VERSITA
DOI: 10.2478/achi-2013-0008

ACTA CHEMICA IASI, **21_2,** 83-92 (2013)

Hosoya-Diudea polynomial in hyper structures

M. P. Vlad[1] and M. V. Diudea[2*]

[1] *Faculty of Economic Sciences,"Dimitrie Cantemir" University, Bucharest, Teodor Mihali Street 56, 400591, Romania*

[2]*Faculty of Chemistry and Chemical Engineering, "Babes-Bolyai" University, Arany Janos Str., 400028 Cluj, Romania*

Abstract. Hosoya polynomial counts finite sequences of distances in a graph G; more exactly, it counts the number of points/atoms lying at a given distance in G. The polynomial coefficients are calculable by means of layer/shell matrices. Shell matrix operator enables the transformation of any square matrix in the corresponding layer/shell matrix, thus generalizing the local property counting according to its distribution by the distances in G. This represents the "Hosoya-Diudea" generalized counting polynomial. We applied this theory to several hypothetical nanostructures with icosahedral symmetry.

Keywords: Hosoya-Diudea polynomial, layer matrix, shell matrix, counting polynomial

Introduction

Let $G(V,E)$ be a connected molecular graph, 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: $G(i)_k = \{v \mid v \in V(G); \quad d_{iv} = k\}$. The collection of all its layers

* M. V. Diudea, *e-mail*: diudea@chem.ubbcluj.ro

defines the partition of G with respect to i: $G(i) = \{G(i)_k \; ; \; k \in [0,1,..,ecc_i]\}$, 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:[1-5]

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

with summation being the most used operation on the collected vertices. The zero column is just the column of vertex properties $[\mathbf{LM}]_{i,0} = p_i$ **.**The Layer matrix **LM** is a collection of the above defined entries:

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

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:[4-6]

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

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:

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

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

An index of *centrality*[2,5] $C(\mathbf{BM})$ is calculated on these matrices (B=L; Sh) as:

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

$$C(\mathbf{BM}) = \sum_i C(\mathbf{BM})_i$$

Counting Polynomials. Define a *distance*-based counting polynomial as:

$$P(x) = \sum_k p(G,k) \cdot x^k$$

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 $d(G)$.[7] The coefficients in Hosoya-Diudea polynomial are calculable from the above defined layer/shell matrices, as the half sums on columns. We use the symbol H(LM,x) for the generalized polynomial computed on a layer matrix LM while Sh(M,x) is the shell-matrix calculated one. 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[8] is recovered.

Some single number descriptors (*i.e.*, topological indices TIs) can be calculated by evaluating the polynomial derivatives (usually in $x = 1$):[9]

$$P^k(G,1) = \sum_k k! \cdot p(G,k)$$

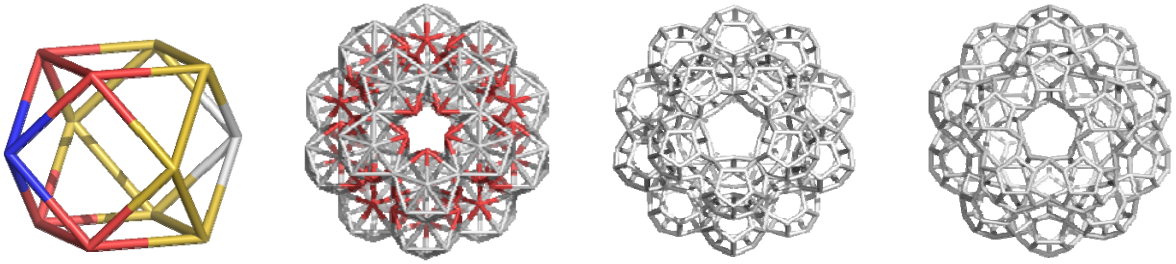
The aim of this work is to apply the generalized Hosoya-Diudea polynomials in counting face/ring surrounding atoms and their shell-distances distribution in three hypothetical nanostructures with icosahedral symmetry.

Results and Discussion

The generalized Hosoya-Diudea polynomials will be calculated on cuboctahedron (as a simple structure to illustrate some matrices and topological indices herein calculated) and three hyper-dodecahedral structures, shown in the Figure 1 below.

Cage design. The object ID@Ico_{20}_180 is made by decorating with icosahedrons Ico the Icosidodecahedron ID, thus any two Ico sharing an

edge. Next, by (Poincaré) dualization[9] one obtains the hyper-cage $S_2(Do)@Do_{20}\_340$, in which the core S2(Do) is decorated with dodecahedra Do, any two Do sharing an edge. In the above, $S_2(Do)$ means the "septupling 2" map operation applied on dodecahedron. Finally, DoX_{20}_340 is made by deleting from $S_2(Do)@Do_{20}\_340$ the shared edge (see X in its name). Such structures in believed to appear by self-assembling of icosahedral and dodecahedral atomic clusters.



CO_12 ID@Ico_{20}_180 $S_2(Do)@Do_{20}$_340 DoX_{20}_340

Figure 1. Cuboctahedron CO and three hyper-dodecahedral nanostructures.

Polynomial examples on cuboctahedron. To exemplify the main matrices[1,9] used in deriving the main results, we have chosen the semi-regular polyhedron named cuboctahedron (Figure 1). In Table 1, the adjacency A matrix (with entries 1 if two vertices are connected by one edge and zero, otherwise) and the distance DI matrix, counting the number of edges on the shortest path joining any two vertices in G, the diagonal elements being zero, are exemplified.

Table 1. Adjacency and Distance matrices in Cuboctahedron CO.

CO_A (adjacency)												
0	1	1	0	0	1	1	0	0	0	0	0	4
1	0	0	1	0	0	1	0	0	0	1	0	4
1	0	0	1	0	1	0	0	0	0	0	1	4
0	1	1	0	0	0	0	0	0	0	1	1	4
0	0	0	0	0	1	1	1	1	0	0	0	4
1	0	1	0	1	0	0	0	1	0	0	0	4
1	1	0	0	1	0	0	1	0	0	0	0	4
0	0	0	0	1	0	1	0	0	1	1	0	4
0	0	0	0	1	1	0	0	0	1	0	1	4
0	0	0	0	0	0	0	1	1	0	1	1	4
0	1	0	1	0	0	0	1	0	1	0	0	4
0	0	1	1	0	0	0	0	1	1	0	0	4
SUM = 48												
1/2SUM = 24												

CO_DI (distance)												
0	1	1	2	2	1	1	2	2	3	2	2	19
1	0	2	1	2	2	1	2	3	2	1	2	19
1	2	0	1	2	1	2	3	2	2	2	1	19
2	1	1	0	3	2	2	2	2	2	1	1	19
2	2	2	3	0	1	1	1	1	2	2	2	19
1	2	1	2	1	0	2	2	1	2	3	2	19
1	1	2	2	1	2	0	1	2	2	2	3	19
2	2	3	2	1	2	1	0	2	1	1	2	19
2	3	2	2	1	1	2	2	0	1	2	1	19
3	2	2	2	2	2	2	1	1	0	1	1	19
2	1	2	1	2	3	2	1	2	1	0	2	19
2	2	1	1	2	2	3	2	1	1	2	0	19
SUM = 228=2W												
1/2SUM = 114=W												

Table 2 illustrates the layer LC and shell Sh(DI) matrices for the cuboctahedron, along with the derived polynomials and corresponding topological indices.

The first derivative (in x=1) of the classical Hosoya polynomial, equal to H(LC,x) polynomial, provides the well-known Wiener index[10] W, that counts all the distances in G (or half-sum of the entries in the DI matrix): $W = H'(1)$. Next, the hyper-Wiener index[11] is calculated as: $WW = H'(1) + (1/2)H''(1)$.

Remark the relations between the H(LC,x) and Sh(DI,x) polynomials, at the bottom of Table 2; the most interesting relation (providing a new topological index) is:

$$H'(\mathbf{LC},1) + H''(\mathbf{LC},1) = [H(\mathbf{LC},x) * (\mathbf{D}^2 / x) = Sh'(\mathbf{DI},x)]_{x=1}$$

D being the vector of distances (D=1, 2,..).

Table 2. Counting H(LC,x) and Sh(DI,x) in Cuboctahedron CO.

	LC(CO)			**Sh**(DI(CO))	
	1 4 6 1 12			1 4 12 3 20	
	1 4 6 1 12			1 4 12 3 20	
	1 4 6 1 12			1 4 12 3 20	
	1 4 6 1 12			1 4 12 3 20	
	1 4 6 1 12			1 4 12 3 20	
	1 4 6 1 12			1 4 12 3 20	
	1 4 6 1 12			1 4 12 3 20	
	1 4 6 1 12			1 4 12 3 20	
	1 4 6 1 12			1 4 12 3 20	
	1 4 6 1 12			1 4 12 3 20	
	1 4 6 1 12			1 4 12 3 20	
	1 4 6 1 12			1 4 12 3 20	
	48 72 12 132			48 144 36 228	
		Sum(x=1)			Sum(x=1)
H(LC,x)	$24x+36x^2+6x^3$	66	Sh(DI,x)=H(LC,x)*D	$24x+72x^2+18x^3$	114=W
H'(LC,x)	$24+72x+18x^2$	114=W	Sh(DI,x)=x*H'(LC,x)		
H"(LC,x)	72+36x	108	Sh(DI,1)=H'(LC,1)		
H'(LC,x)+H"(LC,x)	$96+108x+18x^2$	222	Sh'(DI,x)	$24+144x+54x^2$	222
PD^2S (LC,1)	24+144+54	222	Sh'(DI,x)= H(LC,x)*(D^2/x)		
PD^2S(LC,1)	H'(LC,1)+H"(LC,1)	222	Sh'(DI,1)= PD^2S (LC,1)		

Remark the relations between the H(**LC**,x) and Sh(**DI**,x) polynomials, at the bottom of Table 2; the most interesting relation (providing a *new topological index*) is:

$$H'(\mathbf{LC},1) + H''(\mathbf{LC},1) = [H(\mathbf{LC},x) * (\mathbf{D}^2 / x) = Sh'(\mathbf{DI},x)]_{x=1}$$

D being the vector of distances (D=1, 2,..).

From these relations, we can write the general polynomial inter-changing relations (even ifthe **LM** and **M** matrices, encoding the same topological property,are not counted) and the general formula for the new "Shell-Matrix" index:

$$H(\mathbf{LM},x) = Sh(\mathbf{M},x) / \mathbf{D} = x * Sh'(\mathbf{M},x) / \mathbf{D}^2$$

$$Sh(\mathbf{M},x) = x * H'(\mathbf{LM},x)$$

$$H'(\mathbf{LM},1) + H''(\mathbf{LM},1) = [H(\mathbf{LM},x) * (\mathbf{D}^2 / x) = Sh'(\mathbf{M},x)]_{x=1}$$

Keeping in mind the above results, the Hosoya-Diudea polynomials for **LM** = **LR (**R being the count of rings around each of the points/atoms in the graph/molecule) is written below, in the case of Cuboctahedron (Table 3).

For other properties of Hosoya-Diudea polynomials see refs.[12,13]

Table 3. Counting H(LR,x) and Sh(R,x) in Cuboctahedron CO.

CO_LR;	D 0	1	2	3
1	6	24	36	6
2	6	24	36	6
3	6	24	36	6
4	6	24	36	6
5	6	24	36	6
6	6	24	36	6
7	6	24	36	6
8	6	24	36	6
9	6	24	36	6
10	6	24	36	6
11	6	24	36	6
12	6	24	36	6
	72	288	432	72
Polyn\D	1	2	3	Sum(x=1)
H(LR,x)	144x+	$216x^2$+	$36x^3$	396
H'(LR,x)	144+	432x+	$108x^2$	684
H''(LR,x)	-	432+	216x	648
Sh(R,x)	144x+	$432x^2$+	$108x^3$	684
Sh'(R,x)	144+	864x+	$324x^2$	1332

Table 4. Polynomials and vertex equivalence classes (by layer matrix of rings LR around vertices; signature as vertex centrality) in three hyper-dodecahedral nanostructures (see Figure 1).

Structure	**Topology: vertex equivalence classes**
ID@Ico$_{20}$_180 C(G)=12.99082 C/180=**0.072171** **F_3=400** **400*3=1200** **1200*180 = 216000**	**2H(LR,x)=1200**+8400x+19800x^2+33900x^3+49200x^4+51900x^5+35100x^6+14400x^7+2100x^8; 2H(LR,1)=216000 **2Sh(R,x)=**8400x+39600x^2+101700x^3+196800x^4+259500x^5+210600x^6+100800x^7+16800x^8; **2Sh(R,1)=**934200 2Sh'(R,1)=4581000 1. signature: 0.0920938709199495; | # of elements = 30 | deg = 9 | 3^10 2. signature: 0.0745279687777991; | # of elements = 60 | deg = 5 | 3^5 3. signature: 0.0722421872665493; | # of elements = 30 | deg = 9 | 3^10 4. signature: 0.0598176790970698; | # of elements = 60 | deg = 5 | 3^5
S_2(Do)@Do$_{20}$_340 **C(G)**=16.84805 C/340=**0.049553** **F_5=240** **240*5=1200** **1200*340=408000**	**2H(LR,x)=**1200+4320x+10800x^2+17280x^3+22680x^4+30540x^5+37800x^6+41040x^7+41760x^8+41220x^9+ 40140x^10+37080x^11+31140x^12+24480x^13+15660x^14+8880x^15+1740x^16+240x^17;2H(LR,1)=408000 **2Sh(R,x**)=4320x+21600x^2+51840x^3+90720x^4+152700x^5+226800x^6+287280x^7+334080x^8+370980x^9+ 401400x^10+407880x^11+373680x^12+318240x^13+219240x^14+133200x^15+27840x^16+4080x^17 **2Sh(R,1)**=3425880 2Sh'(R,1)=33416760 1. signature: 0.0524897500026536; | # of elements = 60 | deg = 5 | 5^6 2. signature: 0.0524697638449887; | # of elements = 60 | deg = 3 | 5^3 3. signature: 0.0496528759692478; | # of elements = 20 | deg = 3 | 5^3 4. signature: 0.0489586396313747; | # of elements = 120 | deg = 3 | 5^3 5. signature: 0.0460379516518164; | # of elements = 20 | deg = 3 | 5^3 6. signature: 0.0460271452180233; | # of elements = 60 | deg = 3 | 5^3
DoX$_{20}$_340 C(G)=16.39305 C/340=**0.048215** **F_5=120** **F_8=60** **120*5+60*8=** **1080** **1080*340=367200**	**2H(LR,x)=1080**+3480x^1+7680x^2+13080x^3+19440x^4+23820x^5+28620x^6+32400x^7+35160x^8+35700x^9+ 35760x^10+34080x^11+32220x^12+25920x^13+20220x^14+12000x^15+5460x^16+1020x^17+60x^18; 2H(LR,1)=**367200** **2Sh(R,x)=**3480x+15360x^2+39240x^3+77760x^4+119100x^5+171720x^6+226800x^7+281280x^8+321300x^9+ +357600x^10+374880x^11+386640x^12+336960x^13+283080x^14+180000x^15+87360x^16+17340x^17+ + 1080x^18; **2Sh(R,1)=3280980** 2Sh'(R,1)=33913260 1. signature: 0.0503930947335793; | # of elements = 60 | deg = 3 | 5.8^2 2. signature: 0.0503546980956381; | # of elements = 60 | deg = 4 | 5^2.8^2 3. signature: 0.0477088245398549; | # of elements = 20 | deg = 3 | 8^3 4. signature: 0.0473085257822019; | # of elements = 120 | deg = 3 | 5^2.8 5. signature: 0.047120519066602; | # of elements = 60 | deg = 3 | 5^2.8 6. signature: 0.0444873880198875; | # of elements = 20 | deg = 3 | 5^3

Hosoya-Diudea polynomials in hyper-dodecahedra. The above discussed polynomials and related indices have been calculated for the three hyper-dodecahedral nanostructures, shown in Figure 1; the results are listed in Table 4. In case of H(LR,x), the count at D=0 (i.e., the first term) is also

given and it is useful in checking the topology of the cages: 2H(LR,1)=|V(G)|*Sum(s*F_s), Fs being the number of faces of size s. The computations have been made by TOPOCLUJ[14] and Nano Studio[15] softwares. The matrix LR routine in Nano Studio program also provides the equivalence classes for the atoms (see the signature for each class), according to the values of the centrality index (see above). The global value C(G) is also given; the mean value per atom gives the relative centrality of the structures (0.072171 >0.049553> 0.048215, for ID@Ico_{20}_180, S_2(Do)@Do_{20}_340 and DoX_{20}_340, respectively). It was developed to discriminate the crystallographic networks.

Conclusions

The polynomial coefficients in Hosoya-Diudea generalized polynomials are calculable from layer/shell matrices, as implemented in the TOPOCLUJ software program. We applied this theory to three hypothetical nanostructures with icosahedral symmetry. New relations among the topological parameters were established. Such polynomial description can be useful in structure elucidation analysis and as an alternative to the crystallographic description.

Acknowledgements.

The work was supported by the Romanian Grant PN-II-ID-PCE-2011-3-0346.

References

1. Diudea, M. V.; Gutman, I.; Jäntschi, L. *Molecular Topology*, NOVA: New York, 2001 , pp. 11-51
2. Diudea, M. V. Layer Matrices in Molecular Graphs. *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 1064-1071.

3. Diudea, M. V.; Topan, M. I.; Graovac, A. Layer matrices of walk degrees. *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 1072-1078.
4. Diudea, M. V.; Florescu, M. S.; Khadikar, P. V. *Molecular Topology and Its Applications*, EFICON: Bucharest, 2006, pp 11-46.
5. Diudea M. V.; Ursu, O. Layer matrices and distance property descriptors. *Indian J. Chem.* **2003**, *42A*, 1283-1294.
6. Diudea, M. V. Valences of property. *Croat. Chem.Act.* **1999**, *72*, 835-851.
7. Diudea, M. V. Cluj polynomials. *Studia Univ. "Babes-Bolyai"* **2002**, *47*, 131-139.
8. Hosoya, H. On some counting polynomials in chemistry. *Discrete Appl. Math.* **1988**, *19*, 239-257.
9. Diudea, M. V. Nanomolecules and Nanostructures - Polynomials and Indices. MCM, No. ***10,*** Univ. Kragujevac, Serbia, 2010, pp. 59-71; 169-213.
10. Wiener, H. Structural determination of the paraffin boiling points, *J. Am. Chem. Soc.* **1947**, *69*, 17–20.
11. Randić, M. Novel molecular descriptor for structure-property studies. *Chem. Phys. Lett.* **1993**, *211*, 478-483.
12. Diudea, M. V.; Hosoya-Diudea polynomials revisited. *MATCH Commun. Math.Comput. Chem.* **2013**, *69*, 93-110.
13. Diudea, M. V.; Ashrafi, A. R. Shell-polynomials and Cluj-Tehran index in tori T(4,4)S[5,n]. *Acta Chim. Sloven.* **2010**, *57*, 559-564.
14. Ursu, O.; Diudea, M. V. *TOPOCLUJ software package*, "Babes-Bolyai" University, Cluj, 2002.
15. Nagy, Cs. L.; Diudea, M. V. *Nano Studio software package,* "Babes-Bolyai" University, Cluj, 2009.