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ZAGREB CONNECTION INDICES OF TWO DENDRIMER NANOSTARS

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Abstract: It is well known fact that several physicochemical properties of chemical compounds are closely related to their molecular structure. Mathematical chemistry provides a method to predict the aforementioned properties of compounds using topological indices. The Zagreb indices are among the most studied topological indices. Recently, three modified versions of the Zagreb indices were proposed independently in [Ali, A.; Trinajstić, N. A novel/old modification of the first Zagreb index, *arXiv*:1705.10430 [math.CO] **2017**; *Mol. Inform.* **2018**, *37*, 1800008] and [Naji, A. M.; Soner, N. D.; Gutman, I. On leap Zagreb indices of graphs, *Commun. Comb. Optim.* **2017**, *2*, 99–117], which were named as the Zagreb connection indices and the leap Zagreb indices, respectively. In this paper, we check the chemical applicability of the newly considered Zagreb connection indices on the set of octane isomers and establish general expressions for calculating these indices of two well-known dendrimer nanostars.

***Keywords*:** chemical graph theory; topological index; Zagreb connection indices; leap Zagreb indices; dendrimer nanostar.

Introduction

Predicting physicochemical properties of chemical structures is an interesting issue in theoretical chemistry. Several theoretical methods have

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been developed for this purpose and one of such methods uses topological indices. Topological indices are numbers associated with chemical structures for the purpose of QSPR/ QSAR studies. Their use in lead discovery and optimization for drug design and in correlating and predicting physical properties has been well documented.[1-4]

A molecular graph is a graph of a molecule in which vertices correspond to the atoms while edges represent the covalent bonds between atoms. The following topological indices were firstly appeared[5] within an approximate formula for total π-electron energy of molecule:

$$M_1(G) = \sum_{u \in V(G)} (d_u)^2 \tag{1}$$

$$ZC_1^*(G) = \sum_{u \in V(G)} d_u \tau_u \,, \tag{2}$$

where d_u and τ_u denote degree and connection number (number of those vertices of the (molecular) graph G whose distance from u is 2), respectively, of the vertex $u \in V(G)$. The following topological index was also appeared[6] within the study of molecular branching:

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v \,, \tag{3}$$

where $E(G)$ is the edge set of the (molecular) graph G. The topological indices $M_1$and M_2 are known as the first Zagreb index and second Zagreb index, respectively, and both of these indices have been studied extensively, for example see the recent surveys.[7-10] In contrast, the topological index ZC_1^* was never studied explicitly till 2016.

It is well known that M_1 can be written as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v). \tag{4}$$

It was proved[11,12] that the topological index ZC_1^* can be rewritten as

$$ZC_1^*(G) = \sum_{uv \in E(G)} (\tau_u + \tau_v)\,, \tag{5}$$

which is the connection-number-based version of the first Zagreb index M_1, defined in Eq. (4), and hence it was named as modified first Zagreb connection index.[11,12]

Corresponding to Eq. (1) and Eq. (3), the following connection-number-based version of the Zagreb indices were also put forwarded[11,12]:

$$ZC_1(G) = \sum_{u \in V(G)} (\tau_u)^2, \tag{6}$$

$$ZC_2(G) = \sum_{uv \in E(G)} \tau_u \tau_v\,. \tag{7}$$

The indices ZC_1 and ZC_2 were named as the first Zagreb connection index and second Zagreb connection index, respectively.[11,12] It is worth mentioning here that all the three above-mentioned Zagreb connection indices were independently introduced in Ref. [13] and were referred as the leap Zagreb indices. Further detail about the Zagreb connection indices or leap Zagreb indices can be found in the Refs. [14-20].

Dendrimer nanostar is one of the main objects in nanotechnology. This is a part of a new group of macromolecules that appear to be photon funnels just like artificial antennas. It consists of three major architectural components: core, branches and end groups. Details about dendrimer nanostar can be found in the Refs. [21,22].

The problem of computing topological indices of dendrimer nanostars has attracted a considerable attention from researchers, for example see[23] for the Padmakar-Ivan, Szeged, edge Szeged indices and their polynomials; see[24] for the Cluj index; see[25,26] for several distance-based topological

indices; see[27] for total-Szeged index; see[28] for Hosoya polynomial; see[29] for the Harary index; see[30-32] for some degree based indices including Zagreb indices and see[33] for some distance based indices. In this paper, we continue such type of study for the Zagreb connection indices.

Results and Discussion

Firstly, we check the chemical applicability of the newly considered Zagreb connection indices on the set of octane isomers. In Ref. [12], the modified first Zagreb connection index ZC_1^* was tested against the thirteen physicochemical properties (whose experimental values were taken from the website www.moleculardescriptors.eu.) on the aforementioned set of molecules and it was concluded that ZC_1^* correlates well with the entropy and acentric factor (absolute values of the correlation coefficient are approximately equal to 0.892 and 0.949, respectively). Here, we perform a similar test for the other two Zagreb connection indices ZC_1 and ZC_2, and found that ZC_1 has better correlating ability than both the indices ZC_1^* and ZC_2 in the cases of entropy, enthalpy of vaporization, standard enthalpy of vaporisation and acentric factor, see Table 1.

Table 1. Those absolute values of the correlation coefficient between six certain physicochemical properties of octane isomers and Zagreb connection indices which are greater than 0.8.

Property	ZC_1	ZC_1^*	ZC_2
Entropy (S)	**0.9197**	0.892	0.8362
Density (DENS)	---	---	0.8384
Enthalpy of Vaporization (HVAP)	**0.9135**	---	---
Standard Enthalpy of Vaporisation (DHVAP)	**0.9551**	---	---
Acentric Factor (AcenFac)	**0.9514**	0.949	0.8619
Molar Volume (MV)	---	---	0.8586

Now, we establish general expressions for calculating Zagreb connection indices of two well-known dendrimer nanostars. Before going further, we define some parameters first. Denote by $c_i(G)$ the number of vertices (in the graph G) with connection number i and $y_{i,j}(G)$ the number of edges (in G) connecting the vertices with connection numbers i, j. The formulas for the Zagreb connection indices, given in Equations (6), (7), (5), can be rewritten as

$$ZC_1(G) = \sum_{0\le i\le n-2} c_i(G)\cdot i^2 \ , \tag{8}$$

$$ZC_2(G) = \sum_{0\le i\le j\le n-2} y_{i,j}(G)\cdot ij \ , \tag{9}$$

$$ZC_1^*(G) = \sum_{0\le i\le j\le n-2} y_{i,j}(G)\cdot (i+j) \ , \tag{10}$$

respectively, where n is the number of vertices in G. Firstly, we establish formulas for calculating the Zagreb connection indices of first type of dendrimer nanostar $D_1[n]$, where n is the steps of growth. For $n = 1,2,3$, skeletal formula of $D_1[n]$ (together with the connection number of each atom) is depicted in Figures 1, 2, 3, respectively.

A hexagon of $D_1[n]$ is said to be terminal hexagon if it contains exactly five vertices of degree 2, central hexagon if it contains only vertices with connection number 3 and θ-hexagon if it is neither terminal nor central. Those vertices of $D_1[n]$ which do not lie on any hexagon are said to be α-type vertices. By an (a,b)-type edge, we mean the edge connecting the vertices with connection numbers a and b. Now, we are ready to state and prove the first main result of this paper.

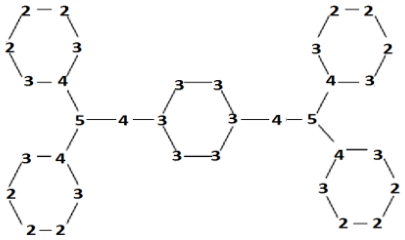

Figure 1. The skeletal formula of $D_1[n]$ (together with the connection number of each atom) for $n = 1$.

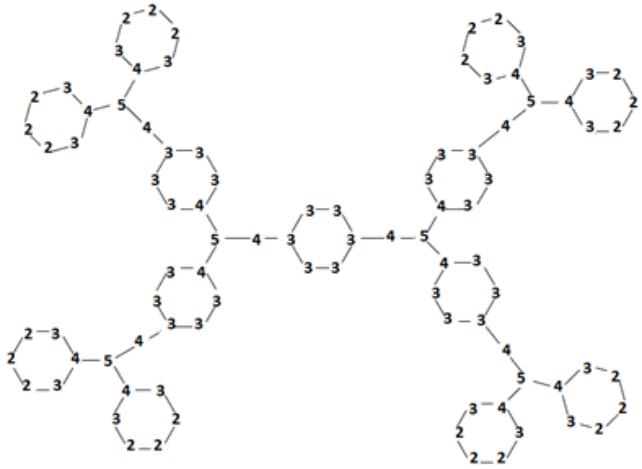

Figure 2. The skeletal formula of $D_1[n]$ (together with the connection number of each atom) for $n = 2$.

Theorem 1. The Zagreb connection indices of the molecular graph G of $D_1[n]$ (see Figures 1, 2 and 3) are given as

i. $ZC_1(G) = 296 \times 2^n - 272$,

ii. $ZC_2(G) = 352 \times 2^n - 330$,

iii. $ZC_1^*(G) = 208 \times 2^n - 184$.

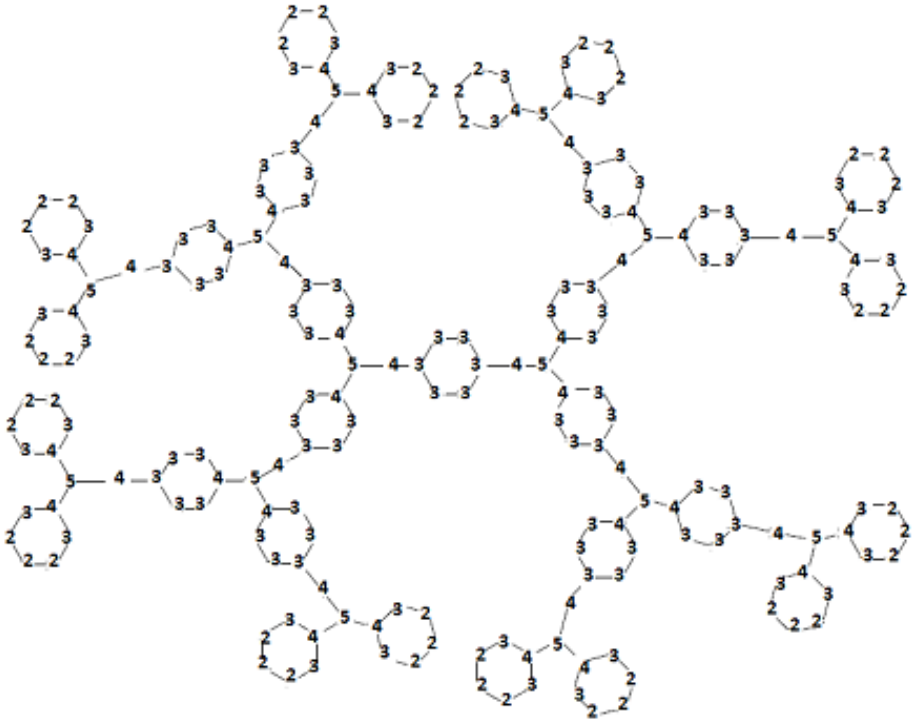

Figure 3. The skeletal formula of $D_1[n]$ (together with the connection number of each atom) for $n = 3$.

Proof: i. Firstly, we evaluate $c_2(G)$. It can be easily observed that only terminal hexagons contain vertices having connection number 2. But, there are exactly three vertices whose connection number is 2 in every terminal hexagon. Hence, $c_2(G)$ must be equal to 3 times the number of terminal hexagons in G. Simple observation yields that, the number of terminal hexagons is 2^{n+1}. Therefore,

$$c_2(G) = 3 \times 2^{n+1}.$$

Now, we calculate $c_3(G)$. In the graph G, there are exactly 2 vertices in every terminal hexagons having connection number 3. Hence, total number of vertices in terminal hexagons with connection number 3 is $2 \times 2^{n+1}$. Also, all the vertices of central hexagon have connection number 3. The

number of θ-hexagons is $0, 4, 12, 28, \ldots$ for $n = 1, 2, 3, 4 \ldots$ respectively. The n^{th} term of the sequence 0,4,12,28, ... is $2^{n+1} - 4$. Each θ-hexagon contains five vertices with connection number 3. Hence, total number of vertices with connection number 3 in θ-hexagons is $5(2^{n+1} - 4)$. Consequently, we have

$$c_3(G) = 14 \times 2^n - 14.$$

Next, we calculate $c_4(G)$. There is exactly one vertex with connection number 4 in every terminal hexagon as well as in θ-hexagon. So, total number of vertices with connection number 4 in terminal hexagons and θ-hexagons is $2^{n+1} + 2^{n+1} - 4 = 4 \times 2^n - 4$. We note that half of the α-type vertices have connection number 4 and the half have connection number 5. The number of α-type vertices with connection number 4 is 2,6,14, ... for $n = 1,2,3, \ldots$ respectively. The n^{th} term of the sequence 2,6,14, ... is $2^{n+1} - 2$. Hence,

$$c_4(G) = 3 \times 2^{n+1} - 6.$$

Finally, we calculate $c_5(G)$. In graph G only α-type vertices have connection number 5 and it is mentioned above that half of α-type vertices have connection number 5. So,

$$c_5(G) = 2^{n+1} - 2.$$

By using definition of the first Zagreb connection index, we get

$$ZC_1(G) = 296 \times 2^n - 272.$$

ii. To derive the second formula, we calculate $y_{2,2}(G)$, $y_{2,3}(G)$ and $y_{3,3}(G)$ first. From the graph G, it is observed that the (2,2)-type, (2,3)-type and (3,3)-type edges lies on only hexagons. The number of hexagons of each type has already been calculated in part (i) and hence after routine computation, we get

$$y_{2,2}(G) = y_{2,3}(G) = 2 \times 2^{n+1}, y_{3,3}(G) = 8 \times 2^n - 10.$$

Now, we calculate $y_{3,4}(G)$. In the graph G, there are exactly 2 edges of (3,4)-type in every terminal hexagon. Hence, total number of (3,4)-type edges in terminal hexagons is $2 \times 2^{n+1}$.

Also, each θ-hexagon contains two edges of $(3,4)$-type. Hence, total number of $(3,4)$-type edges in θ-hexagons is $2(2 \times 2^n - 4)$. We note that the number of those $(3,4)$-type edges which do not lie on any hexagon is same as the number of α-type vertices with connection number 4, which is $2^{n+1} - 2$. So,

$$y_{3,4}(G) = 10 \times 2^n - 10.$$

Next, we calculate $y_{4,5}(G)$. We note that the number of $(3,5)$-type edges is same as the 3 times the number of α-type vertices having connection number 5. Hence,

$$y_{4,5}(G) = 3(2^{n+1} - 2).$$

By substituting the values of $y_{i,j}(G)$ in Eq. (9), we get the desired result.

iii. Substitution of the values of $y_{i,j}(G)$ in Eq. (10), gives the required formula.

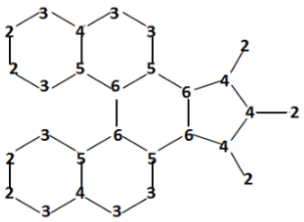

Figure 4. The skeletal formula of $D_2[n]$ (together with the connection number of each atom) for $n = 1$.

Now, we establish formulas for calculating the Zagreb connection indices of the second type of dendrimer nanostar $D_2[n]$ where n is the steps of growth. For $n = 1, 2, 3$, the skeletal formula of $D_2[n]$ (together with the connection number of each atom) is depicted in Figures 4, 5, 6, respectively. A pentagon of $D_2[n]$ is said to be terminal pentagon if it contains exactly three vertices with connection number 4, and non-terminal otherwise. A hexagon of $D_2[n]$ is said to be α-hexagon (or terminal hexagon), θ-hexagon, β-hexagon, γ-hexagon if it has exactly 2, 3, 4, 6 vertices of degree 3, respectively.

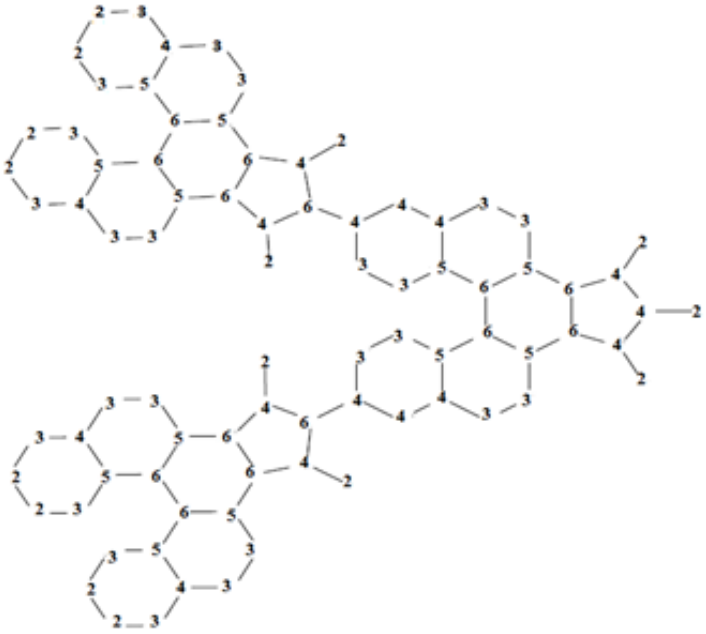

Figure 5. The skeletal formula of $D_2[n]$ (together with the connection number of each atom) for $n = 2$.

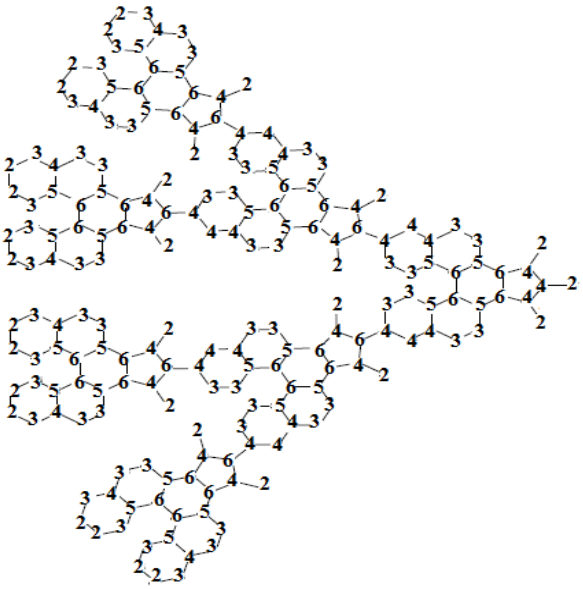

Figure 6. The skeletal formula of $D_2[n]$ (together with the connection number of each atom) for $n = 3$.

Theorem 2. The Zagreb connection indices of the molecular graph G of $D_2[n]$ (see Figures 4, 5 and 6) are given below

i. $ZC_1(G) = 464 \times 2^n - 504$,

ii. $ZC_2(G) = 611 \times 2^n - 668$,

iii. $ZC_1^*(G) = 278 \times 2^n - 294$.

Proof: i. From Figure 6, one can easily observe that the number of α-hexagons, β-hexagons, θ-hexagons and γ-hexagons is 2^n, $2(2^n - 1)$, $2(2^{n-1} - 1)$ and $2^n - 1$, respectively. Also, the number of non-terminal pentagons is $2^n - 2$. Simple calculations yield

$$c_2(G) = 4 \times 2^n - 1, c_3(G) = 8(2^n - 1), c_4(G) = 6 \times 2^n - 7,$$

$$c_5(G) = 4(2^n - 1), c_6(G) = 5 \times 2^n - 6.$$

After substituting the above values in Equation (8), we get

$$ZC_1(G) = 464 \times 2^n - 504.$$

ii. Again, bearing in mind Figure 6 and after routine computations, we have

$y_{2,2}(G) = 2^n$, $y_{2,3}(G) = 2^{n+1}$, $y_{2,4}(G) = 2^{n+1} - 1$, $y_{3,3}(G) = 3 \times 2^n - 4$,

$y_{3,4}(G) = y_{3,5}(G) = 4(2^n - 1)$, $y_{4,4}(G) = y_{4,5}(G) = y_{6,6}(G) = 2(2^n - 1)$

$$y_{4,6}(G) = 5 \times 2^n - 8, y_{5,6}(G) = 6(2^n - 1)$$

After putting the above values in Equation (9), we get

$$ZC_2(G) = 611 \times 2^n - 668.$$

iii. Substitution of the values of $y_{i,j}(G)$, calculated in part (ii), in Equation (10) gives the desired result.

Concluding Remarks

Three recently considered Zagreb connection indices, namely the first Zagreb connection index, modified first Zagreb connection index and the second Zagreb connection index, have been tested in this paper on the set of

octanes isomers for their chemical applicability. It has been found that the first Zagreb connection index has better predictive ability than the other two Zagreb connection indices in the cases of entropy, enthalpy of vaporization, standard enthalpy of vaporisation and acentric factor.

Also, general expressions for calculating all the three Zagreb connection indices of two dendrimer nanostars have been established here. These expressions depend only on the steps of growth of the considered dendrimers.

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