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Dedicated to Professor Ionel Haiduc
on the occasion of his 65th birthday

CLUJ POLYNOMIALS

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ABSTRACT. A novel class of distance property polynomials *P*(*G*,*x*) is proposed, as an extension of the well-known Hosoya polynomial. The polynomial coefficients are calculated by means of layer/shell matrices, built up according to the vertex distance partitions of a graph. Basic definitions and properties for the Cluj matrices and corresponding polynomials, as particular cases of the distance property polynomial, are given.

INTRODUCTION

A graph can be described by: a connection table, a sequence of numbers, a derived number (called sometimes a topological index), a matrix, or a polynomial. Quantum chemistry was the first field in Chemistry that used the polynomial description of a molecular graph. In the early Hűckel theory, the roots of the most studied *characteristic polynomial*:

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

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 are: Topological Resonance Energy TRE, Topological Effect on Molecular Orbitals, TEMO, the Aromatic Sextet Theory, AST, the Kekulé Structure Count, KSC, *etc*.[1-3]

The coefficients a_k of the characteristic polynomial of order N are calculable from the graph G on N vertices:

$$Ch(G,x) = \sum_{k=0}^{N} a_k(G) \cdot x^{N-k} \tag{2}$$

Relation (2), found independently by Sachs, Harary, Milić, Spialter, *etc*.,[2] makes use of the *Sachs graphs*, contained as subgraphs in *G*. More efficient are the numeric methods of linear algebra, such as the recursive algorithms of Le Verier, Frame, or Fadeev.[4,5]

An extension of relation (1) was made by Hosoya[6] and others[7-10] by changing the adjacency matrix with the distance matrix and next by any square topological matrix.

A different field using the polynomial description is that of finite sequences[2] 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 polynomial roots and coefficients are used for characterization of the topological nature of hydrocarbons.[2,3,11]

The present paper introduces novel distance-based sequence polynomials whose coefficients are calculable from two kinds of layer matrices.

BASIC DEFINITIONS

Define a *distance property polynomial* as:

$$P(G,x) = \sum_{k=0}^{d(G)} p(G,k) \cdot x^k \tag{3}$$

with $p(G,0) = P = \sum_i p_i$. In relation (1), $p(G,k)$ is twice the contribution to the global (molecular) property $P=P(G)$ of the vertex pairs located at distance k from each other, in the graph G. The summation runs from zero to $d(G)$, which is the *diameter* of G or the longest distance in the graph.[2,12]

When the local property p_i = 1 (*i.e.*, the vertex cardinality), $p(G,k)$ denotes the number of pair vertices separated by distance k in G, and the classical Hosoya polynomial[13] (more exactly twice this polynomial) is recovered. In this case, $p(G,0) = N$, where N stands for the number of vertices in the hydrogen depleted molecular graph.

The polynomial coefficients $p(G,k)$ are calculable as the column sums in the layer matrices **LM** and **SM**. They are non-square arrays collecting *shells of property*, located at distance k around each vertex.

Let us define the k^{th} layer/shell of vertices v with respect to the vertex i as:

$$G(i)_k = \left\{ v \middle| \; v \in V(G); \quad d_{iv} = k \right\} \tag{4}$$

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

$$G(i) = \left\{ G(i)_k \; ; \, k \in [0,1,..,ecc_i] \right\} \tag{5}$$

with ecc_i being the *eccentricity* of i (*i.e.*, the largest distance from i to the other vertices in G). Since **LM** was defined elsewhere,[14] (see also ref. 15) we give here only the *shell matrix* **SM**, the entries of which are defined as:

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

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:

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

The zero column vector $[\mathbf{SM}]_{i,0}$ collects the diagonal entries in the parent square matrix. In the case that they are zero, by definition, $[\mathbf{SM}]_{i,0}$ =1. The property p_i is usually introduced by means of the zero column. An example is given for the shell Cluj matrix of the graph 1 (see below).

The name of a property polynomial is built up by exchanging the letter *P* for a string including: L (or S) for the type of layer matrix, symbol of the *info matrix* **M**, and the local property p_i. For example, *SUCJ*(*G,x*) reads: the polynomial of the Shell, Unsymmetric Cluj matrix (see below). In the case of a graph theoretical property, p_i is implicitly 1, and therefore omitted.

Vertex contributions to the global polynomial can be written as:

$$P(i,x) = \sum_{k=0}^{d(G)} p(i,k) \cdot x^k \tag{8}$$

where *p*(*i,k*) is the contribution of vertex *i* to the partition *p*(*G,k*) of the global molecular property *P*. Note that *p*(*i,k*)'s are just the entries in **LM** or **SM**.

Usually, the contribution of vertices (*i.e.*, atoms) to the molecular property vary in a molecular graph, so that the polynomial for the whole molecule is obtained by summing all atomic contributions:

$$P(G,x) = \sum\nolimits_i P(i,x) \tag{9}$$

In a vertex transitive graph, the vertex contribution is simply multiplied by *N*:

$$P(G,x) = N \cdot P(i,x) \tag{10}$$

A *distance-extended property* can be calculated by evaluating the *first derivative* of the polynomial, for *x* = 1:

$$P'(G,1) = \sum_{k=1}^{d(G)} k \cdot p(G,k) = D\_P(G) \tag{11}$$

Any square matrix can be used as an info matrix for the layer 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 scheme (*i.e.*, transformed by the sequence: **W**-operator **W**(**M**1,**M**2,**M**3), **W**(**M**) matrix, **LM**/**SM**).[2] In the present paper we limit discussion to some graph theoretical properties. Various property polynomials, using physico-chemical properties are exposed in a following paper.[16]

HOSOYA-LIKE POLYNOMIAL

In the case: $p_i = 1$, **LM** = **LC**, (*i.e.*, layer matrix of cardinalities) and the property polynomial, called the cardinality polynomial $C(G,x)$, is twice the Hosoya polynomial. The formulas given in the following represent well-known results.[13,17,18]

The index calculated as the polynomial first derivative[13,19] is (twice) the well-known Wiener index,[20] W. It is just a distance-extended property.

$$C'(G,1) = \sum_{k=1}^{d(G)} k \cdot p(G,k) = 2 \cdot W \qquad (12)$$

The hyper-Wiener index WW, originated by Randić,[21] is calculated as:

$$WW(G) = W(G) + \Delta(G) \qquad (13)$$

where $\Delta(G)$ is the non-Wiener part[22,23] of the hyper-Wiener number, calculable from the second derivative[17] of the Hosoya polynomial.

$$WW(G) = H'(G,1) + (1/2)H''(G,1) \qquad (14)$$

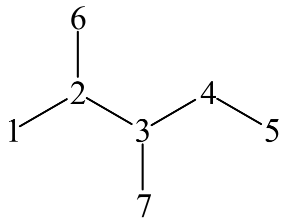
In terms of $C(G,x)$, the relation is trivially deduced from (14):

$$WW(G) = (1/2) \cdot C'(G,1) + (1/4)C''(G,1) \qquad (15)$$

For the graph G_1, the Cardinality polynomial is:

$$C(G,x) = LC(G,x) = 7 + 12x + 14x^2 + 12x^3 + 4x^4 \qquad (16)$$

Real Roots = -0.723, -0.723, -0.134, -0.134.



G_1

CLUJ POLYNOMIALS

Cluj polynomials, as particular cases of the distance property polynomial, make use of the shell matrix **SM** for re-arrange the basic Cluj matrices.

Define the *Cluj fragments*[2,23] $CJ_{i,j,p}$ as the set of vertices v lying closer to i than to j and at least one path $p(i,v)$ exists so that it intersects the path $p(i,j)$ at most in i.

$$CJ_{i,j,p} = \left\{v \middle| v \in V(G);\, d(G)_{i,v} < d(G)_{j,v};\, \text{and } \exists\ p(i,v) \cap p(i,j) = \{i\}\right\} \quad (17)$$

The above definition holds in any undirected graph. The intersecting condition means at least one path $p(i,v)$ is external to the "prohibited" path $p(i,j)$. In trees, due to the unicity of paths joining any two vertices, $CJ_{i,j,p}$ means the number of paths going to j through i. In this way, we characterize the path $p(i,j)$, designed as p hereafter, by a single endpoint, that suffices for the unsymmetric Cluj matrix **UCJ**.[23]

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/sets:

$$[\mathbf{UCJ}]_{\boldsymbol{i,j}} = \max_{p} \left| CJ_{i,j,p} \right| \quad (18)$$

When the path p belongs to the set of *distances* (*i.e.*, geodesics) $D(G)$, the corresponding Cluj matrix is designed as **UCJDi**. When $p \in \Delta(G)$ (*i.e.*, detours), the symbol will be **UCJDe**.

A variant of Cluj fragmentation,[2,24] called $CF_{i,j,p}$ considers all the paths $p(i,v)$ external to $p(i,j)$. It is possible by cutting the "prohibited" path $p(i,j)$, excepting its endpoints. Thus, relation (17) becomes:

$$CF_{i,j,p} = \left\{v \middle| v \in V(G);\, d(G_p)_{i,v} < d(G_p)_{j,v};\ G_p = G - p(i,j)\right\} \quad (19)$$

Relation (18) also holds, in terms of *CF* fragments. The corresponding matrices, denoted by **UCFDi** and **UCFDe**, are in general unsymmetric, apart from some symmetric graphs. This is also true for the **CJ** matrices. They can be made symmetric by the Hadamard multiplication with their transposes:

$$\mathbf{M}_p = \mathbf{UM} \bullet (\mathbf{UM})^{\mathrm{T}} \quad (20)$$

$$\mathbf{M}_e = \mathbf{M}_p \bullet \mathbf{A} \quad (21)$$

The subscript p means that the matrix is defined on paths (*i.e.*, on all pair vertices) while e designates an edge defined matrix. Note that, in trees, the four variants of Cluj matrices are one and the same, so that the symbol **CJ** (unless otherwise specified) will hereafter be used. Only tree graphs are considered here. The shell matrix and its parent **UCJ** for the graph 1 are illustrated in Table 1. Relations for the column sums are given in the bottom of the table.

Table 1

SUCJ(G_1)								**UCJ**(G_1)							
i \ *k*	0	1	2	3	4	$\sum_{k=1}^{d(G)}$		1	2	3	4	5	6	7	*RS*
1	1	1	2	2	1	6		0	1	1	1	1	1	1	6
2	1	15	6	3	0	24		6	0	3	3	3	6	3	24
3	1	15	13	0	0	28		4	4	0	5	5	4	6	28
4	1	8	4	4	0	16		2	2	2	0	6	2	2	16
5	1	1	1	2	2	6		1	1	1	1	0	1	1	6
6	1	1	2	2	1	6		1	1	1	1	1	0	1	6
7	1	1	2	3	0	6		1	1	1	1	1	1	0	6
CS	7	42	30	16	4	92[a]	*CS*	15	10	9	12	17	15	14	92
CS·k		42	60	48	16	166[b]									

(a) 2x*W*; (b) 2x*WW*

For the graph G_1, several Cluj polynomials are exemplified:

$$SUCJ(G,x) = 7 + 42x + 30x^2 + 16x^3 + 4x^4 \tag{22}$$

Real roots = -5.264 -0.389 -0.173 -0.173

$$SURCJ(G,x) = 7 + 8.656x + 5.645x^2 + 3.642x^3 + 0.916x^4 \tag{23}$$

Real roots = -0.783 -0.391 -0.031 -0.031

$$SCJ(G,x) = 7 + 92x + 50x^2 + 20x^3 + 4x^4 \tag{24}$$

Real roots = -12.593 -0.305 -0.122 -0.122

$$SIUCJ(G,x) = -3.975 - 1.804x + 2.464x^2 + 3.225x^3 + x^4 \tag{25}$$

Real roots = -0.515 -0.515 -0.486 1.061

$$SWUCJ(G,x) = 92 + 42x + 30x^2 + 16x^3 + 4x^4 \tag{26}$$

Real roots = -0.324 -0.324 0.096 0.096

In the above polynomials, the matrices are as follows: unsymmetric Cluj (22); unsymmetric reciprocal Cluj (23); symmetric Cluj (24); inverse unsymmetric Cluj (25) and walk (of rank 1) of unsymmetric Cluj (26). The free term in (22) to (24) equals the number of vertices in *G*, which is taken by definition for the zero diagonal matrices. The different free term in the last two examples indicates matrices having non-zero diagonals. The diagonal entries in the walk matrix of rank *e* (relation 26) equals the row sum in the matrix **M** raised to the power *e*, $[{}^{e}\mathbf{WM}]_{ii} = R(\mathbf{M}^{e})_i$. Note that in (26) the free term is twice the Wiener number.

The walk matrix **W**(**M**) is constructed by following the $^{e}\mathbf{WM}$ algorithm,[14] extended for walk count in general graphs and any square matrix. The walk matrix together with the triple matrix walk operator[25] **W**(**M**1,**M**2,**M**3) is used for mixing the info matrices and weighting the topological descriptors (property polynomials included) by various physico-chemical attributes. Details are given in a following paper of this topic.[16] The calculations were performed by the TOPOCLUJ software package.

* * *

Reverting to the polynomials, the distance-extended property, calculated on the Cluj polynomial (*cf*. (11)), is, in trees, twice the hyper-Wiener index:

$$SUCJ'(G,1) = 2 \cdot WW \tag{27}$$

The sum of polynomial coefficients (for $k > 0$) gives twice the Wiener index:

$$SUCJ(G,1,)_{k>0} = 2 \cdot W \tag{28}$$

In case of *SUCJ*(*G*,*x*), the non-Wiener part of the hyper-Wiener index is:

$$2 \cdot \Delta(G) = SUCJ'(G,1) - SUCJ(G,1,)_{k>0} \tag{29}$$

In case of a symmetric Cluj matrix, the sum of polynomial coefficients gives twice the hyper-Wiener index:

$$SCJ(G,1)_{k>0} = 2 \cdot WW \tag{30}$$

The distance-extended property leads, in this case, to twice the Tratch index.[26]

The non-Wiener part of the hyper-Wiener index $\Delta(G)$ (see eq 13) is now obtained as the difference of the Cluj polynomial coefficients for the symmetric **CJ** and unsymmetric **UCJ** matrices.

$$2 \cdot \Delta(G) = SCJ(G,1) - SUCJ(G,1) \tag{31}$$

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*(*G*,*x*). The polynomial coefficients are obtained as the column sums in the layer/shell matrices. The polynomial roots and coefficients can be used for the topological (and chemical) characterization of chemical structures. Examples were given for the Cluj matrices and corresponding polynomials.

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