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Computing ABC_4 index of nanostar dendrimers

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The *ABC* index is a topological index was defined as $ABC(G)=\sum_{uv\in E}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}$, where $d_G(u)$ denotes degree of vertex *u*. Now we define a new version of *ABC* index as $ABC_4(G)=\sum_{uv\in E(G)}\sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}}$, where $\delta_G(u)=\sum_{uv\in E(G)} d_G(v)$. The goal of this paper is further the study of the ABC_4 index.

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1. Introduction

A graph is a collection of points and lines connecting a subset of them. The points and lines of a graph also called vertices and edges of the graph, respectively. If *e* is an edge of *G*, connecting the vertices *u* and *v*, then we write *e* = *uv* and say "*u* and *v* are adjacent". A connected graph is a graph such that there is a path between all pairs of vertices. A simple graph is an unweighted, undirected graph without loops or multiple edges. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted.

Molecular descriptors play a significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [1]. One of the best known and widely used is the connectivity index, introduced in 1975 by Milan Randić [2], who has shown this index to reflect molecular branching. Recently Furtula et al. [3] introduced atom-bond connectivity (*ABC*) index, which it has been applied up until now to study the stability of alkanes and the strain energy of cycloalkanes. This index is defined as follows:

$$ABC(G)=\sum_{e=uv\in E(G)}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}},$$

where $d_G(u)$ stands for the degree of vertex *u*. Now we define a new version of *ABC* indices as follows:

$$ABC_4(G)=\sum_{uv\in E(G)}\sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}},$$

in which $\delta_G(u)=\sum_{v\in N_G(u)} d_G(v)$ and $N_G(u)=\{v\in V(G)\mid uv\in E(G)\}$.

Here our notation is standard and mainly taken from standard books of chemical graph theory [4]. All graphs considered in this paper are finite, undirected, simple and connected. For background materials, see references [5-7].

2. Main results and discussion

In this section we compute the truncated ABC_4 index of chain graphs. Then we use this method to compute the ABC_4 index of an infinite class of nanostar dendrimers. To do this let $U=\{u_1,u_2,\dots,u_k\}$ be a subset of *V*(*G*). The truncated ABC_4 index $ABC_4^{(U)}$ defines as

$$ABC_4^{(u_1,u_2,\dots,u_k)}(G)=\sum_{\substack{uv\in E(G)\\ u,v\neq u_1,u_2,\dots,u_k}}\sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}}$$

i. e.,

$$ABC_4^{(U)}(G)=\sum_{\substack{uv\in E(G)\\ u,v\notin U}}\sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)d_G(v)}}.$$

It should be noticed that in the case $U=\emptyset$, $ABC_4^{(U)}(G)=ABC_4(G)$. At first, we consider some examples:

Example 1. Let K_n be the complete graph on *n* vertices. Then, for every $v\in V(K_n)$, $d_G(v)=n-1$ and so

$\delta_G(v) = (n-1)^2$. This implies that $ABC_4(K_n) = \frac{n(n-1)}{2}\sqrt{\frac{2\left((n-1)^2-1\right)}{(n-1)^4}}$.

Example 2. Let C_n denote the cycle of length *n*. Then $d_G(v) = 2$ and $\delta_G(v) = 4$. Hence, $ABC_4(C_n) = \frac{n}{4}\sqrt{6}$.

Example 3. Let P_n be a path of length *n*. Then one can see that $ABC_4(P_n) = \frac{(n-5)}{4}\sqrt{6} + \sqrt{2} + \sqrt{\frac{5}{3}}$, $(n \geq 5)$.

Let G_i $(1 \le i \le n)$ be some graphs and $v_i \in V(G_i)$. A chain graph denoted by $G = G(G_1,...,G_n,v_1,...,v_n)$ is obtained from the union of the graphs G_i, $i = 1,2,...,n$, by adding the edges v_iv_{i+1} $(1 \le i \le n-1)$, see Fig. 1. Then $|V(G)| = \sum_{i=1}^{n}|V(G_i)|$ and $|E(G)| = (n-1) + \sum_{i=1}^{n}|E(G_i)|$.

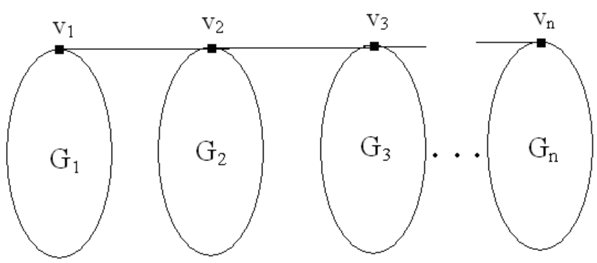

Fig. 1. The chain graph $G = G(G_1,...,G_n,v_1,...,v_n)$.

It is worth noting that the above specified class of chain graphs embraces, as special cases, all trees (among which are the molecular graphs of alkanes) and all unicyclic graphs (among which are the molecular graphs of monocycloalkanes). Also the molecular graphs of many polymers and dendrimers are chain graphs.

Lemma 1. Suppose that $G = G(G_1,G_2,...,G_n,v_1,v_2,...,v_n)$ is a chain graph and for a vertex *u* in *V*(*G*), $N_G[u] = N_G(u) \cup \{u\}$. Then:

(i) $G(G_1,G_2,...,G_n,v_1,v_2,...,v_n)$ is connected if and only if G_i $(1 \le i \le n)$ are connected.

(ii)

$$\mathrm{d}_G(a) = \begin{cases} \mathrm{d}_{G_i}(a) & a \in V(G_i) \text{ and } a \neq v_i \\ \mathrm{d}_{G_i}(a) + 1 & a = v_i,\ i = 1, n \\ \mathrm{d}_{G_i}(a) + 2 & a = v_i,\ 2 \le i \le n-1 \end{cases},$$

(iii) if $u \in V(G_i)$ and $v_i \notin N_{G_i}[u]$ then $\delta_G(u) = \delta_{G_i}(u)$.

Theorem 2. If $U = \{u_1,u_2,...,u_k\}$ be a subset of *V*(*G*) and $v_1,...,v_n \notin U$, then for $G = G(G_1,G_2,...,G_n,v_1,v_2,...,v_n)$ it holds:

$$ABC_4^{(u_1,...,u_k)}(G) = \sum_{i=1}^{n} ABC_4^{\left(U \cup N_{G_i}[v_i]\right)}(G_i) + \sum_{i=1}^{n}\sum_{\substack{uv \in E(G_i) \\ u \in N_{G_i}[v_i] \\ u,v \notin U}} \sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}} + \sum_{i=1}^{n-1}\sqrt{\frac{\delta_G(v_i)+\delta_G(v_{i+1})-2}{\delta_G(v_i)\delta_G(v_{i+1})}}.$$

Proof. By using the definition of the truncated ABC_4 index one can see that

$$ABC_4^{(u_1,u_2,...,u_k)}(G) = \sum_{\substack{uv \in E(G) \\ u,v \notin U}} \sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}} = \sum_{i=1}^{n}\sum_{\substack{uv \in E(G_i) \\ u,v \notin U}} \sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}} + \sum_{i=1}^{n-1}\sqrt{\frac{\delta_G(v_i)+\delta_G(v_{i+1})-2}{\delta_G(v_i)\delta_G(v_{i+1})}}$$

$$= \sum_{i=1}^{n}\sum_{\substack{uv \in E(G_i) \\ u,v \notin U \cup N_{G_i}[v_i]}} \sqrt{\frac{\delta_{G_i}(u)+\delta_{G_i}(v)-2}{\delta_{G_i}(u)\delta_{G_i}(v)}} + \sum_{i=1}^{n}\sum_{\substack{uv \in E(G_i) \\ u \in N_{G_i}[v_i] \\ u,v \notin U}} \sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}} + \sum_{i=1}^{n-1}\sqrt{\frac{\delta_G(v_i)+\delta_G(v_{i+1})-2}{\delta_G(v_i)\delta_G(v_{i+1})}}$$

$$= \sum_{i=1}^{n} ABC_4^{\left(U \cup N_{G_i}[v_i]\right)}(G_i) + \sum_{i=1}^{n}\sum_{\substack{uv \in E(G_i) \\ u \in N_{G_i}[v_i] \\ u,v \notin U}} \sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}}$$

$$+\sum_{i=1}^{n-1}\sqrt{\frac{\delta_G(v_i)+\delta_G(v_{i+1})-2}{\delta_G(v_i)\delta_G(v_{i+1})}}\,.$$

Corollary 3. The truncated ABC_4 index of the chain graph $G=G(G_1,G_2,v_1,v_2)$ $\left(v_1,v_2\notin U, U=\{u_1,u_2,...,u_k\}\subseteq V(G)\right)$ is:

$$ABC_4^{(u_1,...,u_k)}(G)=\sum_{i=1}^{2}ABC_4^{\left(U\cup N_{G_i}[v_i]\right)}(G_i)+\sum_{i=1}^{2}\sum_{\substack{uv\in E(G_i)\\ u\in N_{G_i}[v_i]\\ u,v\notin U}}\sqrt{\frac{\delta_G(u)+\delta_G(v)-2}{\delta_G(u)\delta_G(v)}}+\sqrt{\frac{\delta_{G_1}(v_1)+d_{G_2}(v_2)+\delta_{G_2}(v_2)+d_{G_1}(v_1)}{\left(\delta_{G_1}(v_1)+d_{G_2}(v_2)+1\right)\left(\delta_{G_2}(v_2)+d_{G_1}(v_1)+1\right)}}\,.$$

We use from this Corollary in the next section.

Example 4. Consider the graph G_1 shown in *Fig*. 2. It is easy to see that

$$ABC_4(G_1)=\frac{3}{2}\sqrt{6}+\sqrt{2}+3\sqrt{\frac{7}{5}}+6\sqrt{\frac{2}{7}}\,,$$

$$ABC_4^{(N_{G_1}[v_1])}(G_1)=ABC_4^{(N_{G_1}[v_2])}(G_1)=ABC_4^{(N_{G_1}[v_3])}(G_1)$$

$$=ABC_4^{(N_{G_1}[v])}(G_1)=\sqrt{6}+\sqrt{2}+2\sqrt{\frac{7}{5}}+6\sqrt{\frac{2}{7}}\,,$$

and so, for $1\le i,j\le 3, i\neq j$,

$$ABC_4^{(N_{G_1}[v_i]\cup N_{G_1}[v_j])}(G_1)=\frac{1}{2}\sqrt{6}+\sqrt{2}+\sqrt{\frac{7}{5}}+6\sqrt{\frac{2}{7}}\,.$$

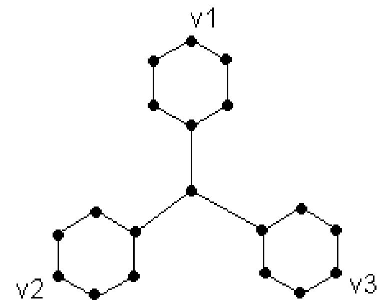

Fig. 2. The graph of nanostar G_n for n=1.

Consider now the chain graph $G_n=G(G_{n-1},H_1,v_1,u_1)$, shown in Fig. 2 (for $n=1$) and Fig. 3, respectively. It is easy to see that $H_i\cong G_1$ ($1\le i\le n-1$) and

$$G_n=G(G_{n-1},H_1,v_1,u_1)$$
$$G_{n-1}=G(G_{n-2},H_2,v_2,u_2)$$
$$\vdots$$
$$G_{n-i}=G(G_{n-i-1},H_{i+1},v_{i+1},u_{i+1})$$
$$\vdots$$
$$G_2=G(G_1,H_{n-1},v_{n-1},u_{n-1})\,.$$

Then by using Corollary 3, we have the following relations:

$$ABC_4(G_n)=ABC_4^{(N_{G_{n-1}}[v_1])}(G_{n-1})+ABC_4^{(N_{H_1}[u_1])}(H_1)+c$$
$$ABC_4^{(N_{G_{n-1}}[v_1])}(G_{n-1})=ABC_4^{(N_{G_{n-2}}[v_2])}(G_{n-2})+ABC_4^{(N_{H_2}[v_1]\cup N_{H_2}[u_2])}(H_2)+c$$
$$\vdots$$
$$ABC_4^{(N_{G_{n-i}}[v_i])}(G_{n-i})=ABC_4^{(N_{G_{n-i-1}}[v_{i+1}])}(G_{n-i-1})+ABC_4^{(N_{H_{i+1}}[v_i]\cup N_{H_{i+1}}[u_{i+1}])}(H_{i+1})+c$$
$$\vdots$$
$$ABC_4^{(N_{G_2}[v_{n-2}])}(G_2)=ABC_4^{(N_{G_1}[v_{n-1}])}(G_1)+ABC_4^{(N_{H_{n-1}}[v_{n-2}]\cup N_{H_{n-1}}[u_{n-1}])}(H_{n-1})+c\,,$$

in which $c=\frac{2}{7}\sqrt{3}+\frac{8}{5}\sqrt{2}+4\sqrt{\frac{2}{7}}$. Summation of these relations yields

$$ABC_4(G_n)=ABC_4^{(N_{G_1}[v_{n-1}])}(G_1)+ABC_4^{(N_{H_1}[u_1])}(H_1)+\sum_{i=2}^{n-1}ABC_4^{(N_{H_i}[v_{i-1}]\cup N_{H_i}[u_i])}(H_i)+(n-1)c\,,$$

and so by using example 4, it is easy to obtain

$$ABC_4(G_n)=2ABC_4^{(N_{G_1}[v_1])}(G_1)+\left(n-2\right)ABC_4^{(N_{G_1}[v_1]\cup N_{G_1}[v_2])}(G_1)+(n-1)c$$
$$=\left(\frac{1}{2}\sqrt{6}+\frac{2}{7}\sqrt{3}+\frac{13}{5}\sqrt{2}+\sqrt{\frac{7}{5}}+10\sqrt{\frac{2}{7}}\right)n+\left(\sqrt{6}-\frac{2}{7}\sqrt{3}-\frac{8}{5}\sqrt{2}+2\sqrt{\frac{7}{5}}-4\sqrt{\frac{2}{7}}\right).$$

In other words we arrived at the following:

Theorem 4. Consider the chain graph $G_n = G(G_{n-1}, H_1, v_1, u_1)$ $(n \geq 2)$, shown in Fig. 3. Then,

$$ABC_4(G_n) = \left(\frac{1}{2}\sqrt{6}+\frac{2}{7}\sqrt{3}+\frac{13}{5}\sqrt{2}+\sqrt{\frac{7}{5}}+10\sqrt{\frac{2}{7}}\right)n + \left(\sqrt{6}-\frac{2}{7}\sqrt{3}-\frac{8}{5}\sqrt{2}+2\sqrt{\frac{7}{5}}-4\sqrt{\frac{2}{7}}\right).$$

Corollary 5. Consider the nanostar dendrimer D, shown in Fig. 4. Then,

$$ABC(D) = \left(\frac{1}{2}\sqrt{6}+\frac{2}{7}\sqrt{3}+\frac{13}{5}\sqrt{2}+\sqrt{\frac{7}{5}}+10\sqrt{\frac{2}{7}}\right)n + \left(\sqrt{6}-\frac{2}{7}\sqrt{3}-\frac{8}{5}\sqrt{2}+2\sqrt{\frac{7}{5}}-4\sqrt{\frac{2}{7}}\right),$$

where n is the number of repetition of the fragment G_1.

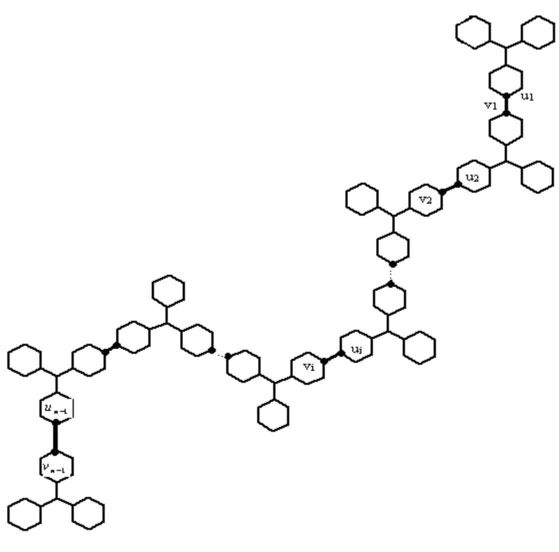

Fig. 3. The chain graph G_n and the labeling of its vertices.

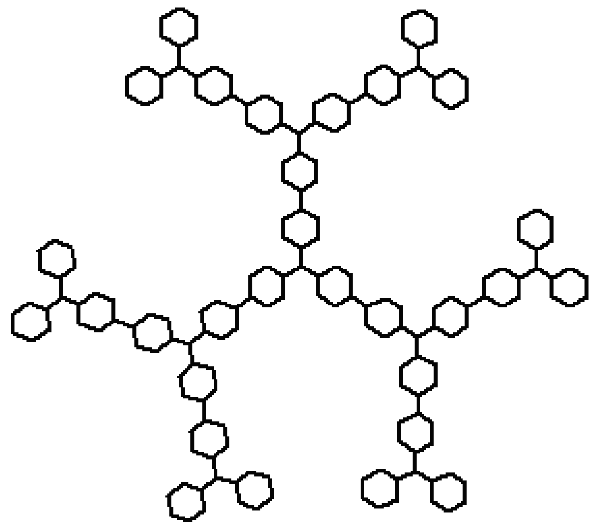

Fig. 4. The graph of the nanostar dendrimer D.

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