Scientific paper

Counting Polynomials in Tori T(4,4)S[*c*,*n*]

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This paper is dedicated to Professor Milan Randić on the occasion of his 80th birthday

Abstract

A counting polynomial $P(x)$ is a description of a graph property $P(G)$ in terms of a sequence of numbers so that the exponents express the extent of its partitions while the coefficients are related to the number of partitions of a given extent. Basic definitions and some properties are given for two classes of polynomials, called here polynomials of vertex proximity and edge proximity, respectively. Formulas to calculate these polynomials in T(4,4)[c,n] tori are derived by a cutting procedure.

Keywords: counting polynomials, Cluj polynomial, Omega polynomial, cutting procedure.

1. Polynomials in Chemistry

A single number, representing a chemical structure, in graph-theoretical terms, is called a topological index TI. It must be a structural invariant, do not depending on the labeling or the pictorial representation of a graph. TIs have found broad applications in the correlation (estimation and prediction) with various molecular properties.[1]

Another representation which has gained particular attention, both from theoretical point of view and applications is by polynomials.

In Quantum Chemistry, the early Hückel theory calculates the levels of π-electron energy of the molecular orbitals, in conjugated hydrocarbons, as roots of the *characteristic polynomial*:[1–4]

$$Ch(x) = \det[x\mathbf{I} - \mathbf{A}] \quad (1)$$

In the above, **I** is the unit matrix of a pertinent order and **A** the adjacency matrix of the graph *G*. The characteristic polynomial is involved in the evaluation of topological resonance energy TRE, the topological effect on molecular orbitals TEMO, the aromatic sextet theory, the Kekulé structure count, *etc*.[4–8]

The coefficients *m(k)* in the polynomial expression:

$$P(\mathbf{M}, x) = \sum_k m(k) \cdot x^k \quad (2)$$

are calculable from the graph *G* by a method making use of the *Sachs graphs*, which are subgraphs of *G*. Some numeric methods of linear algebra, can eventually be more efficient in large graphs.[9,10]

The spectrum $Sp(\mathbf{M})$ represents the eigenvalues of the matrix $\mathbf{M}(G)$ (or the solutions of its related polynomial $P(\mathbf{M}, x)$); its extreme values $MaxSp(\mathbf{M})$ and $MinSp(\mathbf{M})$ are used as topological indices in correlating studies. Other numbers of interest are the values (in $x = 1$) of the polynomial $P(\text{M},1)$ (or the sum of (absolute values) of the polynomial coefficients, see Hosoya's *Z* index[11]) and its first two derivatives P'(M,1) and P''(M,1). More about the characteristic polynomial, the reader can find in ref.[1]

Relation (2) is a general expression of a ***counting polynomial*** (in fact a sequence of numbers), with the exponents showing the extent of partitions $p(G)$, $\cup\, p(G) = P(G)$ of a graph property $P(G)$ while the coefficients *m(k)* are related to the number of partitions of extent *k*.

In the Mathematical Chemistry literature, the counting polynomials have firstly been introduced by Hosoya:[11,12] $Z(x)$ counts independent edge sets while $H(x)$ (initially called Wiener and later Hosoya)[12–14] counts the distances in *G*. Further, Hosoya also proposed the sextet polynomial[15–18] for counting the resonant rings in a benzenoid molecule.[19,20] Other counting polynomials have later been proposed: *independence*, *king*, *color*, *star* or *clique polynomials*.[21–28]

2. Polynomials of Vertex Proximity

Cluj polynomials are defined,[29–32] on the basis of vertex proximities p_i, as in (2): summation runs over all $k = \{p\}$ in G with p being the proximity of the vertex i with respect to any vertex j in G, joined to i by an edge $\{p_{e,i}\}$ (the Cluj-edge polynomials) or by a path $\{p_{p,i}\}$ (the Cluj-path polynomials), taken as the shortest (*i.e.*, distance DI) or the longest (*i.e.*, detour DE) paths.

In (2), the coefficients $m(k)$ can be calculated from the entries of unsymmetric Cluj matrices (as provided by the TOPOCLUJ software program),[33] which represent vertex proximities. To define these, we need some theoretical background, as follows.

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.[34] The distance function in the n-cube is the Hamming distance. A hypercube can also be expressed as the Cartesian product of n edges: $Q_n = \square_n K_2$, K_2 being the complete graph on two points or simply an edge. A subgraph $K \subseteq G$ is called *isometric*, if $d_H(u, v) = d_G(u, v)$, for any $(u, v) \in H$; it is *convex* if any shortest path in G between vertices of H belongs to H.

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.[35]

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 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 the orthogonal edge-cutting procedure:[32,36–39] take a straight line segment, orthogonal to the edge e, and intersect e and all its parallel edges (in a polygonal plane graph). The set of these intersections is called an *orthogonal cut* c_k, $k = 1,2,..,k_{max}$ of G, with respect to the edge e (Figure 1). To any orthogonal cut c_k, two numbers are associated: first one represents the *number of edges* e_k "cut-off", or the cutting cardinality $|c_k|$ while the second (in round brackets, in Figure 1) is v_k or the number of points lying to the left hand with respect to c_k.

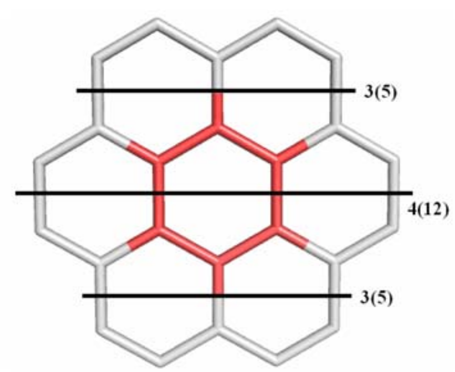
Cluj polynomials and some related ones are calculable from the semicubes in G (see the polynomial exponents, Figure 1), they differing only in the mathematical operation used in composing the edge contributions to the global graph property. Because, in a bipartite graph, the opposite semicubes define 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.

The coefficients of these descriptors are calculated (with some exceptions) as the product of three numbers (in the front of brackets – right hand part of Figure 1) with the meaning: (i) symmetry of G; (ii) occurrence of c_k (in the whole structure) and (iii) e_k.

According to the mathematical operation used in composing the graph semicubes, four polynomials can be defined:

(i) *Summation*, and the polynomial is called *Cluj-Sum*, by Diudea *et al.*[29–32,38–40] (and symbolized CJ_eS):

$$CJ_eS(x) = \sum_e \left(x^{v_k} + x^{v-v_k} \right) \quad (3)$$



$$CJ\,S(x) = 3 \cdot 3 \cdot 2(x^5 + x^{19}) + 3 \cdot 4 \cdot 1(x^{12} + x^{12})$$
$$CJ\,S'(1) = 720;$$
$$PI_v(x) = 3 \cdot 3 \cdot 2(x^{5+19}) + 3 \cdot 4 \cdot 1(x^{12+12}) = 30x^{24};$$
$$PI_v'(1) = 720;$$
$$CJ\,P(x) = 3 \cdot 3 \cdot 2(x^{5 \cdot 19}) + 3 \cdot 4 \cdot 1(x^{12 \cdot 12}) = 18x^{95} + 12x^{144} = SZ(x)$$
$$CJ\,P'(1) = 3438;$$
$$W(x) = 3 \cdot 2(x^{5 \cdot 19}) + 3 \cdot 1(x^{12 \cdot 12})$$
$$W'(1) = 1002;$$
$$\Omega(x) = 3 \cdot 2x^3 + 3x^4$$
$$\Omega(x) = 30 = e = |E(G)|$$
$$CI(G) = 798;$$
$$\Theta(x) = 3(3 \cdot 2)x^3 + 4(3)x^4$$
$$\Theta(1) = 102;$$
$$\Pi(x) = 3(3 \cdot 2)x^{27} + 4(3)x^{26}$$
$$\Pi(1) = 798 = PI'(1)$$

Figure 1. Calculating of several topological descriptors by the Cutting procedure

(ii) *Pair-wise summation*, with the polynomial called (vertex) Padmakar-Ivan[41] by Ashrafi[42–45] (and symbolized PI_v):

$$PI_v(x) = \sum_e x^{v_k + (v - v_k)} \quad (4)$$

(iii) *Pair-wise product*, while the polynomial is called *Cluj-Product* (and symbolized CJ_eP)[32,38,46–50] or also *Szeged* polynomial (and symbolyzed *SZ*):[43–45]

$$CJ_eP(x) = SZ(x) = \sum_e x^{v_k (v - v_k)} \quad (5)$$

(iv) *Single edge pair-wise product*; the polynomial is called *Wiener* and symbolized *W*:[39]

$$W(x) = \sum_k x^{v_k \cdot (v - v_k)} \quad (6)$$

The first derivative (in $x = 1$) of a (graph) counting polynomial provides single numbers, often called topological indices.

It is not difficult to 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:[31]

$$CJ_eS'(1) = PI_v'(1)\,;\; CJ_eS''(1) \neq PI_v''(1) \quad (7)$$

The number of terms is given by the value of the polynomial in $x = 1$: it is $CJ_eS(1) = 2e$ and $PI_v(1) = e$, respectively, because in the last case the two endpoint contributions are pair-wise summed for any edge in a bipartite graph.

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

$$PI_v'(1) = e \cdot v = |E(G)| \cdot |V(G)| \quad (8)$$

It can also be seen by considering the definition of the corresponding index, as written by Ilić:[51]

$$PI_v(G) = PI_v'(1) = \sum_{e=uv} n_{u,v} + n_{v,u} = |V| \cdot |E| - \sum_{e=uv} m_{u,v} \quad (9)$$

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 *vs*. any edge, so that the last term in (8) will miss. The value of $PI_v(G)$ is thus maximal in bipartite graphs, among all graphs on the same number of vertices; the result of (7) can be used as a criterion for checking the "bipatity" of a graph.

The third polynomial uses the pair-wise product; notice that Cluj-Product $CJ_eP(x)$ is precisely the (vertex) Szeged polynomial $SZ_v(x)$, defined by Ashrafi *et al*.[43–45] This comes out from the relations between the basic Cluj (Diudea[46–48,52,53]) and Szeged (Gutman[53,54]) indices:

$$CJ_eP'(1) = CJ_eDI(G) = SZ(G) = SZ_v'(1) \quad (10)$$

The first three above polynomials (and their derived indices) do not count the equidistant vertices, an idea introduced in Chemical Graph Theory by Gutman.[54]

The last polynomial was called Wiener by Diudea, 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):

$$W(G) = W'(1) = \sum_k v_k \cdot (v - v_k) \quad (11)$$

where v_k and $v–v_k$ are the cardinalities of the disjoint semicubes forming a partition with respect to each edge in c_k taken, however, as a "single edge" (as in trees).

A graph in which the following inequality holds is not a partial cube:[38,39]

$$W(G) > |S(G)| \cdot (v/2)^2 \quad (12)$$

The quantity $|S(G)|$ is the cardinality of the sets of all cuts in *G*. An example of equality in (12), which represents the upper bond in the cutting procedure, will be given in the next section. However, a value of $W(G)$ lower than the upper bond does not ensure *G* is a partial cube. In such a case, trying to perform the cutting procedure, a value $v_k > v/2$ will indicate a non-convex, non-isometric subgraph and thus a graph which is not a partial cube. According to Klavžar,[37] $W(G)$ is calculable by the cutting procedure only in partial cubes.

A last remark on $W(x)$: in partial cubes, its exponents are identical to those in $CJP(x) = SZ(x)$ while the coefficients are those in the above polynomials, divided by e_k. When subscript letter is missing, $SZ(x)$ is $SZ_v(x)$.

3. Polynomials of Vertex Proximity in Square-tiled Tori

The cutting procedure we applied on square-tiled tori T(4,4)[c,n]. It can be seen (Figure 2), there are only two cutting types: circular "cir"(around the large hollow) and across "acr" the tube. Accordingly, the proximities are easily calculable from the net parameters *c* (the number of atoms/points across the tube) and *n* (the number of cross-sections around the torus large hollow). Formulas are given in Table 1, for the four polynomials and their topological indices, along with some examples.

Note, in Table 1, entry 4, the coefficients of $W(x)$ are just the number of cuts across the tube ($n/2$) and the circular cuts ($c/2$), respectively: $n/2 + c/2 = |S(G)|$, while the exponent is the pair-wise product of the graph semicubes

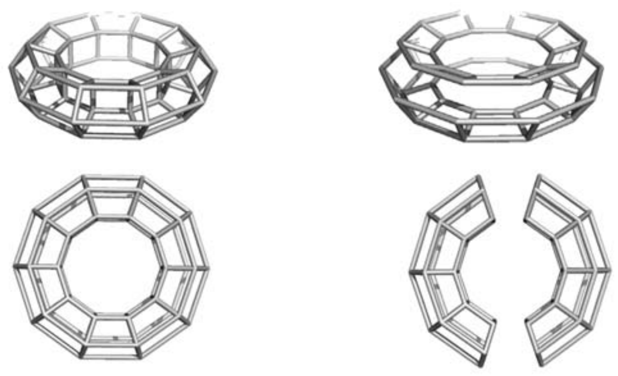


Figure 2. Cutting procedure in square-tiled tori T(4,4)[c,n]: circular (top) and across (bottom) cuttings

$((v/2)^2)$, of which first derivative (in $x = 1$) equals the upper bond (11) in the cutting procedure. Also note, $W(x)$ is defined only in "all even" tori, which are partial cubes.

4. Polynomials of Edge Proximity

Let $G = (V(G),E(G))$ be a connected graph, with the vertex set $V(G)$ and edge set $E(G)$. Two edges $e = (u,v)$ and $f = (x,y)$ of G are called *co-distant* (briefly: $e\ co\ f$) if the notation can be selected such that[35,55]

$$e\ co\ f \Leftrightarrow d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y) \quad (13)$$

where d is the usual shortest-path distance function. Relation *co* is reflexive, that is, $e\ co\ e$ holds for any edge e of G and it is also symmetric: if $e\ co\ f$ then also $f\ co\ e$. In general, *co* is not transitive. A graph is called a *co-graph* if the relation *co* is transitive and thus an equivalence relation.

For an edge $e \in E(G)$, let $c(e) := \{f \in E(G); f\ co\ e\}$ be the set of edges codistant to e in G. The set $c(e)$ can be obtained by an *orthogonal cut oc* of G, with respect to e. If G is a *co-graph* then its orthogonal cuts form a partition in G (see above). A bipartite graph G is a *co-graph* if and on-

Table 1. Formulas for the Polynomials of Vertex Proximity in Square-tiled Tori T(4,4)[c,n]

	Formulas
1	$CJS(x) = cn[x^{c(n-p_n)/2} + x^{c(n-p_n)/2}]_{acr} + cn[x^{n(c-p_c)/2} + x^{n(c-p_c)/2}]_{cir}$ $CJS(x) = cn \cdot 2x^{cn/2} + cn \cdot 2x^{cn/2}$; c,n – *even* $CJS'(1) = cn(2cn - c - n$; c,n – *odd* $CJS'(1) = 2c^2\ 2n^2$; c,n – *even* $CJS'(1) = cn^2\ (2c - 1)$; c – *odd*; n – *even* $CJS'(1) = c^2n^2(2n - 1)$; c – *even*; n – *odd*
Examples	H[7,35]; CJS(x) = $490x^{119} + 490x^{105}$; CJS'(1) = 109760 H[8,40]; CJS(x) = $1280x^{160}$; CJS'(1) = 204800 H[7,20]; CJS(x) = $280x^{70} + 280x^{60}$; CJS'(1) =36400 H[8,35]; CJS(x) = $560x^{140} + 560x^{136}$; CJS'(1) = 154560
2	$CJP(x) = cn \cdot x^{[c(n-p_n)/2]^2} + cn \cdot x^{[n(c-p_c)/2]^2}$ $CJP(x) = cn \cdot x^{(cn/2)^2} + cn \cdot x^{(cn/2)^2}$ c, n – *even* $CJP'(1) = (cn/4)(2c^2n^2 - 2c^2n + c^2 - 2cn^2 + n^2)$; c, n – *odd* $CJP'(1) = cn(c^2n^2/4) + cn(c^2n^2/4)$; c, n – *even* $CJP'(1) = (cn^3/4)(2c^2 - 2c + 1)$; c – *odd*, n – *even* $CJP'(1) = (c^3n/4)(2n^2 - 2n + 1)$; c – *even*, n – *odd*
Examples	H[7,35]; CJP(x) = $245x^{11025}+245x^{14161}$; CJP'(1) = 6170570 H[8,40]; CJP(x) = $320x^{25600}+320x^{25600}$; CJP'(1) = 16384000 H[7,20]; CJP(x) = $140x^{3600}+140x^{4900}$; CJP'(1) = 1190000 H[8,35]; CJP(x) = $280x^{18496}+280x^{19600}$; CJP'(1) = 10666880
3	$PI_v(x) = cn \cdot x^{c(n-p_n)} + cn \cdot x^{n(c-p_c)}$ $PI_v(x) = 2cn \cdot x^{cn}$; c, n – *even* $PI'_v(1) = cn(2cn - c - n)$; c, n – *odd* $PI'_v(1) = 2c^2n^2$; c, n – *even* $PI'_v(1) = cn^2(2c - 1)$; c – *odd*, n – *even* $PI'_v(1) = c^2n(2n - 1)$; c – *even*, n – *odd*
Examples	H[7,35]; $PI_v(x) = 245x^{238} + 245x^{210}$; PI_v'(1) = 109760 H[8,40]; $PI_v(x) = 640x^{320}$; PI_v'(1) = 204800 H[7,20]; $PI_v(x) = 140x^{140} + 140x^{120}$; PI_v'(1) = 36400 H[8,35]; $PI_v(x) = 280x^{280} + 280x^{272}$; PI_v'(1) = 154560
4	$W(x) = (cn/2c) \cdot x^{(v/2)^2} + (cn/2n) \cdot x^{(v/2)^2}$ $= (n/2 + c/2) \cdot x^{(cn/2)^2}$; c, n – *even* $W'(1) = (n/2 + c/2)(c^2n^2/4)$; c, n – *even* $\nu = \|V(G)\| = e = \|E(G)\| = 2cn$
Example	H[8,40]; W(x)= $20x^{25600}+4x^{25600}$; W'(1)= 614400

ly if it is a *partial cube*, and all its semicubes are convex. However, a *co*-graph can also be non-bipartite[39] (*e.g.*, it shows a transitive *co*-relation but has at least one odd cycle, thus being no more a partial cube). It was proven that relation *co* is a *theta* (Djoković[56]) and Winkler[57]) relation.

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). If *G* is a *co*-graph, then its opposite edge strips *ops* $\{s_k\}$ superimpose over the orthogonal cut sets *ocs* $\{c_k\}$ and $|c_k| = |s_k|$.

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*.[55] implicitly used the "*op*" relation in defining the Cluj-Ilmenau index *CI* (see below).

Let us denote by *m*(*s*) or simply *m* the number of *ops* of length $s = |s_k|$ and define the Omega polynomial as:[35,58–67]

$$\Omega(x) = \sum_s m \cdot x^s \tag{14}$$

The exponents count just the intersected edges by the cut-line (in a cutting procedure), which does not need to be orthogonal on all the edges of an *ops.*

A second polynomial which is calculated from the ops in *G*, but counting non-opposite edges, is the *Sadhana Sd* polynomial[68,69]

$$Sd(x) = \sum_s m \cdot x^{e-s} \tag{15}$$

In *co*-graphs/partial cubes, other two related polynomials[70] can be calculated on *ops*:

$$\Theta(x) = \sum_s ms \cdot x^s \tag{16}$$

$$\Pi(x) = \sum_s ms \cdot x^{e-s} \tag{17}$$

The above polynomials count codistant and non-codistant edges, respectively. Thus, non-co-distance is related to edge-proximity, and the name of these polynomials is immediate.

In arbitrary connected graphs, the strips *ops* $\{s_k\}$ does not fit the orthogonal cuts *ocs* $\{c_k\}$ any more; then, in formulas (15) and (16) *s* must be changed by *c* (now with the meaning of the cardinality of co-distant edges in *G*) and the coefficients, accordingly.

The first derivative (computed at *x* = 1) of these counting polynomials provide interesting topological indices:[35,70,71]

$$\Omega'(1) = \sum_s ms = e = |E(G)| \tag{18}$$

$$Sd'(1) = \sum_s m(e-s) = Sd(G) \tag{19}$$

$$\Theta'(1) = \sum_s ms^2 = \Theta(G) \tag{20}$$

$$\Pi'(1) = \sum_s ms(e-s) = \Pi(G) \tag{21}$$

On Ω(*x*) an index, called Cluj-Ilmenau[55] *CI*(*G*), was defined

$$CI(G) = \left\{[\Omega'(1)]^2 - [\Omega'(1) + \Omega''(1)]\right\} \tag{22}$$

In *co*-graphs, there is the equality:[35,70] *CI*(*G*) = *Π*(*G*). It can be obtained applying the definition (21):

$$\begin{aligned} CI(G) &= \left(\sum_s ms\right)^2 - \left[\sum_s ms + \sum_s ms(s-1)\right] = \\ &= e^2 - \sum_s ms^2 = \Pi(G) \end{aligned} \tag{23}$$

Relation (22) is just the formula proposed by John *et al.*[72] to calculate the Khadikar's *PI* index.[28] According to Ashrafi's notations,[73] PI_e (to difer from PI_v) can be written as:

$$PI_e(G) = \sum_{e \in E(G)} \left[n(e,u) + n(e,v)\right] - m(u,v) \tag{24}$$

where *n*(*e*,*u*) is the number of edges lying closer to the vertex *u* than to the *v* vertex while *m*(*u*,*v*) is the number of edges equidistant from *u* and *v*.

Ashrafi defined the equidistance *eqd* of edges by considering the distance from a vertex *z* to the edge *e* = *uv* as the minimum distance between the given point and the two endpoints of that edge:[59,73]

$$d(z,e) = \min\{d(z,u), d(z,v)\} \tag{25}$$

Then, for two edges *e* = (*uv*) and *f* = (*xy*) of *G*,

$$e\ eqd\ f(iii) \Leftrightarrow d(x,e) = d(y,e) \text{ and } d(u,f) = d(v,f) \tag{26}$$

In bipartite graphs (26) superimposes to (13) but not in general graphs, thus appearing a difference between the index *Π*(*G*) and $PI_e(G)$ (hereafter denoted *Π*(*G*)_Diu and $PI_e(G)$_Ash).

The problem of equidistance of vertices was firstly put by Gutman when defined the Szeged index[54] *SZ*(*G*) of which calculation leaves out the equidistant vertices. Similarly, the index $PI_e(G)$ does not account for the equidistant edges.

This index can be calculated as the first derivative, in *x* = 1, of the polynomial defined by Ashrafi[73] as:

$$PI_e(x) = \sum_{e \in E(G)} x^{n(e,u)+n(e,v)} \tag{27}$$

In bipartite graphs, either *co*-graphs or not, the equality: $\Pi(G) = PI_e(G)$ is true, but not in general graphs. In partial cubes, since they are also bipartite, the previous equality can be expanded to the triple one

$$CI(G) = \Pi(G) = PI_e(G) \qquad (28)$$

a relation precisely true in partial cubes but not in all *co*-graphs (namely those being non-bipartite).

Table 2. Formulas for the Polynomials of Edge Proximity in Square-tiled Tori T(4,4)[*c*,*n*]

	Formulas
1	$\Omega(x) = n \cdot x^c + c \cdot x^n$ $\Omega'(1) = 2nc;\ \Omega''(1) = cn(c + n - 2)$ $CI\ (G) = cn(4cn + c - n)$
Examples	H[5,15]; $15x^5 + 5x^{15}$; CI = 21000 H[5,20]; $20x^5 + 5x^{20}$; CI = 37500 H[8,40]; $40x^8 + 8x^{40}$; CI = 394240
2	$Sd(x) = n \cdot x^{e-c} + c \cdot x^{e-n}$ $Sd'(1) = n(e - c) + c(e - e)$
Examples	H[5,15]; $15x^{145} + 5x^{135}$; Sd'(1) = 2850 H[5,20]; $20x^{195} + 5x^{180}$; Sd'(1) = 4800 H[8,40]; $40x^{632} + 8x^{600}$; Sd'(1) = 30080
3; *c*,*n*-odd;	$\Theta(x) = cn \cdot x^{(c + pc_n)} + cn \cdot x^{(n + p_n)}$; c, n – odd $\Theta'(1) = cn(c + n + 2);\ c, n - odd$ $\Pi_{Diu}(x) = cn \cdot x^{[2cn - (c + p_c)]} + cn \cdot x^{[2cn - (n + p_n)]}$; c, n – odd $\Pi'_{Diu}(x) = cn(4cn - c - n - 2);\ c, n - odd$ $Pl_{e,Ash}(x) = \Pi_{Diu}(x) - [m \cdot x^{(e_{acr} - \mathrm{c} + 1)} + m \cdot x^{(e_{acr} - n + 1)}]$ $= cn \cdot x^{[2cn - (2c + p_c) + 1]} + cn \cdot x^{[2cn - (2n + p_n) + 1]}$; c, n – odd $Pl'_{e,Ash}(x) = cn(4cn - 2c - 2n);\ c, n - odd$
Examples	H[7,35]; $\Theta(x) = 245x^8 + 245x^{36}$; $\Theta'(1) = 10780$ $\Pi_{Diu}) = 245x^{454} + 245x^{482}$; $\Pi'_{Diu}(1) = 229320$ $Pl_{e,Ash}(x) = 245x^{476} + 245x^{420}$; $Pl'_{e,Ash}(1) = 219520$
4; *c*,*n*-even; bipartite	$\Theta(x) = cn \cdot x^{2c} + cn \cdot x^{2n};\ c, n - even$ $\Theta'(1) = cn(2c + 2n);\ c, n - even$ $\Pi_{Diu}(x) = cn \cdot x^{2c(n - 1)} + cn \cdot x^{2n(c - 1)}$; c, n – even $\Pi'_{Diu}(1) = 2cn(2cn - c - n);\ c, n - even$ $Pl_{e,Ash}(x) = \Pi_{Diu}(x);\ c, n - even$
Examples	H[8,40]; $\Theta(x) = 320x^{16} + 320x^{80}$; $\Theta'(1) = 30720$ $\Pi_{Diu}\ (x) = 320x^{560} + 320x^{624}$; $\Pi'_{Diu}(1) = 37888$ $Pl_{e,Ash}(x) = 320x^{624} + 320x^{560}$; $Pl'_{e,Ash}(1) = 37888$
5; *c*-odd; *n*-even	$\Theta(x) = cn \cdot x^{2c} + cn \cdot x^n;\ c - odd;\ n - even$ $\Theta'(1) = cn(2c + n);\ c - odd;\ n - even$ $\Pi_{Diu}\ (x) = cn \cdot x^{2c(n - 1)} + cn \cdot x^{n(2c - 1)};\ c - odd;\ n - even$ $\Pi'_{Diu}(1) = cn(4cn - 2c - n);\ c - odd;\ n - even$ $Pl_{e,Ash}(x) = \Pi_{Diu} - m \cdot x^{(e_{cir} - n)}$ $= cn \cdot x^{2c(n - 1)} + cn \cdot x^{2n(c - 1)};\ c - odd;\ n - even$ $Pl'_{Ash}(1) = 2cn(2cn - c - n);\ c - odd;\ n - even$
Examples	H[7.20]; $\Theta(x) = 140x^{14}+140x^{20}$; $\Theta'(1) = 4760$ $\Pi_{Diu} = 140x^{260}+140x^{266}$; $\Pi'_{Diu}(1) = 73640$ $Pl_{e,Ash}(x) = 140x^{266} + 140x^{240}$; $Pl'_{e,Ash}(1) = 70840$
6; *c*-even; *n*-odd	$\Theta(x) = cn \cdot x^c + cn \cdot x^{2n};\ c - even;\ n - odd$ $\Theta'(1) = cn(c + 2n);\ c - even;\ n - odd$ $\Pi_{Diu}\ (x) = cn \cdot x^{c(2n - 1)} + cn \cdot x^{2n(c - 1)};\ c - even;\ n - odd$ $\Pi'_{Diu}(1) = cn(4cn - c - 2n);\ c - even;\ n - odd$ $Pl_{e,Ash}(x) = \Pi_{Diu} - m \cdot x^{(e_{acr} - c)}$ $= cn \cdot x^{2c(n - 1)} + cn \cdot x^{2n(c - 1)};\ c - even;\ n - odd$ $Pl'_{Ash}(1) = 2cn(2cn - c - n);\ c - even;\ n - odd$
Examples	H[8,35]; $\Theta(x) = 280x^8+280x^{70}$; $\Theta'(1) = 21840$ $\Pi_{Diu} = 280x^{490}+280x^{552}$; $\Pi'_{Diu}(1) = 291760$ $Pl_{e,Ash}(x) = 280x^{544} + 280x^{490}$; $Pl'_{e,Ash}(1) = 289520$

Resuming, in bipartite graphs, an orthogonal edge-cutting procedure[36–39] can be used to generate the *ops*. Formulas for the above four polynomials in square-tiled tori T(4,4)[*c*,*n*] are given in Table 2, along with some examples. In formulas of $\Theta(x)$, $\Pi(x)$ and $PI(x)$, more cases must be considered to account for the net parameter parity.

The cutting procedure is limited to bipartite graphs, particularly to planar polyhex structures. In such molecular graphs, the descriptors derived from Cluj and Omega polynomials have been successfully used to predict the boiling points, index of chromatographic retention or their resonance energy.[30,47,74–76]

Among the single number descriptors provided by the Omega polynomial, one is of particular importance: n_p, which equals the coefficient at the first power term, and also the number of *pentagon fusions*. This number accounts for more than 90% of variance in the heat of formation or in the strain energy of small fullerenes, *e.g.*, C_{40} and C_{50}.[67]

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6. References

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Povzetek

Števni polinom *P*(*x*) opisuje lastnost grafa *P*(*G*) v obliki zaporedja številk, tako da eksponenti izražajo obseg njegovih porazdelitev, medtem ko so koeficienti povezani s številom porazdelitev pri danem obsegu. Podane so osnovne definicije in nekaj lastnosti za dva razreda polinomov, tako imenovanih polinomov za opis bližnjosti vozlov in robov. Formule za izračun teh polinomov v T (4,4) [*c,n*] torih so izpeljane z metodo rezanja.