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ORIGINAL PAPER

Cluj polynomials

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Abstract A novel class of counting polynomials, called Cluj polynomials is proposed on the ground of Cluj matrices. The polynomial coefficients are calculated from the above matrices or by means of orthogonal edge-cuts, in case of distance-based edge-calculated version. Basic definitions and properties of the Cluj matrices and corresponding polynomials are given. Relation with other counting polynomials is evidenced. Utility of Cluj descriptors in predicting the resonance energy of a set of planar polyhexes is exemplified.

Keywords Cluj matrices · Cluj polynomials · Cluj descriptors · Omega polynomial · QSPR

1 Introduction

It is well-known that a graph can be described by: a connection table, a sequence of numbers, a matrix, a polynomial or a derived number (called a topological index). In Quantum Chemistry, the early Hűckel theory calculates the levels of π-electron energy, of the molecular orbitals in conjugated hydrocarbons, as roots of the *characteristic polynomial* [1–3]:

$$P(G, x) = \det[x\mathbf{I} - \mathbf{A}(G)] \tag{1}$$

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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 [1–8].

The coefficients $m(G, k)$ in the polynomial expression:

$$P(G, x) = \sum_k m(G, k) \cdot x^k \tag{2}$$

are calculable from the graph G by a method making use of the *Sachs graphs*, which are subgraphs of G. Relation (2) was found independently by Sachs, Harary, Milić, Spialter, Hosoya, etc [2]. The above method is useful in small graphs but, in larger ones, the numeric methods of linear algebra, such as the recursive algorithms of Le Verier, Frame, or Fadeev, are more efficient [9,10].

An extension of relation (1) was made by Hosoya et al. [11] and others [12–15] by changing the adjacency matrix with the distance matrix and next by any square topological matrix.

Relation (2) is a general expression of a counting polynomial, written as 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 $m(G, k)$ are related to the occurrence of partitions of extent k.

Counting polynomials have been introduced, in Mathematical Chemistry literature, by Hosoya [16,17] with his Z-counting (independent edge sets) and the distance degree (initially called Wiener and later Hosoya) [18,19] polynomials. Their roots and coefficients are used for the characterization of topological nature of hydrocarbons.

Hosoya also proposed the sextet polynomial [20–23] for counting the resonant rings in a benzenoid molecule. The sextet polynomial is important in connection with the Clar aromatic sextets [24,25] expected to stabilize the aromatic molecules.

The independence polynomial [26–30] counts selections of k-independent vertices of G. Other related graph polynomials are the *king*, *color* and *star polynomials* [31–37].

If instead of sets of independent vertices one counts sets of mutually adjacent vertices, one obtains the *clique polynomial* [38–40]. More about polynomials the reader can find in Ref. [2].

In the case of some distance-related properties, the polynomial coefficients are calculable from the layer and shell matrices [41–45] built up according to the vertex distance partitions of a graph and calculable by the TOPOCLUJ software package [46].

The present paper introduces a novel class of counting polynomials based on vertex proximities, as given by the Cluj fragments, calculated by the above mentioned software. The article is organized as follows. Section 2 gives the definitions of Cluj matrices and some examples. In Sect. 3, the Cluj polynomials are introduced while their properties are discussed, in connection with other counting polynomials, in Sect. 4. In Sect. 5, an example of using descriptors derived from Cluj matrices/polynomials in

predicting the resonance energy of some polyhex hydrocarbons is given. Conclusions and references will close the paper.

2 Cluj matrices

A Cluj fragment, [2,47–52] symbolized $CJ_{i,j,p}$, collects vertices v lying closer to i than to j, the endpoints of a path $p(i, j)$. In other words, such a fragment collects the vertex proximity of i against any vertex j, joined by the path p, with the distances measured in the subgraph $G-p$, as shown in the following equation:

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

In cycle-containing graphs, 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). By definition, the entries in the Cluj matrix are taken as the maximum cardinality among all such fragments:

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

In trees, due to the unicity of paths joining any two vertices, $CJ_{i,j,p}$ means the set of paths going to j through i. In this way, we characterize the path $p(i,j)$ by means of a single endpoint, that suffices for the unsymmetric matrix **UCJ**.

When the path p belongs to the set of *distances* $DI(G)$, the suffix **DI** is added to the name of matrix, as **UCJDI**. When path p belongs to the set of *detours* $DE(G)$, the suffix is **DE**. The Cluj matrices are defined in any graph and are, in general, unsymmetric, excepting some symmetric graphs. They can be symmetrized by the Hadamard multiplication with their transposes [2,52]

$$\mathbf{SM_p} = \mathbf{UM} \cdot (\mathbf{UM})^{\mathrm{T}} \tag{5}$$

$$\mathbf{SM_e} = \mathbf{SM_p} \cdot \mathbf{A} \tag{6}$$

The subscript p means the matrix calculated on paths (*i.e.*, on all pairs of vertices) while e refers to an edge-calculated (*i.e.*, on all adjacent vertices) matrix. Basic properties and applications of the above matrices and derived descriptors have been presented elsewhere [47–51]. Figure 1 and Tables 1–4 give examples of Cluj matrices, calculated on distance and detour, respectively.

3 Cluj polynomials

The Cluj polynomials are defined, on the basis of Cluj matrices, as

$$CJ(G, x) = \sum_{k} m(G, k) \cdot x^k \tag{7}$$

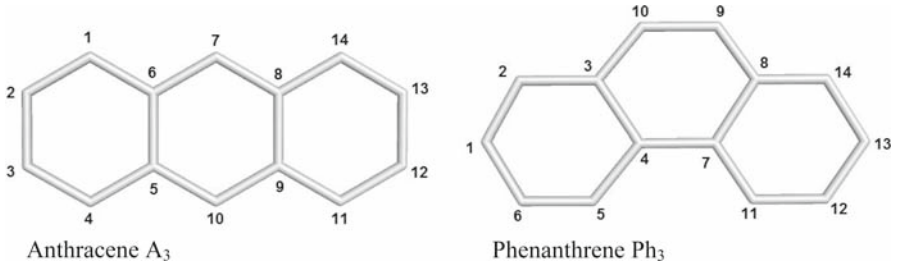


Fig. 1 Numbering anthracene and phenanthrene molecular graphs

Table 1 $\mathbf{UCJDI_p}$(Anthracene A_3)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	*RS*
1	0	11	6	6	2	3	4	4	4	4	6	6	5	5	66
2	3	0	7	2	2	2	4	3	3	3	5	5	4	5	48
3	2	7	0	3	2	2	3	3	3	4	5	4	5	5	48
4	6	6	11	0	3	2	4	4	4	4	5	5	6	6	66
5	10	10	10	11	0	7	6	6	6	7	8	7	7	7	102
6	11	10	10	10	7	0	7	6	6	6	7	7	7	8	102
7	8	8	8	8	4	7	0	7	4	4	8	8	8	8	90
8	8	7	7	7	6	6	7	0	7	6	10	10	10	11	102
9	7	7	7	8	6	6	6	7	0	7	11	10	10	10	102
10	8	8	8	8	7	4	4	4	7	0	8	8	8	8	90
11	6	6	5	5	4	4	4	2	3	4	0	11	6	6	66
12	5	5	4	5	3	3	3	2	2	4	3	0	7	2	48
13	5	4	5	5	3	3	4	2	2	3	2	7	0	3	48
14	5	5	6	6	4	4	4	3	2	4	6	6	11	0	66
CS	84	94	94	84	53	53	60	53	53	60	84	94	94	84	1,044

Table 2 $\mathbf{UCJDI_e}$(Anthracene A_3)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	*RS*
1	0	11	0	0	0	3	0	0	0	0	0	0	0	0	14
2	3	0	7	0	0	0	0	0	0	0	0	0	0	0	10
3	0	7	0	3	0	0	0	0	0	0	0	0	0	0	10
4	0	0	11	0	3	0	0	0	0	0	0	0	0	0	14
5	0	0	0	11	0	7	0	0	0	7	0	0	0	0	25
6	11	0	0	0	7	0	7	0	0	0	0	0	0	0	25
7	0	0	0	0	0	7	0	7	0	0	0	0	0	0	14
8	0	0	0	0	0	0	7	0	7	0	0	0	0	11	25
9	0	0	0	0	0	0	0	7	0	7	11	0	0	0	25
10	0	0	0	0	7	0	0	0	7	0	0	0	0	0	14
11	0	0	0	0	0	0	0	0	3	0	0	11	0	0	14
12	0	0	0	0	0	0	0	0	0	0	3	0	7	0	10
13	0	0	0	0	0	0	0	0	0	0	0	7	0	3	10
14	0	0	0	0	0	0	0	3	0	0	0	0	11	0	14
CS	14	18	18	14	17	17	14	17	17	14	14	18	18	14	224

Table 3 **UCJDE$_p$**(Phenanthrene Ph_3)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	RS
1	0	1	1	2	1	1	2	3	3	3	2	2	2	2	25
2	1	0	1	2	2	1	1	2	2	1	1	1	1	1	17
3	1	1	0	3	2	2	3	2	1	1	3	3	3	2	27
4	2	2	3	0	1	1	1	1	6	3	1	2	1	1	25
5	1	2	2	1	0	1	1	1	1	1	2	2	2	2	19
6	1	1	2	1	1	0	3	2	2	2	3	3	3	3	27
7	1	1	1	1	1	2	0	3	3	6	1	1	2	2	25
8	3	2	2	3	3	3	3	0	1	1	2	2	1	1	27
9	2	2	1	4	2	2	1	1	0	1	1	1	2	1	21
10	2	1	1	1	1	1	4	1	1	0	2	2	2	2	21
11	2	2	1	1	2	2	1	2	1	1	0	1	1	2	19
12	3	3	2	3	3	3	1	2	2	2	1	0	1	1	27
13	2	2	3	2	2	2	2	1	3	3	1	1	0	1	25
14	1	1	2	1	1	1	2	1	1	2	2	1	1	0	17
CS	22	21	22	25	22	22	25	22	27	27	22	22	22	21	322

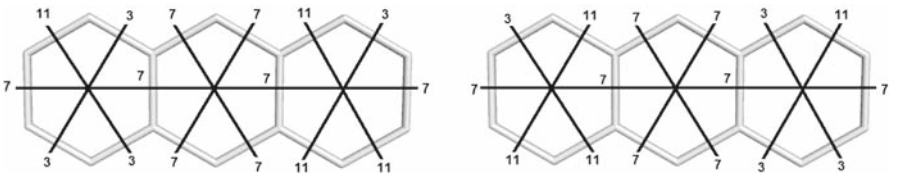
Table 4 **UCJDE$_e$**(Phenanthrene Ph_3)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	RS
1	0	1	0	0	0	1	0	0	0	0	0	0	0	0	2
2	1	0	1	0	0	0	0	0	0	0	0	0	0	0	2
3	0	1	0	3	0	0	0	0	0	1	0	0	0	0	5
4	0	0	3	0	1	0	1	0	0	0	0	0	0	0	5
5	0	0	0	1	0	1	0	0	0	0	0	0	0	0	2
6	1	0	0	0	1	0	0	0	0	0	0	0	0	0	2
7	0	0	0	1	0	0	0	3	0	0	1	0	0	0	5
8	0	0	0	0	0	0	3	0	1	0	0	0	0	1	5
9	0	0	0	0	0	0	0	1	0	1	0	0	0	0	2
10	0	0	1	0	0	0	0	0	1	0	0	0	0	0	2
11	0	0	0	0	0	0	1	0	0	0	0	1	0	0	2
12	0	0	0	0	0	0	0	0	0	0	1	0	1	0	2
13	0	0	0	0	0	0	0	0	0	0	0	1	0	1	2
14	0	0	0	0	0	0	0	1	0	0	0	0	1	0	2
CS	2	2	5	5	2	2	5	5	2	2	2	2	2	2	40

They count vertex proximities of vertices 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 (distance DI) or the longest (detour DE) paths. In Eq. 7, the coefficients $m(G,k)$ are calculated from the entries of Cluj matrices, as provided by TOPOCLUJ software program [46]. The summation runs up to the maximum $k = |\{p\}|$ in G. The above published [42] Cluj polynomials referred to some partitions of the Cluj matrices given by the layer/shell matrices, with no direct interpretation of the counting content.

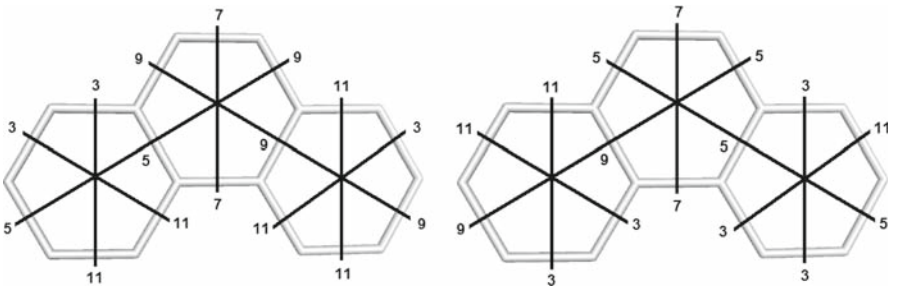
In the case of $CJDI_e$ polynomial, an orthogonal edge-cutting procedure can be used, as suggested in Tables 5 and 6. The same procedure was prior used by Gutman and Klavžar [53] for calculating the Szeged index of polyhex graphs.

Table 5 Edge cut procedure for calculating Cluj polynomial in anthracene A_3



$CJDI_{e\_i}(A_3,x)$=$4x^3$+$8x^7$+$4x^{11}$; $D1|_{x=1}$=112 $CJDI_{e\_j}(A_3,x) = 4x^3 + 8x^7$+$4x^{11}$; $D1|_{x=1}$=112
$CJDI_e(A_3,x) = 8x^3 + 16x^7 + 8x^{11}$; $P1|_{x=1} = 32 = 2e$; $D1|_{x=1} = 224$
$CJDI_p(A_3,x)$=$16x^2$+$20x^3$+$30x^4 + 20x^5 + 28x^6 + 28x^7 + 20x^8 + 12x^{10} + 8x^{11}$; $D1|_{x=1} = 1044$
$CJDE_e(A_3,x) = 28x + 4x^3$; $D1|_{x=1} = 40$
$CJDE_p(A_3,x) = 84x + 60x^2 + 24x^3 + 10x^4 + 4x^6$; $D1|_{x=1} = 340$

Table 6 Edge cut procedure for calculating Cluj polynomial in phenanthrene Ph_3



$CJDI_{e\_i}(Ph_3,x)$=$3x^3$+$2x^5$+$2x^7$+$4x^9 + 5x^{11}$ $CJDI_{e\_j}(Ph_3,x) = 5x^3 + 4x^5 + 2x^7 + 2x9 + 3x^{11}$
$D1|_{x=1} = 124$ $D1|_{x=1} = 100$
$CJDI_e(Ph_3,x) = 8x^3 + 6x^5 + 4x^7 + 6x^9 + 8x^{11}$; $P1|_{x=1} = 32 = 2e$; $D1|_{x=1} = 224$
$CJDI_p(Ph_3,x)$=$18x^2$+$20x^3$+$36x^4$+$20x^5$+$14x^6$+$20x^7$+$28x^8 + 6x^9$+$12x^{10}$+$8x^{11}$; $D1|_{x=1}$=1050
$CJDE_e(Ph_3,x) = 28x + 4x^3$; $P1|_{x=1} = 32 = 2e$; $D1|_{x=1} = 40$
$CJDE_p(Ph_3,x) = 84x + 64x^2 + 30x^3 + 2x^4 + 2x^6$; $D1|_{x=1} = 322$

Since the Cluj matrices are unsymmetric, two polynomials, one with respect to the endpoint i (and to the first triangle of $\mathbf{UCJDI_e}$) and the other one referring to the endpoint j of the edge $e(i,j)$ (and to the second triangle of the mentioned matrix) can be written. However, they depend on the numbering and only their sum polynomial is invariant (see Tables 5 and 6). This last polynomial will only be taken into consideration in the following discussion.

4 Properties of the Cluj polynomials

Among the properties of counting polynomials, the value in $x = 1$ and the first derivative in $x = 1$ are the most important. In the case of $CJDI_e$ polynomial, the value in $x = 1$, $P|_{x=1} = 2e$. It is evident, since every edge is visited twice.

The first derivative, in $x = 1$, $D1|_{x=1}$, gives the meaning of the topological property collected by a matrix/polynomial. In this case, the following theorem holds:

Theorem 1 *In a bipartite graph, the sum of all edge-counted vertex proximities equals the product v×e of the number of vertices and edges in G.*

Demonstration In a bipartite, planar graph, permitting orthogonal edge-cuts, for every edge $e(i, j) \in E(G)$ there is a clear separation of proximities $\{p_{e,i}\}$ and $\{p_{e,j}\}$ of its endpoints. Let's denote by $p_{e,i}$ and $p_{e,j}$ the cardinalities of the above sets. In a bipartite graph, we always can write

$$p_{e,i} + p_{e,j} = v \tag{8}$$

It follows that, for all edges, $e \in E(G)$, the total of edge-counted vertex proximities p_e equals the product $v \times e$, thus demonstrating the theorem.

Recall that an orthogonal (or an elementary) edge-cut of a (polycyclic) bipartite planar graph G, is a straight line segment, passing through the centers of some edges of the graph, being orthogonal to these edges, and intersecting the perimeter of G exactly two times, so that at least one polygon lies between these two intersection points [2,52,53]. Note that trees also allow elementary edge-cuts.

In the orthogonal edge-cut procedure for calculating the $CJDI_e$ index, (*i.e.*, the sum of all entries in the matrix $\mathbf{UCJDI_e}$), the total of edge-counted vertex proximities $p_e = CJDI_e(G, x)D1|_{x=1}$ is calculated as:

$$p_e = \sum_c m(G, c) \cdot c \cdot (p_{e,i} + p_{e,j}) = v \cdot \sum_c m(G, c) \cdot c = v \times e \tag{9}$$

where the coefficients $m(G, c)$ are related to the occurrence of edge-cuts (see below) of extent c and $\sum_c m(G, c) \cdot c = e(G)$. The above theorem can be extended to 3D bipartite molecular structures, although the separation of the proximities is not so evident. Numerical results provided by the Cluj matrix support this extension.

Corollary to Theorem 1. *In bipartite graphs there are no equidistant vertices with respect to the two endpoints of any edge.*

The Cluj matrix counts the vertices lying closer to each of the endpoints of any edge and leaves the equidistant vertices uncounted. Because of relation (8), it follows that, in bipartite graphs, all vertices are counted and *no equidistant vertices* exist. Next, for all of the edges in G, one obtains the total of vertex proximities, p_e, equal to $v \times e$. This is the main result provided by the Cluj matrix/polynomial. The vertex proximity calculation could be of interest in calculating the *bond polarity* and molecular dipole moments. In this respect, weighted molecular graphs must be used.

Recall that, in calculating the Szeged index [53–61] (a topological index related to the Wiener index, [62] which counts all the shortest distances in a graph), equidistant vertices are also not counted.

Table 7 Formulas for Cluj-edge (and related) polynomials in acenes A_h; h = no. of hexagons in molecule

$CJDI_e(A_{h-even}, x) = 8 \cdot \sum_{k=1}^{h/2} x^{(4k-1)} + 2(h+1) \cdot x^{(2h+1)} + 8$
$\times \sum_{k=(h+2)/2}^{h} x^{(4k-1)};\ D1|_{x=1} = 2(2h+1)(5h+1) = v \cdot e$
$CJDI_e(A_{h-odd}, x) = 8 \cdot \sum_{k=1}^{(h-1)/2} x^{(4k-1)} + (2(h-3)+16) \cdot x^{(2h+1)} + 8$
$\times \sum_{k=(h+3)/2}^{h} x^{(4k-1)};\ D1|_{x=1} = v \cdot e$
$CJDE_e(A_{h-even}, x) = (8h+4) \cdot x + 4 \cdot \sum_{k=2}^{h/2} x^{(2k-1)} + 2 \cdot x^{(h+1)};\ D1|_{x=1} = h^2 + 10h + 2$
$CJDE_e(A_{h-odd}, x) = (8h+4) \cdot x + 4 \cdot \sum_{k=2}^{(h+1)/2} x^{(2k-1)};\ D1|_{x=1} = h^2 + 10h + 1$
$\Omega(A_h, x) = 2h \cdot x^2 + x^{(h+1)};\ |D1|_{x=1} = e = 5h + 1;\ D2|_{x=1} = h(h+5)$
$CI(A_h) = (\Omega'(A_h))^2 - (\Omega'(A_h) + \Omega''(A_h)) = (5h+1)^2 - (5h + 1 + h(h+5)) = 24h^2$
$\Omega(A_h, x)|_{x=1} = v/2 = 2h + 1$
$\Pi(A_h, x) = 4h \cdot x^{(5h-1)} + (h+1) \cdot x^{4h};\ D1|_{x=1} = 24h^2$

Table 8 Formulas for Cluj-edge (and related) polynomials in phenacenes Ph_h; h =no. of hexagons in molecule

$CJDI_e(Ph_{h-even/odd}, x) = 8 \cdot x^3 + 4 \cdot \sum_{k=2}^{h-1} x^{(4k-1)} + 6 \cdot \sum_{k=1}^{h-1} x^{(4k+1)} + 8 \cdot x^{4h-1};\ D1|_{x=1} = v \cdot e$
$CJDI_e(A_h/Ph_h) = D1|_{x=1} = v \cdot e = 2(2h+1) \cdot (5h+1) = 2(10h^2 + 7h + 1)$
$CJDE_e(Ph_{h-even}, x) = (8h+4) \cdot x + h \cdot x^3 + 2 \cdot \sum_{k=2}^{h/2} x^{(4k-1)};\ D1|_{x=1} = h^2 + 12h - 2$
$CJDE_e(Ph_{h-odd}, x) = (8h+4) \cdot x + (h+1) \cdot x^3 + 2 \cdot \sum_{k=2}^{(h-1)/2} x^{(4k-1)};\ D1|_{x=1} = h^2 + 10h + 1$
$\Omega(Ph_h, x) = (h+2) \cdot x^2 + (h-1) \cdot x^3;\ D1|_{x=1} = e = 5h + 1;\ D2|_{x=1} = 8h - 2$
$CI(Ph_h) = (5h+1)^2 - (5h + 1 + 8h - 2) = 25h^2 - 3h + 2$
$\Omega(Ph_h, x)|_{x=1} = v/2 = 2h + 1$
$\Pi(Ph_h, x) = 2(h+2) \cdot x^{(5h-1)} + 3(h-1) \cdot x^{(5h-2)};\ D1|_{x=1} = 25h^2 - 3h + 2$

Theorem 2 *In a tree graph, the sum of all path-counted vertex proximities is twice the sum of all distances in G or twice the Wiener W index:*

$$p_p = CJDI_p(G, x)D1|_{x=1} = 2W.$$

Demonstration The column sums in the **UCJDI**$_p$ matrix equals the column sums in the matrix of distances while the row sums in **UCJDI**$_p$ matrix are identical to those in the Wiener matrix [2,52]. It is well-known that the half sum of entries in these matrices counts all the distances in a tree graph, or the Wiener index. Since the first derivative of the $CJDI_p$ polynomial is the sum of all entries in **UCJDI**$_p$, and this sum is twice the the Wiener index, the theorem is thus demonstrated.

In cycle-containing graphs, the Cluj index $CJDI_p$ is different from both the Wiener and Szeged indices [2,52].

Formulas for calculating the Cluj polynomial $CJDI_e$ in acenes A_h and phenacenes Ph_h, function of the number of their hexagons h, are given in Tables 7 and 8, respectively.

Theorem 3 *A full Hamiltonian graph FH shows the minimal exponent value, 1, and the minimal value of the first derivatives of Cluj-detour polynomials:*

$$CJDE_p(G,x)D1|_{x=1} = v(v-1) \text{ and } CJDE_e(G,x)D1|_{x=1} = 2e.$$

Demonstration Recall that a full Hamiltonian FH graph [48] has any pair of its vertices joined by a Hamiltonian path (*i.e.*, a path visiting all the vertices of G). Considering that the Cluj fragments/proximities are counted by deleting the path $p(i, j)$ excepting its endpoints, the proximity of i is always 1, *vs.* any other vertex j in G. Thus, the exponent takes the minimal (unity) value. The coefficient of this unique term of $CJDE_p$ polynomial is $v(v-1)$, as counted from the **CJDE**$_\mathrm{p}$ matrix (which shows all its non-diagonal entries equal to unity). For $CJDE_e$, the demonstration is immediate. Any FH graph shows all the non-diagonal entries in **CJDE**$_\mathrm{p}$ matrix equal to unity but the reciprocal is not always true.

Corollary to Theorem 3. *If the FH graph is a complete graph, then:* $CJDE_p(G,x)D1|_{x=1}..... = CJDE_e(G,x)D1|_{x=1} = 2e$.

In complete graphs, all the vertices are adjacent. Thus, the two polynomials, defined on edges and paths, respectively, coincide, thus $v(v-1) = 2e$.

Two related polynomials are included in the above tables. One is the Omega polynomial, [63] $\Omega(G,x)$, which counts orthogonal edge-cuts and the second one is the Π polynomial $\Pi(G,x)$, which is somehow complementary to the above one. It was shown elsewhere [64,65] that the edges forming an edge-cut strip are locally co-distant, or equidistant or also "topologically" parallel.

Let $m(G,c)$ denote the occurrence of the edge-cut sequence of length c (*i.e.*, the number of edges cut-off) in G. In a bipartite, planar graph, the two polynomials are defined as

$$\Omega(G,x) = \sum_c m(G,c)\cdot x^c \tag{10}$$

$$\Pi(G,x) = \sum_c m(G,c)\cdot c\cdot x^{(e-c)} \tag{11}$$

Their $D1|_{x=1}$ give the total number of equidistant and non-equidistant edges vs each edge in G

$$\Omega(G,x)\ D1|_{x=1} = e = |E(G)| \tag{12}$$

$$\Pi(G,x)\ D1|_{x=1} = \Pi(G) \tag{13}$$

where $\Pi(G)$ equals (in partial cubes) the Khadikar's *PI* topological index [66]. Note that Ashrafi et al. [67] proposed the *PI* polynomial $PI(G,x)$, which first derivative always gives the Khadikar's *PI* topological index.

Two indices have been defined on Omega polynomial. The first one, *CI*, is derived from the first and second derivatives, in $x = 1$, as

$$CI(G) = (\Omega(G,x)D1)^2 - (\Omega(G,x)D1 + \Omega(G,x)D2)\,|_{x=1} \tag{14}$$

The second descriptor is calculable from all possible derivatives *Dn*, in $x = 1$, and normalized to the first one (which equals the number of edges in G)

$$I_\Omega(G) = (1/\Omega(G,x)D1) \cdot \sum_n (\Omega(G,x)Dn)^{1/n}\,|_{x=1} \tag{15}$$

Theorem 4 *In a bipartite planar graph (in a partial cube, in general), CI and PI indices are identical.*

Demonstration From (14) and writing $m(G,c)$ as simply m, *CI* is calculable as

$$\begin{aligned} CI(G) &= \sum_c \{(m\cdot c)^2 - [m\cdot c + m\cdot c(c-1)]\} \\ &= \sum_c [(m\cdot c)^2 - m\cdot c^2] = e^2 - \sum_c m\cdot c^2 \end{aligned} \tag{16}$$

On the other hand, from (11) and (13), *PI* is calculated as

$$PI(G) = \sum_c m\cdot c\cdot(e-c) = e\sum_c m\cdot c - \sum_c m\cdot c^2 = e^2 - \sum_c m\cdot c^2 \tag{17}$$

Clearly, the two indices are identical, because they transform into one and the same ultimate expression, also proposed by John et al. [68] for calculating *PI* in benzenoid hydrocarbon graphs. In the above, the following relation holds

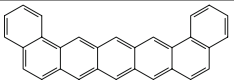
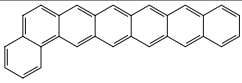
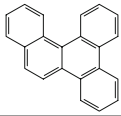
$$e(G) = \sum_c m\cdot c = \Omega(G,x)D1|_{x=1} = \Pi(G,x)|_{x=1} \tag{18}$$

However, relation (11) is not always valid, so that *CI* is, in general, different from *PI*, excepting the case of bipartite planar graphs (partial cubes, in general) [69].

In bipartite graphs embeddable in surfaces of $g > 0$, *e.g.*, in toroidal polyhexes, relation (11) is still more hidden, despite $CI = PI$. In case of the torus T(6,3)H [8,12]: $\Omega(G,x) = 12x^4 + 4x^{24}$; $e = 144$; $CI = 18240$; $\Pi(G,x) = 96x^{122} + 48x^{136}$; $PI = 18240$. According to (11) the polynomial would be: $\Pi(G,x) = 96x^{120} + 48x^{140}$ that gives the same *PI* index value. At this moment no generalization of this case was found.

We stress here that polynomials *CJDI*(G,x) and $\Pi(G,x)$ count, in a same manner, non-equidistant subgraphs (vertices and edges, respectively). An application of these descriptors is presented below.

Table 9 Structure of polyhex hydrocarbons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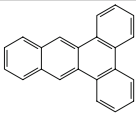
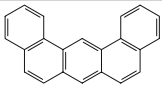
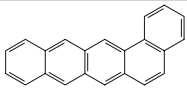
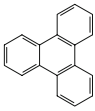
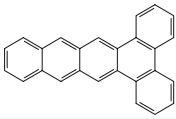
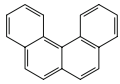
		
4	5	6
		
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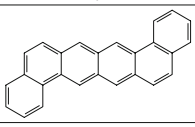
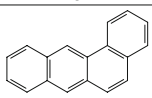
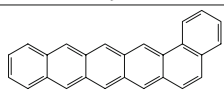
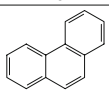
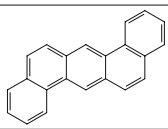
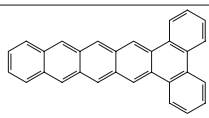
		
10	11	12
		
13	14	15

5 Predicting the resonance energy of planar polyhexes

For testing the correlating ability of descriptors derived from Cluj and Omega polynomials, a data set of 15 planar polyhex hydrocarbons (Table 9), with at least one phenanthrenic unit, have been selected from the Randić's review [70]. The predicted property was the resonance energy, which is claimed for supporting the aromatic character of such molecules. Topological descriptors and the corresponding energetic data are listed in Table 10. The plot of resonance energy vs calculated values (by the best regression equation (19)) is presented in Fig. 2. The calculations were performed by the TopoCluj [46] and Omega [71] software packages.

$$RE_{calc} = 5.02357 - 0.00025 \cdot CJDI_p + 0.00489 \cdot CI - 2.68146 \cdot I_\Omega \qquad (19)$$
$$n = 15;\ R^2 = 0.984;\ F = 228.358$$

6 Conclusions

A novel class of counting polynomials, called Cluj polynomials was proposed on the ground of previous Cluj matrices.

Table 10 Topological and energetic data for molecules in Table 9

Molecule	I	CI	$UCJDI_p$	RE (eV)	RE calc.
1	1.498	1,200	11,200	4.085	4.040
2	1.675	1,194	11,237	3.515	3.526
3	1.348	612	4,373	3.209	3.294
4	1.455	610	4,392	3.111	2.993
5	1.455	610	4,290	2.986	3.019
6	1.638	606	4,301	2.531	2.506
7	1.386	390	2,352	2.708	2.619
8	1.558	878	7,350	3.361	3.278
9	1.386	390	2,306	2.506	2.630
10	1.558	878	7,248	3.27	3.304
11	1.523	388	2,303	2.311	2.254
12	1.765	872	7,219	2.671	2.727
13	1.436	218	1,050	1.955	1.973
14	1.455	610	4,318	2.986	3.012
15	1.675	1194	11,404	3.45	3.484

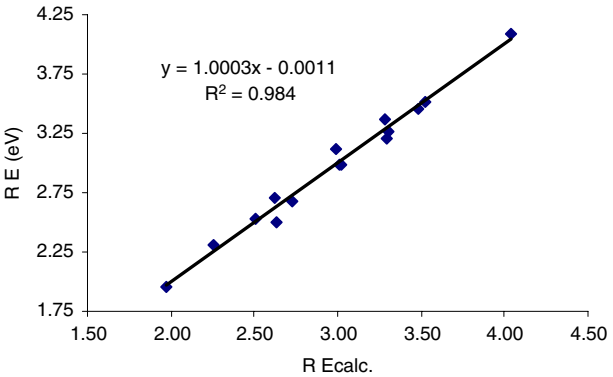


Fig. 2 Resonance energy versus calculated values (Eq. 18)

It was shown that the polynomial coefficients are calculable from the above matrices or by means of orthogonal edge-cuts, in case of $CJDI_e$ version.

Basic definitions and properties of the Cluj matrices and corresponding polynomials were given. The meaning of Cluj descriptors, as vertex proximity descriptors, was clearly evidenced.

It was demonstrated that, in bipartite graphs, the sum of all edge-counted vertex proximities equals the number $v \times e$, of vertices and edges in the graph. In trees, the sum of all path-counted vertex proximities is twice the Wiener index.

A full Hamiltonian graph FH was shown to have the minimal exponent value, 1, and the minimal value of the first derivatives of Cluj-detour polynomials.

The relation of Cluj polynomials with the Π and PI polynomials was recognized.

The descriptors derived from the Cluj and Omega polynomials were used in predicting the resonance energy of a set of planar polyhexes. The use of vertex proximity

calculation in evaluating the bond polarity and molecular dipole moments was suggested.

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References

1. M.V. Diudea, O. Ivanciuc, *Molecular Topology* (in Romanian) (Comprex, Cluj, 1995)
2. M.V. Diudea, I. Gutman, L. Jäntschi, *Molecular Topology* (Nova Science, Huntington, New York, 2001)
3. N. Trinajstić, *Chemical Graph Theory*, 2nd edn. (CRC Press, New York, 1992)
4. I. Gutman, M. Milun, N. Trinajstić, MATCH, Commun. Math. Comput. Chem. **1**, 171–175 (1975)
5. J. Aihara, J. Am. Chem. Soc. **98**, 2750–2758 (1976)
6. I. Gutman, M. Milun, N. Trinajstić, J. Am. Chem. Soc. **99**, 1692–1704 (1977)
7. A. Tang, Y. Kiang, S. Di, G. Yen, *Graph Theory and Molecular Orbitals* (in Chinese) (Science Press, Beijing, 1980)
8. A. Tang, Y. Kiang, G. Yan, S. Tai, *Graph Theoretical Molecular Orbitals* (Science Press, Beijing, 1986)
9. P.S. Dwyes, *Linear Computations* (Wiley, New York, 1951)
10. D.K. Fadeev, I.S. Sominskii, *Problems in Higher Algebra* (Freeman, San Francisco, 1965)
11. H. Hosoya, M. Murakami, M. Gotoh, Natl Sci. Rept. Ochanomizu Univ. **24**, 27–34 (1973)
12. R.L. Graham, L. Lovasz, Adv. Math. **29**, 60–88 (1978)
13. M.V. Diudea, O. Ivanciuc, S. Nikolić, N. Trinajstić, MATCH, Commun. Math. Comput. Chem. **35**, 41–64 (1997)
14. O. Ivanciuc, M.V. Diudea, P.V. Khadikar, Indian J. Chem. **37A**, 574–585 (1998)
15. O. Ivanciuc, T. Ivanciuc, M.V. Diudea, Roum. Chem. Quart. Rev. **7**, 41–67 (1999)
16. H. Hosoya, Bull. Chem. Soc. Japan **44**, 2332–2339 (1971)
17. H. Hosoya, Discrete Appl. Math. **19**, 239–257 (1988)
18. E.V. Konstantinova, M.V. Diudea, Croat. Chem. Acta, **73**, 383–403 (2000)
19. I. Gutman, S. Klavžar, M. Petkovšek, P. Žigert, MATCH,Commun. Math. Chem. **43**, 49–66 (2001)
20. H. Hosoya, T. Yamaguchi, Tetrahedron Lett. 4659–4662 (1975)
21. N. Ohkami, H. Hosoya, Theoret. Chim. Acta **64**, 153–170 (1983)
22. N. Ohkami, A. Motoyama, T. Yamaguchi, H. Hosoya, Tetrahedron **37**, 1113–1122 (1981)
23. H. Hosoya, Topics Curr. Chem. **153**, 255–272 (1990)
24. E. Clar, *Polycyclic Hydrocarbons* (Academic Press, London, 1964)
25. E. Clar, *The Aromatic Sextet* (Wiley, New York, 1972)
26. I. Gutman, H. Hosoya, Z. Naturforsch **45a**, 645–648 (1990)
27. I. Gutman, MATCH, Commun. Math. Chem. **28**, 139–150 (1992)
28. I. Gutman, Publ. Inst. Math. (Beograd) **50**, 19–23 (1991)
29. I. Gutman, Rev. Roum. Chim. **36**, 379–388 (1991)
30. D. Stevanović, Graph Theory Notes New York **34**, 31–36 (1998)
31. A. Motoyama, H. Hosoya, J. Math. Phys. **18**, 1485–1490 (1977)
32. K. Balasubramanian, R. Ramaraj, J. Comput. Chem. **6**, 447–454 (1985)
33. E.J. Farrell, Canad. Math. Bull. **2**, 35–46 (1978)
34. E.J. Farrell, C. De Matas, Ark. Math. **26**, 185–190 (1988)
35. E.J. Farrell, C. De Matas, Util. Math. **33**, 33–45 (1988)
36. E.J. Farrell, C. De Matas, Int. J. Math. Math. Sci. **11**, 87–94 (1988)
37. E.J. Farrell, Proc. Caribb. Acad. Sci. **5**, 163–168 (1994)
38. E.J. Farrell, Int. J. Math. Math. Sci. **12**, 77–84 (1989)
39. C. Hoede, X.L. Li, Discr. Math. **125**, 219–228 (1994)
40. D. Stevanović, Publ. Elektrotehn. Fac. (Beograd) Ser. Mat. **8**, 84–87 (1997)
41. M.V. Diudea, J. Chem. Inf. Comput. Sci. **34**, 1064–1071 (1994)
42. M.V. Diudea, Studia Univ. "Babes-Bolyai" **47**, 131–139 (2002)
43. M.V. Diudea, MATCH, Commun. Math. Comput. Chem. **45**, 109–122 (2002)
44. M.V. Diudea, O. Ursu, Indian J. Chem. **42A**, 1283–1294 (2003)

45. M. Stefu, M.V. Diudea, in: *Nanostructures–Novel Architecture*, ed. by M. V. Diudea (Nova, New York, 2005), pp. 127–165
46. O. Ursu, M.V. Diudea, TOPOCLUJ software program, Babes-Bolyai University, Cluj (2005), http://chem.ubbcluj/~diudea
47. M.V. Diudea, J. Chem. Inf. Comput. Sci. **37**, 300–305 (1997)
48. M.V. Diudea, B. Parv, I. Gutman, J. Chem. Inf. Comput. Sci. **37**, 1101–1108 (1997)
49. M.V. Diudea, G. Katona, I. Lukovits, N. Trinajstic, Croat. Chem. Acta **71**, 459–471 (1998)
50. L. Jäntschi, G. Katona, M.V. Diudea, MATCH, Commun. Math. Comput. Chem. **41**, 151–188 (2000)
51. D. Opris, M.V. Diudea, SAR/QSAR Environ. Res. **12**, 159–179 (2001)
52. M.V. Diudea, M.S. Florescu, P. Khadikar, *Molecular Topology and it's Applications* (EfiCon Press, Bucharest, Romania, 2006)
53. I. Gutman, S. Klavžar, J. Chem. Inf. Comput. Sci. **35**, 1011–1014 (1995)
54. I. Gutman, Graph Theory Notes of New York **27**, 9–15 (1994)
55. A.A. Dobrynin, I. Gutman, Publ. Inst. Math. (Beograd) **56**, 18–22 (1994)
56. A.A. Dobrynin, I. Gutman, Graph Theory Notes of New York **2**(8), 21–23 (1995)
57. A.A. Dobrynin, I. Gutman, G. Domotor, Appl. Math. Lett. **8**, 57–62 (1995)
58. P.V. Khadikar, N.V. Deshpande, P.P. Kale, A. Dobrynin, I. Gutman, G. Domotor, J. Chem. Inf. Comput. Sci. **35**, 547–550 (1995)
59. S. Klavžar, A. Rajapakse, I. Gutman, Appl. Math. Lett. **9**, 45–49 (1996)
60. J. Žerovnik, Croat. Chem. Acta **69**, 837–843 (1996)
61. A.A. Dobrynin, I. Gutman, Croat. Chem. Acta **69**, 845–856 (1996)
62. H. Wiener, Structural determination of paraffin boiling points. J. Am. Chem. Soc. **69**, 17–20 (1947)
63. M.V. Diudea, Carpath. J. Math. **22**, 43–47 (2006)
64. M.V. Diudea, S. Cigher, A.E. Vizitiu, O. Ursu, P.E. John, Croat. Chem. Acta **79**, 445–448 (2006)
65. A.E. Vizitiu, S. Cigher, M.V. Diudea, M.S. Florescu, MATCH Commun. Math. Comput. Chem. **57**, 457–462 (2007)
66. P.V. Khadikar, Nat. Acad. Sci. Lett. **23**, 113–118 (2000)
67. A.R. Ashrafi, M. Manoochehrian, H. Yousefi Azari, Util. Math. **71**, 97–108 (2006)
68. P.E. John, P.V. Khadikar, J. Singh, J. Math. Chem. **42**, 37–45 (2007)
69. S. Klavžar, MATCH Commun. Math. Comput. Chem. **59**, 217–222 (2008)
70. M. Randić, Chem. Rev. **103**, 3449–3605 (2003)
71. S. Cigher, M.V. Diudea, Omega 1.1, software program, "Babes-Bolyai" (University, Cluj, Romania, 2005)