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Counting Polynomials and Related Indices by Edge Cutting Procedures

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Abstract. A topological index is a numeric quantity derived from the structure of a graph $G(V,E)$ which is invariant up to automorphisms of the considered graph. One of the most famous topological indices is the Wiener index $W(G)$; it equals the sum of distances between all unordered pairs of vertices of G. A related number is the Szeged index $SZ(G)$, which is the sum of all products of non-equidistant, proximal vertices $n_u(e)$, $n_v(e)$ with respect to the two ends of any edge $e=(u,v)$ in G. Third is the Cluj index $CJ_eS(G)$, calculated from the first derivative of $CJ_e(x)$ polynomial.

A forth index, called Cluj-Ilmenau $CI(G)$, is calculated from the first and second derivatives of the Omega $\Omega(x)$ polynomial, which counts the opposite edge strips in G. All these indices and related polynomials are derived here by edge cutting procedures in some bipartite graphs and/or partial cubes. A clear relatedness among these descriptors was established and exemplified. Their use in correlating various physico-chemical or biological properties with the molecular structure have been extensively proven.

1. Introduction

One of the most famous topological indices is the Wiener index, introduced by Harold Wiener.[1] The Wiener index equals the sum of topological distances between all unordered pairs of vertices of G:

$$W(G) = \sum\nolimits_{(u,v)\in V(G)} d_G(u,v) \tag{1}$$

The Szeged index is another topological index defined by Ivan Gutman[2] as:

$$Sz(G) = \sum\nolimits_{(u,v)\in E(G)} n_u(e)\cdot n_v(e) \tag{2}$$

where $n_u(e)$ is the number of vertices of G lying closer to u than to v and $n_v(e)$ is the number of vertices of G lying closer to v than to u.

We proposed Cluj matrices and indices in view of extending the definition of Wiener matrices, proposed by Randić[3,4] to cycle-containing graphs, other than the Szeged index did.

A Cluj fragment[5-9] $CJ_{i,j,p}$ collects vertices v lying closer to i than to j, the endpoints of a path $p(i,j)$. Such a fragment collects the *vertex proximities* of i against any vertex j, joined by the path p, with the distances measured in the subgraph $D_{(G-p)}$:

$$CJ_{i,j,p} = \left\{ v \middle| v \in V(G);\, D_{(G-p)}(i,v) < D_{(G-p)}(j,v) \right\} \tag{3}$$

In trees, $CJ_{i,j,p}$ denotes sets of (connected) vertices v joined with j by paths p going through i. The path $p(i,j)$ is characterized by a single endpoint, which is sufficient to calculate the unsymmetric matrix UCJ.

In graphs containing rings, the choice of the appropriate path is quite difficult, thus that path which provides the fragment of maximum cardinality is considered:

$$[\mathrm{UCJ}]_{i,j} = \max_{p} \left| CJ_{i,j,p} \right| \tag{4}$$

When path p belongs to the set of distances $DI(G)$, the suffix DI is added to the name of matrix, as in UCJDI. When path p belongs to the set of detours $DE(G)$, the suffix is DE. When the matrix symbol is not followed by a suffix, it is implicitly DI. The Cluj matrices are defined in any graph and, except for some symmetric graphs, are unsymmetric and can be symmetrized by the Hadamard (pair-wise) multiplication[10] with their transposes:

$$\mathrm{SM}_p = \mathrm{UM} \bullet (\mathrm{UM})^{\mathrm{T}} \tag{5}$$

If the matrices calculated on edges (*i.e.*, on adjacent vertex pairs) are required, the matrices calculated on paths must be multiplied by the adjacency matrix **A** (which has the non-diagonal entries of 1 if the vertices are joined by an edge and, otherwise, zero):

$$\mathrm{SM}_e = \mathrm{SM}_p \bullet \mathrm{A} \tag{6}$$

The Cluj indices, calculated as *half sum* of the matrix entries, previously used in correlating studies published by TOPO GROUP Cluj, were calculated in the symmetric matrices, thus involving a multiplicative operation. Also, the symbol CJ

(Cluj) is used here for the previously denoted CF (Cluj fragmental) matrices and indices.

In this paper, the unsymmetric matrix defined on distances and calculated on edges UCJ_e will be used to compare the coefficients of the Cluj polynomials[11,12] with those obtained by a cutting procedure (see below):

$$UCJ_e = UCJ_p \bullet A \tag{7}$$

2. Basic definitions

Let $G(V,E)$ be a connected bipartite plane graph, with the vertex set $V(G)$ and edge set $E(G)$. Two edges $e=(x,y)$ and $f=(u,v)$ of G are in relation *opposite, e op f,* if they are opposite edges of a face in G. Assuming that faces are isometric subgraphs of G, the relation *op* implies the condition of "topologically parallel edges":[13]

$$d(x,v) = d(x,u) + 1 = d(y,v) + 1 = d(y,u) \tag{8}$$

Relation *op* is reflexive and symmetric but, in general, is not transitive. It will partition the edges set E(G) into *opposite* edge *strips ops,* $S(G)=\{s_1, s_2, ..., s_k\}$, as follows. (i) Any two subsequent edges of an *ops* are in *op* relation; (ii) Any three subsequent edges of such a strip belong to adjacent faces; (iii) The *ops* is taken as maximum possible, irrespective of the starting edge. (iv) The choice about the maximum size of face/ring, and the face/ring mode counting, will decide the length of the strip.

There are graphs in which *op* is transitive and *ops* superimpose over the *orthogonal cut* strips *ocs,* $C(G)=\{c_1, c_2, ..., c_k\}$, defined by relation *co.*[13,14] In such a graph, relation *op*, defined locally (on faces), becomes a global property, like the *co*-relation and the graph is a *co*-graph or a partial cube. Then its orthogonal cuts form a partition of the edges in G: $E(G) = c_1 \cup c_2 \cup ... \cup c_k,\ c_i \cap c_j = \varnothing, i \neq j$. The *ocs* can be obtained by an orthogonal edge-cutting procedure (see below).

A subgraph $H \subseteq G$ 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.

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.[15] The distance function in the n-cube is the Hamming distance. A hypercube can also be expressed as the Cartesian product: $Q_n = {}_{i=1}^{n} K_2$

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 *opposite* and disjoint ones.[16,17]

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 the Cluj polynomials count (see below).

The relation *co* is related to ~ (Djoković[18]) and Θ (Winkler[19]) relations:[20] in a connected bipartite graph, co = ~ = Θ. For two edges e=(u,v) and f=(x,y) of G the theta relation is defined as: $e \Theta f$ if $d(u,x) + d(v,y) \neq d(u,y) + d(v,x)$.

A bipartite graph G is a *co-graph* if and only if it is a *partial cube*, and all its semicubes are convex; relation co / Θ is then transitive.[17] A *co*-graph can also be non-bipartite.

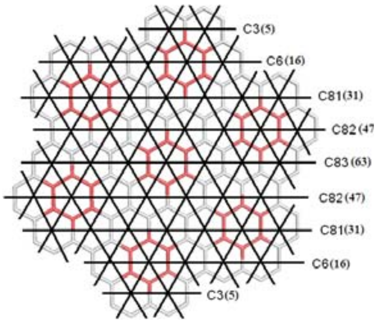
3. Cluj and related polynomials by the cutting procedure

The Cluj polynomials are defined[11,12,21,22] on the basis of Cluj matrices as:

$$CJ(x) = \sum_k m(k) \cdot x^k \tag{9}$$

They count the semicube or proximity p 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 eq. (9), the coefficients $m(k)$ can be calculated from the entries of unsymmetric Cluj matrices by the TOPOCLUJ software program.[23] The summation runs over all $k = |\{p\}|$ in G.

In bipartite graphs, the semicubes counted by CJ_e polynomial can be estimated by an orthogonal edge-cutting procedure.[22,24-26] To perform it, 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* (*oc* for short) of G, with respect to e (Figure 1).



$$CJ_e\,S(x) = 3\cdot2\cdot3(x^5+x^{121})+ 3\cdot2\cdot6(x^{16}+x^{110})+ 3\cdot2\cdot8(x^{31}+x^{95})+ 3\cdot2\cdot8(x^{47}+x^{79})+ 3\cdot1\cdot8(x^{63}+x^{63})$$

$$CJ_e\,S'(1) = 21924;\ CJ_e\,S''(1) = 1762320$$

$$PI_v(x) = 3\cdot2\cdot3(x^{5+121})+ 3\cdot2\cdot6(x^{16+110})+ 3\cdot2\cdot8(x^{31+95})+ 3\cdot2\cdot8(x^{47+79})+ 3\cdot1\cdot8(x^{63+63})$$

$$PI_v{}'(1) = 21924;\ PI_v{}''(1) = 2740500$$

$$CJ_e\,P(x) = 3\cdot2\cdot3(x^{5.121})+ 3\cdot2\cdot6(x^{16.110})+ 3\cdot2\cdot8(x^{31.95})+ 3\cdot2\cdot8(x^{47.79})+ 3\cdot1\cdot8(x^{63.63})$$

$$CJ_e\,P'(1) = 489090$$

$$W(x) = 3\cdot2(x^{5.121})+ 3\cdot2(x^{16.110})+ 3\cdot2(x^{31.95})+ 3\cdot2(x^{47.79})+ 3\cdot1(x^{63.63})$$

$$W'(1) = H'(1) = 66045$$

$$\Omega(x) = 3\cdot2x^3+3\cdot2x^6+(3\cdot4+3\cdot1)x^8 = 6x^3+6x^6+15x^8$$

$$CI(G) = 29046$$

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

To any orthogonal cut c_k, k=1,2,..,$k_{\max}$ two numbers are associated: first one represents the *number of edges* e_k intersected 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.

Out of CJ_e polynomial, there are other topological descriptors that count the semicubes in G (see Figure 1, the polynomial exponents), they differing only in the mathematical operation used in re-composing the edge contributions to the global graph property. Because the opposite semicubes define a partition of vertices in a bipartite graph, it is easily to identify the two semicubes: $n_{uv}= v_k$ and $n_{vu}= v\text{-}v_k$ 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.

Resuming to the mathematical operation used in re-composing the graph semicubes, four polynomials can be defined according to:

(i) *Summation*, and the polynomial is called *Cluj-Sum*, by Diudea *et al.*[11,12,21,22,27] (and symbolized CJ_eS):

$$CJ_eS(x) = \sum_e \left(x^{v_k} + x^{v-v_k} \right) \qquad (10)$$

(ii) *Pair-wise summation*, with the polynomial called (vertex) Padmakar-Ivan[28] by Ashrafi[29-32] (and symbolized PI_v):

$$PI_v(x) = \sum_e x^{v_k+(v-v_k)} \qquad (11)$$

(iii) *Pair-wise product*, while the polynomial is called *Cluj-Product* (and symbolized CJ_eP)[5-9,22,26] or also *Szeged* polynomial (and symbolyzed *SZ*):[30-32]

$$CJ_eP(x) = SZ(x) = \sum_e x^{v_k(v-v_k)} \qquad (12)$$

(iv) *Single edge pair-wise product* and the polynomial is called *Wiener* $W(x)$:

$$W(x) = \sum_k x^{v_k \cdot (v-v_k)} \qquad (13)$$

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

Some comments are now welcome. 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 (see Figure 1) and the following relations hold in any graph:[21]

$$CJ_eS'(1) = PI_v'(1)\,;\; CJ_eS''(1) \neq PI_v''(1) \qquad (14)$$

The number of terms, given by $CJ_eS(1)=2e$ is twice the number given by $PI_v(1)$ because, in the last case, the two endpoint contributions are pair-wise summed for any edge in a bipartite graph (see (10) and (11)).

It is not difficult to observe the first derivative (in x=1) of $PI_v(x)$ takes the maximal value in bipartite graphs:

$$PI_v{}'(1) = e \cdot v = |E(G)| \cdot |V(G)| \tag{15}$$

It can also be seen by considering the definition of the corresponding index, as written by Ilić:[33]

$$PI_v(G) = PI_v{}'(1) = \sum_{e=uv} n_{u,v} + n_{v,u} = |V| \cdot |E| - \sum_{e=uv} m_{u,v} \tag{16}$$

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 (16) 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 (16) 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*.[30-32] This comes out from the relations between the basic Cluj (Diudea[5,34,35]) and Szeged (Gutman[2,35] -see relation (2)) indices:

$$CJ_eP'(1) = CJ_eDI(G) = SZ(G) = SZ_v{}'(1) \tag{17}$$

All the first three polynomials (and their derived indices) do not count the equidistant vertices, an idea introduced in Chemical Graph Theory by Gutman.[2]

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

$$W(G) = W'(1) = \sum_k v_k \cdot (v - v_k) \tag{18}$$

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). In fact, the relation (18) counts paths "external" to the orthogonal cuts c_k, as the Wiener matrix W, proposed by Randić, does. The both descriptors are restrictively defined: only in trees (the matrix W) and only in partial cubes (the polynomial $W(x)$). Note that tree graphs are partial cubes. The both above descriptors count vertices (not edges).

In the opposite, the Hosoya polynomial[36-40] $H(x)$ counts edges (not vertices), by working on the Distance D matrix:[15,35]

$$H(x) = \sum_k m(k) \cdot x^k \tag{19}$$

where the exponent denotes the shortest paths (between pairs of vertices in G) of extent k, while $m(k)$ counts the number of k-paths. The definition of $W(G)$, as given in relation (1), is thus related to the (first derivative $H'(1)$ of) Hosoya polynomial.

Clearly, the both polynomials will provide the same value of $W(G)$ in trees/partial cubes, according to the theorem of Klein, Gutman and Lukovits,[41] which states the equality of sums of the internal paths (collected by D_e&D_p matrices) and the external paths (given by W_e &W_p matrices):[42]

$$W(G) = W'(1) = H'(1) \tag{20}$$

Klavžar[25] stated that, in calculating the index $W(G)$, the orthogonal cut procedure is applicable only in partial cubes. Thus, we can write the following

Proposition 1: A bipartite graph in which the relation (20) holds is a partial cube.

From the above discussion, the proposition appears at least conceivable. More over, the upper bond of the products in relation (18) is reached for $v_k = v/2$ and the number of these maximal length *ocs* is limited by the symmetry of G. Thus, a graph in which the following inequality holds is not a partial cube:[26]

$$W(G) > |S(G)| \cdot (v/2)^2 \tag{21}$$

However, a value of $W(G)$ lower than the above bond and, 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. The final proof is the checking of transitivity of *co*-relation.

A last remark on $W(x)$: in partial cubes, its exponents are identical to those in $CJ_eP(x) = SZ(x)$ while the coefficients are those in the above polynomials, divided by e_k.

4. Omega and related polynomials by the cutting procedure

Let's now return to Figure 1 and introduce the last descriptor: the Omega polynomial.

Denote by $m(s)$ or simply m the number of *ops* of length $s=|s_k|$ and define the Omega polynomial as:[16,17,43-52]

$$\Omega(x)=\sum_{s} m(s)\cdot x^{s} \tag{22}$$

The exponents count just the intersected edges by the cut-line, which is not needed to be orthogonal on all the edges of an *ops* (see above); the coefficients m(s) are easily counted from the symmetry of G.

In partial cubes, other two related polynomials[16,17] can be calculated on *ops*:

$$\Theta(x)=\sum_{s} ms\cdot x^{s} \tag{23}$$

$$\Pi(x)=\sum_{s} ms\cdot x^{e-s} \tag{24}$$

The $\Theta(x)$ counts equidistant edges while $\Pi(x)$ non-equidistant edges. Thus, Omega and its related polynomials count edges not vertices. Their first derivative (in x=1) provides single number topological descriptors:

$$\Omega'(1)=\sum_{s} m\cdot s=e=\left|E(G)\right| \tag{25}$$

$$\Theta'(1)=\sum_{s} m\cdot s^{2}=\theta(G) \tag{26}$$

$$\Pi'(1)=\sum_{s} ms\cdot(e-s)=\Pi(G) \tag{27}$$

On Omega polynomial, the Cluj-Ilmenau index,[13] CI=CI(G), was defined:

$$CI(G)=\left\{[\Omega'(1)]^{2}-[\Omega'(1)+\Omega''(1)]\right\} \tag{28}$$

A polynomial related to $\Pi(x)$ was defined by Ashrafi[53] as:

$$PI_{e}(x)=\sum_{e\in E(G)} x^{n(e,u)+n(e,v)} \tag{29}$$

where $n(e,u)$ is the number of edges lying closer to the vertex u than to the v vertex. Its first derivative (in x=1) provides the $PI(G)$ index proposed by Khadikar.[28,54]

Proposition 2. In *co*-graphs/partial cubes, the equality $CI(G)=\Pi(G)$ holds.

This can be demonstrated by expanding definition (28), *CI* calculation leading to $\Pi(G)$:[16,17]

$$CI(G)=\left(\sum_{s} m\cdot s\right)^{2}-\left[\sum_{s} m\cdot s+\sum_{s} m\cdot s\cdot(s-1)\right]=e^{2}-\sum_{s} m\cdot s^{2}=\Pi(G) \tag{30}$$

Relation (30) is valid only in the assumption $\left|c_{k}\right|=\left|s_{k}\right|$, which provides the same value for the exponent s and this is precisely achieved in *co*-graphs/partial cubes.

A graph, of which $\Theta(x)$ can be written exactly in the terms of $\Omega(x)$, according to the pair relations {(22)&(23)}, will precisely show the equality $CI(G) = \Pi(G)\ cf$ (30). The relatedness of the two polynomials (and identity $CI(G) = \Pi(G)$) is provided rather by the equality of cardinalities $|s_k| = |c_k|$ than by the corresponding sets superposition $\{s_k\} \equiv \{c_k\}$, the condition {(22)&(23)} being thus necessary but not sufficient in order a graph to be declared *co*-graph/partial cube. Finally, the transitivity of *ops*/*ocs* must be proven. Note that there is not known a simple procedure to establish the partial cube status.[17]

The equality $CI(G) = \Pi(G)$ can appear even the pair relations {(22)&(23)} are not related. This is because the equidistance relation *eqd* involves both conditions for topologically "parallel" (relation (8)) and "perpendicular" (relation (31)) edges:

$$d(u,x) = d(u,y) = d(v,x) = d(v,y) \qquad (31)$$

In such a case, the index equality can be considered as a case of degeneracy.

If the graph is *co*-graph/partial cube, then all of its semicubes are convex.[17,20] Further, an orthogonal edge-cutting procedure can be used to get the *ops*.

In general, $\Pi(G) \neq PI(G)$, the difference between the two indices originating in the different definition (Ashrafi[44]) of edge distance: the distance from a vertex *z* to an edge $e = (u,v)$ is taken as the minimum distance between the given point and the two endpoints of *e*:

$$d(z,e) = \min\{d(z,u), d(z,v)\} \qquad (32)$$

Then, the edge *e*=(*u*,*v*) and *f*=(*x*,y) are in relation *e eqd f* if:

$$d(x,e) = d(y,e) \text{ and } d(u,f) = d(v,f) \qquad (33)$$

Relations (8)&(31) are stronger than relations (32)&(33), in bipartite graphs they superimposing to each other (but not in general graphs) and $\Pi(G) = PI(G)$. Since any partial cube is also a bipartite graph, then in partial cubes/*co*-graphs the following triple equality holds:[16,17,26]

$$CI(G) = \Pi(G) = PI_e(G) \qquad (34)$$

In the opposite, in general graphs, the equality changes to the corresponding inequality:

$$CI(G) \neq \Pi(G) \neq PI_e(G) \qquad (35)$$

Resuming, the status of *co*-graph/partial cube cannot be decided by a simple and rapid criterion/condition. Out of various algorithms proposed to reach this task, the testing of transitivity of *ocs* is the last proof. To reduce the number of graphs tested, the conditions {(20)&(30)}, can be considered, under the reserve they are necessary but not sufficient.

5. Applications

In the following, we apply the cutting procedure on two classes of structures: (i) pcu cubic net and (ii) "topological nanocones". Formulas are given symbolically, in view of easily understanding the cutting procedures (in association with the graphs in figures) and only in final, at the first derivative calculation, the net parameter are substituted. Numerical examples are given.

5.1. Cutting procedure in pcu cubic net

We apply now the orthogonal cutting procedure in the *pcu* cubic network, appearing in crystal structure (Figure 2); among various *ocs*, the central one is denoted by k=0. The formulas for the net parameters and topological descriptors are given in Table 1.

C(3,3,3) $C_{k=1}$ $C_{k=0}$

Figure 2. Cutting procedure in *pcu* cubic net

Table 1. Net parameters and topological descriptors in *pcu* cubic lattice.

Type	Formulas
$v(C(a))$	$v(C(a)) = \|V(C(a))\| = (a+1)^3$
$e(C(a))$	$e(C(a)) = \|E(G)\| = 3a(a+1)^2$
v_k	$v_k(C(a)) = k(a+1)^2$

v_0	$v_0(C(a)) = (a+1)^3 / 2$
$e_k = s_k$	$e_k(C(a)) = (a+1)^2$
Wiener	$W(C(a,odd),x) = 3x^{((v/2)^2} + 6\sum_{k=1}^{(a-1)/2} x^{v_k\cdot(v-v_k)}$ $W(C(a,odd),x) = 3x^{((a+1)^3/2)^2} + 6\sum_{k=1}^{(a-1)/2} x^{k(a+1)^2\cdot[(a+1)^3-k(a+1)^2]}$ $W'(C(a,odd),1) = 3[(a+1)^3/2]^2 + 6\sum_{k=1}^{(a-1)/2} k(a+1)^2\cdot[(a+1)^3-k(a+1)^2]$ $W(C(a,even),x) = 6\sum_{k=1}^{a/2} x^{v_k\cdot(v-v_k)}$ $W(C(a,even),x) = 6\sum_{k=1}^{a/2} x^{k(a+1)^2\cdot[(a+1)^3-k(a+1)^2]}$ $W'(C(a,even),1) = 6\sum_{k=1}^{a/2} k(a+1)^2\cdot[(a+1)^3-k(a+1)^2]$ $W'(C(a),1) = (1/2)a(a+2)(a+1)^5$ Examples: a=4; $W(x) = 6x^{2500} + 6x^{3750}$; $W'(1) = 37500$. a=5; $W(x) = 6x^{6480}+6x^{10368}+3x^{11664}$; $W'(1) = 136080$.
Szeged	$SZ(C(a),x) = e_k(C(a))\cdot W(C(a),x) = (a+1)^2\cdot W(C(a),x)$ $SZ'(1) = (a+1)^2\cdot W(C(a)) = (1/2)a(a+2)(a+1)^7$ Examples: a=4; $SZ(x)=150x^{2500}+150x^{3750}$; $SZ'(1) = 937500$. a=5; $SZ(x)=216x^{6480}+216x^{10368}+108x^{11664}$; $SZ'(1) = 4898880$.
Cluj CJ_eS	$CJ_eS(C(a,odd),x) = 6e_k\cdot[x^{v/2} + \sum_{k=1}^{(a-1)/2}(x^{v_k} + x^{v-v_k})]$ $CJ_eS(C(a,odd),x) = 6(a+1)^2\cdot[x^{(a+1)^3/2} +$ $\sum_{k=1}^{(a-1)/2}(x^{k(a+1)^2} + x^{[(a+1)^3-k(a+1)^2]})]$ $CJ_eS(C(a,even),x) = 6e_k\sum_{k=1}^{a/2}(x^{v_k} + x^{v-v_k})$ $CJ_eS(C(a,even),x) = 6(a+1)^2\sum_{k=1}^{a/2}(x^{k(a+1)^2} + x^{[(a+1)^3-k(a+1)^2]})$ $CJ_eS(C(a),x) = 6e_k\cdot\sum_{k=1}^{a} x^{v_k}$ $CJ_eS(C(a),x) = 6(a+1)^2\cdot\sum_{k=1}^{a} x^{k(a+1)^2}$ $CJ_eS'(1) = e\cdot v = 3a(a+1)^2\cdot(a+1)^3 = 3a(a+1)^5$ Examples: a=4; $CJ_eS(x)=150x^{100} + 150x^{75} + 150x^{50} + 150x^{25}$; $CJ_eS'(1)=37500$. a=5; $CJ_eS(x)=216x^{180} + 216x^{144} + 216x^{108}+216x^{72} + 216x^{36}$; $CJ_eS'(1)=116640$.

Omega	$\Omega(\mathrm{C}(a,b,c),x) = a \cdot x^{(b+1)(c+1)} + b \cdot x^{(a+1)(c+1)} + c \cdot x^{(a+1)(b+1)}$
	$\Omega(\mathrm{C}(a,a,c),x) = 2a \cdot x^{(a+1)(c+1)} + c \cdot x^{(a+1)^2}$
	$\Omega(\mathrm{C}(a,a,a),x) = 3a \cdot x^{(a+1)^2}$
	$\Omega'(C(a),1) = e = 3a(a+1)^2$
	$\Omega''(C(a),1) = 3a^2(a+1)^2(a+2)$
	$CI(C(a)) = 3a(3a-1)(a+1)^4$
	Examples:
	a=4; $\Omega(x) = 12x^{25}; \Omega'(1) = 300; CI = 82500$.
	a=5; $\Omega(x) = 15x^{36}; \Omega'(1) = 540; CI = 272160$.

5.2. Cutting procedure in nanocones

Conical nano-structures have been reported in Nanoscience since 1968,[55,56] before the discovery of fullerenes. If a graphite sheet is divided into six sectors, each with an angle of 60º, and if *m* of these sectors (with *m*=1 to 3) are deleted sequentially, the dangling bonds being fused together, three classes of graphs, associated to single-walled nanocones, are obtained; their apex polygon will be a pentagon (*a*=5), a square (*a*=4) or a triangle (*a*=3), respectively. One can extend the construction principle and accept in the family of "topological cones" structures having the apex polygon $a \geq 6$; of course, that "cone" with *a*=6 is just the plane graphite sheet while those having larger polygons will show a saddle shape. In the recent years, several researchers have considered the mathematical properties of such nanostructures.[57-59]

Figure 3 gives three examples of such "topological cones", with the application of the cutting procedures in view of deriving some important topological descriptors.

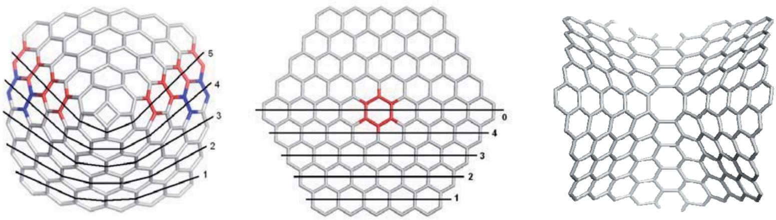


Figure 3. Cutting procedure in nanocones of apex *a*=4,6 and 8

Formulas, referring to net parameters and descriptors are given in the Tables 2 and 3, along with some numerical examples, in Table 4.

Table 2. Net parameters and topological descriptors in bipartite (partial cubes) nanocones

Type	Formulas for Cones C(a,n); a=even; a>4.
$v(a,n)$	$v(a,n)=a(n+1)^2$
$e(a,n)$	$e(a,n)=(a/2)(3n^2+5n+2)$
h_k	$h_k=n+k$
h_0	$h_0=2n+1$
v_k	$v_k=\sum_{i=1}^{k}(2n+2i+1)=k(2n+k+2)$
$e_k=s_k$	$e_k=n+k+1$
e_0	$e_0=2(n+1)$
$CJ_eS(x)$	$CJ_eS(x)=CJ_eS_0(x)+CJ_eS_k(x)$ $CJ_eS_0(x)=[(a/2)(h_0+1)+(a-6)(n+1)]\cdot(x^{v/2}+x^{v/2})$ $CJ_eS_0(x)=(a/2)e_0\cdot(x^{v/2}+x^{v/2})$ $CJ_eS_k(x)=a\sum_{k=1}^{n}(h_k+1)\cdot(x^{v_k}+x^{v-v_k})$ $CJ_eS_k(x)=a\sum_{k=1}^{n}e_k\cdot(x^{v_k}+x^{v-v_k})$ $CJ_eS(x)=(a/2)e_0\cdot(x^{v/2}+x^{v/2})+a\sum_{k=1}^{n}e_k\cdot(x^{v_k}+x^{v-v_k})$ $CJ_eS'(1)=e\times v=(a/2)(3n^2+5n+2)\times a(n+1)^2=(a^2/2)(n+1)^3(3n+2)$
$PI_v(x)$	$PI_v(x)=e\cdot x^v=(a/2)(3n^2+5n+2)\cdot x^{a(n+1)^2}$ $PI_v{}'(1)=CJ_eS'(1)=e\cdot v=(a^2/2)(n+1)^3(3n+2)$
$CJ_eP(x)$	$CJ_eP(x)=(a/2)e_0\cdot(x^{(v/2)^2})+a\sum_{k=1}^{n}e_k\cdot x^{v_k(v-v_k)}$ $CJ_eP'(1)=(a/4)(n+1)^2(-18n^4+9an^4-36n^3+a^2n^3+24an^3+$ $21an^2-19n^2+3a^2n^2+3a^2n-2n+6an+a^2)$ $CJ_eP(,x)=s_k\cdot W(x)$
Wiener	$W(x)=(a/2)(x^{(v/2)^2})+a\sum_{k=1}^{n}x^{v_k(v-v_k)}$ $W'(1)=(a/2)(v/2)^2+a\sum_{k=1}^{n}v_k(v-v_k)$ $W'(C_{a,n},1)=(1/120)a(n+1)(-304n^4+160an^4+460an^3-676n^3+$ $15a^2n^3-444n^2+440an^2+45a^2n^2+45a^2n-76n+$ $140an+15a^2)$

	$W'(C_{2s,n},1)=(1/15)s(n+1)(80sn^4-76n^4-169n^3+15s^2n^3+230sn^3-111n^2+45s^2n^2+220sn^2-19n+45s^2n+70sn+15s^2)$
	$W'(C_{2\cdot 3,n},1)=(1/5)(n+1)(164n^4+656n^3+954n^2+596n+135)$
Omega	$\Omega(x)=(a/2)\cdot x^{2(n+1)}+\sum_{k=2}^{n+1}a\cdot x^{n+k}$ $\Omega'(1)=(a/2)(3n^2+5n+2)$ $CI((a,n)=(1/12)a(n+1)(27an^3-28n^2+63an^2-50n+48an+12a-24)$

Table 3. Net parameters and topological descriptors in bipartite (non-partial cubes) nanocones

Type	Formulas for Cones *C*(4,*n*).	
$v(4,n)$	$v(4,n)=4(n+1)^2$	
$e(4,n)$	$e(4,n)=2(3n^2+5n+2)$	
$e_k=s_k$	$e_k=n+k+1$	
v_k	$v_k=k(2n+k+2)$	
	n=odd:	*n*=even:
last normal cut	$k_0=(n+1)/2$	$k_0=n/2$
corrected cut	$k_c=k_0+1=(n+3)/2$	$k_c=k_0+1=(n+2)/2$
correction	$c_k=2(k-k_c)+2=2k-n-1$	$c_k=2(k-k_c)+2=2k-n-1$
CJ$CJ_eS(x)$	$CJ_eS(C(4,n),x)=4(n+1)(x^{v/2}+x^{v/2})+4\sum_{k=1}^{k_c-1}e_k\cdot(x^{v_k}+x^{v-v_k})+4\sum_{k=k_c}^{n}(e_k-2c_k)\cdot(x^{v_k}+x^{v-v_k})+4\sum_{k=k_c}^{n}2c_k\cdot(x^{v_k-(c_k)^2}+x^{v-v_k+(c_k)^2})$ $CJ_eS'(C(4,n),1)=e\cdot v=2(3n^2+5n+2)\cdot 4(n+1)^2=8(3n+2)(n+1)^3$	
$CJ_eP(x)$	$CJ_eP(C(4,n),x)=4(n+1)\cdot x^{(v/2)^2}+4\sum_{k=1}^{k_c-1}e_k\cdot x^{v_k(v-v_k)}+4\sum_{k=k_c}^{n}(e_k-2c_k)\cdot x^{v_k(v-v_k)}+4\sum_{k=k_c}^{n}2c_k\cdot x^{(v_k-(c_k)^2)(v-v_k+(c_k)^2)}$ $CJ_eP'(C(4,n_{even}),1)=16+(538/5)n+(4129/15)n^2+370n^3+(1669/6)n^4+(557/5)n^5+(557/30)n^6$ $CJ_eP'(C(4,n_{odd}),1)=(31/2)+(523/5)n+(8213/30)n^2+370n^3+(1669/6)n^4+(557/5)n^5+(557/30)n^6$	
Omega	$\Omega(x)=(a/2)\cdot x^{2(n+1)}+\sum_{k=2}^{n+1}a\cdot x^{n+k}$ $\Omega'(1)=(a/2)(3n^2+5n+2)$ $CI((a,n)=(1/12)a(n+1)(27an^3-28n^2+63an^2-50n+48an+12a-24)$	

As can be seen from Tables 2 and 3, Omega polynomial is calculated by the same general formula in any cones with $a\geq 4$, *a*=even.

It is important to see that if G allows an "orthogonal cut" then $\{e_k\} \equiv \{c_k\} \equiv \{s_k\}$; however, in cones with a=4 and a=odd, a detail on these sets is needed.

In all cones, with $a \geq 4$, a=integer, the equality $CI(G) = \Pi(G)$ holds, by the following reasons: (i) cones with even $a > 4$ are partial cubes; (ii) cones with odd $a > 4$ are unions of partial cubes in non-bipartite graphs ($\{c_k\} \equiv \{s_k\}$ and co is transitive, thus the cones are co-graphs, but not partial cubes); (iii) cones with $a = 4$ show $|s_k| = |c_k|$ (but $\{c_k\} \neq \{s_k\}$, c_k is non-transitive and the bipartite graphs are not co-graphs or partial cubes), the last case being considered as a case of degeneracy.

In cones with a=3, $CI(G) \neq \Pi(G)$ because $|s_k| \neq |c_k|$ (and the non-bipartite graphs are not co-graphs or partial cubes). In any cone with a=even (*i.e.*, bipartite graphs), the equality $\Pi(G) = PI(G)$ holds.

Table 4. Examples for the formulas in Tables 2 and 3.

a	n	Polynomial	Index
4	3	$CJ_eS(x) = 20x^{55} + 24x^{44} + 16x^{35} + 12x^{33} + 32x^{32} + 12x^{31} +$	$CJ_eS'(1) = 5632$
		$16x^{29} + 24x^{20} + 20x^{9}$	
		$PI_v(x) = 88x^{64}$	$PI_v'(1) = 5632$
		$SZ_v(x) = 20x^{495} + 24x^{880} + 16x^{1015} + 12x^{1023} + 16x^{1024}$	$SZ_v'(1) = 75920$
		$\Omega(x) = 4x^5 + 4x^6 + 4x^7 + 2x^8$	CI=7176
4	4	$CJ_eS(x) = 24x^{89} + 28x^{76} + 8x^{62} + 24x^{61} + 12x^{56} + 24x^{53} +$	$CJ_eS'(1) = 14000$
		$40x^{50} + 24x^{47} + 12x^{44} + 24x^{39} + 8x^{38} + 28x^{24} + 24x^{11}$	
		$PI_v(x) = 140x^{100}$	$PI_v'(1) = 14000$
		$SZv(x) = 24x^{979} + 28x^{1824} + 8x^{2356} + 24x^{2379} + 12x^{2464} + 24x^{2491}$	$SZv'(1) = 289864$
		$+20x^{2500}$	
		$\Omega(x) = 4x^6 + 4x^7 + 4x^8 + 4x^9 + 2x^{10}$	CI= 18480
6	3	$CJ_eS(x) = 30x^{87} + 36x^{76} + 42x^{63} + 48x^{48} + 42x^{33} + 36x^{20} + 30x^{9}$	$CJ_eS'(1) = 12672$
		$PI_v(x) = 132x^{96}$	
		$SZ_v(x) = 30x^{783} + 36x^{1520} + 42x^{2079} + 24^{2304}$	$PI_v'(1) = 12672$
		$W(x) = 6x^{783} + 6x^{1520} + 6x^{2079} + 3^{2304}$	$SZ_v'(1) = 220824$
		$\Omega(x) = 6x^5 + 6x^6 + 6x^7 + 3x^8$	W'(1)=33204
			CI= 16572
6	4	$CJ_eS(x) = 36x \quad + 42x^{126} + 48x \quad + 54x^{94} + 60x^{75} + 54x^{56} +$	$CJ_eS'(1) = 31500$
		$48x^{39} + 42x^{24} + 36x^{11}$	
		$PI_v(x) = 210x^{150}$	$PI_v'(1) = 31500$

		$SZ_v(x)= 36x^{1529}+42x^{3024}+48x^{4329}+54x^{5264}+30x^{5625}$	$SZ_v'(1)= 842850$
		$W(x)=6x^{1529}+6x^{3024}+6x^{4329}+6x^{5264}+3x^{5625}$	$W'(1)=101751$
		$\Omega(x) =6x^6+6x^7+6x^8+6x^9+3x^{10}$	CI= 42420
8	3	$CJ_eS(x)=40x + 48x + 56x^{95} + 64x^{64} + 56x^{33} + 48x^{20} + 40x^9$	$CJ_eS'(1)= 22528$
		$PI_v (x) = 176x^{128}$	$PI_v'(1) =22528$
		$SZ_v(x)=40x^{1071}+48x^{2160}+56x^{3135}+32x^{4096}$	$SZ_v'(1)=453152$
		$W(x)=8x^{1071}+8x^{2160}+8x^{3135}+4x^{4096}$	$W'(1)=67312$
		$\Omega(x) = 8x^5+8x^6+8x^7+4x^8$	CI= 29840
8	4	$CJ_eS(x)=48x^{189} + 56x^{176} + 64x + 72x^{144} + 80x + 72x^{56} + 64x^{39} + 56x^{24} + 48x^{11}$	$CJ_eS'(1)= 56000$
		$PI_v(x) = 280x^{200}$	$PI_v' (1)= 56000$
		$SZ_v(x)=48x^{2079}+56x^{4224}+64x^{6279}+72x^{8064}+40x^{10000}$	$SZ_v'(1)=1718800$
		$W(x)= 8x^{2079}+8x^{4224}+8x^{6279}+8x^{8064}+4x^{10000}$	$W'(1)=205168$
		$\Omega(x) = 8x^6+8x^7+8x^8+8x^9+4x^{10}$	CI= 76160

In graphs which are not partial cubes, like the cones C(4,*n*),) one can use a procedure based on Θ^* which is the transitive closure of Winkler's Θ relation.[60,61]

Numerical calculation were done by our original software programs TOPOCLUJ,[23] Omega counter[62] and Nano Studio.[63]

The use of the herein discussed descriptors in correlating of various physico-chemical or biological properties with the molecular structure have been extensively proven, thus we only invite the reader to consult some monographs in the field.[54,64-67]

Conclusions

The most used topological indices: Wiener index $W(G)$, Szeged index $SZ(G)$, Cluj indices $CJ(G)$ and the more recently defined Cluj-Ilmenau $CI(G)$, were derived here by edge cutting procedures in some bipartite graphs and/or partial cubes. The analytical formulas enabled us to find a clear relatedness among these topological descriptors. Numerical examples were given.

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