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Hosoya-Diudea Polynomials Revisited

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Abstract

A novel class of property-distance counting polynomials was proposed in ref. *Studia Univ. "Babes-Bolyai"*, 2002, *47*, 131-139**.** The polynomial coefficients are calculated by means of layer/shell matrices, built up according to the vertex distance partitions of a graph. The old results are revisited and put in a new light. More focused was the polynomial constructed on the Cluj matrix acted by the shell matrix operator.

1. Introduction

In the early Hűckel theory, the roots of the graph *characteristic polynomial*:[1]

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

with **I** being the unit matrix of a pertinent order and **A** the adjacency matrix, are assimilated to the π-electron energy levels of the molecular orbitals in conjugated hydrocarbons. Other related topics: Topological Resonance Energy TRE, Topological Effect on Molecular Orbitals, TEMO, the Aromatic Sextet Theory, AST, the Kekulé Structure Count, KSC, *etc*. [1,2] also used the information provided by $Ch(x)$.

The coefficients of the characteristic polynomial are calculable from the graph G as shown by Sachs, Harary, Milić, Spialter, *etc*. [1], by using the Sachs subgraphs or by some more efficient numeric methods of linear algebra, (see the recursive algorithms of Le Verier, Frame, or Fadeev) [3,4].

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Hosoya[5] and others[6-10] have extended the above definition (1) by changing the adjacency matrix with the distance matrix and next by any topological square matrix.

A different field in the polynomial description is that of finite sequences of some graph invariants, such as the distance degree sequence or the sequence of the number of k-independent edge sets. The polynomial corresponding to the last sequence was introduced by Hosoya as the Z-counting polynomial [11].

The present paper is organized as follows. After the above introduction, basic definitions are given in a second section, as preliminaries for the main study on Hosoya-Diudea polynomials, detailed in the third section. In the forth section, the Cluj-Centrality CJC index is introduced while its dicriminating ability is presented in the fifth section. Conclusions and References will close the article.

2. Basic definitions

Let $G(V,E)$ be a connected molecular graph, [12] without directed and multiple edges and without loops, the vertex and edge-sets of which being represented by V(G) and E(G), respectively. Let's next define the k^{th} layer/shell of vertices v lying at distance k with respect to the reference vertex i as [13]:

$$G(i)_k = \{ v |\ v \in V(G);\quad d_{iv} = k \} \tag{2}$$

The collection of all its layers defines the partition of G with respect to i:

$$G(i) = \{ G(i)_k \ ; k \in [0,1,..,ecc_i] \} \tag{3}$$

with ecc_i being the *eccentricity* of i (*i.e.*, the largest distance from i to the other vertices in G).

Layer Matrices

The entries in a layer matrix (of a vertex property) **LM**, are defined as [13-15]:

$$[\mathbf{LM}]_{i,k} = \sum_{v | d_{i,v}=k} p_v \tag{4}$$

with summation being the most used operation on the collected vertices. The zero column is just the column of vertex properties $[\mathbf{LM}]_{i,0} = p_i$. Any atomic/vertex property can be considered as p_i. More over, any square matrix M can be taken as *info matrix*, *i.e.*, the matrix supplying local/vertex properties as *row sum RS*, *column sum CS* or *diagonal entries* given by the *Walk* matrix [13], as developed by TOPOCLUJ software package [16].

The Layer matrix **LM** is a collection of the above defined entries:

$$\mathbf{LM} = \left\{ [\mathbf{LM}]_{i,k} ; i \in V(G); k \in [0,1,..,d(G)] \right\} \tag{5}$$

with $d(G)$ being the diameter of the graph or the largest distance in G.

Shell Matrices

The entries in a *shell matrix* **ShM** are defined as [13, 17]:

$$[\mathbf{ShM}]_{i,k} = \sum_{v | d_{i,v}=k} [\mathbf{M}]_{i,v} \tag{6}$$

where **M** is any square topological matrix. Any other operation over the square matrix entries $[\mathbf{M}]_{i,v}$ can be used. The shell matrix is a collection of the above defined entries:

$$\mathbf{ShM} = \left\{ [\mathbf{ShM}]_{i,k} ; i \in V(G); k \in [0,1,..,d(G)] \right\} \tag{7}$$

The zero column $[\mathbf{ShM}]_{i,0}$ is just the diagonal entries in the info matrix **M**.

Counting Polynomials

Define a *distance*-based polynomial as:

$$P(x) = \sum\nolimits_k p(G,k) \cdot x^k \tag{8}$$

with $p(G,k)$ being sets of local contributions (of extent k) to the global (molecular) property $P(G) = \cup p(G,k)$ and summation running up to $d(G)$ [1,18].

The polynomial coefficients are calculable from the above defined layer/shell matrices, as the half sums on columns. When $p(v)$=1 (*i.e.*, the vertex counting), $p(G,k)$ denotes the number of pair vertices separated by distance k in G, and the classical Hosoya polynomial [19] is recovered (see below).

Some single number descriptors (*i.e.*, topological indices TIs) can be calculated by evaluating the polynomial derivatives (usually in x = 1):

$$P^k(G,1) = \sum\nolimits_k k! \cdot p(G,k) \tag{9}$$

Any square matrix can be used as an info matrix for the layer/shell matrices, thus resulting in an unlimited number of property polynomials. The property P can be taken either as a crude property (*i.e.*, column zero in **LM**) or within some weighting schemes. In the present paper we limit discussion to some graph theoretical properties.

3. Hosoya-Diudea polynomials

In the following, a polynomial will be named by specifying the info square matrix (if any) and the layer/shell matrix used to compute it.

Hosoya Polynomial

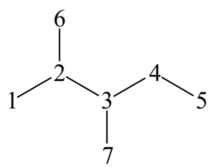
In the case: $p(v)=1$, **LM** = **LC**, (*i.e.*, layer matrix of counting) and the property polynomial $P(\mathbf{LC},x)$ is just the Hosoya $H(x)$ polynomial. The formulas given in the following represent well-known results. The index calculated as the polynomial first derivative is the well-known Wiener index [20], *W*.

$$W(G) = P'(\mathbf{LC},1) \tag{10}$$

The hyper-Wiener index *WW*, patterned by Randić [21], is calculated as

$$WW(G) = P'(\mathbf{LC},1) + (1/2)P''(\mathbf{LC},1) \tag{11}$$

For the graph G_1, the $P(\mathbf{LC},x)$ polynomial is given in Figure 1.



G_1

i/k	1	2	3	4
1	1	2	2	1
2	3	2	1	0
3	3	3	0	0
4	2	2	2	0
5	1	1	2	2
6	1	2	2	1
7	1	2	3	0
C	1	1	1	4
S	2	4	2	

Figure 1. The graph G_1 and its Hosoya polynomial

$$P(\mathbf{LC},x) = 6x + 7x^2 + 6x^3 + 2x^4$$

$$P'(\mathbf{LC},1) = W = 46;\ P''(\mathbf{LC},1) = 74;\ WW = 46 + 74/2 = 83$$

Shell Polynomials

Any square matrix **M**, taken as the info matrix to be treated by the Shell-operator [13,18,22], will provide a Shell matrix **ShM** and a corresponding Hosoya-Diudea polynomial, weighted by the property of info matrix. The polynomial coefficients are calculable from the shell matrices, as the half sums on columns. Hereafter, such a polynomial will be called a Shell-polynomial and symbolized $P(\mathbf{ShM},x)$ or $ShM(x)$.

Next, a new topological index, calculated on the first two Shell-polynomial derivatives (by analogy to WW - see (11)), was proposed [23-25]:

$$CT(ShM,G)=P'(\mathbf{ShM},1)+(1/2)P''(\mathbf{ShM},1) \quad (12)$$

It was named the ***Cluj-Tehran*** index and symbolized $CT(ShM,G)$ (with the specification of the info matrix **M**). Examples will be given in the following.

Info Matrix: DI (Distance)

The polynomial defined on the Sell of Distance matrix **ShDI** (given at the middle of Table 1) has the coefficients already multiplied by (topological) distance and then $P(\mathbf{ShDI},1)=P'(\mathbf{LC},1)=W$. Recall the half sum of entries in the Distance matrix D gives the well-known Wiener index W.

The Hyper-Wiener index is calculable on $P(\mathbf{ShDI},x)$ as:

$$WW(G)=[P(\mathbf{ShDI},1)+P'(\mathbf{ShDI},1)]/2 \quad (13)$$

and the relation is valid in any graph.

Table 1. Polynomial $P(\mathbf{ShDI},x)$ and CT index in G_1.

	ShDI(G_1)					**DI**(G_1)							
i \ *k*	1	2	3	4	*RS*	1	2	3	4	5	6	7	*RS*
1	1	4	6	4	15	0	1	2	3	4	2	3	15
2	3	4	3	0	10	1	0	1	2	3	1	2	10
3	3	6	0	0	9	2	1	0	1	2	2	1	9
4	2	4	6	0	12	3	2	1	0	1	3	2	12
5	1	2	6	8	17	4	3	2	1	0	4	3	17
6	1	4	6	4	15	2	1	2	3	4	0	3	15
7	1	4	9	0	14	3	2	1	2	3	3	0	14
CS	12	28	36	16	92	15	10	9	12	17	15	14	92

P(**ShDI**,x)	$6x +14x^2 +18x^3 +8x^4$	
P(1)	46	= W
P'(1)	120	= WW=(46+120)/2=83
P''(1)	232	
CT (*ShDI*)	236	

Info Matrix: $\mathbf{DI_p}$ (Distance path)

The matrix $\mathbf{DI}_p$ was proposed by Diudea [26] to count the “internal” paths existing between any pair of vertices (i,j) in G; it is provided, within the TOPOCLUJ software package [16], by the combinatorial matrix operator. The half sum of entries in the matrix $\mathbf{DI}_p$ gives the well-known hyper-Wiener index *WW*. More about this and other related matrices the reader can find in our recent book [25]. The derived polynomial $P(\mathbf{ShDI_p},x)$ shows $P(1)=WW$ (Table 2) while the 1[st] derivative is related to that of other polynomials (see below).

Table 2. Polynomial $P(\mathbf{ShDI_p},x)$ and corresponding *CT* index in G_1.

	ShDI$_\mathbf{p}$(G_1)					**DI**$_\mathbf{p}$(G_1)							
i \ *k*	1	2	3	4	*RS*	1	2	3	4	5	6	7	*RS*
1	1	6	12	10	29	0	1	3	6	10	3	6	29
2	3	6	6	0	15	1	0	1	3	6	1	3	15
3	3	9	0	0	12	3	1	0	1	3	3	1	12
4	2	6	12	0	20	6	3	1	0	1	6	3	20
5	1	3	12	20	36	10	6	3	1	0	10	6	36
6	1	6	12	10	29	3	1	3	6	10	0	6	29
7	1	6	18	0	25	6	3	1	3	6	6	0	25
CS	12	42	72	40	166	29	15	12	20	36	29	25	166

Table 2. (continued)

P(**ShDI**$_\mathbf{p}$,*x*)	6x	+21x^2	+36x^3	+20x^4
P(1)	83 = *WW*			
P'(1)	236			
P''(1)	498			
CT(*ShDI*$_p$)	485			

Info Matrix: $\mathbf{W}_p$ (Wiener path)

The matrix $\mathbf{W}_p$ was proposed by Randić [27], to count the "external" paths joining any pair of vertices (*i*,*j*) in *G*. This matrix is defined only in tree graphs and it is provided, within the TOPOCLUJ software package [16], as the **SCJ** matrix (see below). The half sum of entries in the matrix $\mathbf{W_p}$ gives the well-known hyper-Wiener index *WW*.

The polynomial $P(\mathbf{ShW}_p,x)$ shows $P(1)=WW$ (Table 3) while the 1[st] derivative is also related to that of other polynomials, as will be see in the following section.

Table 3. Polynomial $P(\mathbf{ShW_p},x)$ and corresponding *CT* index in G_1.

	ShW$_\mathbf{p}$(G$_1$)					**W**$_\mathbf{p}$(G$_1$)							
i \ *k*	1	2	3	4	*RS*	1	2	3	4	5	6	7	*RS*
1	6	5	3	1	15	0	6	4	2	1	1	1	15
2	24	9	3	0	36	6	0	12	6	3	6	3	36

3	28	13	0	0	41	4	12	0	10	5	4	6	41
4	16	8	4	0	28	2	6	10	0	6	2	2	28
5	6	5	4	2	17	1	3	5	6	0	1	1	17
6	6	5	3	1	15	1	6	4	2	1	0	1	15
7	6	5	3	0	14	1	3	6	2	1	1	0	14
CS	92	50	20	4	166	15	36	41	28	17	15	14	166

P(**ShW$_p$**,x)	46 x	+25x^2	+10x^3	+2x^4
P(1)	83 = *WW*			
P'(1)	134			
P''(1)	134			
CT(*ShW$_p$*)	201			

Info Matrix: UCJ (Unsymmetric Cluj)

A Cluj subgraph [1,13,17,22,25,28,29] $CJ_{i,j,p}$ collects the vertex proximities of *i* against any vertex *j*, joined by the path *p*, with the distances measured in the subgraph *G-p*:

$$CJ_{i,j,p} = \left\{ v \middle| v \in V(G); DI_{(G-p)}(i,v) < DI_{(G-p)}(j,v) \right\} \quad (13)$$

By definition, the entries in the Cluj matrix are taken, as the maximum cardinality among all such subgraphs, to limit the possibilities in the choice of p, in cycle-containing graphs:

$$[\mathbf{UCJ}]_{\boldsymbol{i,j}} = \max_{p} \left| CJ_{i,j,p} \right| \quad (14)$$

In trees, the paths joining any two vertices is unique, then $CJ_{i,j,p}$ represents the set of paths going to *j* through *i*. In this way, the path *p*(*i*,*j*) is characterized by a single endpoint, which is sufficient to calculate 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 in UCJDI. When path *p* belongs to the set of detours DE(G), the suffix is DE. In trees, due to the uniqueness of the paths, the two variants of Cluj matrices superimpose. When the matrix symbol is not followed by a suffix, it is implicitly DI. Thus, **UCJ** can be calculated on path $\mathbf{UCJ}_p$ or on edges $\mathbf{UCJ}_e$., the last one being obtained as the Hadamard pair-wise product of $\mathbf{UCJ}_p$ with the adjacency matrix A (having the entries 1 if the pair (*i*,*j*) belongs to *E*(*G*) or zero, otherwise):

$$\mathbf{UCJ}_a = \mathbf{UCJ}_p \bullet \mathbf{A} \quad (15)$$

The Cluj matrices are defined in any graph and, except for some symmetric graphs, are unsymmetric. They can be made symmetric by the Hadamard multiplication with their transposes:

$$\mathbf{SCJ}_p = \mathbf{UCJ}_p \bullet (\mathbf{UCJ}_p)^{\mathrm{T}} \quad (16)$$

The matrix $\mathbf{SCJ}_p$ is identical to $\mathbf{W_p}$ matrix (see above).

The Shell-Cluj polynomial $P(\mathbf{ShUCJ},x)$ is calculated only on the unsymmetric, on path calculated, matrix $\mathbf{UCJ}_p$ (or simply **UCJ**). The matrix **UCJ** and its corresponding shell for the graph G_1 are illustrated in Table 4.

In trees, there is interesting meaning of the descriptors derived from the Shell-Cluj polynomial (see the bottom of Table 4). These originate in the mixing information (both as in $\mathbf{DI_p}$ and $\mathbf{W_p}$) contained in **UCJ** matrix, which demonstrates the well-known theorem of Klein, Lukovits and Gutman [30], saying that, in a tree graph, the number of internal paths (given by $\mathbf{DI_p}$) equal that of external paths (calculated by $\mathbf{W_p}$).

In trees, the following relation is true:

$$m_k(\mathbf{ShUCJ}) = m_k(\mathbf{ShW}_\mathrm{p}) - m_{k+1}(\mathbf{ShW}_\mathrm{p}) \tag{17}$$

which says the coefficients of Shell-Cluj polynomial $P(\mathbf{ShUCJ},x)$ can be deduced from those of $P(\mathbf{ShW_p},x)$ polynomial. Also, the hyper-Wiener index can be expressed from the derivatives of the two above polynomials:

$$WW = (1/2)[3P'(\mathbf{ShW}_\mathrm{p}) - P'(\mathbf{ShDI}_\mathrm{p})] \tag{18}$$

In cycles, the above relations are no more valid, firstly because the matrix $\mathbf{W_p}$ is not defined. The meaning of the above descriptors is deeply different in cycle-containing graphs compared to trees [25].

Table 4. Polynomial $P(\mathbf{ShUCJ},x)$ and corresponding CT index in G_1.

	ShUCJ(G_1)					**UCJ**(G_1)							
i \ *k*	1	2	3	4	*RS*	1	2	3	4	5	6	7	*RS*
1	1	2	2	1	6	0	1	1	1	1	1	1	6
2	15	6	3	0	24	6	0	3	3	3	6	3	24
3	15	13	0	0	28	4	4	0	5	5	4	6	28
4	8	4	4	0	16	2	2	2	0	6	2	2	16
5	1	1	2	2	6	1	1	1	1	0	1	1	6
6	1	2	2	1	6	1	1	1	1	1	0	1	6
7	1	2	3	0	6	1	1	1	1	1	1	0	6
CS	42	30	16	4	92	15	10	9	12	17	15	14	92

P(**ShUCJ**,x)	$21x + 15x^2 + 8x^3 + 2x^4$	
P(1)	46	= W
P'(1)	83	= WW
P''(1)	102	= P' ($\mathbf{ShDI_p}$)-P'($\mathbf{ShW_p}$)
$CT(ShUCJ)$	134	= P'($\mathbf{ShW_p}$)

Info Matrix: DDI (Degree Distance)

The Cramer product of the diagonal matrix of vertex degrees **D** with the Distance matrix **DI** provides the matrix of degree distances denoted as **DDI**.

$$\mathbf{D}(G) \times \mathbf{DI}(G) = \mathbf{DDI}(G) \tag{19}$$

The above Cramer product (19) is equivalent (gives the same half sum of entries) with the pair-wise (Hadamard) product of the vectors "row sum" *RS* in the Adjacency **A** and Distance **DI** matrices, respectively [22,25].

$$RS(\mathbf{A}) \bullet RS(\mathbf{DI}) = RS(\mathbf{DDI}) \tag{20}$$

Next, by applying the Shell operator, we obtain the Shell matrix of *Degree-Distance*s **ShDDI**, of which column half sums are just the coefficients of the corresponding Shell-polynomial [25] $P(\mathbf{ShDDI}, x)$ (an example is given in Table 5)

Irrespective the above Cramer product (19) is performed "to the left" or "to the right", the Shell-polynomial $P(\mathbf{ShDDI}, x)$ remains always the same.

The half sum of entries in the **D**×**DI** or **DI**×**D** matrices is the well-known Degree-Distance *DDI*(*G*) index, defined by Dobrynin and Kochetova [31].

Table 5. Degree-Distance matrix **DDI** of the graph G_1 and its Shell matrix

	ShDDI(G_1)						**DDI**(G_1)							
i \ *k*	0	1	2	3	4	*RS*	1	2	3	4	5	6	7	*RS*
1	0	1	4	6	4	15	0	1	2	3	4	2	3	15
2	0	9	12	9	0	30	3	0	3	6	9	3	6	30
3	0	9	18	0	0	27	6	3	0	3	6	6	3	27
4	0	4	8	12	0	24	6	4	2	0	2	6	4	24
5	0	1	2	6	8	17	4	3	2	1	0	4	3	17
6	0	1	4	6	4	15	2	1	2	3	4	0	3	15
7	0	2	4	9	0	14	3	2	1	2	3	3	0	14
CS	0	26	52	48	16	142								14
							24	14	12	18	28	24	22	2

P(**ShDDI**,*x*)	13x	+26x^2	+24x^3	+8x^4	
P(1)					71
P'(1)					169
P"(1)					292
CT(*ShDDI*)					315

$$DDI(G) = \sum_{v \in V(G)} D(v) DI(v), \qquad (21)$$

where $D(v)$ and $DI(v)$ are just $RS(\mathbf{A}(v))$ and $RS(\mathbf{DI}(v))$, see (20). This index is in fact the non-trivial part of the Schultz index [25,32-34]. Accordingly, this index can be calculated as the half sum of entries within the matrices **A**×**DI** or **DI**×**A**. Next, by applying the Shell operator, we obtain the matrices **Sh(A×DI)** and **Sh(DI×A)** which differ from **ShDDI** and **ShDID** by the non-zero diagonals, of which information is lost in the first derivative of the corresponding Shell-polynomial. Even the $P(1)$ values are the same and equal to the values of index $DegD(G)$, in the following we will only calculate the polynomial $P(\mathbf{ShDDI},x)$.

Another reason is that the entries in **DDI** matrix have just the property defined by Dobrynin in (21). This matrix can also be obtained by Diudea's Walk operator [25,35]

$$\mathbf{D}(k)\mathbf{DI}(G) = \mathbf{W}_{(\mathbf{A},\mathbf{K},\mathbf{DI})} \qquad (22)$$

where **K** stands for the square matrix, of a pertinent order, having all the non-diagonal entries k while the diagonal entries zero; in case k=1, the classical $DDI(G)$ index is recovered. The walk operator $\mathbf{W}_{(\mathbf{M}1,\mathbf{M}2,\mathbf{M}3)}$ is defined as

$$[\mathbf{W}_{(\mathbf{M}_1,\mathbf{M}_2,\mathbf{M}_3)}]_{i,j} = RS(\mathbf{M}_1^{[\mathbf{M}_2]_{i,j}})_i [\mathbf{M}_3]_{i,j}. \qquad (23)$$

It works by Hadamard algebra and was extensively exemplified in refs [22,25,35]. (see also ref. [36]). The shell matrix of the walk operator $\mathbf{W}_{(\mathbf{A},\mathbf{K},\mathbf{DI})}$ is next illustrated in Table 6 (for k=1).

Relation (22), by setting k=1,..d(G), with $d(G)$ being the diameter of the graph, defines *Extended-Degree-Distance* matrices and corresponding Shell-polynomials $P(\mathbf{ShW}_{(\mathbf{A},\mathbf{K},\mathbf{DI})},x)$, recalling the "extended connectivity" developed at the pioneering age of Chemical Graph Theory by Balaban *et al*. [37-40] or by Morgan [41], for the Chemical Abstracts CA service.

Table 6. Shell matrix of $\mathbf{W}_{(\mathbf{A},\mathbf{K},\mathbf{DI})}$

$\mathbf{W}_{(\mathbf{A},1,\mathbf{DI})}(G_1)$

	1	2	3	4	5	6	7	RS
1	0	1	2	3	4	2	3	15
2	3	0	3	6	9	3	6	30
3	6	3	0	3	6	6	3	27
4	6	4	2	0	2	6	4	24
5	4	3	2	1	0	4	3	17
6	2	1	2	3	4	0	3	15

$\mathbf{ShW}_{(\mathbf{A},1,\mathbf{DI})}(G_1)$

	0	1	2	3	4	RS
1	0	1	4	6	4	15
2	0	9	12	9	0	30
3	0	9	18	0	0	27
4	0	4	8	12	0	24
5	0	1	2	6	8	17
6	0	1	4	6	4	15

7	3	2	1	2	3	3	0	14	7	0	1	4	9	0	14
CS	24	14	12	18	28	24	22	142	CS	0	26	52	48	16	142
1/2SUM = 71									P(1)	0	13	26	24	8	71
									P'(1)		13	52	72	32	169

Info Matrix: Shell-Degree-Cluj Polynomials

In full analogy to the Shell-degree-distance polynomial, one can write a modified relation (22), with the Cluj matrix instead of Distance matrix [25]:

$$\mathbf{D}(k)\mathbf{UCJ}(G) = \mathbf{W}_{(\mathbf{A},\mathbf{K},\mathbf{UCJ})} \tag{24}$$

The corresponding Shell-extended-degree-Cluj polynomial $P(\mathbf{ShW}_{(\mathbf{A},\mathbf{K},\mathbf{UCJ})},x)$ and derived indices are exemplified (for k=1) in Table 7.

Table 7. Shell matrix of $\mathbf{W}_{(\mathbf{A},\mathbf{K},\mathbf{UCJ})}$

$\mathbf{W}_{(\mathbf{A},1,\mathbf{UCJ})}(G_1)$

	1	2	3	4	5	6	7	*RS*
1	0	1	1	1	1	1	1	6
2	18	0	9	9	9	18	9	72
3	12	12	0	15	15	12	18	84
4	4	4	4	0	12	4	4	32
5	1	1	1	1	0	1	1	6
6	1	1	1	1	1	0	1	6
7	1	1	1	1	1	1	0	6
CS	37	20	17	28	39	37	34	212

1/2SUM = 106

$\mathbf{ShW}_{(\mathbf{A},1,\mathbf{UCJ})}(G_1)$

	0	1	2	3	4	*RS*
1	0	1	2	2	1	6
2	0	45	18	9	0	72
3	0	45	39	0	0	84
4	0	16	8	8	0	32
5	0	1	1	2	2	6
6	0	1	2	2	1	6
7	0	1	2	3	0	6
CS	0	110	72	26	4	212
P(1)	0	55	36	13	2	106
P'(1)	0	55	72	39	8	174
P''(1)		0	72	78	24	174
CT=261						

Since the matrix UCJ is a non-symmetric one, we can use in (24) its transpose. The corresponding Shell-extended-degree-Cluj-T polynomial $P(\mathbf{ShW}_{(\mathbf{A},\mathbf{K},\mathbf{UCJT})},x)$ and derived indices are exemplified (for k=1) in Table 8.

Table 8. Shell matrix of $\mathbf{W}_{(\mathbf{A},\mathbf{K},\mathbf{UCJT})}$

$\mathbf{W}_{(\mathbf{A},1,\mathbf{UCJT})}(G_1)$

	1	2	3	4	5	6	7	*RS*
1	0	6	4	2	1	1	1	15
2	3	0	12	6	3	3	3	30
3	3	9	0	6	3	3	3	27
4	2	6	10	0	2	2	2	24
5	1	3	5	6	0	1	1	17
6	1	6	4	2	1	0	1	15
7	1	3	6	2	1	1	0	14
CS	11	33	41	24	11	11	11	142

1/2SUM = 71

$\mathbf{ShW}_{(\mathbf{A},1,\mathbf{UCJT})}(G_1)$

	0	1	2	3	4	*RS*
1	0	6	5	3	1	15
2	0	18	9	3	0	30
3	0	18	9	0	0	27
4	0	12	8	4	0	24
5	0	6	5	4	2	17
6	0	6	5	3	1	15
7	0	6	5	3	0	14
CS	0	72	46	20	4	142
P(1)	0	36	23	10	2	71
P'(1)	0	36	46	30	8	120
P''(1)		0	46	60	24	130

CT=185

Info Matrix: D(k_r)M (Remote Degree Matrix)

Let's now consider the remote valences $D(k_r)$ defined as the number of neighbors at distance $d(i,j)=r$, $r=1,2,...d(G)$ [25]. They can be calculated as row sums *RS* in the corresponding remote Adjacency matrices $\mathbf{A}_r$. Then, the extension of these remote valences can be achieved as

$$\mathbf{D}(k_r)\mathbf{M}(G) = \mathbf{W}_{(\mathbf{A}_r,\mathbf{K},\mathbf{M})} \qquad (25)$$

where $k,r=1,2,...d(G)$; next, r-different Shell-polynomials $P(\mathbf{ShW}_{(\mathbf{A}_r,\mathbf{K},\mathbf{M})},x)$ can be calculated. An example is given, for **M**=**DI**, r=2; k=1, in Table 9.

Table 9. Shell matrix of $\mathbf{W}_{(\mathbf{A2},1,\mathbf{DI})}$

$\mathbf{W}_{(\mathbf{A2},1,\mathbf{DI})}(G_1)$

	1	2	3	4	5	6	7	*RS*
1	0	2	4	6	8	4	6	30
2	2	0	2	4	6	2	4	20
3	6	3	0	3	6	6	3	27
4	6	4	2	0	2	6	4	24
5	4	3	2	1	0	4	3	17
6	4	2	4	6	8	0	6	30
7	6	4	2	4	6	6	0	28

$\mathbf{ShW}_{(\mathbf{A2},1,\mathbf{DI})}(G_1)$

	0	1	2	3	4	*RS*
1	0	2	8	12	8	30
2	0	6	8	6	0	20
3	0	9	18	0	0	27
4	0	4	8	12	0	24
5	0	1	2	6	8	17
6	0	2	8	12	8	30
7	0	2	8	18	0	28

28	18	16	24	36	28	26	176	*CS*	0	26	60	66	24	176
1/2SUM = 88								P(1)	0	13	30	33	12	88
								P'(1)	0	13	60	99	48	220

4. Cluj-centrality CJC index

On the above defined Shell-polynomials, a Centrality super-index was defined [25]:

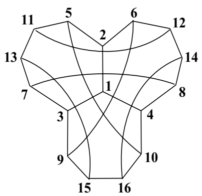
$$\boldsymbol{CJC}(G) = (1/kr)\sum\nolimits_{k,r}[RC(\mathbf{ShW}_{(\mathbf{A}_r,\mathbf{K},\mathbf{M})})]^s \qquad (26)$$

In the above relation, $C(\mathbf{ShM})$ is the centrality function [13-15, 42]:

$$C(\mathbf{ShM})_i = \left[\sum_{k=1}^{ecc_i}\left(\left[\mathbf{ShM}\right]_{ik}^{2k}\right)^{1/(ecc_i)^2}\right]^{-1} \qquad (27)$$

$$RC(\mathbf{ShM}) = (1/|V(G)|\sum_i\{[C(\mathbf{ShM})_i]/\max[C(\mathbf{ShM})_i]\} \qquad (28)$$

The indices of centrality are exemplified, for s=1, in case of graph G_2, in Tables 10 and 11.



G_2. DDS_i: 3 6 6

Table 10. Centrality indices for G_2: **M**=**DI**

	A1,1,DI	A1,2,DI	A1,3,DI	A2,1,DI	A2,2,DI	A2,3,DI	A3,1,DI	A3,2,DI	A3,3,DI
1	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
2	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
3	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
4	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
5	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
6	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
7	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
8	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
9	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
10	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
11	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
12	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
13	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421

14	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
15	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
16	0.048001	0.02512	0.012899	0.021132	0.004545	0.000927	0.0165282	0.002717	0.000421
RC	1	1	1	1	1	1	1	1	1
EC	16	16	16	16	16	16	16	16	16
CJC(DI,G_2)=1									

Table 11. Centrality indices for G_2: **M**=**UCJ**

	A1,1,UCJ	**A1,2,UCJ**	**A1,3,UCJ**	**A2,1,UCJ**	**A2,2,UCJ**	**A2,3,UCJ**	**A3,1,UCJ**	**A3,2,UCJ**	**A3,3,UCJ**
1	0.959767	0.953534	0.948127	0.952041	0.941477	0.934615	0.950032	0.93886	0.932394
2	1	1	1	1	1	1	1	1	1
3	0.983054	0.979570	0.976347	0.978700	0.972171	0.967628	0.977509	0.970446	0.965845
4	0.983054	0.979570	0.976347	0.978700	0.972171	0.967628	0.977509	0.970446	0.965845
5	0.990549	0.986283	0.982176	0.985182	0.976650	0.970513	0.983664	0.974346	0.968310
6	1	1	1	1	1	1	1	1	1
7	0.983054	0.979570	0.976347	0.978700	0.972171	0.967628	0.977509	0.970446	0.965845
8	0.990549	0.986283	0.982176	0.985182	0.976650	0.970513	0.983664	0.974346	0.968310
9	1	1	1	1	1	1	1	1	1
10	0.983054	0.979570	0.976347	0.978700	0.972171	0.967628	0.977509	0.970446	0.965845
11	0.990549	0.986283	0.982176	0.985182	0.976650	0.970513	0.983664	0.974346	0.968310
12	0.990549	0.986283	0.982176	0.985182	0.976650	0.970513	0.983664	0.974346	0.968310
13	0.983054	0.979570	0.976347	0.978700	0.972171	0.967628	0.977509	0.970446	0.965845
14	0.983054	0.979570	0.976347	0.978700	0.972171	0.967628	0.977509	0.970446	0.965845
15	0.990549	0.986283	0.982176	0.985182	0.976650	0.970513	0.983664	0.974346	0.968310
16	0.990549	0.986283	0.982176	0.985182	0.976650	0.970513	0.983664	0.974346	0.968310
RC	0.987587	0.984291	0.981204	0.983458	0.977150	0.972716	0.982317	0.975476	0.971083
EC	1,3,6,6	1,3,6,6	1,3,6,6	1,3,6,6	1,3,6,6	1,3,6,6	1,3,6,6	1,3,6,6	1,3,6,6
CJC(UCJ,G_2)=0.979476									

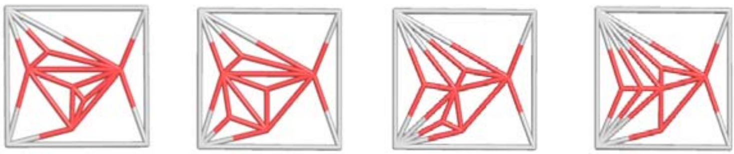
Since the Distance Degree Sequence of any vertex in G_2 is DDS_i: 3 6 6, it is immediate the equivalence of all vertices, the population of this single equivalence class is *EC*=16 and the (global) relative centrality *RC*=1. However, the Cluj matrix **UCJ** is able to discriminate among the vertices of G_2, thus the global centrality is less than unity, by this criterion, as shown in Table 11; deviation to the *full centrality* is rather low (*FCD*=0.020). The population on the equivalence classes is given at the bottom of the above table.

5. Discriminating ability of CJC index

The CJC index can be used to discriminate/compare complex structures, as the quadruplet H10Q(11 to 44 - Figure 2) presented by Hosoya as *isospectral* structures with respect to the adjacency **A** matrix. This quadruplet, identified in the paper of Hosoya *et al.* [43] as: 29368=Q_11; 31037=Q_22; 31706=Q_33 and 31851=Q_44 can not be solved

neither by matrices $ShW_{(A1,1,DI)}$ and $ShW_{(A2,1,DI)}$ nor by their higher analogues, as provided by the *CJN*
super index [25], **M**=**DI**.

This quadruplet, showing degeneracy of $\mathbf{A}_1$ matrix, is not uniform: it consists of two sub-sets, partition depending on the degeneracy of considered matrix: **DI** [(11&44);(22&33)]; **DE** [(11&22)FHD;(33&44)]; **CJDE** [(11&22)FHD;(33&44)] and also $W_{(A1,1,DE)}$(33&44). Correspondingly, are the Distance Degree Sequence *DDS*: [(11&44), 22, 23]; [(22&33), 22, 22, 1]; the Wiener index *W*: [(11&44), 68]; [(22&33), 69]; the Detour index *w*: [(11&22), 405]; [(33&44), 399]; *CJDE*: [(11&22), 45]; [(33&44), 52].



H10Q_11 H10Q_22 H10Q_33 H10Q_44

Figure 2. Isospectral quartet of 10 vertices (Hosoya *et al.*[31])

The values of centrality indices are listed in Tables 12 and 13. As a first remark, our descriptors are able to discriminate this complex set of graphs.

According to the first proximities (r=1): Q_22(**DI**: 0.8910)>Q_33(**DI**: 0.8902)> Q_44(**DI**: 0.8783) > Q_11(**DI**: 0.6191) and to *CJC*: Q_44(**DI**: 0.5834)>Q_33(**DI**: 0.5437)> Q_22(**DI**: 0.5342)> Q_11(**DI**: 0.3556). This means that the remote neighborhoods are distributed by the centrality function in a more diverse manner. The *CJC* index can be used as a test of the homogeny of graphs, in a given criterion (**DI-**criterion, in the above).

In the **UCJ-**criterion (r=1): Q_44(UCJ: 0.8783)>Q_33(UCJ: 0.7802)>Q_22(UCJ: 0.7781)>Q_11(0.7381) and *CJC*: Q_44(UCJ: 0.6163)>Q_33(UCJ: 0.5420)>Q_22(UCJ: 0.5232)>Q_11(0.4396) the distribution at the first proximities is kept to the global *CJC* index and is the same as for *CJC* in the **DI** criterion. It is, perhaps, due to the fact the Cluj subgraphs include information of first and remote proximities at once, so that the distribution by centrality function is quite the same for all included subgraphs.

Table 12. Sums of Relative Centrality ***RC*** , average ***RC_AV*** and ***CJC*** indices for the graphs **H10Q_11** and **H10Q_44**: **M=DI**; **UCJ**

	A1,1,M	**A1,2,M**	**A2,1,M**	**A2,2,M**	***RC_AV***	***CJC***
	DI	**DI**	**DI**	**DI**	**DI**	**DI**
***RC*(Q_11)**	6.190536	4.50088	1.912452	1.619195	3.555766	
	0.619054	0.450088	0.191245	0.161920		0.355577
***RC*(Q_44)**	8.782636	7.331955	3.569239	3.650173	5.833501	
	0.878264	0.733196	0.356924	0.365017		0.583350
	UCJ	**UCJ**	**UCJ**	**UCJ**	**UCJ**	**UCJ**
***RC*(Q_11)**	7.380789	6.187785	2.193209	1.821228	4.395753	
	0.738079	0.618779	0.219321	0.182123		0.439575
***RC*(Q_44)**	8.782636	7.1806206	4.271030	4.418795	6.163271	
	0.878264	0.7180621	0.427103	0.441880		0.616327

Table 13. Sums of Relative Centrality ***RC*** , average ***RC_{AV}*** and ***CJC*** indices for the graphs **H10Q_22** and **H10Q_33**: **M=DI**; **UCJ**

	A1,1,M	**A1,2,M**	**A1,3,M**	**A2,1,M**	**A2,2,M**	**A2,3,M**	**A3,1,M**	**A3,2,M**	**A3,3,M**	***RC_{AV}***	***CJC***
	DI	**DI**	**DI**	**DI**	**DI**	**DI**	**DI**	**DI**	**DI**	**DI**	**DI**
***RC*(Q_22)**	8.9101	8.1153	8.0299	6.1015	5.5904	5.3322	2	2	2	5.3422	
	0.8910	0.8115	0.8030	0.6101	0.5590	0.5332	0.2	0.2	0.2		0.5342
***RC*(Q_33)**	8.9022	8.3069	8.1796	6.0570	5.9529	5.5322	2	2	2	5.4367	
	0.8902	0.8307	0.8180	0.6057	0.5953	0.5532	0.2	0.2	0.2		0.5437
	UCJ	**UCJ**	**UCJ**	**UCJ**	**UCJ**	**UCJ**	**UCJ**	**UCJ**	**UCJ**	**UCJ**	**UCJ**
***RC*(Q_22)**	7.7808	7.4279	7.0557	6.8142	6.2041	5.8741	1.9780	1.9780	1.9780	5.2323	
	0.7781	0.7428	0.7056	0.6814	0.6204	0.5874	0.1978	0.1978	0.1978		0.5232
***RC*(Q_33)**	7.8025	7.4396	7.0704	7.0544	6.9635	6.4716	1.9937	1.9937	1.9937	5.4203	
	0.7802	0.7440	0.7070	0.7054	0.6963	0.6472	0.1994	0.1994	0.1994		0.5420

We can say that the **UCJ**-criterion is a more reliable criterion in searching the homogeny of graphs by our centrality function. Further investigations are needed to find the usefulness of these theoretical tools.

6. Conclusions

Extension of the well-known Hosoya polynomial, grounded on vertex distance partitions of a graph, resulted in a novel class of distance property polynomials *P*(**ShM**,*x*) (called Shell-polynomials) which are Hosoya polynomials weighted by the property enclosed in the info matrix **M**.

The polynomial coefficients are obtained as the column half sums in the shell matrices. Examples were given for each studied case.

The single number descriptors calculated from polynomials defined on any combination **ShM** are actually tested in our labs in QSAR/QSPR studies.

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