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Remarks on Multiplicative Atom-Bond Connectivity Index

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ABSTRACT The atom-bond connectivity (ABC) index is one of the most actively studied degree-based graph invariants that are found in a vast variety of chemical applications. This paper is devoted to establishing some extremal results regarding the variant of the ABC index, the so-called multiplicative ABC index (ABCΠ), which, for a graph G, is defined as $ABC\Pi(G) = \prod_{uv\in E(G)} \sqrt{\frac{d(u)+d(v)-2}{d(u)d(v)}}$. We have shown that the complete graph K_n has a minimum ABCΠ index among connected simple graphs with n vertices, while the star graph S_{n-1} has the maximum ABCΠ index. As S_{n-1} attains the maximum amongst bipartite graphs on n vertices, we additionally show that the bipartite complete balanced graph $K_{\lfloor n/2\rfloor,\lceil n/2\rceil}$ attains the minimum in this class of graphs. As an interesting problem, we propose to characterize the trees with the minimum value of this index, and, here, we have some structural properties of these trees. We conclude this paper with few conjectures for possible further work.

INDEX TERMS Chemical graph theory, atom-bond connectivity, multiplicative atom-bond connectivity index.

I. INTRODUCTION

Atopological index can be considered as a function $f : G \rightarrow \mathbb{R}$ which maps each graph to a real number. In the past 40 years, inspired by the chemical engineering applications, many degree-based or distance-based indices were introduced, such as Wiener index, PI index, Zagreb index, harmonic index, sum connectivity index and so on.

In 1998, Estrada *et al.* [1] defined a new topological index called the atom-bond connectivity index (in short, the *ABC* index). It has a reputation to be one of the most important topological indices which reflect the properties of alkanes. The atom-bond connectivity index of a graph G can be formulated by

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

where $d(x)$ is the degree of vertex x. The *ABC* index has been widely studied by researchers, and a lot of achievements on this index have been obtained. Zhang and Yang [2] determined the maximum *ABC* index of a connected graph of a given order, with a fixed independence number, number of pendent vertices, edge-connectivity, and chromatic number, respectively. In [3], [4] an efficient computation technique of trees with the smallest atom-bond connectivity index were applied. The structural properties of trees with a minimal atom-bond connectivity index were studied in several papers including [5]–[9]. In [2], [10], [11] extremal graph with some given parameters were considered.

In 2010 Graovac and Ghorbani [12] introduced a distance-based analog of the ABC index, the Graovac-Ghorbani (GG) index,

$$GG(G) = \sum_{uv\in E(G)}\sqrt{\frac{n_u+n_v-2}{n_u n_v}},$$

where n_u is defined as the number of vertices of G lying closer to u than to v and similarly n_v as the number of vertices of G lying closer to v than to u. This topological index yielded promising results when compared to analogous descriptors [13]. Some of the properties of the Graovac-Ghorbani index were presented in [14]. Another variant of the ABC

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index, the so-called multiplicative atom-bond connectivity index

$$ABC\Pi(G) = \prod_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}, \quad (1)$$

was introduced by Kulli in [15], where the multiplicative atom-bond connectivity index of $VC_5C_7[p, q]$ and $HC_5C_7[p, q]$ nanotubes were computed. Since the multiplicative atom-bond connectivity index has not been widely studied until now, the results on the multiplicative atom-bond connectivity index are still limited, compared to the atom-bond connectivity index.

It is worthy to mention that the square root in (1) does not play any significant role in the nature of this index regardlessly one study this index empirically or mathematically. Anyway, we decided to keep it, as this index is deduced from the ABC index, though there the square root is much less transparent.

In this article we have characterized extremal graphs with respect to $ABC\Pi$. We have shown that the complete graph K_n has a minimum $ABC\Pi$ index among connected simple graphs with n vertices, while the star graph S_{n-1} has the maximum $ABC\Pi$ index. As S_{n-1} attains the maximum amongst bipartite graphs on n vertices, we additionally show that the bipartite complete balanced graph $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$ attains the minimum in this class of graphs. As an interesting problem, we propose to characterize the trees with minimum value of this index, and here we gave only some structural properties of them.

II. SOME AUXILIARY RESULTS

For a sake of simplicity, let us define

$$\varphi(a, b) = \frac{a + b - 2}{ab}. \quad (2)$$

Then the multiplicative atom-bond connectivity index (1), can be simply rewritten as

$$ABC\Pi(G) = \prod_{uv \in E(G)} \sqrt{\varphi(d(u), d(v))}.$$

As obviously, the expression (2) plays an important role in the definition of the multiplicative atom-bond connectivity index, we will give some basic mathematical properties of it. In our case, as values a and b are degrees of vertices of a connected graphs, i.e., they are positive integers. Moreover, as we consider larger graphs, at least one of a and b is always larger than 1.

Two straightforward properties of φ are the following:

(P1). *$\varphi(x, y) = 0$ only for $x = y = 0$, and in all other cases $0 < \varphi(x, y) < 1$.*

(P2). *$\varphi(x, 2) = \frac{1}{2}$ for every $x \geq 1$.*

As a continuation of the above property, one can easily to show that $\varphi(x, 1)$ is strict increasing function and for $y \geq 3$ being fixed, $\varphi(x, y)$ is a strict decreasing function. This observation implies the next two properties:

(P3). *Let $x \in [1, \Delta_1]$ and $y \in [1, \Delta_2]$. Then $\varphi(x, y)$ attains its minimum when $x = \Delta_1$ and $y = \Delta_2$ with $\varphi(x, y) = (\Delta_1 + \Delta_2 - 2)/(\Delta_1 \Delta_2)$.*

(P4). *Let $x, y \in [1, \Delta]$. Then $\varphi(x, y)$ attains its maximum when $\{x, y\} = \{1, \Delta\}$ with $\varphi(x, y) = 1 - 1/\Delta$.*

(P5). *Let x and y be two positive integers such that $y \geq 3$. Then*

- *$\varphi(x, y)/\varphi(x, y-1) > 1$ for $x = 1$;*
- *$\varphi(x, y)/\varphi(x, y-1) = 1$ for $x = 2$;*
- *$\varphi(x, y)/\varphi(x, y-1) < 1$ for $x \geq 3$.*

As $\varphi(x, y)$ is a symmetric function, the above properties are also valid by interchanging the roles of the first and the second coordinate. Thus, in what follows, we will use the properties in both ways.

III. EXTREMAL FOR GENERAL GRAPHS AND BIPARTITE GRAPHS

In this section, we first characterize the extremal of multiplicative atom-bond connectivity index amongst graphs on n vertices, and next amongst bipartite graphs on n vertices.

Theorem 1: Among all connected graphs on n vertices, the multiplicative atom-bond connectivity index attains minimum at K_n and it attains maximum at S_{n-1}.

Proof: Consider first the minimum value. Let it be attained by some graph G on n vertices and m edges. Then

$$\begin{aligned} ABC\Pi(G)^2 &= \prod_{uv \in E(G)} \varphi(d(u), d(v)) \\ &\geq \prod_{uv \in E(G)} \varphi(n-1, n-1) \\ &= \varphi(n-1, n-1)^m \\ &\geq \varphi(n-1, n-1)^{\binom{n}{2}}. \end{aligned}$$

Notice that the first inequality holds by (P3) and the second inequality by (P1) and the fact that a connected graph has at most $\binom{n}{2}$ edges. Also notice in the first one we have equality if each vertex is of degree $n-1$, i.e., $m = \binom{n}{2}$, and this coincides precisely when the second inequality becomes equality, and this is precisely when G is a complete graph.

Let us now consider the maximum value. Again, assume it is attained by some graph G on n vertices and m edges. Then,

$$\begin{aligned} ABC\Pi(G)^2 &= \prod_{uv \in E(G)} \varphi(d(u), d(v)) \\ &\geq \prod_{uv \in E(G)} \varphi(1, n-1) \\ &= \varphi(1, n-1)^m \\ &\geq \varphi(1, n-1)^{n-1}. \end{aligned}$$

In a same line as before, the first inequality holds by (P4) and the second one by (P1) and the fact that a connected graph has at least $n-1$. At the first one we have equality if every edge has one endvertex of degree 1 and other of degree $n-1$ by (P4). This is only possible when G is the star S_{n-1}. And, in this case simultaneously the second inequality becomes equality holds, since then $m = n-1$. □

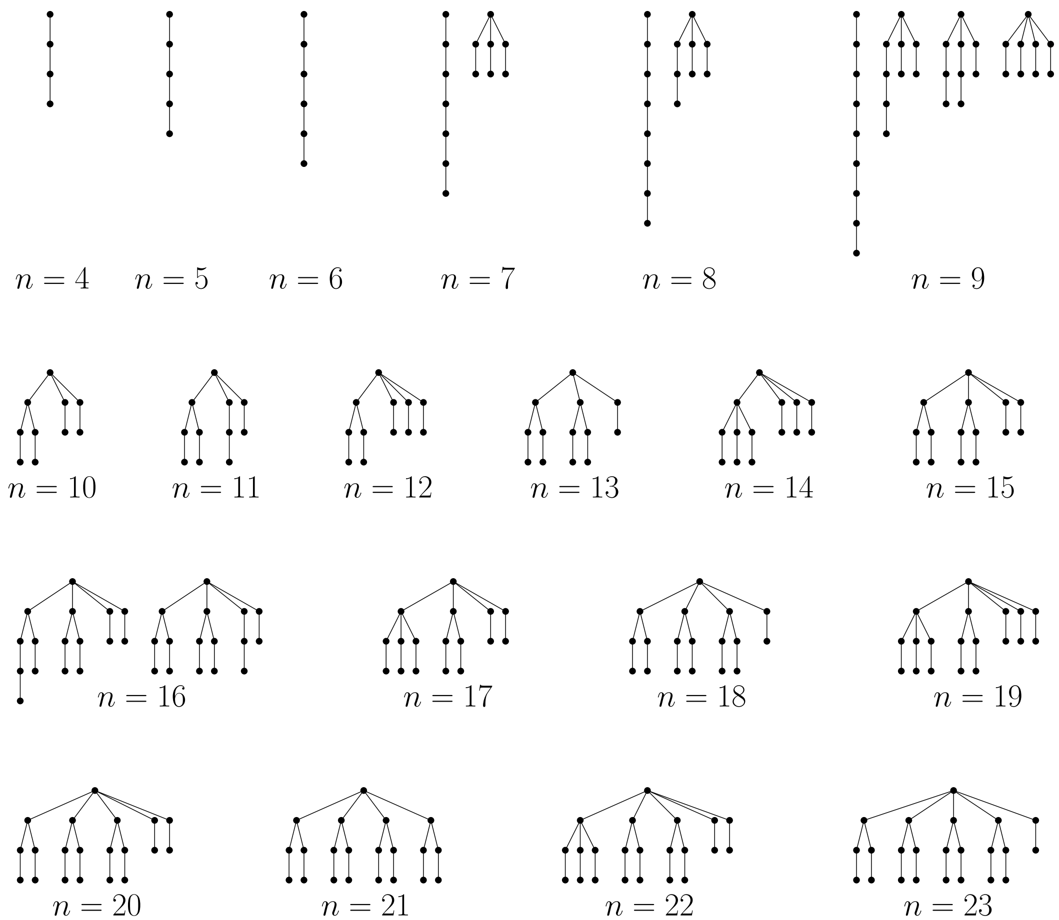

FIGURE 1. The extremal trees up to 23 vertices.

The multiplicative atom-bond connectivity indices of these graphs are

$$ABC\Pi(K_n) = \left(\frac{2n-4}{(n-1)^2}\right)^{\frac{1}{2}\binom{n}{2}}$$

and

$$ABC\Pi(S_{n-1}) = \left(\frac{n-2}{n-1}\right)^{\frac{n-1}{2}}.$$

Proposition 2: Among all bipartite graphs on n vertices the balanced complete bipartite graph $K_{\lfloor n/2\rfloor,\lceil n/2\rceil}$ achieves the minimum multiplicative atom-bond connectivity index.

Proof: Suppose that the minimum is achieved by a bipartite graph G with sizes of bipartitions a and $b = n - a$, where $a \le b$. Notice for an edge uv, it holds $d(u) + d(v) \le n$, and hence

$$\varphi(d(u), d(v)) = \frac{d(u) + d(v) - 2}{d(u)d(v)} \ge \frac{a + b - 2}{ab},$$

and by (P3) the lower bound is achieved for $a = \lfloor n/2\rfloor$ and $b = \lceil n/2\rceil$. Thus,

$$\begin{aligned} ABC\Pi(G)^2 &\ge \prod_{uv\in E(G)} \varphi(a, b) \\ &\ge \varphi(a, b)^{a\cdot b} \ge \varphi(\lfloor n/2\rfloor, \lceil n/2\rceil)^{a\cdot b}. \end{aligned}$$

As $\varphi(\lfloor n/2\rfloor, \lceil n/2\rceil) < 1$ by (P1), we obtain also here minimum for $a = \lfloor n/2\rfloor$ and $b = \lceil n/2\rceil$. Thus, the complete balanced bipartite graph attains the minimum. □

The multiplicative atom-bond connectivity index of this graph is

$$ABC\Pi(K_{\lfloor n/2\rfloor,\lceil n/2\rceil}) = \left(\frac{n-2}{\lfloor n/2\rfloor\lceil n/2\rceil}\right)^{\frac{1}{2}\lfloor n/2\rfloor\lceil n/2\rceil}.$$

IV. EXTREMAL TREES

This section is devoted to trees. As S_{n-1} attains the maximum value of multiplicative atom-bond connectivity index, we will consider the problem of determining the minimum value. It turned that this problem is harder, and we are not able to give a complete solution at this moment. We first state it, and then later we give some properties of the extremal trees.

Problem 3: Find the trees on n vertices with minimum value of multiplicative atom-bond connectivity index.

For a sake of simplicity, in what follows, let us denote by T_n a tree on n vertices with minimum value of multiplicative atom-bond connectivity index. Our computations show that for small values of n, it is not uniquely determined, i.e., there could be several such optimal trees (see Figure 1, where all extremal trees of order up to 23 are depicted).

By the following result we show some basic properties of T_n. Therein we use the following definitions A *thread* in a path in a graph of length ≥ 2 which internal vertices are of degree 2, but the endvertices are not. A thread is *internal* if both of its endvertices are of degree ≥ 3. And, it is *open*, if it has an endvertex of degree 1.

Next we show few properties of the trees with minimal multiplicative atom-bond connectivity index regarding the internal and open threads, vertices of degree at least 2 and the neighborhood of leaves.

Theorem 4: The following properties of T_n holds:

(a) T_n has no internal thread;

(b) If $n \geq 10$, then T_n has at least two vertices of degree ≥ 3;

(c) Every leaf of T_n ($n \geq 4$) is adjacent to a 2-vertex;

(d) T_n has no open thread of length ≥ 4;

(e) T_n has no two open threads of length 3.

Proof: We prove each of the claims separately.

(a). Suppose T_n has an internal thread $u_0u_1 \cdots u_k$. Let degrees of u_0 and u_k be a and b, respectively. Then $a, b \geq 3$, and $d(u_i) = 2$ for $i = 1, \ldots, k-1$. Let ℓ be a leaf attached to a vertex v, whose degree is $s \geq 2$. Observe that v could coincide with u_0 or u_k, but this does not change the proof presented in the sequel.

Construct tree T'_n by removing the path of 2-vertices $u_1 \cdots u_{k-1}$ from T_n and reattaching to ℓ and then connecting u_0 and u_k by an edge. Notice that ℓ is a 2-vertex and u_{k-1} is a leaf in T'_n. See Figure 2 for an illustration.

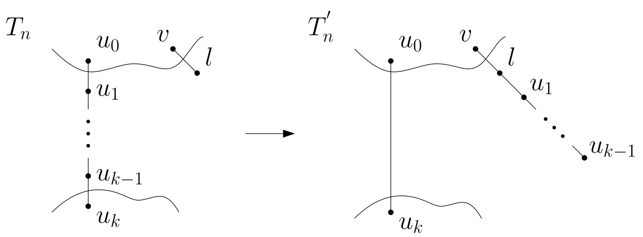

FIGURE 2. The transformation used in the proof of Theorem 4(a).

As vertices $u_1, \ldots, u_{k-1}$ are of degree 2 in T_n and T'_n and the vertex ℓ is of degree 1 in T_n and of degree 2 in T'_n, we obtain by (P2) that

$$\frac{ABC\Pi(T_n)^2}{ABC\Pi(T'_n)^2} = \frac{(\frac{1}{2})^k \varphi(s,1)}{(\frac{1}{2})^k \varphi(a,b)} = \frac{(s-1)}{s}\frac{ab}{a+b-2} \geq \frac{1}{2}\cdot\frac{9}{4} > 1.$$

Observe that the lowest value of the above expression is obtained for $a = b = 3$. Thus, this calculation shows that T'_n has a smaller value of multiplicative atom-bond connectivity index than T_n, a contradiction.

(b). Suppose T_n has at most one vertex of degree ≥ 3. Then for every edge $e = uv$ of T_n, we have $\varphi(d(u), d(v)) = 1/2$ if one of the vertices u, v is of degree 2, and if not, then one of u, v is of degree 1 and the other is of degree $s \geq 3$, which gives $\varphi(d(u), d(v) = 1 - 1/s > 1/2$. Thus, among such trees the path P_n attains $ABC\Pi(P_n)^2 = 1/2^{n-1}$ minimum value. But as $n \geq 10$, we can do better by taking an edge uv and attaching on each of the endvertices u and v two open treads of length ≥ 2, as $n \geq 10$, we have at least 9 edges, so this is possible to construct. Denote this graph by T'_n. Note that in this graph every edge contribute $1/2$ except uv which contributes $1/3$, thus $ABC\Pi(T'_n)^2 = 1/(2^{n-2}3)$, a contradiction to the minimality of T_n.

(c). Suppose that v is a vertex of degree $s \geq 3$ and it is adjacent to a leaf ℓ_1. And, let ℓ_2 be another leaf of T_n, say it is attached to a vertex u of degree $p \geq 2$. We may assume $s \geq p$. Notice that possibly $u = v$. Let T'_n be the tree that obtained from T_n by reattaching ℓ_1 to ℓ_2. Note that v becomes a vertex of degree $s - 1$, and ℓ_1 and ℓ_2 are of degree 1 and 2 in T'_n, respectively (see Figure 3).

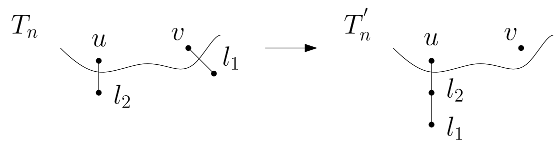

FIGURE 3. The transformation used in the proof of Theorem 4(c).

By (b), we may assume that $u \neq v$. We argue similarly as before. Denote by $a_1, a_2, \ldots, a_{s-1}$ the neighbors of v distinct from ℓ_1. We obtain

$$\frac{ABC\Pi(T_n)^2}{ABC\Pi(T'_n)^2} = \frac{\varphi(p,1)\cdot\varphi(s,1)}{\varphi(p,2)\cdot\varphi(2,1)}\prod_{i=1}^{s-1}\frac{\varphi(d(a_i),s)}{\varphi(d(a_i),s-1)}. \quad (3)$$

Notice that $\varphi(d(a_i), s)/\varphi(d(a_i), s-1) \geq 1$ for $d(a_i) = 1$ and 2 by (P5). If $d(a_i) \geq 3$, then this ratio is smaller than one but we have

$$\frac{\varphi(d(a_i),s)}{\varphi(d(a_i),s-1)} \geq \frac{s-1}{s}\cdot\frac{d(a_i)+s-2}{d(a_i)+s-3} > 1 - \frac{1}{s}.$$

Now by (3), we have

$$\frac{ABC\Pi(T_n)^2}{ABC\Pi(T'_n)^2} > 4\left(1-\frac{1}{s}\right)^s\left(1-\frac{1}{p}\right) > 1.$$

Notice that $(1 - 1/s)^s$ is an increasing function (as the first derivative of this expression is positive for $s \geq 3$), thus it takes minimum at $s = 3$, and since $1 - 1/p \geq 1/2$, we conclude that the expression is bigger than 1. This contradicts the choice of T_n.

(d). Suppose that T_n has such a thread $v_0v_1 \cdots v_k$ with $k \geq 4$, $d(v_0) \geq 3$, and $d(v_k) = 1$. Let $s = d(v_0)$ and denote by $a_1, a_2, \ldots a_{k-1}$ the other neighbors of v_0. Let T'_n be the tree obtained from T_n by reattaching v_{k-1} to v_k. Note that v_0 becomes of degree $s + 1$, and v_{k-2} and v_k are leaves in T'_n. See Figure 4.

As each edge v_iv_{i+1} has at least one endvertex of degree 2, we have $\varphi(d(v_i), d(v_{i+1})) = 1/2$ in both T_n and T'_n. By (c), v_0 has no leaf attached, so each a_i is of degree > 1. This gives that $\varphi(s, d(a_i))/\varphi(s + 1, d(a_i)) \geq 1$ by (P5). By (a) and (b)

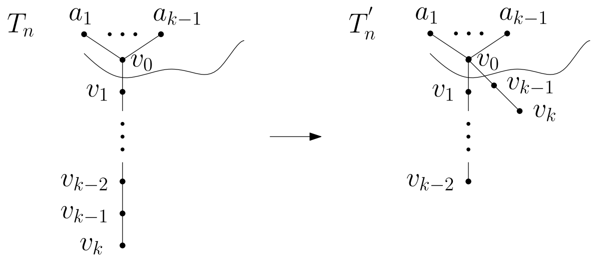

FIGURE 4. The transformation used in the proof of Theorem 4(*d*).

we have that at least one neighboring vertex of v_0, say a_j, has degree at least 3. It follows that $\varphi(s, d(a_j))/\varphi(s+1, d(a_j)) > 1$. Consequently, we have

$$\frac{ABC\Pi(T_n)^2}{ABC\Pi(T_n')^2} = \prod_{i=1}^{s-1} \frac{\varphi(d(a_i), s)}{\varphi(d(a_i), s+1)} > 1,$$

which contradicts the minimality of T_n.

(e). Suppose that T_n has two such threads $v_0v_1v_2v_3$ and $u_0u_1u_2u_3$ with u_0, v_0 being of degree ≥ 3 and u_3, v_3 being leaves. Let T_n' be the tree that obtained from T_n by reattaching v_3 to v_0, and u_3 to v_3. Thus, from the two 3-threads, we are making three 2-threads, two attached at v_0 and one at u_0. Note that each of the thread edges e is incident with a 2-vertex thus it has value $\varphi(e) = 1/2$ by (P5). The degree of v_0 is increased by one, say from s to $s+1$. Again denote by $a_1, a_2, \ldots a_{s-1}$ the other neighbors of v_0.

By the same arguments as in (d), we have also here that each a_i is of degree > 1, which gives that $\varphi(s, d(a_i))/\varphi(s+1, d(a_i)) \geq 1$. Also at least one neighboring vertex of v_0, denoted by a_j, has degree at least 3, which implies $\varphi(s, d(a_j))/\varphi(s+1, d(a_j)) > 1$. This assures that T_n' has smaller value of multiplicative atom-bond connectivity index than T_n

$$\frac{ABC\Pi(T_n)^2}{ABC\Pi(T_n')^2} = \prod_{i=1}^{s-1} \frac{\varphi(d(a_i), s)}{\varphi(d(a_i), s+1)} > 1,$$

a contradiction. □

Due to Theorem 4(a), we have the following immediate consequence.

Corollary 5: For $n \geq 10$, the vertices of T_n with degrees at least 3 induce a tree.

We conclude with the following two, related to each other, conjectures.

Conjecture 6: For $n \geq 17$, the tree T_n is uniquely defined.

Conjecture 7: For $n \geq 17$, the tree T_n has no open thread of length 3.

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