{n-2}s}$
6	$CJS'(1) = 2^{2n-3}s(sn+s-2)$
7	$CJS''(1) = \frac{4^{n-2}}{6}s\left[2^n\left(3s^2n+5s^2-12s+4\right)-12(sn+s-2)\right]$
Szeged polynomial and index	
8	$Sz(TU4s,x) = \sum_{i=1}^{\lfloor \frac{s-1}{2} \rfloor} 2^n x^{4^{n-1}i(s-i)} + \left[2^{n-2}\left(sn-s+1+(-1)^s\right)\right]x^{4^{n-2}s^2}$
9	$Sz(TU4s) = \sum_{i=1}^{\lfloor \frac{s-1}{2} \rfloor} 2^{3n-2}\,i(s-i) + 2^{3n-6}s^2\left(sn-s+1+(-1)^s\right)$

Table 3: Cluj and related polynomials in **TU*rs***

Number of vertices and edges	
1	$\lvert V(TUrs)\rvert = 2^{n-2}rs \quad \lvert E(TU4s)\rvert = 2^{n-3}r(sn+2s-2)$
PIv; PIv`* and *PIv``	
2	$PI_v(TUrs,x) = 2^{n-3}r\,(sn+2s-2)x^{2^{n-2}rs}$
3	$PI_v'(1) = 2^{2n-5}r^2s\,(sn+2s-2)$
4	$PI_v''(1) = 4^{n-3}\,r^2s\,(2^{n-1}rs-2)(sn+2s-2)$
Cluj polynomial and its derivatives	
5	$CJS(TUrs,x) = \sum_{i=1}^{\lfloor \frac{s-1}{2} \rfloor} 2^{n-1}r\left[x^{2^{n-2}ri} + x^{2^{n-2}r(s-i)}\right] + \left[2^{n-2}r\left(sn+1+(-1)^s\right)\right]x^{2^{n-3}rs}$
6	$CJS'(1) = 2^{2n-5}r^2s(sn+2s-2)$
7	$CJS''(1) = \frac{4^{n-4}}{3}r^2s\left[2^n r\left(3s^2n+8s^2-12s+4\right)-24(ns+2s-2)\right]$
Szeged polynomial and index	
8	$Sz(TUrs,x) = \sum_{i=1}^{\lfloor \frac{s-1}{2} \rfloor} 2^{n-1}r\,x^{4^{n-2}r^2i(s-i)} + 2^{n-3}r\left(sn+1+(-1)^s\right)x^{4^{n-3}r^2s^2}$
9	$Sz(TUrs) = \sum_{i=1}^{\lfloor \frac{s-1}{2} \rfloor} 2^{3n-5}\,r^3i\,(s-i) + 2^{3n-9}r^3s^2\left(sn+1+(-1)^s\right)$

Table 4: Examples: *PIv; PIv`* and *PIv``*; number of vertices and edges in TU45

n	*PIv* Polynomial	*PIv`*	*PIv``*	v	e
3	$36x^{20}$	720	13680	20	36
4	$92x^{40}$	3680	143520	40	92
5	$224x^{80}$	17920	1415680	80	224
6	$528x^{160}$	84480	13432320	160	528
7	$1216x^{320}$	389120	124129280	320	1216

Table 5: Examples: Cluj polynomial and its derivatives in TU45

n	Cluj polynomial	*CJ*`(1)	CJ``(1)
3	$8x^{16}+8x^{12}+40x^{10}+8x^{8}+8x^{4}$	720	7120
4	$16x^{32}+16x^{24}+120x^{20}+16x^{16}+16x^{8}$	3680	75040
5	$32x^{64}+32x^{48}+320x^{40}+32x32+32x^{16}$	17920	739840
6	$64x^{128}+64x^{96}+800x^{80}+64x^{64}+64x^{32}$	84480	7001600
7	$128x^{256}+128x^{384}+1920x^{160}+128x^{128}+128x^{64}$	389120	64491520

Table 6: Examples: Szeged polynomial and index in TU45

n	Szeged polynomial	Szeged index
3	$20x^{100}+16x^{384}+8x^{64}$	3280
4	$60x^{400}+16x^{384}+16x^{256}$	34240
5	$160x^{1600}+32x^{1536}+32x^{1024}$	337920
6	$400x^{6400}+64x^{6144}+64x^{4096}$	3215360
7	$960x^{25600}+128x^{24576}+128x^{16384}$	29818880

Table 7: Examples: PI_v; PI_v` and PI_v``; number of vertices and edges in TU68

n	PI_v Polynomial	PI_v`	PI_v``	v	e
2	$90x^{48}$	4320	203040	48	90
3	$228x^{96}$	21888	2079360	96	228
4	$552x^{192}$	105984	20242944	192	552
5	$1296x^{384}$	497664	190605312	384	1296
6	$2976x^{768}$	2285568	1753030656	768	2976

Table 8: Cluj polynomial and its derivatives in **TU68**

n	Cluj polynomial	*CJ*`(1)	CJ``(1)
2	$12\left(x^{42}+x^{36}+x^{30}+x^{18}+x^{12}+x^{6}\right)+108x^{24}$	4320	111456
3	$24\left(x^{84}+x^{72}+x^{60}+x^{36}+x^{24}+x^{12}\right)+312x^{48}$	21888	1125504
4	$48\left(x^{168}+x^{144}+x^{120}+x^{72}+x^{48}+x^{24}\right)+816x^{96}$	105984	10842624
5	$96\left(x^{336}+x^{228}+x^{240}+x^{144}+x^{96}+x^{48}\right)+2016x^{192}$	497664	101246976
6	$192\left(x^{672}+x^{576}+x^{480}+x^{288}+x^{192}+x^{96}\right)+4800x^{384}$	2285568	924917760

Table 9: Examples; Szeged polynomial and index in TU68

n	Szeged polynomial	Szeged index
2	$54x^{576}+12x^{540}+12x^{432}+12x^{252}$	45792
3	$156x^{2304}+24x^{2160}+24x^{1728}+24x^{1008}$	476928
4	$408x^{9216}+48x^{8640}+48x^{6912}+48x^{4032}$	4700160
5	$1008x^{36864}+96x^{34560}+96x^{27648}+96x^{16128}$	44679168
6	$2400x^{147456}+192x^{138240}+192x^{110592}+192x^{64512}$	414056448

CONCLUSION

In this paper we presented the calculation of Cluj polynomial in hypercube hypertubes TU*rs*. Definitions and relations with other polynomials and their corresponding topological indices, were given. Analytical formulas as well as examples were tabulated.

REFERENCES

1. H. Hosoya, *Discrete Appl. Math.*, **1988**, 19, 239.
2. M. V. Diudea, *J. Chem. Inf. Comput. Sci.,* **1997**, 37, 300.
3. M. V. Diudea, *Croat. Chem. Acta.,* **1999**, 72, 835.
4. M. V. Diudea, A. E. Vizitiu and D. Janežič, *J. Chem. Inf. Model.*, **2007**, 47, 864.

5. M. V. Diudea, *J. Math. Chem.*, **2009**, *45*, 295.
6. M. V. Diudea, N. Dorosti, A. Iranmanesh, Cluj Cj Polynomial and Indices in a Dendritic Molecular Graph, *Studia Univ. "Babes-Bolyai"*, *Chemia*, 55 (4), **2010**, 247-253.
7. M. V. Diudea, *Novel Molecular Structure Descriptors-Theory and Applications I*, **2010**, 191.
8. M. V. Diudea, *Novel Molecular Structure Descriptors-Theory and Applications II*, **2010,** 57.
9. I. Gutman and S. Klavžar, *J. Chem. Inf. Comput.,* **1995**, 35, 1011.
10. M. V. Diudea and S. Klavžar, *Acta. Chem. Sloven.*, **2010**, 57, 565.
11. P. V. Khadikar, *Nat. Acad. Sci. Lett.,* **2000**, 23, 113.
12. M. H. Khalifeh, H. Yousefi-Azari and A. R. Ashrafi, *Linear Algebra Appl.*, **2008** 429, 2702.
13. A. R. Ashrafi, M. Ghorbani and M. Jalali, *J. Theor. Comput. Chem.*, **2008**, 7, 221.
14. T. Mansour and M. Schork, *Discr. Appl. Math.*, **2009**, 157, 1600.
15. I. Gutman , *Graph Theory Notes,* **1994**, 27, 9.
16. A. Parvan-Moldovan, M. V. Diudea, *Iran. J. Math. Chem.*, **2015**, 6, 163.
17. K. Fathalikhani, A. Pîrvan-Moldovan, M. V. Diudea, *Studia Univ. Babes-Bolyai, Chemia*, **2016**, 61, 291.
18. O. Ursu, M. V. Diudea, **TOPOCLUJ** software program, *Babes-Bolyai University*, **2005**.