Vertex-degree-based topological indices of some dendrimer nanostars

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A topological index is the number obtained from molecular graph, reflecting certain structural features of the corresponding molecule. A great variety of topological indices are being used in Theoretical Chemistry and many of them depend only on the vertex degree of the molecular graph. In the present study, the authors have obtained general expressions for evaluating the vertex-degree-based topological indices of four types of dendrimer nanostar.

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1. Introduction

Throughout this study, we consider only simple, finite and undirected graphs. For undefined notations and terminologies from Graph Theory, see for example [1]. In molecular graphs, the vertices correspond to atoms while the edges represent covalent bonds between atoms [2]. The number obtained from molecular graph, reflecting certain structural features of the molecule is called ''molecular structure descriptor'' or simply ''topological index'' [3]. A great variety of such indices is being studied and used in theoretical chemistry [3-6]. Among them a large number of indices, depends only on vertex degree of the molecular graph [4-6]. The general form [8-10, 44] of these indices is:

$$TI(G) = \sum_{1\leq i<j\leq \Delta(G)} \theta_{i,j} . x_{i,j}(G) , \qquad (1)$$

where $\Delta(G)$ is the maximum vertex degree in the graph G, $\theta_{i,j}$ is a non-negative real valued function depending on i , j with $\theta_{i,j} = \theta_{j,i}$ and $x_{i,j}(G)$ is the number of edges in G connecting the vertices of degrees i and j. Many well-known topological indices are the special cases of (1):

i). Let $\alpha \neq 0$ is a real number. If $\theta_{i,j} = (ij)^{\alpha}$, then TI is general Randić index [11] (variable second Zagreb index [41]). Moreover, if $\alpha = -\frac{1}{2}, 1, -1$ then TI is Randić index [12], second Zagreb index [13], modified second Zagreb index [14] respectively.
ii). If $\theta_{i,j} = (i+j)^{\beta}$, where $\beta \neq 0$ is a real number, then TI is the general sum-connectivity index [15]. If we take β equal to $-\frac{1}{2}$ or 1, then TI is the sum-connectivity index [16] or the first Zagreb index [13] respectively.
iii). If $\theta_{i,j} = (\frac{i+j-2}{ij})^{\gamma}$, where $\gamma \neq 0$ is a real number, then TI is the general atom-bond connectivity index [17]. If γ is equal to $\frac{1}{2}$ or -3, then TI corresponds to the atom-bond connectivity index [18] or the augmented Zagreb index [19] respectively.
iv). If $\theta_{i,j} = \left(\frac{2\sqrt{ij}}{i+j}\right)^{\lambda}$, where $\lambda > 0$ is a real number, then TI is the ordinary generalized geometric–arithmetic index [20]. For $\lambda = 1$, TI is the first geometric-arithmetic index [21].
v). If $\theta_{i,j} = \frac{2}{i+j}$, then TI is the harmonic index [22].
vi). If $\theta_{i,j} = |i-j|$, then TI is the Albertson index [23].
vii). If $\theta_{i,j} = \frac{lni}{i} + \frac{lnj}{j}$, then TI is logarithm of the first multiplicative Zagreb index [31].
viii). If $\theta_{i,j} = ln(i+j)$, then TI is logarithm of the second multiplicative Zagreb index [31].
ix). If $\theta_{i,j} = ln\, i + lnj$, then TI is logarithm of the modified first multiplicative Zagreb index [32].

There are many other topological indices which can be obtained from (1), see for example [10, 44]

Nanostructured materials are those with at least one dimension falling in nanometer scale, and include nanoparticles (including quantum dots, when exhibiting quantum effects), nanorods and nanowires, thin films, and bulk materials made of nanoscale building blocks or consisted of nanoscale structures [24].

Dendrimer nanostar is one of the main objects in Nano-biotechnology. This is a part of a new group of macromolecules that appear to be photon funnels just like artificial antennas and also is a great resistant of photo bleaching. It consists of three major architectural components: core, branches and end groups. For further details about dendrimer nanostars see [40].

M.V. Diudea [25, 26] was the first chemist who considered the problem of computing topological indices of nanostructures. A.R. Ashrafi and his co-authors [27, 28, 29, 30] continued this pioneering work of M.V. Diudea. Nowadays, there are many researchers [7, 33-43], who have been interested in the problem of computing topological indices of nanostructures. In this paper, we have attempted the aforementioned problem and have been able to find simple general expressions for evaluating the vertex-degree-based topological indices of four types of dendrimer nanostar.

2. Main results and discussion

Let us denote by $NS_1[n]$ and $NS_2[n]$ the graphs of the dendrimer nanostars given in the Fig. 1 and Fig. 2 respectively, where n is the steps of growth.

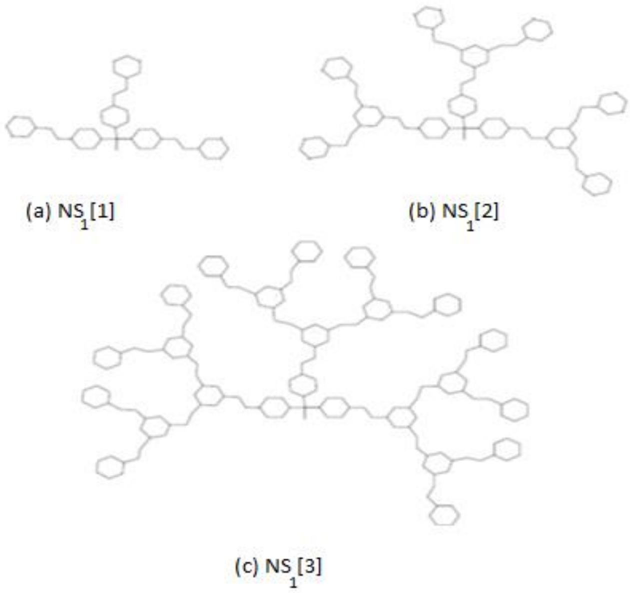

Fig. 1. The dendrimer nanostar $NS_1[n]$ for $n = 1,2,3$.

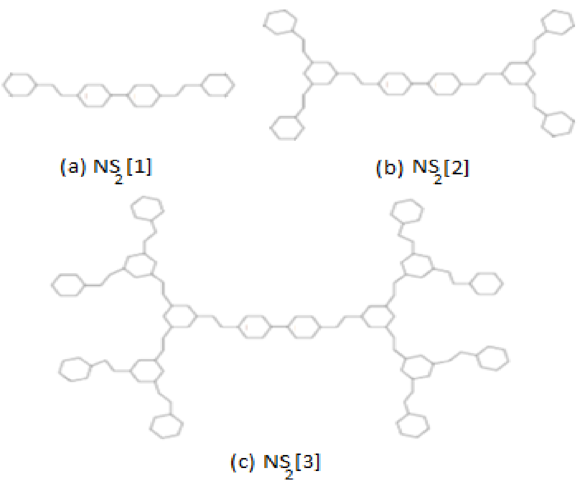

Fig. 2. The dendrimer nanostar $NS_2[n]$ for $n = 1,2,3$.

To establish the general expressions for calculating the vertex-degree-based topological indices of the form (1) for the dendrimer nanostars $NS_1[n]$ and $NS_2[n]$, it is enough to find the non-zero $x_{i,j}(NS_k[n])$ where $k = 1,2$. By simple reasoning and after routine calculations, one have

$$x_{1,4}(NS_1[n]) = 1, \qquad x_{2,2}(NS_1[n]) = 9.2^n + 3,$$

$$x_{2,3}(NS_1[n]) = 18.2^n - 12, \; x_{3,4}(NS_1[n]) = 3,$$

and

$$x_{2,2}(NS_2[n]) = 6.2^n + 2,$$

$$x_{2,3}(NS_2[n]) = 12.2^n - 8, \qquad x_{3,3}(NS_2[n]) = 1.$$

Substituting these values in the Eq.(1), one have

$$TI(NS_1[n]) = \theta_{1,4} + \theta_{2,2}(9.2^n + 3)$$
$$+\theta_{2,3}(18.2^n - 12) + 3\theta_{3,4} \,, \tag{2}$$

and

$$TI(NS_2[n]) = \theta_{2,2}(6.2^n + 2)$$
$$+\theta_{2,3}(12.2^n - 8) + \theta_{3,3} \,. \tag{3}$$

Recall that, if $\theta_{i,j} = ij$ then TI is the second Zagreb index M_2 and hence from the Eq.(2) and Eq.(3), one have

$$M_2(NS_1[n]) = 9.2^{n+4} - 20,$$

and

$$M_2(NS_2[n]) = 3.2^{n+5} - 31.$$

In 2009, A.R. Asharfi and P. Nikzad [33] gave efficient formulae for evaluating the Randić index of the dendrimer nanostars $NS_1[n]$ and $NS_2[n]$. Later on, M. B. Ahmadi and M. Sadeghimehr [34], and S. Alikhani et al. [43] obtained closed form formulae for calculating the atom-bond connectivity index of the dendrimer nanostars $NS_1[n]$ and $NS_2[n]$ respectively. Using Eq.(2) and Eq.(3) we can calculate any vertex-degree-based topological index of the form (1) for the dendrimer nanostars $NS_1[n]$, $NS_2[n]$.

Now, let us find general expressions for calculating the vertex-degree-based topological indices of the form (1) for the dendrimer nanostars $NS_3[n]$ and $NS_4[n]$, see the Fig. 3 and Fig. 4.

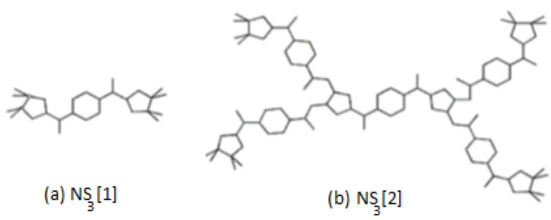

Fig. 3. The dendrimer nanostar $NS_1[n]$ for $n = 1,2$.

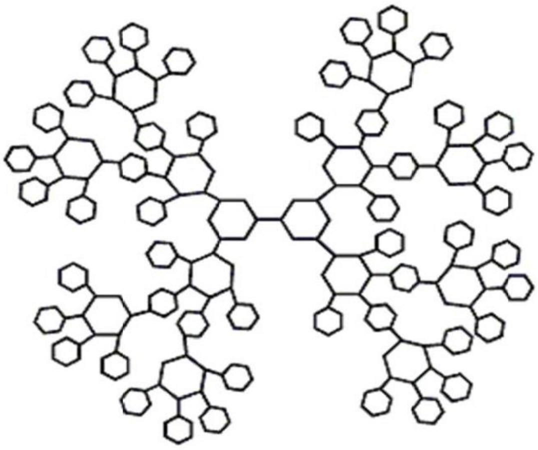

Fig. 4. The dendrimer nanostar NS_4[2].

By simple reasoning and after routine calculations, one have

$$x_{1,3}(NS_3[n]) = 4.2^n - 6, \quad x_{1,4}(NS_3[n]) = 4.2^n,$$

$$x_{2,2}(NS_3[n]) = 4.2^n - 6, x_{2,3}(NS_3[n]) = 18.2^n - 28,$$

$$x_{2,4}(NS_3[n]) = 2.2^n, x_{3,3}(NS_3[n]) = 7.2^n - 10,$$

$$x_{4,4}(NS_3[n]) = 2^n,$$

and

$$x_{2,2}(NS_4[n]) = 56.\,2^n - 48,$$

$$x_{2,3}(NS_4[n]) = 48.\,2^n - 44,$$

$$x_{3,3}(NS_4[n]) = 36.\,2^n - 35.$$

Bearing these values in mind and using Eq.(1), we have the following general expressions

$$TI(NS_3[n]) = (4.2^n - 6)(\theta_{1,3} + \theta_{2,2}) + 4.2^n\theta_{1,4} + (18.\,2^n - 28)\theta_{2,3} + 2.2^n\theta_{2,4} + (7.2^n - 10)\theta_{3,3} + 2^n\theta_{4,4}\,, \quad (4)$$

$$TI(NS_4[n]) = \theta_{2,2}(56.\,2^n - 48) + \theta_{2,3}(48.\,2^n - 44) + \theta_{3,3}(36.\,2^n - 35)\,. \quad (5)$$

If we take $\theta_{i,j} = |i - j|$, then TI is the Albertson index A and from the Eq.(4) and Eq.(5) it follows that

$$A(NS_3[n]) = 2(21.2^n - 20),$$

and

$$A(NS_4[n]) = 4(12.\,2^n - 11).$$

In 2010, A. Madanshekaf and M. Ghaneei, [36] established efficient formulae for calculating the Randić index and atom-bond connectivity index of $NS_3[n]$. In 2012, M. Rostami et al. [35] calculated the sum-connectivity index and first geometric-arithmetic index of $NS_3[n]$ and $NS_4[n]$. Very recently, S. Alikhani et al. [43] gave closed form formula for calculating the atom-bond connectivity index of the dendrimer nanostars $NS_4[n]$. The Eq.(4) and Eq.(5) can be used to calculate any vertex-degree-based topological index of the form (1) for the dendrimer nanostars $NS_3[n]$, $NS_4[n]$.

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