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# ZAGREB CONNECTION INDICES OF SOME NANOSTRUCTURES

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**Abstract:** The first Zagreb index (occurred in an approximate formula of total π-electron energy, communicated in 1972) and the second Zagreb index (appeared in 1975, within the study of molecular branching) are among the most studied topological indices. Recently, three modified versions of the Zagreb indices were proposed independently in [A. Ali, N. Trinajstić, A novel/old modification of the first Zagreb index, arXiv:1705.10430 [math.CO], 2017] and [A. M. Naji, N. D. Soner, I. Gutman, 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 derive formulas for calculating these modified versions of the Zagreb indices of four well known nanostructures.

***Keywords*:** chemical graph theory; topological index; Zagreb connection index; leap Zagreb index; nanostructure

## Introduction

Modeling physicochemical properties of chemical compounds is an interesting issue in theoretical chemistry.

A topological index is a numerical quantity calculated from the molecular graph (a graph representing a chemical compound in which vertices correspond to the atoms while edges represent the covalent bonds

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between atoms) of a chemical compound in such a way that this quantity must remain same under graph isomorphism and also it must be well related to at least one physicochemical property of the considered chemical compound. A recent trend in theoretical chemistry is the use of topological indices in predicting the certain properties of chemical compounds.[1-4]

The first Zagreb index $M_1$, occurred in an approximate formula of total $\pi$-electron energy,[5] and the second Zagreb index $M_2$, appeared within the study of molecular branching,[6] are among the most studied topological indices. These topological index are defined as

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

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v , \tag{2}$$

where $V(G)$ is the vertex set of a graph $G$, $E(G)$ is the edge set of $G$ and $d_u$ denote degree of the vertex $u \in V(G)$. The first and second Zagreb indices have been studied extensively; for example, see the recent survey papers.[7-10]

Corresponding to Equation (1) and Equation (2), the following connection-number-based version of the Zagreb indices were put forwarded,[11-13] independently:

$$ZC_1(G) = \sum_{u \in V(G)} (\tau_u)^2, \tag{3}$$

$$ZC_2(G) = \sum_{uv \in E(G)} \tau_u \tau_v . \tag{4}$$

The indices $ZC_1$ and $ZC_2$ were named as the first Zagreb connection index and second Zagreb connection index, respectively.[12] The following topological index was also appeared in the same formula where $M_1$ was occurred:

$$ZC_1^*(G) = \sum_{u \in V(G)} d_u \tau_u , \tag{5}$$

where $\tau_u$ denote connection number (number of those vertices of $G$ whose distance from $u$ is 2) of the vertex $u \in V(G)$. The index $ZC_1^*$ was never studied explicitly till 2016. Recently, this index has been reconsidered in the Refs.[11,12] and in the Ref.[13], independently. Ali and Trinajstić[12] checked the chemical applicability of $ZC_1^*$ and they found that this topological index correlates well with the entropy and acentric factor of octane isomers. They[12] also determined the graphs having maximum and minimum $ZC_1^*$ values among all molecular trees with $n$ vertices. Naji *et al.*[13] established several bounds on the topological indices $ZC_1^*$, $ZC_1$, $ZC_2$ and they also derived formulas for calculating these three topological indices of join of graphs. Further work on the topological indices $ZC_1^*$, $ZC_1$, $ZC_2$ can be found in the Refs.[14-17].

It is well known fact that $M_1$ can be written as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v). \tag{6}$$

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

$$ZC_1^*(G) = \sum_{uv \in E(G)} (\tau_u + \tau_v)\,, \tag{7}$$

which is the connection-number-based version of first Zagreb index $M_1$, defined in Eq. (3), and hence it was named as modified first Zagreb connection index.

The main purpose of the present paper is to address the problem of computing topological indices of nanostructures. We solve this problem for four nanostructures in case of the Zagreb connection indices $ZC_1^*$, $ZC_1$, $ZC_2$.

## Results and Discussion

In order to obtain the main results, we need to define some parameters. Denote by $c_i(G)$ the number of vertices in $G$ 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 (3), (4) and (7), can be rewritten as

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

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

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

where $n$ is the number of vertices in $G$. Firstly, we establish formulas for calculating the Zagreb connection indices of a dendrimer nanostar, denoted by $D_1[n]$, whose molecular graph is depicted in Figure 1 for $n = 2$. In this Figure, connection numbers are also displayed against every vertex of the molecular graph.

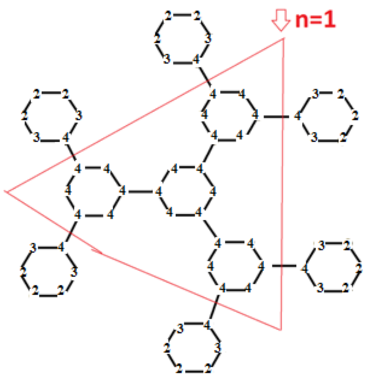


**Figure 1** . The molecular graph of $D_1[2]$ together with the vertex connection numbers.

A hexagon of $D_1[n]$ is said to be terminal hexagon if it contains exactly five vertices of degree 2. A hexagon of $D_1[n]$ containing only vertices with connection number 4 is called non-terminal hexagon. An edge connecting the vertices having degrees $d_1$ and $d_2$ is known as the edge of the type $(d_1, d_2)$.

**Theorem 1.** The Zagreb connection indices of the molecular graph $G$ of $D_1[n]$ (for example, see Figure 1) are given as

**i.** $ZC_1(G) = 213 \times 2^n - 192,$

**ii.** $ZC_2(G) = 258 \times 2^n - 240,$

**iii.** $ZC_1^*(G) = 246 \times 2^n - 240.$

**Proof: i.** Clearly, $|V(G)| = 18 \times 2^n - 12$, $|E(G)| = 21 \times 2^n - 15$ and 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 of the terminal hexagons of $G$. Also, the number of terminal hexagons is $3, 6, 12, \ldots$ for $n = 1, 2, 3, \ldots$ respectively. The $n^{th}$ term of the sequence $3, 6, 12, \ldots$ is $3 \times 2^{n-1}$. So, total number of vertices with connection number 2 in terminal hexagons is $9 \times 2^{n-1}$, that is,

$$c_2(G) = 9 \times 2^{n-1}.$$

Similarly,

$$c_3(G) = 3 \times 2^n.$$

Finally, we calculate $c_4(G)$. In graph $G$, both the terminal hexagons and non-terminal hexagons have vertices with connection number 4. Every terminal hexagon has only one vertex with connection number 4. So, total number of vertices with connection number 4 in terminal hexagons is $3 \times 2^{n-1}$. The number of vertices with connection number 4 in non-terminal hexagons is $6(3 \times 2^{n-1} - 2)$. Hence,

$$c_4(G) = 21 \times 2^{n-1} - 12$$

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

$$ZC_1(G) = 213 \times 2^n - 192.$$

**ii.** We note that only terminal hexagons contain edges of the type $(2,2)$, $(2,3)$ and $(3,4)$ and hence

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

Now, we calculate $y_{4,4}(G)$. Every non-terminal hexagon have 6 edges of the type $(4,4)$ and the number of non-terminal hexagons is $6(3 \times 2^{n-1} - 2)$. The edges which do not lie on any hexagons are also of the type $(4,4)$. These edges are $3 \times 2^n - 3$ in total. Hence,

$$y_{4,4}(G) = 12 \times 2^n - 15.$$

From the definition of the second Zagreb connection index, it follows that

$$ZC_2(G) = 258 \times 2^n - 240$$

**iii.** Substitution of the values of $y_{i,j}(G)$ in the following formula gives the desired result:

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

A hexagon of $D_2[n]$ (see Figure 2) is said to be terminal hexagon if it contains exactly five vertices of degree 2. A hexagon of $D_2[n]$ is called $\alpha$-hexagon if it contains exactly four vertices of degree 2. A hexagon of $D_2[n]$ is said to be $\beta$-hexagon if it contains exactly five vertices of degree 3. A hexagon of $D_2[n]$ containing only vertices with connection number 4 is referred as a central hexagon. Clearly, there are only two central hexagons in $D_2[n]$. Corresponding to every $\beta$-hexagon, there are five edges which connect the $\beta$-hexagon to other five hexagons. From these five edges, two have the type $(4,5)$, which will be called $\theta$-type edges and the other three have the type $(4,6)$, which will be referred as $\omega$-type edges.

**Theorem 2.** The Zagreb connection indices of the molecular graph $G$ of $D_2[n]$ (see Figure 2) are given as

**i.** $ZC_1(G) = 1520 \times 2^n - 1416$,

**ii.** $ZC_2(G) = 1928 \times 2^n - 1808$,

**iii.** $ZC_1^*(G) = 992 \times 2^n - 920$.

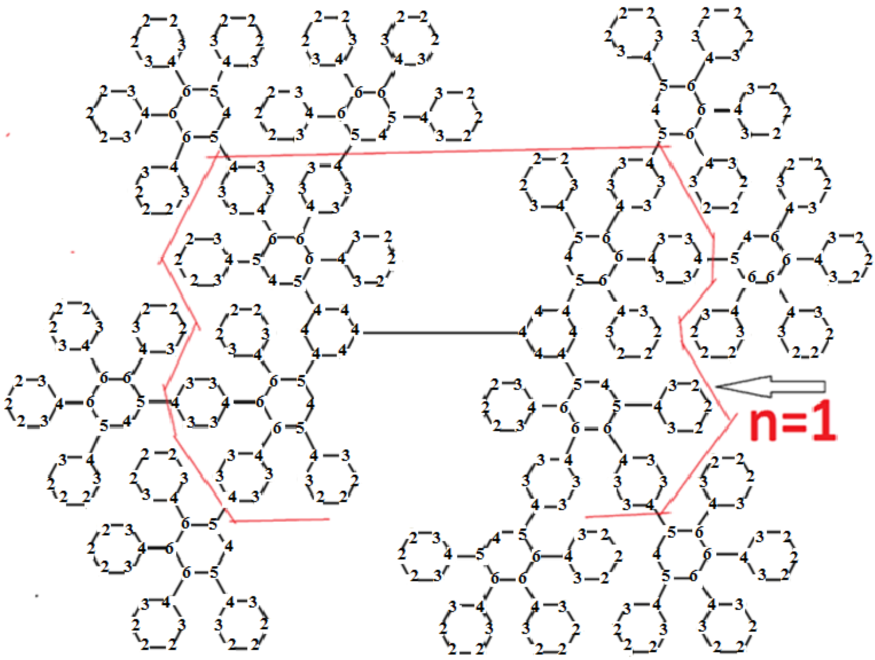


**Figure 2.** The molecular graph of $D_2[2]$.

**Proof: i.** It can be observed that $|V(G)| = 120 \times 2^n - 8, |E(G)| = 140 \times 2^n - 127$ and 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 of the terminal hexagons. It can be easily seen from the graph $G$ that the number of terminal hexagons is $16,40,128,\ldots$ for $n = 1,2,3,\ldots$ respectively. The $n^{th}$ term of the sequence $16,40,128,\ldots$ is $12 \times 2^n - 8$. So, total number of vertices with connection number 2 in terminal hexagons is $3(12 \times 2^n - 8)$. Hence,

$$c_2(G) = 36 \times 2^n - 24$$

Now, we calculate $c_3(G)$. In the graph $G$, only terminal hexagons and $\alpha$-hexagons have vertices with connection number 3. Each terminal hexagons have two vertices with connection number 3. So, total number of vertices with connection number 3 in terminal hexagons is $2(12 \times 2^n - 8)$. Also, the number of $\alpha$-hexagons is $0,8,16,\dots$ for $n = 1,2,3,\dots$ respectively. The $n^{th}$ term of the sequence $0,8,16,\dots$ is $4 \times 2^n - 8$. Each $\alpha$-hexagon have four vertices with connection number 3. Thus, total number of vertices with connection number 3 in $\alpha$-hexagons is $4(4 \times 2^n - 8)$ and hence

$$c_3(G) = 40 \times 2^n - 48.$$

Next, we calculate $c_4(G)$. Clearly, every hexagon has at least one vertex with connection number 4. The number of vertices with connection number 4 in the central hexagons is 12. The number of $\beta$-hexagons is $4 \times 2^n - 4$. Also, the number of vertices with connection number 4 in terminal hexagons and $\beta$-hexagons is $12 \times 2^n - 8 + 4 \times 2^n - 4$. Each $\alpha$-hexagon have two vertices with connection number 4. So, number of vertices with connection number 4 in $\alpha$-hexagons is $2(4 \times 2^n - 8)$. Hence,

$$c_4(G) = 24 \times 2^n - 16.$$

Finally, we calculate $c_5(G)$ and $c_6(G)$. It is clear that every $\beta$-hexagon contain 2 and 3 vertices with connection numbers 5 and 6, respectively. Thus,

$$c_5(G) = 8 \times 2^n - 8.$$

and

$$c_6(G) = 12 \times 2^n - 12.$$

Now, by using the definition of first Zagreb connection index, we get

$$ZC_1(G) = 1520 \times 2^n - 1416.$$

**ii.** It is evident from the graph $G$ that only terminal hexagons contain edges of the types $(2,2)$ and $(2,3)$. But, every terminal hexagon has two edges of the type $(2,2)$ and two edges of the type $(2,3)$. But, the number of terminal hexagons is $12 \times 2^n - 8$. Hence,

$$y_{2,2}(G) = y_{2,3}(G) = 24 \times 2^n - 16.$$

In order to find the desired formula, we calculate the quantities $y_{3,3}(G)$, $y_{3,4}(G), y_{4,4}(G), y_{4,5}(G), y_{4,6}(G), y_{5,6}(G)$ and $y_{6,6}(G)$.

It is obvious from the graph $G$ that only the $\alpha$-hexagons have edges of the type $(3,3)$. But, every $\alpha$-hexagons has two edges of the type $(3,3)$ and the number of $\alpha$-hexagons is $4 \times 2^n - 8$. So,

$$y_{3,3}(G) = 8 \times 2^n - 16.$$

Certainly, only terminal hexagons and $\alpha$-hexagons contain the edges of the type $(3,4)$. But, every terminal hexagon has two edges of the type $(3,4)$ and every $\alpha$-hexagon has four edges of the type $(3,4)$. So, the number of edges of the type $(3,4)$ in $G$ is $2( 12 \times 2^n - 8) + 4(4 \times 2^n - 8)$, that is,

$$y_{3,4}(G) = 40 \times 2^n - 48.$$

It is obvious that

$$y_{4,4}(G) = 13.$$

Since every $\beta$-hexagon has two edges of the type $(4,5)$ and the number of $\beta$-hexagons is $4 \times 2^n - 4$. So, the total number of $(4,5)$-type edges in $\beta$-hexagons is $2( 4 \times 2^n - 4)$. The $\theta$-type edges are $8, 24, 56, \ldots$ for $n = 1, 2, 3 \ldots$ respectively. The $n^{th}$ term of the sequence $8, 24, 56, \ldots$ is $8 \times 2^n - 8$ and hence

$$y_{4,5}(G) = 16 \times 2^n - 16.$$

The $\omega$-type edges are only edges of the type $(4, 6)$, which are $12 \sum_{i=0}^{n-1} 2^i$ in total. Hence,

$$y_{4,6}(G) = 12(2^n - 1).$$

Edges of the type $(5,6)$ exist only on $\beta$-hexagons. Every $\beta$-hexagon contains two $(5,6)$-type edges. So,

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

Similarly,

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

By substituting the values of the quantities $y_{i,j}(G)$ in the formula of the second Zagreb connection index, we get

$$ZC_2(G) = 1928 \times 2^n - 1808.$$

**iii.** Substitution of the values of $y_{i,j}(G)$ in the following formula gives the desired result:

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

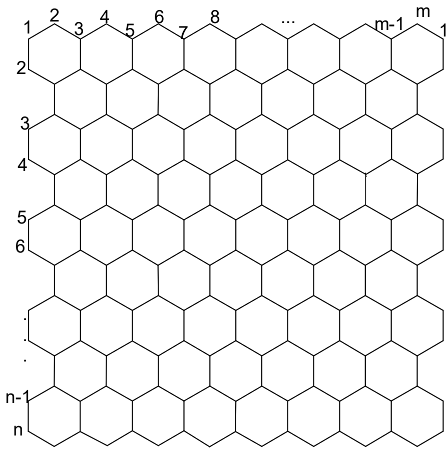


**Figure 3**. The 2-dimensional lattice of a nanotube used in Theorem 3.

The proofs of next four results (Theorems 3, 4, 5 and 6) are similar to that Theorem 2 and hence we omit them.

**Theorem 3.** The Zagreb connection indices of the molecular graph $G_1$ of the nanotube, depicted in Figure 3, are given as

$$ZC_1(G_1) = 36mn - 40m,$$

$$ZC_2(G_1) = 36mn - 76m,$$

$$ZC_1^*(G_1) = 18mn - 16m.$$

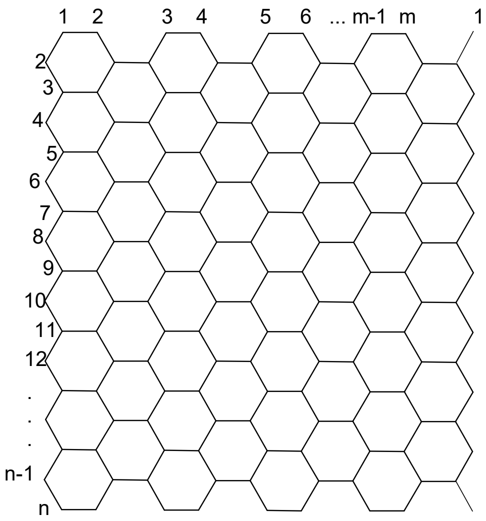


**Figure 4.** The 2-dimensional lattice of a nanotube used in Theorem 4.

**Theorem 4.** The Zagreb connection indices of the molecular graph $G_2$ of the nanotube, shown in Figure 4, are given as

$$ZC_1(G_2) = 36mn - 76m,$$

$$ZC_2(G_2) = 54mn - 128m,$$

$$ZC_1^*(G_2) = 18mn - 30m.$$

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