Degree-Based Multiplicative Atom-bond Connectivity Index of Nanostructures

Wei Gao, Muhammad Kamran Jamil, Waqas Nazeer, and Murad Amin

***Abstract*—There are a lot of nanomaterials and related chemical substances synthesized in the laboratory every year, which makes the test of their performance has become a hard work. The theory of nanoscience from the perspective of graph theory provides an excellent idea, characteristics of the nanomaterials can be obtained by calculating topological indices in their corresponding molecular graphs, and have attracted the attention of scholars in the field of nanoscience. In this paper, we learn the characteristics of nanostructures from mathematical point of view. Some important nanomaterials are selected and their multiplicative atom-bond connectivity indices are determined by edge set divided trick. These theoretical results can be considered as a guideline in nanoengineering.**

***Index Terms*—theoretical nanoscience, multiplicative atom-bond connectivity index, nanotubes, nanotori dendrimer, nanostar.**

I. Introduction

OVER the years, the theoretical nanoscience has attracted more and more attention of scholars, the computational results are applied to nanoscience, biological, and pharmaceutical science fields. One of the important research branch of theoretical nanoscience can be stated as follows: the nanostructures related molecular structure is expressed by graphs, by calculating the topological index we can get the properties of the corresponding nanostructures. This technology can obtain effective results in the absence of experimental conditions, which is interested by the scholars from developing countries and regions. Gradually, as the development computing tricks, it has become an important branch in the field of theoretical nanoscience, and concerned by scientists from various fields (see Balaban [1], Munteanu et al. [2], Buscema et al. [3], Gao et al. [5], [4], Sirimulla et al. [6], Bodlaj and Batagelj [7], Nadeem and Shaker [8], Nistor and Troitsky [9], Arockiaraj et al. [10], Khakpoor and Keshe [11], and Ivanciuc [12] for more details).

We only consider simple nanostructure related molecular graph (each vertex represents as an atom and each edge expresses as a chemical bond) in our paper. Let G be a molecular graph with vertex set $V(G)$ and edge set $E(G)$. For each vertex v, the degree $d(v)$ of v is the number of vertices adjacent to v. A topological index can be regarded as a real function $f : G \rightarrow \mathbb{R}$ which maps each molecular graph to a real number. In the past four decades, inspired by applications from the chemical engineering, many degree-based, spectral-based or distance-based indices were introduced, such as Zagreb index, atom-bond connectivity index, Wiener index, Harary index, Szeged index, PI index, eccentric connectivity index, harmonic index, Zagreb index and so on. Moreover, there are several advancements on distance-based, spectral-based, degree-based indices of special nanomaterial molecular structures which can be referred to Ramane and Jummannaver [13], Zhao and Wu [14], Sardar [15], Gao and Wang [16], [17], Gao et al. [18], [47], [48], Gao and Siddiqui [21], Abdo et al. [22], Basavanagoud [23], Sunilkumar et al. [24], and Guirao and de Bustos [25].

Estrada and Torres [26] introduced a new topological index called the atom-bond connectivity index (in short, the ABC index) which reflect the properties of alkanes. The atom-bond connectivity index of a molecular graph G can be stated as

$$\mathrm{ABC}(G) = \sum_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}.$$

Dehghan-Zadeh et al. [27] determined the first and second maximum values of the atom-bond connectivity index of tetracyclic graphs with n vertex. Ashrafi and Dehghan-Zadeh [28] studied the first and the second maximum values of the ABC index of cactus graphs with fixed vertex number. Goubko et al. [29] raised a counterexample for the previous conclusion. Husin et al. [30] researched the ABC index of two families of nanostar dendrimers. Dehghan-Zadeh and Ashrafi [31] derived the ABC index of quasi-tree graphs. Dimitrov [32] proposed an efficient computation approach of trees with the smallest atom-bond connectivity index. The structural characters of trees with a minimal ABC index were considered [35], [33], [34], [36], [37].

As a variant of the ABC index, the first multiplicative atom-bond connectivity index is formulated by

$$\mathrm{ABC}\Pi(G) = \prod_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}},$$

which was defined in Kulli [38]. In Kulli's work, he determined the first multiplicative atom-bond connectivity index of $VC_5C_7[p,q]$ and $HC_5C_7[p,q]$ nanotubes.

Furthermore, Kulli [39] introduced the fourth multiplicative atom-bond connectivity index which can be represented as

$$\mathrm{ABC}_4\Pi(G) = \prod_{uv\in E(G)} \sqrt{\frac{S(u)+S(v)-2}{S(u)S(v)}},$$

where $S(v) = \sum_{uv\in E(G)} d(u)$ for each $v \in V(G)$.

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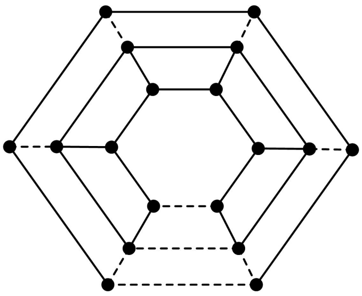

Fig. 1. Web graph Wn, m.

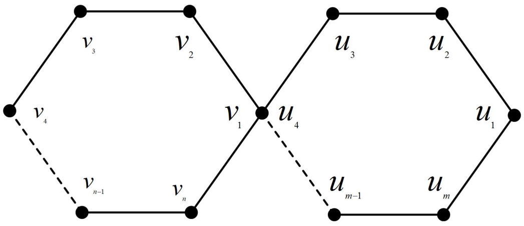

Fig. 2. The structure of $C_{n,m}$.

A. Examples on computing of first multiplicative atom-bond connectivity index

Now, we present some of the examples about the calculating process of the first multiplicative atom bond connectivity index.

Example 1. $W_n = K_1 \vee C_{n-1}$ is called wheel graph. By simple computation, we have $ABC\Pi_1(W_n) = (\frac{2}{3})^{n-1}(\sqrt{\frac{n}{3(n-1)}})^{n-1}$.

Example 2. Let n and m be two positive integers. The web graph $W(n,m)$ is constructed from the Cartesian product of cycle C_n and path P_m (see Figure 1 as an example).

By analyzing the structure of web graph $W(n,m)$, if $m = 2$, it easy to get

$$ABC\Pi_1(W(n,m)) = (\sqrt{\frac{3+3-2}{3\cdot 3}})^{3n} = (\frac{2}{3})^{3n}.$$

If $m \geq 2$, then the first multiplicative atom bond connectivity index of web graph $W(n,m)$ is

$$\begin{aligned} & ABC\Pi_1(W(n,m)) \\ = & (\sqrt{\frac{3+3-2}{3\cdot 3}})^{2n}(\sqrt{\frac{4+4-2}{4\cdot 4}})^{n(2m-5)} \\ & \times(\sqrt{\frac{3+4-2}{3\cdot 4}})^{2n} \\ = & (\frac{2}{3})^{2n}(\frac{\sqrt{6}}{4})^{n(2m-5)}(\sqrt{\frac{5}{12}})^{2n}. \end{aligned}$$

In the following three examples, we show the value of $ABC\Pi_1$ index for three kinds of vertex gluing graphs.

Example 3. Let $C_{n,m}$ be a graph constructed from two cycles C_n and C_m with one common vertex (see Figure 2 as an example).

Using the definition of the first multiplicative atom bond connectivity index, we get

$$\begin{aligned} & ABC\Pi_1(C_{n,m}) \\ = & (\sqrt{\frac{2+2-2}{2\cdot 2}})^{m+n-4}(\sqrt{\frac{2+4-2}{2\cdot 4}})^4 = (\sqrt{\frac{1}{2}})^{n+m}. \end{aligned}$$

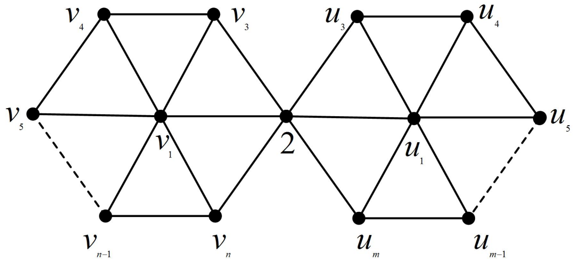

Fig. 3. The structure of $W_{n,m}$.

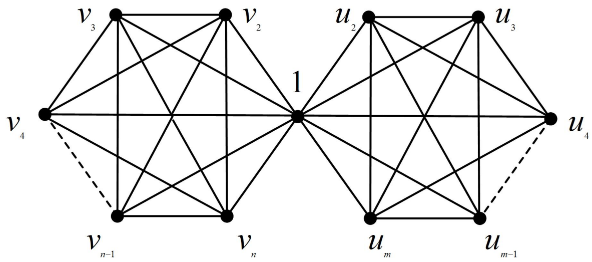

Fig. 4. The structure of $K(n,m)$.

Example 4. Let $W_{n,m}$ be a graph constructed from two wheel graphs W_n and W_m with one common vertex (see Figure 3 as an instance).

According to its graph structure analysis, we obtain

$$\begin{aligned} & ABC\Pi_1(W_{n,m}) \\ = & (\sqrt{\frac{3+3-2}{3\cdot 3}})^{m+n-6}(\sqrt{\frac{6+3-2}{6\cdot 3}})^4 \\ & \times(\sqrt{\frac{(n-1)+3-2}{(n-1)\cdot 3}})^{n-2}(\sqrt{\frac{(m-1)+3-2}{(m-1)\cdot 3}})^{m-2} \\ & \times\sqrt{\frac{(n-1)+6-2}{(n-1)\cdot 6}}\sqrt{\frac{(m-1)+6-2}{(m-1)\cdot 6}} \\ = & (\frac{2}{3})^{m+n-6}(\sqrt{\frac{7}{18}})^4(\sqrt{\frac{n}{3(n-1)}})^{n-2} \\ & \times(\sqrt{\frac{m}{3(m-1)}})^{m-2}\sqrt{\frac{n+3}{6(n-1)}}\sqrt{\frac{m+3}{6(m-1)}}. \end{aligned}$$

Example 5. Let $K(n,m)$ be a graph constructed from two complete graphs K_n and K_m with one common vertex (see Figure 4 as an instance).

By means of simple calculation, we yield

$$\begin{aligned} & ABC\Pi_1(K(n,m)) \\ = & (\sqrt{\frac{(n-1)+(n-1)-2}{(n-1)\cdot(n-1)}})^{\frac{(n-1)(n-2)}{2}} \\ & \times(\sqrt{\frac{(m-1)+(m-1)-2}{(m-1)\cdot(m-1)}})^{\frac{(m-1)(m-2)}{2}} \\ & \times(\sqrt{\frac{(m-1)+(m+n-2)-2}{(m-1)\cdot(m+n-2)}})^{m-1} \\ & \times(\sqrt{\frac{(n-1)+(m+n-2)-2}{(n-1)\cdot(m+n-2)}})^{n-1} \\ = & (\frac{\sqrt{2n-4}}{n-1})^{\frac{(n-1)(n-2)}{2}}(\frac{\sqrt{2m-4}}{m-1})^{\frac{(m-1)(m-2)}{2}} \\ & \times(\sqrt{\frac{2m+n-5}{(m-1)(m+n-2)}})^{m-1} \\ & \times(\sqrt{\frac{2n+m-5}{(n-1)(m+n-2)}})^{n-1}. \end{aligned}$$

B. Organization of the rest paper

So far, there have been numerous theoretical results about ABC index, but on the degree-based multiplication of ABC index is also very small. As a variable of the original ABC index, degree-based multiplication ABC indices have a broad application prospect, it is worthy of further study. This motivates us to calculate some important chemical molecular structure of ABC multiplication index.

The rest of paper is organized as follows: first, we determine the fourth multiplication ABC index of V-phenylenic nanotubes and nanotori; then, the first multiplication ABC index of $TUC_4C_8[p,q]$ and other C_4C_8 net are considered; next, the first multiplication ABC index of $NS_1[n]$ and two classes of dendrimer nanostars ($D_1[n]$ and $D_3[n]$) are computed; at last, the first multiplication ABC index of carbon nanocones $C_m[n]$ are calculated.

II. Main Results and Proofs

In this section, we present the main results and their detail proofs. The trick to get these conclusions is followed by edge set dividing technology.

A. Fourth multiplication ABC index of V-phenylenic nanotubes and nanotori

The aim of this section is to determine the fourth multiplication ABC index of V-phenylenic nanotube and nanotori. The novel phenylenic and naphthylenic lattices consist of a square net embedded on the toroidal surface. As polycyclic conjugated molecules, phenylenes are composed of square and hexagons in which each 4-membered ring is adjacent to two 6-membered cycles, and no two 6-membered rings are adjacent mutually. We denote V-phenylenic nanotube and V-phenylenic nanotorus as $VPHX[m,n]$ and $VPHY[m,n]$, respectively. The representation of these two kinds of nanostructures are manifested in Figure 5 and Figure 6, respectively.

Foregone results on V-phenylenic nanotubes and nanotori can refer to Yousefi-Azari et al. [40], Alamian et al. [41],

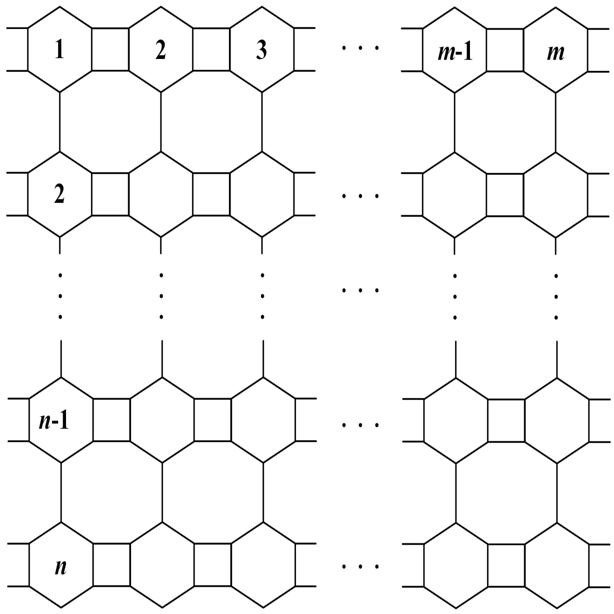

Fig. 5. The structure of V-phenylenic nanotube $VPHX[m,n]$.

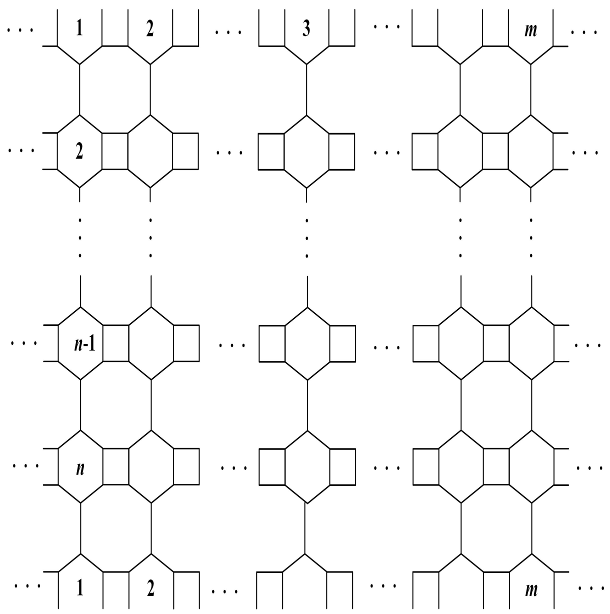

Fig. 6. The structure of V-phenylenic nanotorus $VPHY[m,n]$.

Ashrafi et al. [42], Bahrami and Yazdani [43], Ghorbani et al. [44], Moradi and Baba-Rahim [45], Farahani [46] and Gao et al. [47], [48], [49] and [50]. The main computing conclusion is formulated as follows.

Theorem 1 Let n and m be two positive integers. The fourth multiplication ABC index of V-phenylenic nanotubes and nanotori are

$$\mathrm{ABC}_4\Pi(VPHX[m,n]) = (\frac{1}{2})^{4m}(\frac{7}{32})^m(\frac{5}{24})^m(\frac{4}{9})^{9mn-9m}$$

and

$$\mathrm{ABC}_4\Pi(VPHY[m,n]) = (\frac{4}{9})^{9mn}.$$

Proof. The proof is followed by edge set dividing approach in which the edge set is separated into several subsets according to the value of $S(u)$ and $S(v)$.

By analysis the molecular structure of V-phenylenic nanotubes $VPHX[m,n]$, we see that its edge set can be divided into the following four parts:

- $e = (u, v)$: $S(u) = 6$ and $S(v) = 8$, and there are $4m$ such edges;
- $e = (u, v)$: $S(u) = S(v) = 8$, and there are $2m$ such edges;
- $e = (u, v)$: $S(u) = 8$ and $S(v) = 9$, and there are $2m$ such edges;
- $e = (u, v)$: $S(u) = S(v) = 9$, and there are $9mn - 9m$ such edges.

In light of the definition of the fourth multiplication ABC index, we have

$$\begin{aligned} & \mathrm{ABC}_4\Pi(VPHX[m,n]) \\ = & \prod_{uv\in E(VPHX[m,n])} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \\ = & (\sqrt{\frac{6+8-2}{6\times 8}})^{4m}(\sqrt{\frac{8+8-2}{8\times 8}})^{2m}(\sqrt{\frac{8+9-2}{8\times 9}})^{2m} \\ & \times(\sqrt{\frac{9+9-2}{9\times 9}})^{9mn-9m} \\ = & (\frac{1}{2})^{4m}(\sqrt{\frac{7}{32}})^{2m}(\sqrt{\frac{5}{24}})^{2m}(\frac{4}{9})^{9mn-9m}. \end{aligned}$$

For V-phenylenic nanotori $VPHY[m, n]$, this is a 3-regular molecular graph with $d(v) = 3$ for each $v \in V(VPHY[m, n])$, and thus $S(v) = 9$ for vertex v. In view of the definition of the fourth multiplication ABC index, we get

$$\mathrm{ABC}_4\Pi(VPHY[m,n]) = (\sqrt{\frac{9+9-2}{9\times 9}})^{9mn} = (\frac{4}{9})^{9mn}.$$

Hence, we obtain the desired results. □

B. The first multiplication ABC index of nanostructures

The aim of this section is to yield the first multiplication ABC index of $TUC_4C_8[p, q]$, where q is the number of rows and p is the number of columns. Then we determine this topological index for its nanotubes. At last, the first multiplication ABC index of $TUC_4C_8[p, q]$ (can be seen in Figure 7) is yielded. In this subsection, we always assume $p, q \in \mathbb{N}$.

Theorem 2 Let $G = TUC_4C_8[p, q]$ be the two dimensional molecular lattice structure depicted in Figure 7. Then,

$$\mathrm{ABC}_1\Pi(G) = (\frac{1}{2})^{3p+3q-2}(\frac{2}{3})^{12pq-8(p+q)+4}.$$

Proof. By analysis its structure, its edge set can be divided into three subsets:

- $e = (u, v)$: $d(u) = d(v) = 2$, and there are $2p + 2q + 4$ such edges;
- $e = (u, v)$: $d(u) = 2$ and $d(v) = 3$, and there are $4p + 4q - 8$ such edges;
- $e = (u, v)$: $d(u) = d(v) = 3$, and there are $12pq - 8(p + q) + 4$ such edges.

In term of the definition of the first multiplication ABC index, we infer

$$\begin{aligned} \mathrm{ABC}_1\Pi(G) = & \prod_{uv\in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ = & (\sqrt{\frac{2+2-2}{2\times 2}})^{2p+2q+4}(\sqrt{\frac{2+3-2}{2\times 3}})^{4p+4q-8} \\ & \times(\sqrt{\frac{3+3-2}{3\times 3}})^{12pq-8(p+q)+4} \\ = & (\sqrt{\frac{1}{2}})^{2p+2q+4}(\sqrt{\frac{1}{2}})^{4p+4q-8}(\frac{2}{3})^{12pq-8(p+q)+4}. \end{aligned}$$

Hence, the formula in the theorem is correct. □

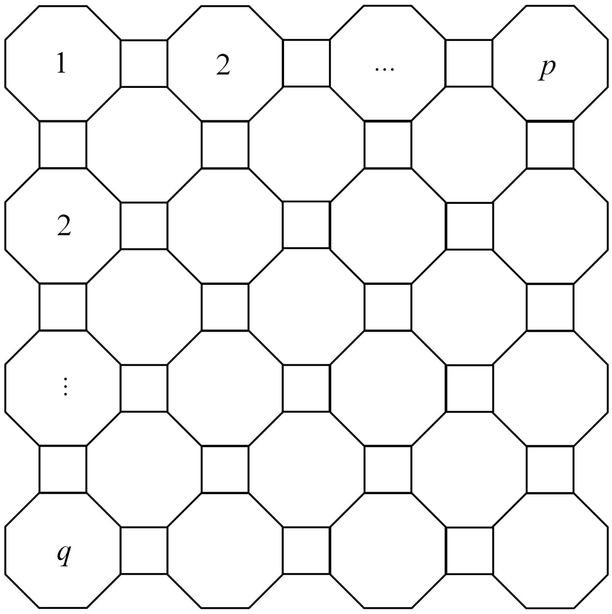

Fig. 7. The structure of 2-D Lattice $C_4C_8[4, 4]$.

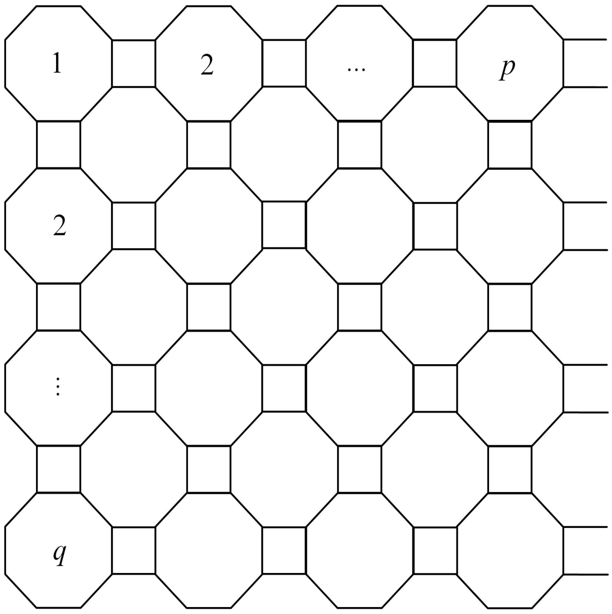

Fig. 8. The structure of 2-D graph of $C_4C_8[4, 4]$ nanotube.

Theorem 3 Let G be the two dimensional $C_4C_8[p, q]$ nanotube described in Figure 8. Then,

$$\mathrm{ABC}_1\Pi(G) = (\frac{1}{2})^{3p}(\frac{2}{3})^{12pq-8p}.$$

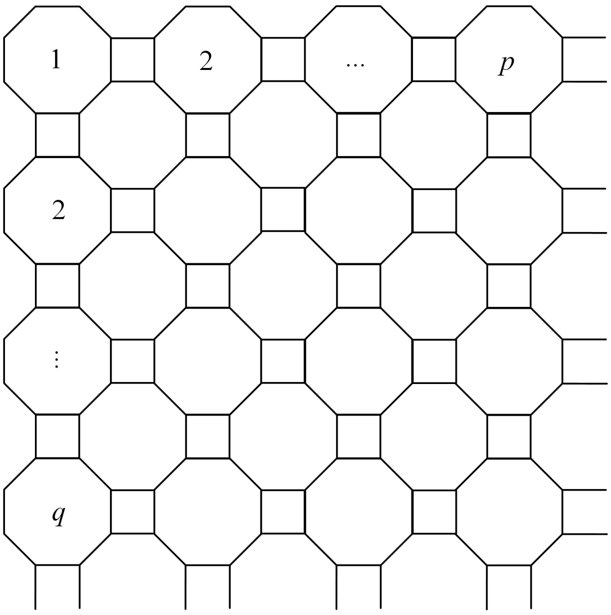

Fig. 9. The structure of 2-D graph of $C_4C_8[4,4]$ nanotorus.

Proof. Similarly, its edge set can be divided into three subsets:
- $e=(u,v)$: $d(u)=d(v)=2$, and there are $2p$ such edges;
- $e=(u,v)$: $d(u)=2$ and $d(v)=3$, and there are $4p$ such edges;
- $e=(u,v)$: $d(u)=d(v)=3$, and there are $12pq-8p$ such edges.

By virtue of the definition of the first multiplication ABC index, we deduce

$$\begin{aligned}\mathrm{ABC}_1\Pi(G) &= (\sqrt{\frac{2+2-2}{2\times 2}})^{2p}(\sqrt{\frac{2+3-2}{2\times 3}})^{4p}\\ &\times(\sqrt{\frac{3+3-2}{3\times 3}})^{12pq-8p}\\ &= (\sqrt{\frac{1}{2}})^{2p}(\sqrt{\frac{1}{2}})^{4p}(\frac{2}{3})^{12pq-8p}.\end{aligned}$$

Therefore, we verify the expected conclusion. □

Theorem 4 Let G be the two dimensional $C_4C_8[p,q]$ nanotori described in Figure 9. Then,

$$\mathrm{ABC}_1\Pi(G) = (\frac{2}{3})^{12pq}.$$

Proof. Since $C_4C_8[p,q]$ nanotori is a 3-regular molecular graph with $12pq$ edges. We directly get the result □

C. The first multiplication ABC index of $NS_1[n]$

In this part, we raise the first multiplication ABC index of an infinite class of $NS_1[n]$ (as examples, the basic structures of $NS_1[n]$ can be seen in Figure 10, Figure 11 and Figure 12).

Theorem 5 Let $n\in\mathbb{N}$ be the step number of growth. The first multiplication ABC index of $NS_1[n]$ is given by

$$\mathrm{ABC}_1\Pi(NS_1[n]) = \frac{\sqrt{3}}{2}(\sqrt{\frac{1}{2}})^{27\cdot 2^n-9}(\sqrt{\frac{5}{12}})^3.$$

Proof. By analysis $E(NS_1[n])$, we have four separate subsets listed as follows:
- $e=(u,v)$: $d(u)=1$ and $d(v)=4$, and there one edge in this subset;
- $e=(u,v)$: $d(u)=d(v)=2$, and there are $9\cdot 2^n+3$ such edges;
- $e=(u,v)$: $d(u)=2$ and $d(v)=3$, and there are

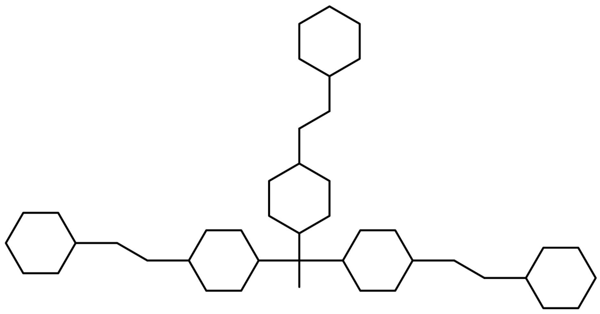

Fig. 10. The molecular structure of $NS_1[1]$.

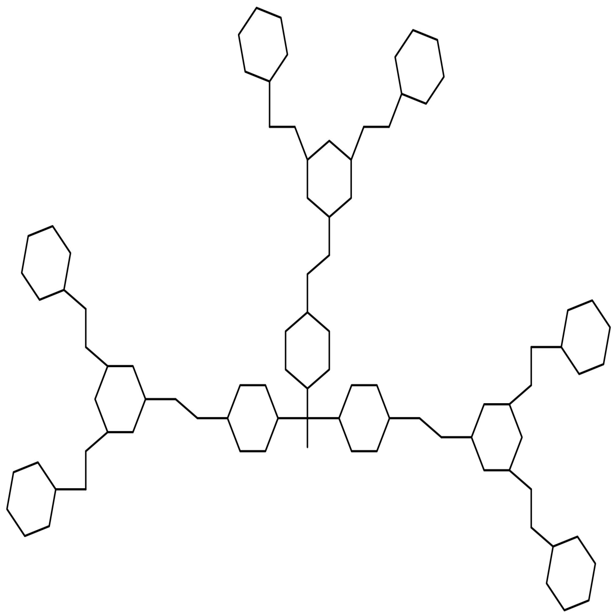

Fig. 11. The molecular structure of $NS_1[2]$.

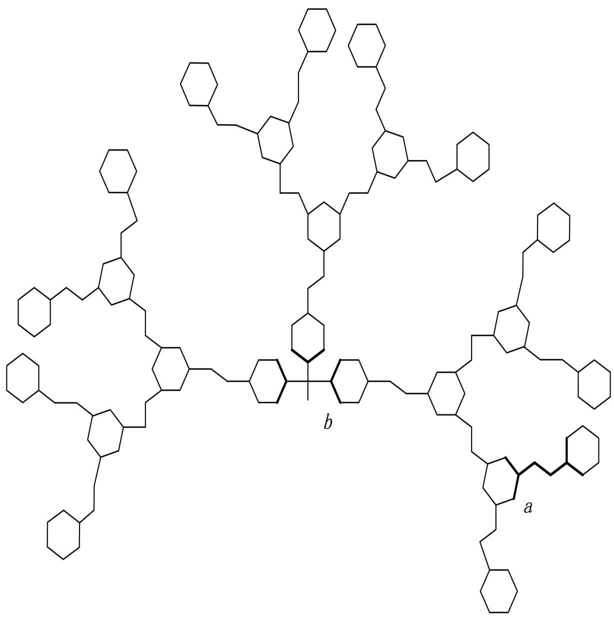

Fig. 12. The molecular structure of $NS_1[3]$.

$18 \cdot 2^n - 12$ such edges;
- $e = (u, v)$: $d(u) = 3$ and $d(v) = 4$, and there are three such edges.

Hence, using the definition of the first multiplication ABC index, we derive

$$\begin{aligned} \mathrm{ABC_1\Pi}(NS_1[n]) &= \prod_{uv \in E(NS_1[n])} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= (\sqrt{\frac{1+4-2}{1\times 4}})(\sqrt{\frac{2+2-2}{2\times 2}})^{9\cdot 2^n+3} \\ &\quad \times(\sqrt{\frac{2+3-2}{2\times 3}})^{18\cdot 2^n-12}(\sqrt{\frac{3+4-2}{3\times 4}})^3 \\ &= \frac{\sqrt{3}}{2}(\sqrt{\frac{1}{2}})^{27\cdot 2^n-9}(\sqrt{\frac{5}{12}})^3. \end{aligned}$$

The proof is completed. □

D. The first multiplication ABC index of dendrimer nanostars $D_1[n]$ and $D_3[n]$

Here, we discuss the first multiplication ABC index of dendrimer nanostars $D_1[n]$ and $D_3[n]$, where these two molecular structures are widely appeared in the chemical compounds, drugs, and nanomaterials.

Theorem 6 Let $n \in \mathbb{N}$ be the number of steps of growth, then the first multiplication ABC index of dendrimer nanostars $D_1[n]$ is stated as

$$\mathrm{ABC_1\Pi}(D_1[n]) = \sqrt{\frac{2}{3}}(\frac{1}{2})^{9\cdot 2^n-6}.$$

Proof. Its edge set can be divided into three subsets:
- $e = (u, v)$: $d(u) = 1$ and $d(v) = 3$, and there one edge in this subset;
- $e = (u, v)$: $d(u) = d(v) = 2$, and there are $6 \cdot 2^n - 2$ such edges;
- $e = (u, v)$: $d(u) = 2$ and $d(v) = 3$, and there are $12 \cdot 2^n - 10$ such edges.

Hence, according to the definition of the first multiplication ABC index, we get

$$\begin{aligned} \mathrm{ABC_1\Pi}(D_1[n]) &= \prod_{uv \in E(D_1[n])} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= (\sqrt{\frac{1+3-2}{1\times 3}})(\sqrt{\frac{2+2-2}{2\times 2}})^{6\cdot 2^n-2} \\ &\quad \times(\sqrt{\frac{2+3-2}{2\times 3}})^{12\cdot 2^n-10} \\ &= \sqrt{\frac{2}{3}}(\sqrt{\frac{1}{2}})^{18\cdot 2^n-12}. \end{aligned}$$

The desired result is obtained. □

As an instance, the molecular structure of $D_3[3]$ is presented in Figure 13.

Theorem 7 Let $n \in \mathbb{N}$ be the number of steps of growth, then the first multiplication ABC index of dendrimer nanostars $D_3[n]$ is stated as

$$\mathrm{ABC_1\Pi}(D_3[n]) = (\sqrt{\frac{2}{3}})^{3\cdot 2^n}(\frac{1}{2})^{18\cdot 2^n-9}(\frac{2}{3})^{9\cdot 2^n-6}.$$

Proof. The set $E(NS_3[n])$ can be divided into following four parts:
- $e = (u, v)$: $d(u) = 1$ and $d(v) = 3$, and there $3 \cdot 2^n$ edges in this subset;
- $e = (u, v)$: $d(u) = d(v) = 2$, and there are $12 \cdot 2^n - 6$ such edges;
- $e = (u, v)$: $d(u) = 2$ and $d(v) = 3$, and there are $24 \cdot 2^n - 12$ such edges;
- $e = (u, v)$: $d(u) = d(v) = 3$, and there are $9 \cdot 2^n - 6$ such edges.

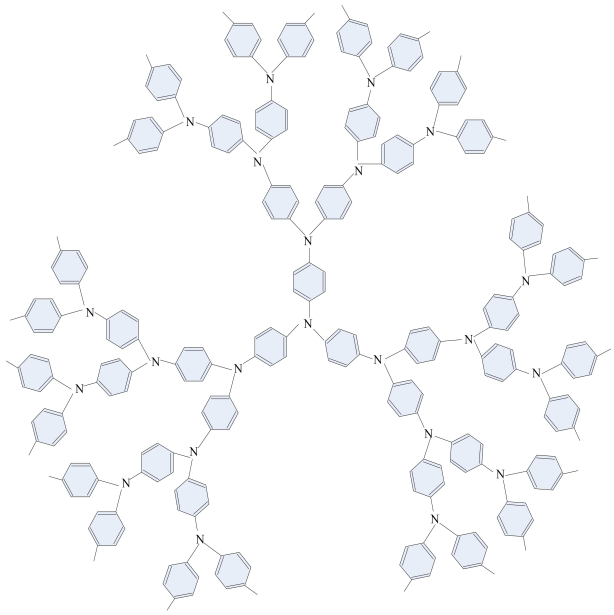

Fig. 13. The example of $D_3[n]$: $n = 3$.

Hence, using the definition of the first multiplication ABC index, we derive

$$\begin{aligned} \mathrm{ABC_1\Pi}(D_3[n]) &= \prod_{uv \in E(D_3[n])} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= (\sqrt{\frac{1+3-2}{1\times 3}})^{3\cdot 2^n}(\sqrt{\frac{2+2-2}{2\times 2}})^{12\cdot 2^n-6} \\ &\quad \times(\sqrt{\frac{2+3-2}{2\times 3}})^{24\cdot 2^n-12}(\sqrt{\frac{3+3-2}{3\times 3}})^{9\cdot 2^n-6} \\ &= (\sqrt{\frac{2}{3}})^{3\cdot 2^n}(\sqrt{\frac{1}{2}})^{36\cdot 2^n-18}(\frac{2}{3})^{9\cdot 2^n-6}. \end{aligned}$$

We complete the proof. □

E. The first multiplication ABC index of carbon nanocones

Now, we compute the first multiplication ABC index of carbon nanocones $CNC_m[n] = C_m[n]$ (see Figure 14 as an example of carbon nanocone).

Theorem 8 Let $m \geq 3$ and $n \geq 1$ be two positive integers, then the first multiplication ABC index of carbon nanocones $C_m[n]$ can be expressed as

$$\mathrm{ABC_1\Pi}(C_m[n]) = (\sqrt{\frac{1}{2}})^{2mn+m}(\frac{2}{3})^{\frac{m(3n^2+n)}{2}}.$$

Proof. By analysis the molecular structure of carbon nanocones $C_m[n]$, we found that its edge set can be divided into three parts:
- $e = (u, v)$: $d(u) = d(v) = 2$, and there are m such edges;
- $e = (u, v)$: $d(u) = 2$ and $d(v) = 3$, and there are $2mn$ such edges;

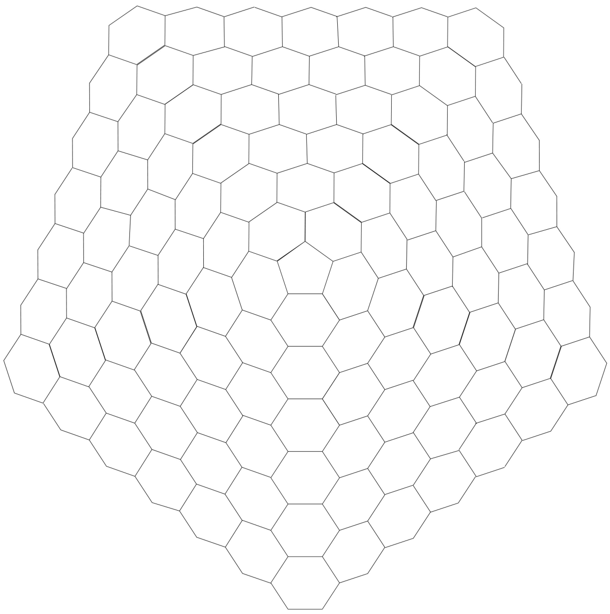

Fig. 14. The example of carbon nanocone $C_m[n]$.

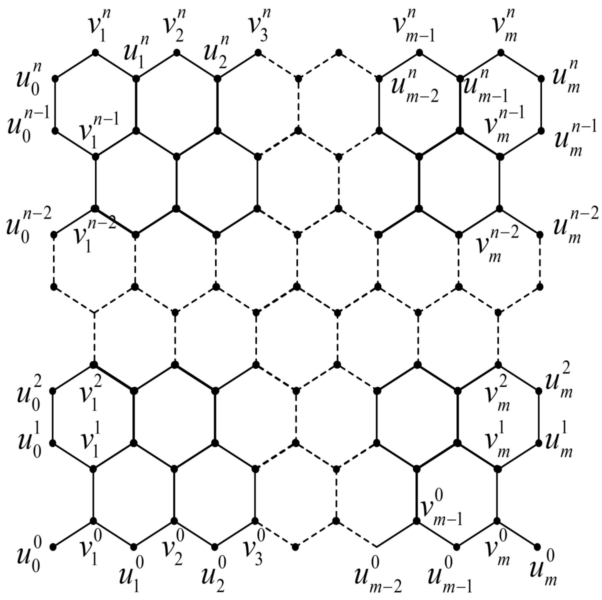

Fig. 15. The structure of NA_m^n nanotubes nanotube.

- $e = (u, v)$: $d(u) = d(v) = 3$, and there are $\frac{m(3n^2+n)}{2}$ such edges.

Then, by means of the definition of the first multiplication ABC index, we derive

$$\begin{aligned} \mathrm{ABC_1\Pi}(C_m[n]) &= \prod_{uv\in E(C_m[n])} \sqrt{\frac{d_u+d_v-2}{d_u d_v}} \\ &= (\sqrt{\frac{2+2-2}{2\times 2}})^m (\sqrt{\frac{2+3-2}{2\times 3}})^{2mn} \\ &\quad \times (\sqrt{\frac{3+3-2}{3\times 3}})^{\frac{m(3n^2+n)}{2}} \\ &= (\sqrt{\frac{1}{2}})^{2mn+m} (\frac{2}{3})^{\frac{m(3n^2+n)}{2}}. \end{aligned}$$

Hence, we check the desired result. □

F. The fifth multiplication ABC index of NA_m^n nanotubes

The eccentricity $ec(u)$ of vertex $u \in V(G)$ is defined as the maximum distance between u and any other vertex in G. Gao et al. [51] introduced the fifth multiplicative atom bond connectivity index which was stated as

$$ABC\Pi_5(G) = \prod_{uv\in E(G)} \sqrt{\frac{ec(u)+ec(v)-2}{ec(u)ec(v)}}.$$

The structure of of NA_m^n nanotubes was discussed by Bac et al. [52] as follows: consider the $m \times n$ quadrilateral section P_m^n with $m \geq 2$ hexagons on the top and bottom sides and $n \geq 2$ hexagons on the lateral sides cut from the regular hexagonal lattice L. If we identify two lateral sides of P_m^n such that we identify the vertices u_0^j and u_m^j, for $j = 0, 1, 2, \cdots, n$, then the NA_m^n nanotubes are obtained. The detailed structure of NA_m^n nanotubes nanotube can refer to Figure 15. In this part, we study NA_m^n nanotube with $n = m$ and it's fifth multiplication ABC index is determined.

Theorem 9 The fifth multiplication ABC index of NA_m^n nanotubes can be expressed as follows:

- If $n \equiv 0$(mod2), then

$$\begin{aligned} \mathrm{ABC_5\Pi}(NA_m^n) &= \prod_{i=1}^{\frac{n}{2}} \prod_{p=\frac{3n}{2}}^{2n-1} (\sqrt{\frac{2p-1}{p^2+p}})^{6i-3} \\ &\quad \times \prod_{p=n} (\sqrt{\frac{4p-1}{4p^2+2p}})^{3n} \prod_{p=n} \frac{4p}{(2p-1)^2} \\ &\quad \times \prod_{i=\frac{n}{2}+3} \prod_{p=2n+1}^{\frac{5n}{2}-1} (\sqrt{\frac{2p-1}{p^2+p}})^{(\frac{n}{2}-1)(6i-16)} \\ &\quad \times \prod_{i=3n+6, j\in\{0,\cdots,\frac{n}{2}-1\}} \prod_{p=\frac{5n}{2}}^{3n-1} (\sqrt{\frac{2p-1}{p^2+p}})^{6n-i}. \end{aligned}$$

- If $n \equiv 1$(mod4), then

$$\begin{aligned} &\mathrm{ABC_5\Pi}(NA_m^n) \\ &= \frac{\sqrt{2p-2}}{p} \prod_{p=\frac{3n+1}{2}}^{\frac{5n-1}{2}, p\equiv 0(mod2)} (\sqrt{\frac{2p-2}{p^2}})^{n-1} \\ &\quad \times \prod_{i=1}^{\frac{n-3}{2}, i\equiv 1(mod2)} \prod_{p=\frac{3n+1}{2}}^{2n-2, p\equiv 0(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{4i} \\ &\quad \times \prod_{i=2}^{\frac{n-1}{2}, i\equiv 0(mod2)} \prod_{p=\frac{3n+3}{2}}^{2n-1, p\equiv 1(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{8i-2} \\ &\quad \times \prod_{p=2n}^{\frac{5n-1}{2}, p\equiv 0(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{\frac{(n+3)(n+1)}{2}} \\ &\quad \times \prod_{p=2n+1}^{\frac{5n-3}{2}, p\equiv 1(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{n(n-1)} \\ &\quad \times \prod_{i=1}^{\frac{n-1}{4}} \prod_{p=\frac{5n+1}{2}}^{3n-2, p\equiv 1(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{16i} \end{aligned}$$

$$\times \prod_{i=1}^{\frac{n-3}{2}, i\equiv 1(mod2)} \prod_{p=\frac{5n+3}{2}}^{3n-1, p\equiv 0(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{4i}.$$

- If $n \equiv 3(\text{mod}4)$, then

$$\begin{aligned}
&\text{ABC}_5\Pi(NA_m^n) \\
= &\prod_{p=\frac{3n+3}{2}}^{\frac{5n+1}{2}, p\equiv 0(mod2)} (\sqrt{\frac{2p-2}{p^2}})^{n+1} \\
&\times \prod_{i=1}^{\frac{n+1}{4}} \prod_{p=\frac{3n+1}{2}}^{2n-1, p\equiv 1(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{16i-10} \\
&\times \prod_{i=1}^{\frac{n+1}{4}} \prod_{p=\frac{3n+3}{2}}^{2n, p\equiv 0(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{8i} \\
&\times \prod_{p=2n+1}^{\frac{5n-1}{2}, p\equiv 1(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{n(n+1)} \\
&\times \prod_{p=2n+2}^{\frac{5n-3}{2}, p\equiv 0(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{\frac{(n+1)(n-3)}{2}} \\
&\times \prod_{i=1}^{\frac{n-3}{4}, n\neq 3} \prod_{p=\frac{5n+3}{2}, n\neq 3}^{3n-2, p\equiv 0(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{16i} \\
&\times \prod_{i=1}^{\frac{n+1}{4}, n\neq 3} \prod_{p=\frac{5n+1}{2}}^{3n-1, p\equiv 0(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{8i-4}.
\end{aligned}$$

Proof. The whole proof can be divided into three parts according to the value of n.

Case 1. $n \equiv 0(\text{mod}2)$.

In this case, the edge set of NA_m^n nanotubes can be divided into five parts according to the value of $ec(u)$ and $ec(v)$:

- $ec(u) = p$ and $ec(v) = p + 1$ where $p \in \{2n - \frac{n}{2}, \cdots, 2n-1\}$, and there are $6i-3$ such edges with $i \in \{1, \cdots, \frac{n}{2}\}$;
- $ec(u) = 2p$ and $ec(v) = 2p+1$ where $p = n \equiv 0(\text{mod}2)$, and there are $3n$ such edges with $n \equiv 0(\text{mod}2)$;
- $ec(u) = ec(v) = 2p+1$ where $p = n \equiv 0(\text{mod}2)$, and there are 2 such edges;
- $ec(u) = p$ and $ec(v) = p + 1$ where $p \in \{2n+1, \cdots, \frac{5n}{2}-1\}$, and there are $(\frac{n}{2}-1)(3n+2)$ such edges;
- $ec(u) = p$ and $ec(v) = p+1$ where $p \in \{\frac{5n}{2}, \cdots, 3n-1\}$, and there are $6n-i$ such edges with $i = 3n+6j$ and $j \in \{0, \cdots, \frac{n}{2}-1\}$.

In terms of the definition of the fifth multiplication ABC index, we have

$$\begin{aligned}
&\text{ABC}_5\Pi(NA_m^n) \\
= &\prod_{uv\in E(NA_m^n)} \sqrt{\frac{ec(u)+ec(v)-2}{ec(u)ec(v)}} \\
= &\prod_{i=1}^{\frac{n}{2}} \prod_{p=\frac{3n}{2}}^{2n-1} (\sqrt{\frac{2p-1}{p^2+p}})^{6i-3} \\
&\times \prod_{p=n}(\sqrt{\frac{4p-1}{4p^2+2p}})^{3n} \prod_{p=n} \frac{4p}{(2p-1)^2} \\
&\times \prod_{i=\frac{n}{2}+3} \prod_{p=2n+1}^{\frac{5n}{2}-1} (\sqrt{\frac{2p-1}{p^2+p}})^{(\frac{n}{2}-1)(6i-16)} \\
&\times \prod_{i=3n+6, j\in\{0,\cdots,\frac{n}{2}-1\}} \prod_{p=\frac{5n}{2}}^{3n-1} (\sqrt{\frac{2p-1}{p^2+p}})^{6n-i}.
\end{aligned}$$

Case 2. $n \equiv 1(\text{mod}4)$.

In this case, the edge set of NA_m^n nanotubes can be divided into eight parts according to the value of $ec(u)$ and $ec(v)$:

- $ec(u) = ec(v) = p$ where $p = n \equiv 0(\text{mod}2)$, and there only one such edge;
- $ec(u) = ec(v) = p$ where $\frac{3n+1}{2} < p \leq \frac{5n-1}{2}$ and $p \equiv 0(\text{mod}2)$, and there $n-1$ such edges;
- $ec(u) = p$ and $ec(v) = p+1$ where $\frac{3n+1}{2} \leq p \leq 2n-2$ and $p \equiv 0(\text{mod}2)$, and there are $4i$ such edges with $i \in \{1, \cdots, \frac{n-3}{2}\}$ and $i \equiv 1(\text{mod}2)$;
- $ec(u) = p$ and $ec(v) = p+1$ where $\frac{3n+3}{2} \leq p \leq 2n-1$ and $p \equiv 0(\text{mod}2)$, and there are $8i-2$ such edges with $i \in \{2, \cdots, \frac{n-1}{2}\}$ and $i \equiv 0(\text{mod}2)$;
- $ec(u) = p$ and $ec(v) = p+1$ where $2n \leq p \leq \frac{5n-1}{2}$ and $p \equiv 0(\text{mod}2)$, and there are $\frac{(n+3)(n+1)}{2}$ such edges;
- $ec(u) = p$ and $ec(v) = p+1$ where $2n+1 \leq p \leq \frac{5n-3}{2}$ and $p \equiv 1(\text{mod}2)$, and there are n^2-n such edges;
- $ec(u) = p$ and $ec(v) = p+1$ where $\frac{5n+1}{2} \leq p \leq 3n-2$ and $p \equiv 1(\text{mod}2)$, and there are $16i$ such edges with $i \in \{1, \cdots, \frac{n-1}{4}\}$;
- $ec(u) = p$ and $ec(v) = p+1$ where $\frac{5n+3}{2} \leq p \leq 3n-1$ and $p \equiv 0(\text{mod}2)$, and there are $4i$ such edges with $i \in \{1, \cdots, \frac{n-3}{2}\}$ and $i \equiv 1(\text{mod}2)$.

In view of the definition of the fifth multiplication ABC index, we get

$$\begin{aligned}
&\text{ABC}_5\Pi(NA_m^n) \\
= &\prod_{uv\in E(NA_m^n)} \sqrt{\frac{ec(u)+ec(v)-2}{ec(u)ec(v)}} \\
= &\frac{\sqrt{2p-2}}{p} \prod_{p=\frac{3n+1}{2}}^{\frac{5n-1}{2}, p\equiv 0(mod2)} (\sqrt{\frac{2p-2}{p^2}})^{n-1} \\
&\times \prod_{i=1}^{\frac{n-3}{2}, i\equiv 1(mod2)} \prod_{p=\frac{3n+1}{2}}^{2n-2, p\equiv 0(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{4i} \\
&\times \prod_{i=2}^{\frac{n-1}{2}, i\equiv 0(mod2)} \prod_{p=\frac{3n+3}{2}}^{2n-1, p\equiv 1(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{8i-2} \\
&\times \prod_{p=2n}^{\frac{5n-1}{2}, p\equiv 0(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{\frac{(n+3)(n+1)}{2}} \\
&\times \prod_{p=2n+1}^{\frac{5n-3}{2}, p\equiv 1(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{n(n-1)} \\
&\times \prod_{i=1}^{\frac{n-1}{4}} \prod_{p=\frac{5n+1}{2}}^{3n-2, p\equiv 1(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{16i}
\end{aligned}$$

$$\times \prod_{i=1}^{\frac{n-3}{2}, i\equiv 1(mod2)} \prod_{p=\frac{5n+3}{2}}^{3n-1, p\equiv 0(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{4i}.$$

Case 3. $n \equiv 3$(mod4).

In this case, the edge set of NA_m^n nanotubes can be divided into seven parts according to the value of $ec(u)$ and $ec(v)$:

- $ec(u) = ec(v) = p$ where $p \in \{\frac{3n+3}{2}, \cdots, \frac{5n+1}{5}\}$, and there $n+1$ such edge;
- $ec(u) = p$ and $ec(v) = p+1$ where $\frac{3n+1}{2} \leq p \leq 2n-1$ and $p \equiv 1$(mod2), and there are $16i - 10$ such edges with $i \in \{1, \cdots, \frac{n+1}{4}\}$;
- $ec(u) = p$ and $ec(v) = p+1$ where $\frac{3n+3}{2} \leq p \leq 2n$ and $p \equiv 0$(mod2), and there are $8i$ such edges with $i \in \{1, \cdots, \frac{n+1}{4}\}$;
- $ec(u) = p$ and $ec(v) = p+1$ where $2n+1 \leq p \leq \frac{5n-1}{2}$ and $p \equiv 1$(mod2), and there are $n(n+1)$ such edges;
- $ec(u) = p$ and $ec(v) = p+1$ where $2n+2 \leq p \leq \frac{5n-3}{2}$, $p \equiv 0$(mod2) and $n \neq 3$, and there are $\frac{(n+1)(n-3)}{2}$ such edges with $n \neq 3$;
- $ec(u) = p$ and $ec(v) = p+1$ where $\frac{5n+3}{2} \leq p \leq 3n-2$, $p \equiv 1$(mod2) and $n \neq 3$, and there are $16i$ such edges with $i \in \{1, \cdots, \frac{n-3}{4}\}$ and $n \neq 3$;
- $ec(u) = p$ and $ec(v) = p+1$ where $\frac{5n+1}{2} \leq p \leq 3n-1$, $p \equiv 0$(mod2), and there are $8i - 4$ such edges with $i \in \{1, \cdots, \frac{n+1}{4}\}$.

In light of the definition of the fifth multiplication ABC index, we infer

$$\begin{aligned}
& \mathrm{ABC}_5\Pi(NA_m^n) \\
= & \prod_{uv\in E(NA_m^n)} \sqrt{\frac{ec(u)+ec(v)-2}{ec(u)ec(v)}} \\
= & \prod_{p=\frac{3n+3}{2}}^{\frac{5n+1}{2}, p\equiv 0(mod2)} (\sqrt{\frac{2p-2}{p^2}})^{n+1} \\
& \times \prod_{i=1}^{\frac{n+1}{4}} \prod_{p=\frac{3n+1}{2}}^{2n-1, p\equiv 1(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{16i-10} \\
& \times \prod_{i=1}^{\frac{n+1}{4}} \prod_{p=\frac{3n+3}{2}}^{2n, p\equiv 0(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{8i} \\
& \times \prod_{p=2n+1}^{\frac{5n-1}{2}, p\equiv 1(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{n(n+1)} \\
& \times \prod_{p=2n+2}^{\frac{5n-3}{2}, p\equiv 0(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{\frac{(n+1)(n-3)}{2}} \\
& \times \prod_{i=1}^{\frac{n-3}{4}, n\neq 3} \prod_{p=\frac{5n+3}{2}, n\neq 3}^{3n-2, p\equiv 0(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{16i} \\
& \times \prod_{i=1}^{\frac{n+1}{4}, n\neq 3} \prod_{p=\frac{5n+1}{2}}^{3n-1, p\equiv 0(mod2)} (\sqrt{\frac{2p-1}{p^2+p}})^{8i-4}.
\end{aligned}$$

From what we have discussed in above three cases, we deduce the desired result. □

III. Conclusion

In this paper, we study the degree-based indices multiplication ABC of several common appeared nanostructures. The exact computational formulas are presented by means of edge set dividing approach. These theoretical results in nanoscience, biology, pharmacy and other fields have a wide application prospect.

Conflict of Interests

The authors hereby declare that there is no conflict of interests regarding the publication of this paper.

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References

[1] A. T. Balaban, “Can topological indices transmit information on properties but not on structures?,” *Journal of Computer-Aided Molecular Design*, 2005, vol. 19, no. 9-10, pp. 651-660, 2005.

[2] C. R. Munteanu, A. L. Magalhaes, A. Duardo-Sanchez, A. Pazos, and H. Gonzalez-Diaz, “S2SNet: a tool for transforming characters and numeric sequences into star network topological indices in chemoinformatics, bioinformatics, biomedical, and social-legal sciences,” *Current Bioinformatics*, vol. 8, no. 4, pp. 429-437, 2013.

[3] M. Buscema, M. Asadi-Zeydabadi, W. Lodwick, and M. Breda, “The H-0 function, a new index for detecting structural/topological complexity information in undirected graphs,” *Physica A-Statistical Mechanics and Its Applications*, vol. 447, pp. 355-378, 2016.

[4] W. Gao, W. F. Wang, and M. R. Farahani, “Topological indices study of molecular structure in anticancer drugs,” *Journal of Chemistry*, vol. 2016, http://dx.doi.org/10.1155/2016/3216327.

[5] W. Gao, W. F. Wang, M. K. Jamil, and M. R. Farahani, “Electron energy studying of molecular structures via forgotten topological index computation,” *Journal of Chemistry*, vol. 2016, http://dx.doi.org/10.1155/2016/1053183.

[6] S. Sirimulla, M. Lerma, and W. C. Herndon, “Prediction of partial molar volumes of amino acids and small peptides: counting atoms versus topological indices,” *Journal of Chemical Information and Modeling*, vol. 50, no. 1, pp. 194-204, 2010.

[7] J. Bodlaj and V. Batagelj, “Network analysis of publications on topological indices from the web of science,” *Molecular Informatics*, vol.33, no. 8, pp. 514-535, 2014.

[8] I. Nadeem and H. Shaker, “On topological indices of tri-hexagonal boron nanotubes,” *Journal of Optoelectronics and Advanced Materials*, vol. 18, no. 9-10, pp. 893-898, 2016.

[9] V. Nistor and E. Troitsky, “Analysis of gauge-equivariant complexes and a topological index theorem for gauge-invariant families,” *Russian Journal of Mathematical Physics*, vol. 22, no. 1, pp. 74-97, 2015.

[10] M. Arockiaraj, S. R. J. Kavitha, and K. Balasubramanian, “Vertex cut method for degree and distance-based topological indices and its applications to silicate networks,” *Journal of Mathematical Chemistry*, vol. 54, no. 8, pp. 1728-1747, 2016.

[11] A. A. Khakpoor and B. A. Keshe, “Physical and electro-optical properties of rylenes as nanostructures using topological indices method,” *Journal of Nanoelectronics and Optoelectronics*, vol. 11, no. 3, pp. 280-283, 2016.

[12] O. Ivanciuc, “Chemical graphs, molecular matrices and topological indices in chemoinformatics and quantitative structure-activity relationships,” *Current Computer-Aided Drug Design*, vol. 9, no. 2, pp. 153-163, 2013.

[13] H. S. Ramane and R. B. Jummannaver, “Note on forgotten topological index of chemical structure in drugs,” *Applied Mathematics and Nonlinear Sciences*, vol. 1, no. 2, pp. 369-374, 2016.

[14] B. Zhao and H. L. Wu, “Pharmacological characteristics analysis of two molecular structures,” *Applied Mathematics and Nonlinear Sciences*, vol. 2, no. 1, pp. 93-110, 2017.

[15] M. S. Sardar, S. Zafar, and Z. Zahid, “Computing topological indices of the line graphs of banana tree graph and firecracker graph,” *Applied Mathematics and Nonlinear Sciences*, vol. 2, no. 1, pp. 83-92, 2017.

[16] W. Gao and W. F. Wang, “The eccentric connectivity polynomial of two classes of nanotubes,” *Chaos, Solitons and Fractals*, vol. 89, pp. 290-294, 2016.

[17] W. Gao and W. F. Wang, "The fifth geometric arithmetic index of bridge graph and carbon nanocones," *Journal of Difference Equations and Applications*, vol. 23, no. 1-2, pp. 100-109, 2017.
[18] W. Gao, L. Yan, and L. Shi, "Generalized zagreb index of polyomino chains and nanotubes," *Optoelectronics and Advanced Materials–Rapid Communications*, vol. 11, no. 1-2, pp. 119-124, 2017.
[19] W. Gao, M. R. Farahani, and L. Shi, "The forgotten topological index of some drug structures," *Acta Medica Mediterranea*, vol. 32, pp. 579-585, 2016.
[20] W. Gao, M. K. Siddiqui, M. Imran, M. K. Jamil, and M. R. Farahani, "Forgotten topological index of chemical structure in drugs," *Saudi Pharmaceutical Journal*, vol. 24, no. 3, pp. 258-264, 2016.
[21] W. Gao and M. K. Siddiqui, "Molecular descriptors of nanotube, oxide, silicate, and triangulene networks," *Journal of Chemistry*, vol. 2017, https://doi.org/10.1155/2017/6540754.
[22] H. Abdo, D. Dimitrov, and W. Gao, "On the irregularity of some molecular structures," *Canadian Journal of Chemistry*, vol. 95, no. 2, pp. 174-183, 2017.
[23] B. Basavanagoud, V. R. Desai, and S. Patil, "(β,α)-Connectivity index of graphs," *Applied Mathematics and Nonlinear Sciences*, vol. 2, no. 1, pp. 21-30, 2017.
[24] M. H. Sunilkumar, B. K. Bhagyashri, G. B. Ratnamma, and M. G. Vijay, "QSPR analysis of certain graph theocratical matrices and their corresponding energy," *Applied Mathematics and Nonlinear Sciences*, vol. 2, no. 1, pp. 131-150, 2017.
[25] J. L. G. Guirao and M. T. de Bustos, "Dynamics of pseudo–radioactive chemical products via sampling theory," *Journal of Mathematical Chemistry*, vol. 50, no. 2, pp. 374-378, 2012.
[26] E. Estrada and L. Torres, "An atom-bond connectivity index: Modelling the enthalpy of formation of alkanes," *Indian Journal of chemistry*, vol. 37, no. 10, pp. 849-855, 1998.
[27] T. Dehghan-Zadeh, A. R. Ashrafi, and N. Habibi, "Maximum values of atom-bond connectivity index in the class of tetracyclic graphs," *Journal of Applied Mathematics and Computing*, vol. 46, pp. 285-303, 2014.
[28] A. R. Ashrafi and T. Dehghan-Zadeh, "Extremal atom-bond connectivity index of cactus graphs," *Communications of the Korean Mathematical Society*, vol. 30, no. 3, pp. 283-295, 2015.
[29] M. Goubko, C. Magnant, P. S. Nowbandegani, and I. Gutman, "ABC index of trees with fixed number of leaves," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 74, pp. 697-702, 2015.
[30] N. M. Husin, R. Hasni, and N. E. Arif, "Atom-bond connectivity and geometric arithmetic indices of dendrimer nanostars," *Australian Journal of Basic and Applied Sciences*, vol. 7, no. 9, pp. 10-14, 2013.
[31] T. Dehghan-Zadeh and A. R. Ashrafi, "Atom-bond connectivity index of quasi-tree graphs," *Rendiconti del Circolo Matematico di Palermo*, vol. 63, pp. 347-354, 2014.
[32] D. Dimitrov, "Efficient computation of trees with minimal atom-bond connectivity index," *Applied Mathematics and Computation*, vol. 224, pp. 663-670, 2013.
[33] M. B. Ahmadi, D. Dimitrov, I. Gutman, and S. A. Hosseini, "Disproving a conjecture on trees with minimal atom-bond connectivity index," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 72, pp. 685–698, 2014.
[34] D. Dimitrov, "On structural properties of trees with minimal atom-bond connectivity index," *Discrete Applied Mathematics*, vol. 172, pp. 28–44, 2014.
[35] D. Dimitrov, "On structural properties of trees with minimal atom-bond connectivity index II: Bounds on B-1- and B-2-branches," *Discrete Applied Mathematics*, vol. 204, pp. 90-116, 2016.
[36] D. Dimitrov, Z. Du, and C. M. da Fonseca, "On structural properties of trees with minimal atom-bond connectivity index III: Trees with pendent paths of length three", *Applied Mathematics and Computation*, vol. 282, pp. 276–290, 2016.
[37] D. Dimitrov, B. Ikica and R. Škrekovski, "Remarks on maximum atom-bond connectivity index with given graph parameters," *Discrete Applied Mathematics*, vol. 222, pp. 222–226, 2017.
[38] V. R. Kulli, "Multiplicative connectivity indices of certain nanotubes," *Annals of Pure and Applied Mathematics*, vol. 12, no. 2, pp. 169-176, 2016.
[39] V. R. Kulli, "Two new multiplicative atom bond connectivity indices," *Annals of Pure and Applied Mathematics*, vol. 13, no. 1, pp. 1-7, 2017.
[40] H. Yousefi-Azari, A. Bahrami, J. Yazdani, and A. R. Ashrafi, "PI index of V-Phenylenic nanotubes and nanotori," *Journal of Computational and Theoretical Nanoscience*, vol. 4, no. 3, pp. 604-605, 2007.
[41] V. Alamian, A. Bahrami, and B. Edalatzadeh, "PI polynomial of V-phenylenic nanotubes and nanotori," *International Journal of Molecular Sciences*, vol. 9, no. 3, pp. 229-234, 2008.
[42] A. R. Ashrafi, M. Ghorbani, and M. Jalali, "Computing Sadhana polynomial of V-phenylenic nanotubes and nanotori," *Indian Journal of Chemistry Secton A-Inorganic Bio-Inorganic Physical Theoretical & Analytical Chemistry*, vol. 47, no. 4, pp. 535-537, 2008.
[43] A. Bahrami and J. Yazdani, "Vertex PI index of V-phenylenic nanotubes and nanotori," *Digest Journal of Nanomaterials and Biostructures*, vol. 4, no. 1, pp. 141-144, 2009.
[44] M. Ghorbani, H. Mesgarani, and S. Shakeraneh, "Computing GA index and ABC index of V-phenylenic nanotube," *Optoelectronics and Advanced Materials-Rapid Communications*, vol. 5, no. 3-4, pp. 324-326, 2011.
[45] S. Moradi and S. Baba-Rahim, "The eccentric connectivity index of V-phenylenic nanotubes and nanotorus," *Fullerenes Nanotubes and Carbon Nanostructures*, vol. 21, no. 4, pp. 326-332, 2013.
[46] M. R. Farahani, "Computing fourth atom-bond connectivity index of V-phenylenic nanotubes and nanotori," *Acta Chimica Slovenica*, vol. 60, no. 2, pp. 429-432, 2013.
[47] W. Gao and L. Shi, "Szeged related indices of unilateral polyomino chain and unilateral hexagonal chain," *IAENG International Journal of Applied Mathematics*, vol. 45, no. 2, pp. 138-150, 2015.
[48] W. Gao, L. Shi, and M. R. Farahani, "Distance-based indices for some families of dendrimer nanostars," *IAENG International Journal of Applied Mathematics*, vol. 46, no. 2, pp. 168-186, 2016.
[49] W. Gao, L. L. Zhu, and Y. Guo, "Multi-dividing infinite push ontology algorithm," *Engineering Letters*, vol. 23, no. 3, pp. 132-139, 2015.
[50] L. L. Zhu, W. G. Tao, X. Z. Min, and W. Gao, "Theoretical characteristics of ontology learning algorithm in multi-dividing setting," *IAENG International Journal of Computer Science*, vol. 43, no. 2, pp. 184-191, 2016.
[51] W. Gao, Y. J. Chen, and W. F. Wang, "The topological variable computation for a special type of cycloalkanes," *Journal of Chemistry*, vol. 2017, https://doi.org/10.1155/2017/6534758.
[52] M. Bac, J. Horvathova, M. Mokrisova, A. Semanicova, and A. Suhanyiova, "On topological indices of carbon nanotube network," *Canadian Journal of Chemistry*, vol. 93, no. 10, pp. 1157-1160, 2015.

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