Scientific paper

Shell-Polynomials and Cluj-Tehran Index in Tori T(4,4)S[5,n]

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This paper is dedicated to Professor Milan Randić on the occasion of his 80th birthday

Abstract

Weighted Hosoya polynomials have been developed by Diudea, in ref. *Studia Univ. "Babes-Bolyai"*, 2002, *47*, 131–139. Among various weighting schemes, those polynomials obtained by using Diudea's Shell matrix operator are far more interesting. We present here the Shell-Distance and Shell-Degree-Distance polynomials and close formulas to calculate them and derived Cluj-Tehran CT index in the family of square tiled tori T(4,4)S[5,n]. Applications of the proposed descriptors are also presented.

Keywords: Weighted Hosoya polynomial; Shell-polynomial; Cluj-Tehran index

1. Introduction

Let $G(V,E)$ be a connected molecular graph,[1] without directed and multiple edges and without loops, the vertex and edge-sets of which being represented by V(G) and E(G), respectively. Define the k^{th} layer/shell of vertices v lying at distance k with respect to the reference vertex i as:[2]

$$G(i)_k = \{v |\ v \in V(G);\quad d_{iv} = k\} \tag{1}$$

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

$$G(i) = \{G(i)_k\ ; k \in [0,1,..,ecc_i]\} \tag{2}$$

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

On the above notions, we define the entries in a layer matrix (of a vertex property) **LM** as:[2–5]

$$[\mathbf{LM}]_{i,k} = \sum_{v|d_{i,v}=k} p_v \tag{3}$$

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.

The information can be taken from any square matrix M (called here the *info matrix*) as *row sum RS*, *column sum CS* or *diagonal entries* given by the *Walk* matrix,[2] as developed by TOPOCLUJ software package.[6]

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

$$\mathbf{LM} = \{[\mathbf{LM}]_{i,k}\ ; i \in V(G); k \in [0,1,..,d(G)]\} \tag{4}$$

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

Similarly, we can define the entries in a *shell matrix* **ShM**:[2,4]

$$[\mathbf{ShM}]_{i,k} = \sum_{v|d_{i,v}=k} [\mathbf{M}]_{i,v} \tag{5}$$

where **M** is any square topological matrix. Any operation, (other than summation) over the square matrix entries $[\mathbf{M}]_{i,v}$, can be used, thus Sh being a true matrix operator. The shell matrix will collect the above defined entries:

$$\mathbf{ShM} = \{[\mathbf{ShM}]_{i,k}\ ; i \in V(G); k \in [0,1,..,d(G)]\} \tag{6}$$

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

2. LM Polynomials

Define a *distance*-based polynomial as:[7]

$$P(x)=\sum_k p(G,k)\cdot x^k \tag{7}$$

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 layer/shell matrices, as the half sums on columns.

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

$$P^k(1)=\sum_k k!\cdot p(G,k) \tag{8}$$

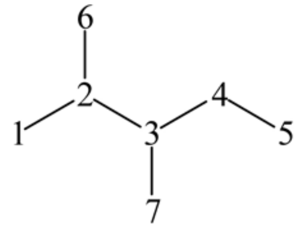
In case: $p(v) = 1$ (*i.e.*, the vertex counting), **LM** = **LC**, (*i.e.*, layer matrix of counting), $p(G,k)$ denotes the number of pair vertices separated by distance k in G, and the classical Hosoya $H(x)$ polynomial is recovered.[8] The index calculated as the polynomial first derivative is the well-known Wiener index,[9] W.

$$W(G)=P'(\mathbf{LC},1) \tag{9}$$

The hyper-Wiener index WW, patterned by Randić,[10] is calculated from $P'(1)$ and $P''(1)$ derivatives as:

$$WW(G)=P'(\mathbf{LC},1)+(1/2)P''(\mathbf{LC},1) \tag{10}$$

Figure 1 illustrates the $P(\mathbf{LC},x)$ polynomial.



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
CS	12	14	12	4

Figure 1. The graph G_1 and its Hosoya polynomial $P(\mathbf{LC},x) = 6x + 7x^2 + 6x^3 + 2x^4$; $P'(\mathbf{LC},1) = W = 46$

3. ShM Polynomials

The weighting in the Shell polynomials is performed by the aid of Diudea's Shell matrix operator[2,4] and the weight is just the property of *info matrix* **M**. Our attention is focused on Shell-Distance and Shell-Degree-Distance polynomials, respectively.

3. 1. Shell-Distance Polynomial

Define the Shell-Distance polynomial[7,11] as

$$P(\mathbf{ShD},x)=\sum_k p(G,k)\cdot x^k \tag{11}$$

where $p(G,k)$ are calculated as the column half sums in the matrix **ShD** (Table 1). The polynomial defined on **ShD** matrix has the coefficients already multiplied by the (topological) distance and clearly $P(\mathbf{ShD},1) = W(G)$, the well-known Wiener index.

The 1st derivative of this polynomial is then weighted by the squared distances in G. An index, called *Cluj-Tehran*[11] $CT(\mathbf{ShM})$ index (with specified **M**) is calculated by relation

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

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

	ShD						**D**							
i \ *k*	1	2	3	4	*RS*		1	2	3	4	5	6	7	*RS*
1	1	4	6	4	16		0	1	2	3	4	2	3	15
2	3	4	3	0	11		1	0	1	2	3	1	2	10
3	3	6	0	0	10		2	1	0	1	2	2	1	9
4	2	4	6	0	13		3	2	1	0	1	3	2	12
5	1	2	6	8	18		4	3	2	1	0	4	3	17
6	1	4	6	4	16		2	1	2	3	4	0	3	15
7	1	4	9	0	15		3	2	1	2	3	3	0	14
CS	12	28	36	16	92	*CS*	15	10	9	12	17	15	14	92
$P(x)$	6x	$14x^2$	$18x^3$	$8x^4$										
$P(1)$					46	=	*W*							
$P'(1)$					120									
$P''(1)$					232									
CT (**ShD**)					236									

The results, for G_1, are given at the bottom of Table 1.

3. 2. Shell-Degree-Distance Polynomials

The Cramer product of the diagonal matrix of vertex degrees **Deg** with the Distance **D** matrix provides the matrix of degree distances, denoted **DegD**.

$$\mathbf{Deg}(G)\times\mathbf{D}(G)=\mathbf{DegD}(G) \qquad (13)$$

The above Cramer product 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 **D** matrices, respectively[12]

$$RS(\mathbf{A})\bullet RS(\mathbf{D})=RS(\mathbf{DegD}) \qquad (14)$$

Next, applying the Shell operator, the matrix **Sh-DegD**, of which column half sums are just the coefficients of the corresponding Shell-polynomial, is obtained

Table 2. Polynomial *P*(**ShDegD**,*x*) and corresponding *CT* index in G_1.

	ShDegD						**DegD**							
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	9	12	9	0	30		3	0	3	6	9	3	6	30
3	9	18	0	0	27		6	3	0	3	6	6	3	27
4	4	8	12	0	24		6	4	2	0	2	6	4	24
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	2	4	9	0	14		3	2	1	2	3	3	0	14
CS	26	52	48	16	142	*CS*	24	14	12	18	28	24	22	142
P(*x*)	13x	$26x^2$	$24x^3$	$8x^4$										
P(1)					71									
$P'(1)$					169									
$P''(1)$					292									
CT (**ShDegD**)					315									

Table 3. Matrix operations of the diagonal Degree **Deg** matrix

Deg × D = DegD									**D × Deg = DDeg**								
	1	2	3	4	5	6	7	RS		1	2	3	4	5	6	7	RS
1	**0**	1	2	3	4	2	3	15	1	**0**	3	6	6	4	2	3	24
2	3	**0**	3	6	9	3	6	30	2	1	**0**	3	4	3	1	2	14
3	6	3	**0**	3	6	6	3	27	3	2	3	**0**	2	2	2	1	12
4	6	4	2	**0**	2	6	4	24	4	3	6	3	**0**	1	3	2	18
5	4	3	2	1	**0**	4	3	17	5	4	9	6	2	**0**	4	3	28
6	2	1	2	3	4	**0**	3	15	6	2	3	6	6	4	**0**	3	24
7	3	2	1	2	3	3	**0**	14	7	3	6	3	4	3	3	**0**	22
CS	24	4	12	18	28	24	22	142	CS	15	30	27	24	17	15	14	42

1/2SUM = 71 1/2SUM = 71

Sh(DegD)							**Sh(DDeg)**						
	0	1	2	3	4	RS		0	1	2	3	4	RS
1	**0**	1	4	6	4	15	1	**0**	3	8	9	4	24
2	**0**	9	12	9	0	30	2	**0**	5	6	3	0	14
3	**0**	9	18	0	0	27	3	**0**	6	6	0	0	14
4	**0**	4	8	12	0	24	4	**0**	4	8	6	0	18
5	**0**	1	2	6	8	17	5	**0**	2	6	12	8	28
6	**0**	1	4	6	4	15	6	**0**	3	8	9	4	24
7	**0**	1	4	9	0	14	7	**0**	3	10	9	0	24
CS	**0**	26	52	48	16	142	CS		26	52	48	16	142
P(1)		13	26	24	8	71	P(1)		13	26	24	8	71
P'(1)		13	52	72	32	169	P'(1)		13	52	72	32	169

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$$P(\mathbf{ShDegD},x)=\sum_{k}p(G,k)\cdot x^{k} \qquad (16)$$

An example is given in Table 2; at the bottom of table, *CT* index is given.

Irrespective CP (11) is performed "to the left" or "to the right", the Shell-polynomial is the same (Table 3).

The half sum of entries in the **Deg** × **D** or **D** × **Deg** matrices is the well-known degree-distance *DegD*(*G*) index, defined by Dobrynin and Kochetova[13]

$$DegD(G)=\sum_{v\in V(G)}Deg(v)D(v) \qquad (17)$$

where Deg(v) and D(v) are just RS(A(v)) and RS(D(v)), see (13). This index is in fact the non-trivial part of the Schultz index.[14–26] Accordingly, this index can be calculated as the half sum of entries in the matrices **A** × **D** or **D** × **A** (Table 4). Next, applying the Shell operator, we obtain the matrices **ShA** × **D/ShD** × **A** which are different from **ShDeg** × **D / ShD** × **Deg**, because of the non-zero diagonal of **A** × **D/D** × **A**, of which information is lost in the further first derivative of the corresponding Shell-polynomial. Even the P(1) values are the same and equal the degree-distance index *DegD*(*G*), in the following we will calculate only the polynomial *P*(**ShDegD**,*x*).

Another reason is that the entries in **DegD** matrix represent precisely the property defined by Dobrynin in (14). This matrix can also be obtained by Diudea's Walk operator[12,16] as

$$\mathbf{DegD}(G)=\mathbf{W}(\mathbf{A},\mathbf{1},\mathbf{D}) \qquad (18)$$

where **1** stands for the square matrix of the pertinent order, having all the non-diagonal entries 1 while the diagonal entries zero.

The walk operator[4,5,12,16] $\mathbf{W}(\mathbf{M}_1,\mathbf{M}_2,\mathbf{M}_3)$ is defined as

$$[\mathbf{W}(\mathbf{M}_1,\mathbf{M}_2,\mathbf{M}_3)]_{i,j}=RS(\mathbf{M}_1^{[\mathbf{M}_2]_{i,j}})_i[\mathbf{M}_3]_{i,j} \qquad (19)$$

It works by Hadamard algebra and was extensively exemplified in refs.[12,16] (see also ref.[27])

4. Shell Polynomials *P*(ShD,*x*) and *P*(ShDegD,*x*) in T(4,4)S[5,*n*]

The above defined Shell-polynomials are calculated for the series of square tiled nanotori T(4,4)S[5,*n*] (Figure 2). Because such graphs are vertex transitive, formulas are given only for the vertex polynomial. At the end of each case, examples are given for the Cluj-Tehran *CT* index. To obtain the global value of *CT* the value per vertex is to be multiplied by *half the number of vertices* in the torus: $v = 5n$.

Table 4. Matrix operations involving **A**×**D** matrix

A × D	1	2	3	4	5	6	7	
1	**1**	0	1	2	3	1	2	10
2	4	**3**	4	7	10	4	7	39
3	7	4	**3**	4	7	7	4	36
4	6	4	2	**2**	2	6	4	26
5	3	2	1	0	**1**	3	2	12
6	1	0	1	2	3	**1**	2	10
7	2	1	0	1	2	2	**1**	9
	24	14	12	18	28	24	22	142
1/2SUM = 71								

D × A	1	2	3	4	5	6	7	
1	**1**	4	7	6	3	1	2	24
2	0	**3**	4	4	2	0	1	14
3	1	4	**3**	2	1	1	0	12
4	2	7	4	**2**	0	2	1	18
5	3	10	7	2	**1**	3	2	28
6	1	4	7	6	3	**1**	2	24
7	2	7	4	4	2	2	**1**	22
	10	39	36	26	12	10	9	142
1/2SUM = 71								

Sh(**A** × **D**)	0	1	2	3	4	RS
1	**1**	0	2	4	3	10
2	**3**	12	14	10	0	39
3	**3**	12	21	0	0	36
4	**2**	4	8	12	0	26
5	**1**	0	1	4	6	12
6	**1**	0	2	4	3	10
7	**1**	0	2	6	0	9
CS	12	28	50	40	12	142
P(1)	614	25	20	6	71	
P'(1)	14	50	60	24	148	

Sh(**D** × **A**)	0	1	2	3	4	RS
1	**1**	4	8	8	3	24
2	**3**	4	5	2	0	14
3	**3**	6	3	0	0	12
4	**2**	4	8	4	0	18
5	**1**	2	7	12	6	28
6	**1**	4	8	8	3	24
7	**1**	4	11	6	0	22
CS	12	28	50	40	12	142
P(1)	6	14	25	20	6	71
P'(1)		14	50	60	24	148

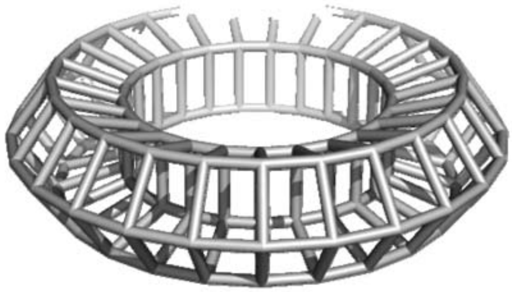

Figure 2. Torus of the series T(4,4)S[5,n].

4. 1. Case: *n* = 5 + 10 *m*.

$$P(\mathbf{ShDI}(i,T(4,4)S[5,5+10m]),x)=4x+16x^2+$$
$$+\sum_{k=1}^{m}\sum_{r=0}^{4}\left[30+50(k-1)+10r\right]\cdot x^{3+5(k-1)+r}+$$
$$+(24+40m)\cdot x^{5(m-1)+8}+(16+20m)\cdot x^{5(m-1)+9}$$

$$P'(\mathbf{ShDI}(i,T(4,4)S[5,5+10m]),1)=\frac{1250m^3}{3}+$$
$$+925m^2+\frac{2125m}{3}+172$$

$$P''(\mathbf{ShDI}(i,T(4,4)S[5,5+10m]),1)=\frac{3125m^4}{2}+$$
$$+\frac{12625m^3}{3}+\frac{8775m^2}{2}+\frac{6245m}{3}+368$$

$$CT(\mathbf{ShDI}(i,T(4,4)S[5,5+10m]))=\frac{3125m^4}{2}+$$
$$+\frac{12625m^3}{3}+\frac{8775m^2}{2}+\frac{6245m}{3}+368$$

Example:

$$CT(\mathbf{ShDI}(i,T(4,4)S[5,5+10m])):$$
$$m(1;2;3)=8526;\ 48996;\ 165016$$

4. 2. Case: *n* = 10 *m*.

$$P(\mathbf{ShDI}(i,T(4,4)S[5,10m])=4x+16x^2+30x^3+40x^4+$$
$$\sum_{k=2}^{m}\sum_{r=0}^{4}\left[50(k-1)+10r\right]\cdot x^{5(k-1)+r}+[45+45(m-1)]\cdot x^{5(m-1)+5}+$$
$$[36+30(m-1)]\cdot x^{5(m-1)+6}+[14+10(m-1)]\cdot x^{5(m-1)+7}$$

$$P'(\mathbf{ShDI}(i,T(4,4)S[5,10m]),1)=\frac{25m(50m^2+36m+13)}{3}$$

$$P''(\mathbf{ShDI}(i,T(4,4)S[5,10m]),1)=$$
$$=\frac{5m(1875m^3+1300m^2+615m+122)}{6}$$

$$CT(\mathbf{ShDI}(i,T(4,4)S[5,10m]))=$$
$$=\frac{5m(1875m^3+2300m^2+1335m+382)}{12}$$

Example:

$$CT(\mathbf{ShDI}(i,T(4,4)S[5,10m])):$$
$$m(2,3,4)=22710;\ 94640;\ 270870$$

Because in T(4,4)S[5,n] the vertices have all the degree 4, all the above formulas must be multiplied by 4 to get the corresponding degree-distance descriptors.

5. Modeling Octane Properties

To test the correlating ability of the descriptors derived from the degree-distance matrices (**ShM**$_k$) and Shell-polynomials we focused on the set of octanes, as one of the benchmark-sets[28–30] in correlating studies by using topological indices.

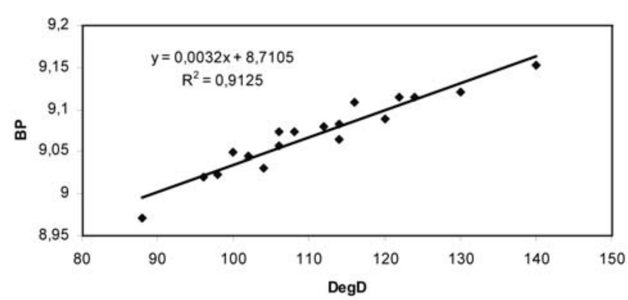

Figure 3. The plot of octanes BP (°C) vs DegD index

Among several physico-chemical properties, the boiling point BP was best modeled, in monovariate regression, by the index DegD (plotted in Figure 3) while in trivariate model, by the other descriptors derived from the Shell-polynomials, the Cluj-Tehran index included. Remark the best monovariate model reported so far is only 0.78 for the BP of octanes.[28] Other applications refer to the discriminating studies in large databases comprising molecular graphs: the super index CJN (Cluj-Niš), including descriptors derived from the Shell-polynomials, succeeded in solving a set of more than five thousands molecules without degeneracy.[11]

6. Conclusions

Weighting a distance-based polynomial is easily achieved by using the Shell-matrix operator. This enables one to calculate a variety of so-called Shell-polynomials. In this article we derived close formulas to calculate the Shell-polynomial $P(\mathbf{ShD},x)$ and $P(\mathbf{ShDegD},x)$ in a family of square tiled tori. Applications of the proposed descriptors demonstrated their utility.

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8. References

1. F. Harary, *Graph Theory*, Addison-Wesley, Reading, M.A., 1969.
2. M. V. Diudea, O. Ursu, *Indian J. Chem*., **2003**, *42A*, 1283–1294
3. M. V. Diudea, M. Topan, A. Graovac, *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 1071–1078.
4. M. V. Diudea, M. S. Florescu, P. V. Khadikar, Molecular Topology and Its Applications, EFICON, Bucharest, 2006.
5. M.V. Diudea, I. Gutman, L. Jäntschi, Molecular Topology, NOVA, New York, 2002.
6. O. Ursu, M. V. Diudea, TOPOCLUJ software package, “Babes-Bolyai” University, Cluj, 2002.
7. M. V. *Diudea, Studia Univ. “Babes-Bolyai”,* **2002,** *47,* 131–139.
8. H. Hosoya, *Discrete Appl. Math.,* **1988***, 19,* 239–257.
9. H. Wiener, *J. Amer. Chem. Soc.* **1947**, *69*, 17–20.
10. M. Randić, *Chem. Phys. Lett.* **1993**, *211*, 478–483.
11. M. V. Diudea, Nanomolecules and Nanostructures – Polynomials and Indices, Mathematical Chemistry Monographs, No. 10, University of Kragujevac and Faculty of Science Kragujevac, 2010.
12. M. V. Diudea, *Croat. Chem. Acta*, **1999**, *72*, 835–851.
13. A. A. Dobrynin, A. A. Kochetova, *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 1082–1086.
14. H. P. Schultz, *J. Chem. Inf. Comput. Sci.* **1989***, 29,* 227–228
15. E. Estrada, L. Rodriguez, *MATCH Commun. Math.Comput. Chem.*, **1997**, *35*,157–167.
16. M. V. Diudea, M. Randić, *J. Chem. Inf. Comput. Sci*. **1997**, *37*, 1095–1100.
17. M. V. Diudea, *MATCH Commun. Math. Comput. Chem.*, **1995**, *32*, 85–103.
18. M. V. Diudea, C. M. Pop, *Indian J. Chem*. **1996**, *35A*, 257–261.
19. I. Gutman, *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 1087–1089.
20. D. J. Klein, Z. Mihalić, D. Plavšić, N. Trinajstić, *J. Chem. Inf. Comput. Sci.* **1992**, *32*, 304–305.
21. D. Plavšić, S. Nikolić, N. Trinajstić, D. J. Klein, *Croat. Chem. Acta*, **1993**, *66*, 345–353.
22. A. I. Tomescu, *Discrete Appl. Math*, **2008**, *156*, 125–130.
23. O. Bucicovschi, S. M. Cioaba, *Discrete Appl. Math*, **2008**, *156*, 3518–3521.
24. P. Dankelmann, I. Gutman, S. Mukewembi, H. C. Swart, *Discrete Appl. Math*, **2009**, *157*, 2773–2777
25. Sh. Chen, Zh. Guo, *Int*. *J. Contemp. Math. Sciences*, **2010**, *5*, 649–652.
26. A. Ilić, S. Klavžar, D. Stevanović, *MATCH Commun. Math. Comput. Chem*., **2010**, *63*, 411–424.
27. M. Randić, *Theor. Chim. Acta,* **1995**, *92*, 97–106.
28. http://www.moleculardescriptors.eu/dataset/dataset.htm; http://www.iamc-online.org
29. D. Vukičević, *Croat.Chem. Acta*, submitted.
30. D. Stevanović, A. Ilić, C. Onişor and M. V. Diudea, *Acta Chim. Slovenica*, **2009,** *56* (2) 410–417.

Povzetek

Utežene Hosoya polinome je razvil Diudea (v ref.: *Studia Univ. “Babes-Bolyai”*, 2002, *47*, 131–139). Med raznolikimi utežitvenimi shemami so precej bolj zanimivi polinomi, dobljeni z uporabo Diudejevega operatorja matrike lupin (obodov) grafa. Tu so predstavljeni polinomi obodnih razdalj in stopnje obodnih razdaj (Shell-Distance, Shell-Degree-Distance) in izpeljane formule za njihov izračun ter za Cluj-Tehran CT indeks v družini »kvadratno-razdeljenih« torusov T(4,4)S[5,n]. Predstavljena je tudi uporaba predlaganih deskriptorjev.