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Atom bond connectivity index of an infinite class $NS_1[n]$ of dendrimer nanostars

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A topological index of a graph G is a numeric quantity related to G which is describe molecular graph G. The nanostar dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers [5]. In this paper the Atom Bond Connectivity (ABC) Index of some graphs and an infinite class of nanostar dendrimers are computed.

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1. Introduction

Molecular descriptors have found a wide application in QSPR/QSAR studies [4]. Among them, topological indices have a prominent place. One of the best known and widely used is the connectivity index, χ, introduced in 1975 by Milan Randic [1, 6], who has shown this index to reflect molecular branching. To keep the spirit of the Randic index, Ernesto Estrada et al. proposed an index, nowadays known as the Atom Bond Connectivity (ABC) index [2]. The introduction of graph theoretic concepts in chemistry is well known and the reader is referred to the following references for definitions and notations [7, 8].

The ABC index of graph G is defined as follows [1]:

$$ABC(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u + d_v - 2}}{\sqrt{d_u d_v}},$$

where the summation goes over all edges of G, d_u and d_v are the degrees of the terminal vertices u and v of edge uv and $E(G)$ is the edge set of G with cardinality $m = |E(G)|$.

2. Main results and discussion

Lemma 1. Consider the complete graph K_n of order n. The atom bond connectivity index of this graph is computed as follow:

$$ABC(K_n) = \frac{1}{2} n \sqrt{2(n-2)}$$

Proof. The degree of all the vertices of a complete graph of order n is $n-1$ and the number of edges for K_n is equal to $\frac{1}{2}n(n-1)$, i.e., $|E(K_n)| = \frac{1}{2}n(n-1)$. Thus

$$ABC(K_n) = \frac{1}{2}n(n-1)\frac{\sqrt{2(n-1)-2}}{\sqrt{(n-1)^2}} = \frac{1}{2}n\sqrt{2(n-2)}.$$

Lemma 2. Suppose C_n is a cycle of length n labeled by $1, 2, \ldots, n$. Then the atom bond connectivity (ABC) index of this cycle is

$$ABC(C_n) = \frac{\sqrt{2}}{2} n$$

Proof. The degree of all the vertices of C_n is two, so we can write

$$ABC(C_n) = n\frac{\sqrt{2+2-2}}{\sqrt{2.2}} = \frac{n\sqrt{2}}{2}.$$

Lemma 3. if S_n is the star on n vertices, then $ABC(S_n) = \sqrt{(n-1)(n-2)}$.

Proof. See [1].

Lemma 4. If G is a regular graph of degree $r > 0$, then $ABC(G) = \frac{1}{2} n \sqrt{2r-2}$.

Proof. A regular graph G on n vertices, having degree r, possesses $\frac{nr}{2}$ edges, thus

$$ABC(G) = \frac{nr}{2}\frac{\sqrt{r+r-2}}{\sqrt{r.r}} = \frac{1}{2}n\sqrt{2r-2}.$$

3. ABC index for infinite class $NS_1[n]$ of dendrimer nanostars

Consider the molecular graph $G(n) = NS_1[n]$, where n is steps of growth in this type of dendrimer nanostars, see Fig. 1. $NS_1[n]$ can be divided to three parts in each step. Define d_{ij} to be the number of edges connecting a vertex of degree *i* with a vertex of degree *j*. Also $d_{ij}^{(n)}$ means the value of d_{ij} in the n^{th} step.

Using a simple calculation, we can show that $|V(NS_1[n])| = 24 \times 2^n - 4$ and $|E(NS_1[n])| = 27 \times 2^n - 5$.

Theorem 4: The Atom Bond Connectivity index of $G(n) = NS_1[n]$ is computed as follows

$$ABC(NS_1[n]) = \frac{\sqrt{3}}{2} + \frac{\sqrt{15}}{2} + \frac{(6+9\sum_{i=1}^{n} 2^i)\sqrt{2}}{2} + \frac{(6+3(2^{n+1}+\sum_{i=1}^{n} 2^{i-1}))\sqrt{2}}{2}.$$

Proof: There is only one vertex of degree 1, and the number of vertices of degree 4 is also 1. Since there is an edge between the vertices of degree one and four, we have $d^{(n)}_{14} = 1$ (for all *n*) and it is easy to see that $d_{34} = 3$ for all the steps of growth.

On the other hand the number of the new branches in n^{th} step is equal to $3 \times .2^{n-1}$ (the number of new branches in each step organize a geometric progression).

We can show that $d_{22}^{(n)} = 6 + 3(2^{n+1} + \sum_{i=1}^{n} 2^{i-1})$, because $NS_1[n]$ can be divided to exactly three parts in each step and the number of edges connecting two vertices of degree 2 (except the edges of the hexagon) in each part is 3, on the other hand the number of the new hexagon in each step is 3.2^{n-1} and each of them has 4 edges that connecting two vertices of degree 2, also there are three hexagons in all of the steps and each of them have 2 edges that connecting two vertices of degree 2. So we have

$$d_{22}^{(n)} = 3 \times 2 + 3 \times 4 \times 2^{n-1} + 3\sum_{i=1}^{n} 2^{i-1} = 6 + 3(2^{n+1} + \sum_{i=1}^{n} 2^{i-1}).$$

Also the number of edges connecting a vertex of degree 2 with a vertex of degree 3 in each branch of each step is 6 (see Fig. 1), and there are 6 joint edges that connect a vertex of degree 2 with a vertex of degree 3, so we have $d_{23}^{(n)} = 6 + 6\sum_{i=1}^{n} 3 \times 2^{i-1} = 6 + 9\sum_{i=1}^{n} 2^i$.

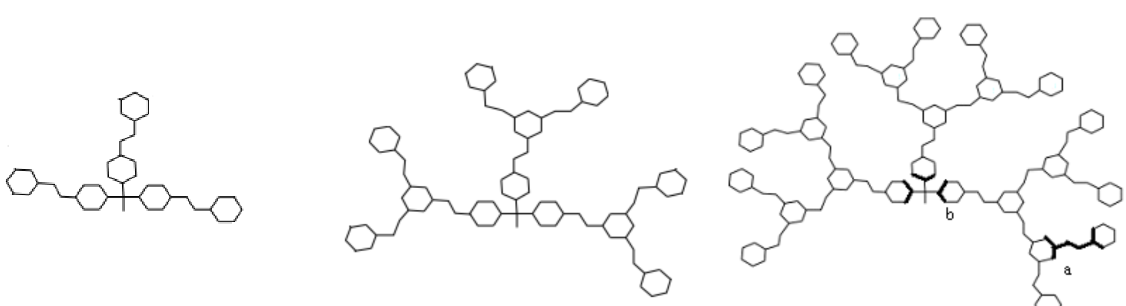
Thus we have

$$ABC(NS_1[n]) = \frac{\sqrt{3}}{2} + \frac{\sqrt{15}}{2} + \frac{(6+9\sum_{i=1}^{n} 2^i)\sqrt{2}}{2} + \frac{(6+3(2^{n+1}+\sum_{i=1}^{n} 2^{i-1}))\sqrt{2}}{2}.$$

Now the proof is complete.

Table 1. Computing A.B.C index for $NS_1[i],\ i \le 5$.

	d_{14}	d_{34}	d_{22}	d_{23}	$ABC(NS_1[n])$
$NS_1[1]$	1	3	39	60	72.81
$NS_1[2]$	1	3	75	132	149.17
$NS_1[3]$	1	3	147	276	301.91
$NS_1[4]$	1	3	291	564	1211.95
$NS_1[5]$	1	3	39	60	72.81



c. $NS_1[1]$ *b. $NS_1[2]$* *c. $NS_1[3]$*

Fig. 1. The molecular graph of $NS_1[n]$.

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