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Some Basic Results on the Second Multiplication Atom-Bond Connectivity Index

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Abstract. As the atom-bond connectivity index kept expanding, the multiplicative atom-bond connectivity indices were introduced to measure the stability of alkanes and strain energy of cycloalkanes. Let $ABC\Pi(G) = \prod_{uv\in E(G)} \sqrt{\frac{n_u+n_v-2}{n_u n_v}}$ denote the first multiplicative atom-bond connectivity index (ABCΠ) of a graph G, in which n_u represents the number of vertices which are closer to vertex u than vertex v. Similarly, n_v is defined in this way. In this paper, we study the basic mathematical characters of the second multiplicative atom-bond connectivity index.

Key words: theoretical chemistry, molecular graph, second multiplicative atom-bond connectivity index

2010 Mathematics Subject Classification: 05C70.

1. Introduction

As the improvement of the experimental skills as well as the experimental conditions, compounds materials, and the drugs have been emerging in the laboratory every year. These new material needs the experimental methods to detect their physical, chemical, material or pharmacological properties, which greatly increases the cost of the test and workload to analyze new compounds. Indeed, this work needs put plenty of experimental instruments and reagents, so it has gradually become an important expense. On the other hand, the

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experimental results of the early years show that there is closely relationship between chemical structure of compounds and their related characteristics. The theoretical chemistry provides a new way of thinking and help researchers indirectly acquire the properties of compounds by means of mathematical deduction and calculation. The basic idea is to represent a graph for each molecular structure, and topological index is defined on the graph. The characteristics of molecular structure are determined by calculation of the corresponding topological index. The laws are not subject to the experimental conditions and have been welcomed by the less developed countries and regions. At present, in Iran, Pakistan and India, a large number of scholars use mathematical methods to study the properties of compounds. For the contributions on the topological index computation and its engineering applications one can refer to Balaban [1], Buscema et al. [2], Gao et al. [3–5], Bodlaj and Batagelj [6], Lokesha et al. [7], Khakpoor and Keshe [8], and Ivanciuc [9].

This paper only covers simple (molecular) graphs. Let $G = (V(G), E(G))$ be a connected graph with vertex set $V(G)$ and edge set $E(G)$ respectively. The degree $d(v)$ of a vertex v is the number of edges incident to v. A topological index is a function $f : G \to \mathbb{R}$ which maps each graph to a real number. In around recent 40 years, motivated by the chemical, material and pharmaceutical engineering applications, lots of degree-based, distance-based and spectrum-based indices were introduced, such as Wiener index, graph energy, PI index, Randić energy, Zagreb index, resolvent energy, harmonic index, signless Laplacian estrada index sum connectivity index, etc. In addition, some advancements on distance-based, degree-based and spectrum-based indices of special molecular structures are contributed, and they can be in reference to Sardar et al. [10], Gao and Wang [11, 12], Abdo et al. [13], Hosamani et al. [14], Carballosa et al. [15], Hernandez-Gomez et al. [16], Bermudo et al. [17], and Guirao and de Bustos [18].

The atom-bond connectivity index (in short, the ABC index) was proposed by Estrada and Torres [19] and it is a graph invariant suitable for stability of alkanes and the strain energy of cycloalkanes. As a graph G, the atom-bond connectivity index can be formulated as

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

For this famous index, it has been widely studied by researchers and an amount of conclusions have been obtained. The first and second maximum values of the atom-bond connectivity index of tetracyclic graphs with n vertex were calculated by Dehghan-Zadeh et al. [20]. Ashrafi and Dehghan-Zadeh [21] studied the first and second maximum values of the ABC index of cactus graphs with order n. Goubko et al. [22] presented a counterexample to the main result of the previous conclusion. Dehghan-Zadeh and Ashrafi [23] determined the atom-bond connectivity index of quasi-tree graphs. Besides, an efficient computation trick of trees with the smallest atom-bond connectivity index are raised by Dimitrov [24].

As the multiplicative version of the ABC index, the first multiplicative atom-bond connectivity index

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

was introduced by Kulli [27]. Inspired by this multiplicative index, Zhong et al. [28] characterized extremal graphs with respect to the first multiplicative atom-bond connectivity index. In the same way, the multiplicative atom-bond connectivity index of a catacondensed hexagonal system was determined as well.

The second multiplication ABC index is also introduced by Kulli [27] which is formulated as follows:

$$\mathrm{ABC}_2\Pi(G) = \prod_{uv \in E(G)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}},$$

where

$$n_u = |\{x \in V(G) | d(u,x) < d(v,x)\}|$$

and

$$n_v = |\{x \in V(G) | d(u,x) < d(v,x)\}|.$$

Let K_n, S_n and P_n be the complete graph, star and path on n vertices, respectively. And let $K_{n,m}$ also be the complete bipartite graph on $n+m$ vertices. A tree is said to be star-like if exactly one of its vertices has degree greater than two. By $S(2r,s)$, $r,s \geq 1$, we denote a star-like tree with diameter less than or equal to 4, which has a vertex v_1 of degree $r+s$ and

$$S(2r,s) - \{v_1\} = \underbrace{p_2 \cup \cdots \cup p_2}_{r} \cup \underbrace{p_1 \cup \cdots \cup p_1}_{s}.$$

One can prove that, this tree has $2r+s+1 = n$ vertices. We say that the star-like tree $S(2r,s)$ has $r+s$ branches, where the lengths of them are $\underbrace{2,\cdots,2}_{r},\underbrace{1,\cdots,1}_{s}$ respectively. For $n,m \geq 2$, denoted by $S_{m,n}$ which means a tree with $n+m$ vertices formed by adding a new edge connecting the centers of the stars S_n and S_m. Finally, if and only if they are not adjacent in G, the complement G of a simple graph G is a simple graph with vertex set V and two vertices are close to each other in G.

Although there are abundant known result on ABC index, the theoretical results on the second multiplicative atom-bond connectivity index are still limited. In the article, we demonstrate several basic mathematical features of the second multiplicative atom-bond connectivity index.

2. Main results and proofs

The aim of this part is to demonstrate the main results and their proofs in details.

Theorem 1. *Let G be a connected graph of order n with m edges and p pendent vertices, then*

$$\mathrm{ABC}_2\Pi(G) < (\sqrt{\frac{n-2}{n-1}})^p.$$

Proof. Clearly, we can assume that $n \geq 3$. For each pendent edge uv of graph G we have $n_u = 1$ and $n_v = n-1$. For each non-pendent edge uv of graph G we have $\frac{n_u+n_v-2}{n_u n_v} < 1$. So

$$\mathrm{ABC}_2\Pi(G) = \prod_{uv\in E(G),d(u)=1} \sqrt{\frac{n_u+n_v-2}{n_u n_v}} \times \prod_{uv\in E(G),d(u),d(v)\neq 1} \sqrt{\frac{n_u+n_v-2}{n_u n_v}} < (\sqrt{\frac{n-2}{n-1}})^p.$$

A simple calculation shows that the Diophantine equation $x + y - 2 = xy$ does not have any integer solution. Then the upper bound does not happen. $\square$

Theorem 2. *Let T a tree of order $n > 2$ with p pendent vertices. Then*

$$\mathrm{ABC}_2\Pi(T) \leq \left(\sqrt{\frac{n-2}{n-1}}\right)^p \left(\frac{\sqrt{2}}{2}\right)^{n-p-1}$$

with equality if and only if $T \cong K_{1,n-1}$ or $T \cong S(2r, s)$ where $n = 2r + s + 1$.

Proof. For any edge of trees we have $n_u + n_v = n$. Now we assume, the tree T have p pendent vertex, then there exists p edge that $n_u = 1$ and $n_v = n - 1$. For each non-pendent edge uv of tree T, $2 \leq n_u, n_v \leq n - 2$ and then $n_u n_v \geq 2(n-2)$. This implies that $\sqrt{n_u n_v} \geq \sqrt{2(n-2)}$ and so

$$\frac{1}{\sqrt{n_u n_v}} \leq \frac{1}{\sqrt{2(n-2)}}.$$

Hence,

$$\begin{aligned} \mathrm{ABC}_2\Pi(T) &= \prod_{uv \in E(T), d(u)=1} \sqrt{\frac{n-2}{n_u n_v}} \times \prod_{uv \in E(T), d(u), d(v) \neq 1} \sqrt{\frac{n-2}{n_u n_v}} \\ &\leq \left(\sqrt{\frac{n-2}{n-1}}\right)^p \left(\sqrt{\frac{n-2}{2(n-2)}}\right)^{n-p-1}. \end{aligned} \tag{1}$$

Suppose now that equality holds in (1), we can consider the following cases:

Case (a): $p = n - 1$. From equality in (1), we must have $n_u = n - 1$ and $n_v = 1$ for each edge $uv \in E(T)$ and $n_u \geq n_v$, that is, each edge uv must be pendent. Since T is a tree, $T \cong K_{1,n-1}$.

Case (b): $p < n - 1$. In this case the diameter of T is strictly greater than 2. So there is a neighbor of a pendent vertex, say u, adjacent to some non-pendent vertex k. Since $n_u = n - 2$ and $n_v = 2$ for each non-pendent edge $uv \in E(T)$, $n_u \geq n_v$, we conclude that the degree of each neighbor of a pendent vertex is two and each vertex is adjacent to vertex k. In addition, also the remaining pendent vertices are adjacent to vertex k. Hence T is isomorphic to $T \cong S(2r, s)$ where $n = 2r + s + 1$.

In contrast, it is easy to see that the equality in (1) holds for star $K_{1,n-1}$ or $S(2r, s)$ where $n = 2r + s + 1$. $\square$

Theorem 3. *Let G be a graph on $n > 2$ vertices, m edges and p pendent vertices. Then*

$$\mathrm{ABC}_2\Pi(G) \leq \left(\sqrt{\frac{n-2}{n-1}}\right)^p$$

with equality if and only if $G \cong K_{1,n-1}$ or $G \cong K_n$.

Proof. For each pendant edge uv, $n_u = 1$, $n_v = n-1$ and for the others n_u, $n_v \geq 1$. This implies that

$$\begin{aligned} \mathrm{ABC}_2\Pi(G) &= \prod_{uv\in E(G)} \sqrt{\frac{n_u+n_v-2}{n_u n_v}} \\ &= \prod_{uv\in E(G),d(u)=1} \sqrt{\frac{n_u+n_v-2}{n_u n_v}} \times \prod_{uv\in E(G),d(u),d(v)\neq 1} \sqrt{\frac{n_u+n_v-2}{n_u n_v}} \\ &= \left(\sqrt{\frac{n-2}{n-1}}\right)^p \times \prod_{uv\in E(G),d(u),d(v)\neq 1} \sqrt{\frac{n_u+n_v-2}{n_u n_v}} \leq \left(\sqrt{\frac{n-2}{n-1}}\right)^p. \end{aligned}$$

For equality we should consider two cases:

Case(a) $p = 0$, in this case for all edges $e = uv$, $n_u = n_v = 1$ and this implies $G \cong K_n$.

Case(b) $p = m$, in this case all edges are pendant and so $G \cong K_{1,n-1}$. □

Theorem 4. *Let T be a tree of order $n > 2$ with p pendent vertices. Then*

$$\mathrm{ABC}_2\Pi(T) \geq \left(\sqrt{\frac{n-2}{n-1}}\right)^p \left(\frac{2\sqrt{n-2}}{n}\right)^{n-p-1}$$

with equality if and only if $T \cong K_{1,n-1}$ or $T \cong S_{\frac{n}{2},\frac{n}{2}}$.

Proof. It is clear that in a tree for every edge uv, $n_u + n_v = n$ and hence

$$\mathrm{ABC}_2\Pi(T) = \prod_{uv\in E(G)} \sqrt{\frac{n-2}{n_u n_v}}.$$

Now we assume that T have p pendent vertices, then there exist p edges such as $e = uv$ where $n_u = 1$ and $n_v = n - 1$. Also, for each non-pendant edge uv, $n_u n_v \leq \dfrac{n^2}{4}$ and so

$$\begin{aligned}
\mathrm{ABC}_2\Pi(T) &= \prod_{uv\in E(G),d(u)=1}\sqrt{\frac{n-2}{n_un_v}}\times\prod_{uv\in E(G),d(u),d(v)\neq 1}\sqrt{\frac{n-2}{n_un_v}}\\
&= \left(\sqrt{\frac{n-2}{n-1}}\right)^p\times\prod_{uv\in E(G),d(u),d(v)\neq 1}\sqrt{\frac{n-2}{n_un_v}}\\
&\geq \left(\sqrt{\frac{n-2}{n-1}}\right)^p\left(\frac{2\sqrt{n-2}}{n}\right)^{n-p-1}.
\end{aligned}$$

Let the equality of the formula above holds, we can consider two following cases:
Case(a) $p = n-1$, in this case all edges are pendant. Therefore $T \cong K_{1,n-1}$ and so $\mathrm{ABC}_2\Pi(T) = \left(\sqrt{\frac{n-2}{n-1}}\right)^{n-1}$.
Case(b) $p < n-1$, in this case equality holds if and only if for all non-pendant edges, $n_u = n_v = \frac{n}{2}$ and this completes the proof. □

Theorem 5. *Let G and $\overline{G}$ are connected graphs on n vertices with p and $\overline{p}$ pendent vertices, respectively. Then*

$$\mathrm{ABC}_2\Pi(G) + \mathrm{ABC}_2\Pi(\overline{G}) < \left(\sqrt{\frac{n-2}{n-1}}\right)^p + \left(\sqrt{\frac{n-2}{n-1}}\right)^{\overline{p}}.$$

Proof. The result is obtained directly from Theorem 1. □

Conflict of Interests

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

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