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Cluj-Tehran Index

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Abstract

A novel topological index, called Cluj-Tehran *CT*, is defined on the ground of Shell polynomials. The polynomial coefficients are calculated by means of Shell matrices, built up according to the vertex distance partitions of a graph. Close formulas for calculating the Shell polynomial in case of Cluj matrices and the corresponding Cluj-Tehran *CT* index in several particular classes of graphs are given.

Introduction

Finite sequences of some graph invariants, such as the distance degree sequence or the sequence of the number of *k*-independent edge sets can be written as polynomials, as was introduced by Hosoya with his Z-counting polynomial.[1] Later, a variety of counting polynomials have been defined and their properties investigated.[2-6] Interested readers are invited to consult some recent books in the field.[7-10]

Among the counting polynomial, of particular interest proved to be the Shell polynomials, proposed by Diudea,[11] which are Hosoya polynomials[12] weighted with

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topological or physico-chemical local properties, useful in Mathematical Chemistry and correlating studies.

Let's define the entries in a *Shell matrix* **ShM** as:[8,13]

$$[\mathbf{ShM}]_{i,k} = \sum_{v|d_{i,v}=k} [\mathbf{M}]_{i,v} \tag{1}$$

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:

$$\mathbf{ShM} = \left\{ [\mathbf{ShM}]_{i,k}\,;\, i \in V(G);\, k \in [0,1,..,d(G)] \right\} \tag{2}$$

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

Define now the Shell polynomial[10,11] as:

$$ShM(x) = \sum_k p(G,k) \cdot x^k \tag{3}$$

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 $d(G)$.

The polynomial coefficients are calculable from the above defined shell matrices, as the half sums on columns. Any square matrix M can be used as info matrix in calculating the Shell-polynomials.

Cluj-Tehran index

On the ground of Shell polynomials and the first two derivatives, in x=1, we define here the Cluj-Tehran index[10] as:

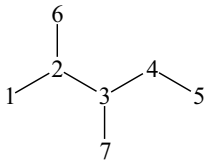
$$CT(ShM,G) = ShM'(1) + (1/2)ShM''(1) \tag{4}$$

The formula is the same as that used in calculating the Hyper-Wienner *WW* index[14] on Hosoya polynomial, with the difference the actual index is more general; in the name of actual index, the name/symbol of the info matrix must be specified.

The index *WW* can be obtained from the *ShD(x)* as the half sum of the zero and first derivatives, in x=1:

$$WW(G) = [ShD(1) + ShD'(1)]/2 \tag{5}$$

Relation (5) is true in any graph. Note, the value of *ShD(x)*, in x=1, equals the Wiener index[15] $W(G)$. The above formulas are exemplified on the graph G_1 in Table 1.



G_1

Table 1. Polynomial $ShD(x)$ and CT index in G_1.

	ShD(G_1)					**D**(G_1)							
$i \setminus k$	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

$ShD(x)$	$6x$ $+14x^2$ $+18x^3$ $+8x^4$		
$P(1,G_1)$	46	*W*	
$P^{`}(1,G_1)$	120	*WW*=(46+120)/2=83	
$P^{``}(1,G_1)$	232		
CT (*ShD*)	236		

Shell-Cluj polynomial

A Cluj fragment[7,10,16] $CJ_{i,j,p}$ collects vertices v lying closer to i than to j, the endpoints of a path $p(i,j)$. It collects the vertex proximities of i against any vertex j, joined by the path p, with the distances measured in the subgraph G-p:

$$CJ_{i,j,p} = \left\{ v \middle| v \in V(G);\, D_{(G-p)}(i,v) < D_{(G-p)}(j,v) \right\} \tag{6}$$

In graphs containing rings, 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). The entries in the Cluj matrix are taken, by definition, as the maximum cardinality among all such fragments:

$$\mathbf{[UCJ]}_{\boldsymbol{i,j}} = \max_{p} \left| CJ_{i,j,p} \right| \tag{7}$$

In trees, due to the unique nature of paths joining any two vertices, $CJ_{i,j,p}$ 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):

$$\mathbf{UCJ}_e = \mathbf{UCJ}_p \bullet \mathbf{A} \tag{8}$$

The Cluj matrices are defined in any graph; they are non-symmetric matrices, excepting some symmetric graphs, when are symmetric ones. They can be symmetrized by the Hadamard multiplication with the corresponding transposes:

$$\mathbf{SCJ}_p = \mathbf{UCJ}_p \bullet (\mathbf{UCJ}_p)^{\mathrm{T}} \tag{9}$$

To calculate the Shell-Cluj polynomial $ShUCJ(x)$, only the unsymmetric matrix **UCJ** will be used. It is worthy mentioned that, in tree graphs, the polynomial derivatives, in x=1, are: $P(1,G)=W(G)$ and $P'(1,G)=WW(G)$, properties which come out from the properties of Cluj matrices. The above formulas are exemplified on the graph G_1 in Table 2.

Table 2. Polynomial $ShUCJ(x)$ and CT index in G_1.

	ShUCJ(G_1)					**UCJ**(G_1)							
$i \setminus k$	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
$ShUCJ(x)$	$21x$	$+15x^2$	$+8x^3$	$+2x^4$									
$P(1,G_1)$					46	*W*							
$P'(1,G_1)$					83	*WW*							
$P''(1,G_1)$					102								
$CT(ShUCJ)$					134								

For cycles, an example of the Shell-Cluj polynomial is given in Table 3. It can be seen that the relations with W and WW indices are not obeyed in cycle-containing graphs.

Table 3. Polynomial *ShUCJ*(x) and *CT* index in the simple cycle C_6.

	ShUCJ(C_6)				**UCJ(C_6)**						
$i \setminus k$	1	2	3	*RS*	1	2	3	4	5	6	*RS*
1	6	4	2	12	0	3	2	2	2	3	12
2	6	4	2	12	3	0	3	2	2	2	12
3	6	4	2	12	2	3	0	3	2	2	12
4	6	4	2	12	2	2	3	0	3	2	12
5	6	4	2	12	2	2	2	3	0	3	12
6	6	4	2	12	3	2	2	2	3	0	12
CS	36	24	12	72	12	12	12	12	12	12	72

ShUCJ(x)	$18x + 12x^2 + 6x^3$		
P(1)		36	Compare:
P'(1)		60	W=27
P''(1)		60	WW=42
CT(*ShUCJ*)		90	

Shell-Cluj polynomial and CT-index in particular graphs

Three classes of graphs are next investigated to find close formulas for calculating the Shell-*Cluj ShUCJ*(x) polynomial and Cluj-Tehran *CT* index: paths $\boldsymbol{P_n}$, stars $\boldsymbol{S_{1,m}}$, and simple cycles $\boldsymbol{C_n}$.

Paths $\boldsymbol{P_n}$

$$ShUCJ(P_n,x)=\sum_{k=0}^{n-2}\binom{n-k}{2}\cdot x^{k+1}$$

$$ShUCJ(P_n,1)=\sum_{k=0}^{n-2}\binom{n-k}{2}=\binom{n}{2}\left(\frac{n+1}{3}\right)=\frac{n(n-1)(n+1)}{6}$$

$$ShUCJ'(P_n,1)=\sum_{k=0}^{n-2}(k+1)\binom{n-k}{2}=\binom{n}{2}\frac{(n+1)(n+2)}{12}=\frac{n(n-1)(n+1)(n+2)}{24}$$

$$ShUCJ''(P_n,1)=\sum_{k=1}^{n-2}k(k+1)\binom{n-k}{2}=\binom{n}{2}\frac{(n+1)(n-2)(n+2)}{30}=\frac{n(n-1)(n+1)(n-2)(n+2)}{60}$$

$$CT(ShUCJ(P_n))=P^1+P^2/2=\binom{n}{2}\frac{(n+1)(n+2)(n+3)}{60}=\frac{n(n-1)(n+1)(n+2)(n+3)}{120}$$

Examples: $CT(ShUCJ(P_n))$; $n=\overline{2,10}$: 1; 6; 21; 56; 126; 252; 462; 792; 1287.

Stars $\boldsymbol{S_{1,m}}$; n=1+m.

$$ShUCJ(S_{1,m},x)=\binom{n+1}{2}\cdot x+\binom{n}{2}\cdot x^2$$

$$ShUCJ(S_{1,m},1)=\binom{n+1}{2}+\binom{n}{2}=n^2$$

$$ShUCJ'(S_{1,m},1)=\binom{n+1}{2}+2\binom{n}{2}=\frac{n(3n-1)}{2}$$

$$ShUCJ''(S_{1,m},1)=2\binom{n}{2}=n(n-1)$$

$$CT(ShUCJ(S_{1,m}))=P^1+P^2/2=\binom{n+1}{2}+3\binom{n}{2}=n(2n-1)$$

Examples: $CT(ShUCJ(S_{1,m}))$; $n=\overline{3,10}$: 15; 28; 45; 66; 91; 120; 153; 190.

Cycles C_n

Case: 0(mod 4).

$$ShUCJ(C_n,x)=\frac{n^2}{2}\cdot x+\sum_{k=1}^{\frac{n-4}{4}}n\left(\frac{n}{2}-k\right)\cdot\left(x^{2k}+x^{2k+1}\right)+\frac{n^2}{8}\cdot x^{\frac{n}{2}}$$

$$ShUCJ(C_n,1)=n^2(3n+8)/32$$

$$ShUCJ'(C_n,1)=n^2(4n^2+3n-4)/96$$

$$ShUCJ''(C_n,1)=n^3(5n^2-12n-8)/384$$

$$CT(ShUCJ(C_n(0(\mathrm{mod}\,4)))=n^2(5n^3+20n^2+16n-32)/768$$

Examples: $CT(ShUCJ(C_n,0(\mathrm{mod}4)))$; n=8,12,16: 328; 2190; 8608

Case: 1(mod 4).

$$ShUCJ(C_n,x)=\sum_{k=0}^{\frac{n-5}{4}}\left[n\frac{n-(2k+1)}{2}\right]\cdot\left(x^{2k+1}+x^{2k+2}\right)$$

$$ShUCJ(C_n,1)=n(n-1)(3n+1)/32$$

$$ShUCJ'(C_n,1)=n(n-1)(4n^2+7n+9)/96$$

$$ShUCJ''(C_n,1)=n(n-1)(5n^3-7n^2-9n-21)/384$$

$$CT(ShUCJ(C_n(1(\mathrm{mod}\,4)))=n(n-1)(n+3)(5n^2+10n+17)/768$$

Examples: $CT(ShUCJ(C_n,1(\mathrm{mod}4)))$; n=9,13,17: 576; 3224; 11560

Case: 2(mod 4).

$$ShUCJ(C_n,x)=\frac{n^2}{2}\cdot x+\sum_{k=1}^{\frac{n-6}{4}}n\left(\frac{n}{2}-k\right)\cdot\left(x^{2k}+x^{2k+1}\right)+\frac{n(n+2)}{4}\cdot\left(x^{\frac{n}{2}-1}+\frac{1}{2}x^{\frac{n}{2}}\right)$$

$$ShUCJ(C_n,1) = n(n+2)(3n+2)/32$$

$$ShUCJ'(C_n,1) = n(n+2)(4n^2-5n+6)/96$$

$$ShUCJ''(C_n,1) = n(n-2)(n+2)(5n^2-12n+12)/384$$

$$CT(ShUCJ(C_n(2(\mathrm{mod}\,4))) = n(n+2)(5n^3+10n^2-4n+24)/768$$

Examples: $CT(ShUCJ(C_n,2(\mathrm{mod}4)))$; n=6, 10,14: 90; 935; 4564

Case: 3(mod 4).

$$ShUCJ(C_n,x) = \sum_{k=0}^{\frac{n-7}{4}} \left[n\frac{n-(2k+1)}{2} \right] \cdot \left(x^{2k+1} + x^{2k+2} \right) + \frac{n(n+1)}{4} \cdot x^{\frac{n-1}{2}}$$

$$ShUCJ(C_n,1) = n(n+1)(3n-1)/32$$

$$ShUCJ'(C_n,1) = n(n+1)(4n^2-n-9)/96$$

$$ShUCJ''(C_n,1) = n(n+1)(n-3)(5n^2-2n-15)/384$$

$$CT(ShUCJ(C_n(3(\mathrm{mod}\,4))) = n(n+1)^2(5n^2+10n-27)/768$$

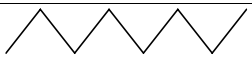
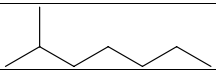
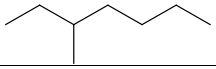
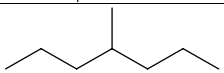
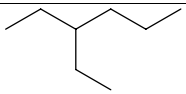
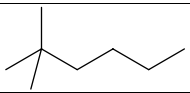
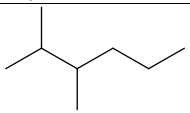
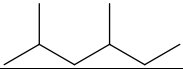
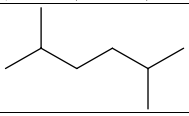
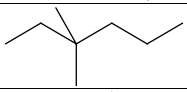
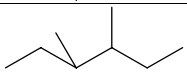
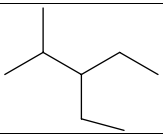
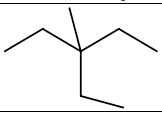
Examples: $CT(ShUCJ(C_n,3(\mathrm{mod}4)))$; n=7, 11,15: 168; 1419; 6240

In the above, the last row in each case gives examples of *CT* index. The calculations were performed by the TOPOCLUJ software package.

Correlating ability of CT index

Topological indices *TI*s are among the simplest and efficient descriptors for *QSPR*/*QSAR*. We tested the newly proposed Cluj-Tehran CT index, namely CT(Sh(DegDI) in predicting some physico-chemical properties of Octane alkanes.[17] The best correlations have been obtained with the values of boiling point BP, entropy S and total surface area TSA (Table 5). The results were compared with those obtained for the simple Degree-Distance DegDI index and with those available online in the IAMC database.[18]

Table 4. Octanes and their boiling point BP, entropy S and total surface area TSA values

	Molecule	BP	S	TSA	CT(ShDegDI)
1		9.153	111.67	415.3	1470
2		9.120	109.84	407.85	1155
3		9.115	111.26	397.34	978
4		9.114	109.32	396.04	921
5		9.108	109.43	379.04	744
6		9.065	103.42	405.11	767
7		9.079	108.02	384.93	693
8		9.082	106.98	388.11	727
9		9.088	105.72	395.08	875
10		9.056	104.74	389.79	585
11		9.074	106.59	376.91	602
12		9.073	106.06	368.1	545
13		9.049	101.48	366.99	460

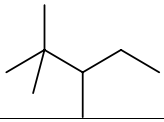
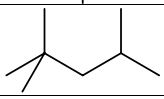
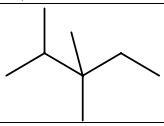
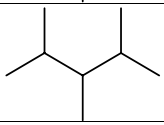
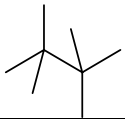
14		9.023	101.31	371.75	443
15		9.031	104.09	392.19	545
16		9.020	102.06	377.4	409
17		9.044	102.39	368.93	494
18		8.971	93.06	390.47	307

Table 5. Statistics of QSPR study on Octanes

	R^2	BP	S	TSA
1	DegDI[17]	0.913	0.771	0.520
2	**CT(ShDegDI)[17]**	**0.8182**	**0.6460**	**0.613**
3	Best in Octanes[18] (monovariate)	0.782	0.920	0.721

One can see, CI index shows a moderately good ability in predicting some physico-chemical properties of alkanes, which could be useful in multi-variate regression studies.

Conclusions

A novel topological index, called Cluj-Tehran *CT*, is defined on the ground of Shell polynomials. The polynomial coefficients are calculated as the column half sums of Shell matrices, built up according to the vertex distance partitions of a graph. Close formulas to calculate the Shell-Cluj polynomial and the corresponding Cluj-Tehran index in several particular classes of graphs were given.

The *CT* descriptors have been tested in prediction of some physico-chemical properties of octane alkanes, with promising results, particularly those defined on combination **ShDegDI**

and are continuing tested in our labs on any combination **ShM** for correlating and discriminating abilities.

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