The fifth version of atom bond connectivity index (ABC_5) of an ınfinite class of dendrimers

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The atom-bond connectivity index-5(ABC_5) is a new topological index defined as; $ABC_5(G)=\sum_{uv\in E(G)}\sqrt{\frac{M_u+M_v-2}{M_uM_v}}$ where M_u denotes the product of the degrees of adjacent vertices of *u*. In this paper we compute this new topological index for an infinite class of dendrimers.

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1. Introduction

Dendrimers are spheroid or globular nanostructures that are precisely engineered to carry molecules encapsulated in their interior void spaces or attached to the surface. Size, shape, and reactivity are determined by generation (shells) and chemical composition of the core, interior branching, and surface functionalities. Dendrimers are constructed through a set of repeating chemical synthesis procedures that build up from the molecular level to the nanoscale region under conditions that are easily performed in a standard organic chemistry laboratory. The dendrimer diameter increases linearly whereas the number of surface groups increases geometrically. Dendrimers are very uniform with extremely low polydispersities, and are commonly created with dimensions incrementally grown in approximately nanometer steps from 1 to over 10 nm. The control over size, shape, and surface functionality makes dendrimers one of the "smartest"or customizable nanotechnologies commercially available.

Dendrimers provide polyvalent interactions between surfaces and bulk materials for applications such as adhesives, surface coatings, or polymer cross-linking.

Dendrimers are recognized as one of the major commercially available nanoscale building blocks. Nanotechnology encompasses sizes that are much larger than most molecules but much smaller than cells. Dendrimers are so versatile that they can be synthesized to the same dimensions as bimolecular such as hemoglobin. Dendrimer diameters increase linearly per generation, whereas the number of surface groups increases geometrically.

Molecular descriptors have found a wide application in QSPR/QSAR studies [1]. Çalımlı, proposed the new atom bond connectivity (ABC_5) index [2]. This index is defined as follows:

as $ABC_5(G)=\sum_{uv\in E(G)}\sqrt{\frac{M_u+M_v-2}{M_uM_v}}$ where M_u denotes the product of the degrees of adjacent vertices of *u*. Some topological indices for infinite class of dendrimers were computed in [3-5]. In this paper we compute this new topological index for an infinite class of dendrimers.

2. Theorem and proof

Structure of dendrimers, which are used in this study is as depicted in Fig. 1 and Fig. 2. Here *n* is the step of growth in the type of dendrimer.

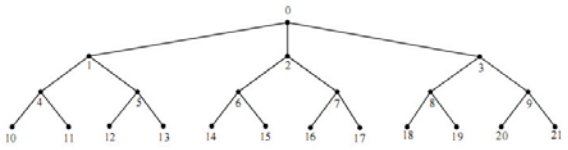

Fig. 1. The Dendrimer Molecule whit 22 vertices.

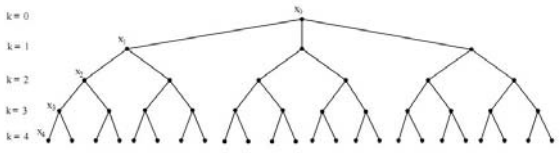

Fig. 2. The Dendrimer Molecule D4.

Table 1. Dendrimers and their edges.

D[1]	$3.2^0=3$
D[2]	$3.2^1=6$
D[3]	$3.2^2=12$
D[4]	$3.2^3=24$
D[5]	$3.2^4=48$
D[n]	3.2^{n-1}

Theorem: The ABC_5 index of the nanostar dendrimer *D[n]* is computed as;

$$ABC_5(D[n]) = \frac{2.(2^{n-2}-1)\sqrt{13}}{9} + \frac{2^{n-1}\sqrt{7}}{3} + 2^n$$

Proof: We can directly from the definition of the ABC_5 index and from the Table 1;

$$ABC_5(D[n]) = 3.\sqrt{\frac{3^3+3^3-2}{3^6}} + 6.\sqrt{\frac{3^3+3^3-2}{3^6}} + \ldots + 3.2^{n-3}\sqrt{\frac{3^3+3^3-2}{3^6}}$$

$$+3.2^{n-2}\sqrt{\frac{3^3+3-2}{3^4}} + 3.2^{n-2}\sqrt{\frac{3+3-2}{3^2}}$$

$$= \frac{3\sqrt{52}}{3^3} + \frac{6\sqrt{52}}{3^3} + \ldots + \frac{3.2^{n-3}\sqrt{52}}{3^3} + \frac{3.2^{n-2}\sqrt{28}}{3^2} + \frac{3.2^{n-3}\sqrt{4}}{3}$$

$$= \frac{2\sqrt{13}}{9} + \frac{4\sqrt{13}}{9} + \ldots + \frac{2^{n-2}\sqrt{13}}{9} + \frac{2^{n-1}\sqrt{7}}{3} + 2^n$$

$$= \frac{\sqrt{13}}{9}(2+2^2+\ldots+2^{n-2}) + \frac{2^{n-1}\sqrt{7}}{3} + 2^n$$

$$= \frac{2.(2^{n-2}-1)\sqrt{13}}{9} + \frac{2^{n-1}\sqrt{7}}{3} + 2^n$$

3. Concluding remarks

The fifth version of Atom Bond Connectivity Index (ABC_5) is a novel connectivity index and in this paper we defined and found exact formulas for the fifth version of Atom Bond Connectivity Index of an infinite class of dendrimers. It would be interesting, the investigation of its mathematical properties and quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) for future study. It would be also inetersting to investigate relationships between the fifth version of Atom Bond Connectivity Index of dendrimers and structures of dendrimers and their physicochemical properties.

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