# On the Difference of Atom-Bond Sum-Connectivity and Atom-Bond-Connectivity Indices

### Akbar Ali<sup>a,\*</sup>, Ivan Gutman<sup>b</sup>, Izudin Redžepović<sup>c</sup>, Jaya Percival Mazorodze<sup>d</sup>, Abeer M. Albalahi<sup>a</sup>, Amjad E. Hamza<sup>a</sup>

<sup>a</sup>Department of Mathematics, College of Science, University of Ha'il, Ha'il, Saudi Arabia <sup>b</sup>Faculty of Science,

University of Kragujevac, Kragujevac, Serbia <sup>c</sup>Department of Natural Sciences and Mathematics, State University of Novi Pazar, Novi Pazar, Serbia <sup>d</sup>Department of Mathematics, University of Zimbabwe, Harare, Zimbabwe akbarali.maths@gmail.com, gutman@kg.ac.rs, iredzepovic@np.ac.rs,

mazorodzejava@gmail.com, a.albalahi@uoh.edu.sa,

aboaljod2@hotmail.com

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#### Abstract

The atom-bond connectivity (ABC) index is one of the wellinvestigated degree-based topological indices. The atom-bond sumconnectivity (ABS) index is a modified version of the ABC index, which was introduced recently. The primary goal of the present paper is to investigate the difference between the aforementioned two indices, namely ABS - ABC. It is shown that the difference ABS - ABC is positive for all graphs of minimum degree at least 2

<sup>\*</sup>Corresponding author

as well as for all line graphs of those graphs of order at least 5 that are different from the path and cycle graphs. By means of computer search, the difference ABS - ABC is also calculated for all trees of order at most 15.

#### 1 Introduction

In this paper we consider finite simple graphs (i.e., graphs without directed, weighted, and multiple edges, and without self-loops). Let G be such a graph. In order to avoid trivialities, it will be assumed that G is connected. Its vertex set is  $\mathbf{V}(G)$  and its edge set is  $\mathbf{E}(G)$ . The order and size of Gare  $|\mathbf{V}(G)| = n$  and  $|\mathbf{E}(G)| = m$ , respectively. By an *n*-vertex graph, we mean a graph of order n. The degree  $d_u = d_u(G)$  of the vertex  $u \in \mathbf{V}(G)$ is the number of vertices adjacent to u. The edge connecting the vertices u and v will be denoted by uv. A vertex with degree one is known as a pendent vertex.

For graph-theoretical terminology and notation used without being defined, we refer the readers to the books [8,9,27]

In the early years of mathematical chemistry, Milan Randić invented a topological index [25] that eventually became one of the most successfully applied graph-based molecular structure descriptors [21, 22, 26]. It is nowadays called "connectivity index" or "Randić index" and is defined as

$$R = R(G) = \sum_{uv \in \mathbf{E}(G)} \frac{1}{\sqrt{d_u \, d_v}} \,.$$

Much later, Zhou and Trinajstić [28] proposed to consider the variant of the connectivity index, in which multiplication is replaced by summation, named "sum-connectivity index", defined as

$$SC = SC(G) = \sum_{uv \in \mathbf{E}(G)} \frac{1}{\sqrt{d_u + d_v}}.$$

The same authors examined the relations between R and SC [29].

In 1998, Estrada et al. [12] conceived another modification of the con-

nectivity index, called "atom-bond-connectivity index", defined as

$$ABC = ABC(G) = \sum_{uv \in \mathbf{E}(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \, d_v}} \,.$$

This structure descriptor differs from the original connectivity index by the term  $d_u + d_v - 2$ , which is just the degree of the edge uv (= number of edges incident to uv).

Soon it was established that the ABC index has valuable applicative properties [16]. Its mathematical features were also much investigated, see the recent papers [11, 14, 20], the review [3], and the references cited therein. Especially intriguing is the fact that the apparently simple problem of finding the connected *n*-vertex graph(s) with minimum ABC index remained unsolved for about a decade [18].

Quite recently, the sum-connectivity analogue of the ABC index was put forward, defined as

$$ABS = ABS(G) = \sum_{uv \in \mathbf{E}(G)} \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}}$$

and named "atom-bond sum-connectivity index" [4]. Until now, only a limited number of properties of the ABS index were determined. In [4], the authors determined graphs having the minimum/maximum values of the ABS index among all (i) general graphs (ii) (molecular) trees, with a fixed order; parallel results for the case of unicyclic graphs were obtained in the paper [5], where chemical applications of the ABS index were also reported. (The general ABS index corresponding to the general ABC index [6,10,13] was also proposed in [5]; besides, see [1,2].) Alraqad et al. [7] addressed the problem of finding graphs attaining the minimum ABS index over the class of all trees having given order or/and a fixed number of pendent vertices. Additional detail about the known mathematical properties can be found in the recent papers [15, 19, 23, 24].

As well known, if a graph G has components  $G_1$  and  $G_2$ , then  $ABC(G) = ABC(G_1) + ABC(G_2)$  and  $ABS(G) = ABS(G_1) + ABS(G_2)$ . As a consequence of this, denoting by  $P_2$  the graph of order 2 and size 1, the

following holds.

(a) If G is any graph, and  $G^+$  is a graph whose components are G, an arbitrary number of isolated vertices, and an arbitrary number of  $P_2$ -graphs, then  $ABC(G) = ABC(G^+)$  and  $ABS(G) = ABS(G^+)$ .

(b) if  $G^{++}$  is a graph whose components are G, an arbitrary number of isolated vertices, an arbitrary number of  $P_2$ -graphs, and an arbitrary number of cycles of arbitrary size, then  $ABC(G) - ABS(G) = ABC(G^{++}) - ABS(G^{++})$ .

In order to avoid these trivialities, in what follows we consider only connected graphs. An obvious question is how the two closely related structure descriptors ABC and ABS are related. In this paper, we provide some answers to this question. More precisely, we prove that the difference ABS - ABC is positive for all graphs of minimum degree at least 2 as well as for all line graphs of those graphs of order at least 5 that are different from the path and cycle graphs. We also calculate the difference ABS - ABC for all trees of order at most 15 by utilizing computer software.

### 2 Main Results

We start this section with a simple but notable result that if the minimum degree of a graph G is at least 2 then the ABS index of G cannot be lesser than the ABC index of G.

**Proposition 2.1.** Let G be a connected non-trivial graph of order n, without pendent vertices. Then

$$ABC(G) \le ABS(G).$$

Equality holds if and only if  $G \cong C_n$ , where  $C_n$  is the n-vertex cycle.

*Proof.* For every edge  $uv \in E(G)$ , note that  $d_u d_v \ge d_u + d_v$  with equality if and only if  $d_u = d_v = 2$  because  $\min\{d_u, d_v\} \ge 2$ .

If the order of a graph G is one or two, then the equality ABG(G) =

ABS(G) = 0 holds in a trivial manner.

**Proposition 2.2.** Let G be a connected graph possessing a vertex x of degree 2. Construct the graph  $G^*$  by inserting a new vertex y on an edge incident to x. Evidently, the degree of y is also 2. Then

$$ABC(G) - ABS(G) = ABC(G^*) - ABS(G^*).$$
(1)

*Proof.* Bearing in mind the way in which the graph  $G^*$  was constructed, we see that

$$ABC(G^{\star}) = ABC(G) + \sqrt{\frac{d_x + d_y - 2}{d_x d_y}} = ABC(G) + \frac{1}{\sqrt{2}}$$

and

$$ABS(G^{\star}) = ABS(G) + \sqrt{\frac{d_x + d_y - 2}{d_x + d_y}} = ABS(G) + \frac{1}{\sqrt{2}}.$$

Proposition 2.2 implies that if there is a graph G of order n, possessing a vertex of degree 2, for which  $ABC(G) - ABS(G) = \Theta$ , then for any  $p \ge 1$  there exist graphs of order n + p with the same  $\Theta$ -value.

The situation with graphs possessing pendent vertices is much less simple. In what follows we present our results pertaining to trees. By means of computer search we established the following.

**Observation 2.3.** (a) All trees of order n,  $3 \le n \le 10$ , have the property ABC > ABS.

(b) The smallest tree for which ABC < ABS is depicted in Fig. 1. For n = 11, this tree is unique satisfying ABC < ABS.

(c) For n = 12, 13, 14, and 15, there exist, respectively, 6, 31, 134, and 564 distinct n-vertex trees for which ABC < ABS.

(d) The tree depicted in Fig. 1 possess vertices of degree 2. Therefore, from Proposition 2.2 it follows that there exist n-vertex trees with property ABS > ABC for any  $n \ge 11$ .



Figure 1. The smallest tree for which ABC < ABS.

**Observation 2.4.** No tree of order n,  $3 \le n \le 15$ , has the property ABC = ABS. However, there is a family of four 15-vertex trees, shown in Fig. 2, whose ABC- and ABS-values are remarkably close. For each of these trees:  $ABC \approx 10.184232$  and  $ABS \approx 10.184135$ .



Figure 2. A family of trees with nearly equal ABC- and ABS-values.

Next, we show that the inequality ABS > ABC is satisfied by a reasonably large class of graphs, namely by the line graphs. If G is the line graph of a connected n-vertex graph K such that  $2 \le n \le 4$ , then from the discussion made in the previous part of this section one can directly obtain the classes of graphs satisfying (i) ABS(G) > ABC(G), (ii) ABS(G) = ABC(G). Consequently, we assume that  $n \ge 5$ .

**Theorem 2.5.** If G is the line graph of a connected n-vertex graph K such that  $n \ge 5$  and that  $K \notin \{P_n, C_n\}$ , then ABS(G) > ABC(G).

In order to prove Theorem 2.5, we need some preparations.

A decomposition of a graph G is a class  $S_G$  of edge-disjoint subgraphs of G such that  $\bigcup_{S \in S_G} \mathbf{E}(S) = \mathbf{E}(G)$ . By a clique in a graph G, we mean a maximal complete subgraph of G. A pendent (resp. branching) vertex in a graph is a vertex of degree 1 (resp. of degree at least 3). By a pendent edge of a graph, we mean an edge whose one of the end-vertices is pendent and the other one is non-pendent. for  $r \ge 2$ , a path  $u_1 \cdots u_r$  in a graph is said to be pendent if  $\min\{d_{u_1}, d_{u_r}\} = 1$ ,  $\max\{d_{u_1}, d_{u_r}\} \ge 3$ , and  $d_{u_i} = 2$ for  $2 \le i \le r - 1$ . If  $P : u_1 \cdots u_r$  is a pendent path in a graph with  $d_{u_r} \ge 3$ , we say that P is attached with the vertex  $u_r$ . Two pendent paths of a graph are said to adjacent if they have a common (branching) vertex.

For the proof of Theorem 2.5 we need the following well-known result:

**Lemma 2.6.** [17] A graph G is the line graph of a graph if and only if the star graph of order 4 is not an induced subgraph of G.

We can now start with the proof of Theorem 2.5.

proof of Theorem 2.5. Since  $K \not\cong P_n$ , the graph G has at least one cycle. If G is one of the two graphs  $H_1, H_2$ , depicted in Fig. 3, then one can directly verify that ABS > ABC holds. In what follows, we assume that  $G \notin \{H_1, H_2\}$ .



Figure 3. The graphs  $H_1$  and  $H_2$  mentioned in the proof of Theorem 2.5.

Consider the difference

$$ABS(G) - ABC(G) = \sum_{uv \in \mathbf{E}(G)} \left( \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}} - \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \right)$$

and define a function f of two variables x and y as

$$f(x,y) = \sqrt{\frac{x+y-2}{x+y}} - \sqrt{\frac{x+y-2}{xy}}$$

where  $y \ge x \ge 1$  and  $y \ge 2$ . Note that the function f is strictly increasing (in both x and y). Also, if x and y are integers satisfying the inequalities  $y \ge x \ge 1$  and  $y \ge 2$ , then the inequality f(x, y) < 0 holds if and only if x = 1. Thus,

$$-0.129757 \approx \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} = f(1,2) \le f(1,y) < 0$$

for every  $y \ge 2$ . Also,

$$f(x,y) \ge f(2,3) = \sqrt{\frac{3}{5}} - \frac{1}{\sqrt{2}} \approx 0.0674899 > f(2,2) = 0$$

for  $y \ge x \ge 2$  and  $y \ge 3$ . Furthermore, we have f(1,2) + f(2,y) > 0 for every  $y \ge 5$ . Thus, if either G has no pendent paths or every pendent path of G has length at least 2, which is attached with a vertex of degree at least 5, then ABS(G) - ABC(G) > 0. In the remaining proof, we assume that  $G \notin \{H_1, H_2\}$  and that G either has at least one pendent path of length 1 or it has at least one pendent path of length at least 2, which is attached with a vertex of degree 3 or 4.

Let H' be the graph depicted in Fig. 4, i.e., H' is obtained from two disjoint graphs  $H_1$  and H by identifying their vertices z and z'.

**Fact 1.** If  $G \cong H'$ , then the sum of the contributions of the edges of  $H_1$ in G to the difference ABS(G) - ABC(G) is positive.

It is a well-known fact that the line graph G can be decomposed into cliques, such that every edge of G lies on exactly one clique and every non-pendent vertex of G lies on exactly two cliques. Also, by Lemma 2.6, G contains no pair of adjacent pendent paths/edges and hence the number of pendent edges/paths of G is at most  $\lfloor |\mathbf{E}(G)|/2 \rfloor$ . Bearing this in mind, we decompose G into connected subgraphs  $G_1, \ldots, G_k$  in such a way that



**Figure 4.** The graphs  $H_1$ , H, and H' mentioned in the proof of Theorem 2.5.

every  $G_i$  contains at most one pendent path of G, such that:.

- (a) if  $G_i$  contains a pendent path of G of length 1 such that the branching vertex (in G) of the considered path has at least one neighbor of degree 2 in G, then  $G_i$  consists of the mentioned path together with all the edges incident with the branching vertex (in G) of the mentioned path (for an example, see Fig. 5);
- (b) if  $G_i$  has a pendent path of length at least 2 in G or if  $G_i$  contains a pendent path of G of length 1 such that the branching vertex (in G) of the considered path has no neighbor of degree 2 in G, then  $G_i$ consists of the mentioned path together with exactly one additional edge incident with the branching vertex (in G) of the mentioned path (for an example, see Fig. 5).

In order to complete the proof, it is enough to show that the contribution of any edge of  $G_i$  (in G) to the difference ABS(G) - ABC(G) is positive. If a subgraph  $G_i$  of G contains no pendent vertex of G then certainly, the contribution of all edges of  $G_i$  (in G) to the difference ABS(G) - ABC(G) is positive.



Figure 5. (a) A tree T, its line graph L(T), and a decomposition of L(T) into three connected subgraphs  $G_1, G_2, G_3$ . (b) A tree T, its line graph L(T), and a decomposition of L(T) into four connected subgraphs  $G_1, G_2, G_3, G_4$ .

**Case 1:** a subgraph  $G_i$  contains a pendent path of G of length 1, such that the branching vertex (in G) of the considered path has at least one neighbor of degree 2 in G.

Let  $P: v_1v_2$  be the pendent path of G contained in  $G_i$ , where  $d_{v_1}(G) = 1$  and  $d_{v_2}(G) \geq 3$ . Note that every neighbor of  $v_2$  different from  $v_1$  in G has degree at least  $d_{v_2}(G) - 1$  in G. Thus,  $d_{v_2}(G) = 3$  in the case under consideration. Recall that  $G \notin \{H_1, H_2\}$  (see Fig. 3). Consequently,  $G_i \cong H_1$  and hence by Fact 1, the contribution of all edges of  $G_i$  to the difference ABS(G) - ABC(G) is positive.

**Case 2:** a subgraph  $G_i$  has a pendent path of G of length 1, such that the branching vertex (in G) of the considered path has no neighbor of degree 2 in G.

Note that  $G_i$  is itself a path in this case. Let  $G_i : v_1v_2v'$ , where  $v_1v_2$  is a pendent path of G,  $d_{v_1}(G) = 1$ , and  $d_{v_2}(G) \ge 3$ . If  $d_{v_2}(G) \ge 4$ , then the contribution of all edges of  $G_i$  to the difference ABS(G) - ABC(G) is positive because  $d_{v'}(G) \ge d_{v_2}(G) - 1$  and f(1, y) + (y - 1, y) > 0 for every  $y \ge 4$ . Next, assume that  $d_{v_2}(G) = 3$ . Since  $d_{v'}(G) \ge 3$  in the considered case, the contribution of all edges of  $G_i$  to the difference

ABS(G) - ABC(G) is again positive because f(1,3) + f(3,y) > 0 for all  $y \ge 3$ .

**Case 3:** a subgraph  $G_i$  has a pendent path of length at least 2 in G.

Note that  $G_i$  is itself a path. Let  $G_i : v_1 v_2 \cdots v_r v'$ , where  $v_1 v_2 \cdots v_r$  $(r \ge 3)$  is a pendent path of G,  $d_{v_1}(G) = 1$ , and  $d_{v_r}(G) \in \{3, 4\}$ , because G has no pendent path of length at least 2, which is attached with a vertex of degree at least 5 (see the paragraph before Fact 1).

#### Subcase 3.1: $d_{v_r}(G) = 3$ .

The vertex v' has degree at least 2 and  $f(1,2) + f(2,3) + f(3,y) \ge f(1,2) + f(2,3) + f(2,3) > 0$  for  $y \ge 3$ . Thus, the contribution of all edges of  $G_i$  (in G) to the difference ABS(G) - ABC(G) is positive.

#### **Subcase 3.2:** $d_{v_r}(G) = 4$ .

In this case, the vertex v' has degree at least 3 and  $f(1,2) + f(2,4) + f(4,y) \ge f(1,2) + f(2,4) + f(3,4) > 0$  for  $y \ge 4$ . Thus, the contribution of all edges of  $G_i$  (in G) to the difference ABS(G) - ABC(G) is again positive.

This completes the proof of Theorem 2.5.

**Theorem 2.7.** Let G be a connected graph of size m. If the number of pendent vertices of G is at most  $\lfloor m/2 \rfloor$  and the number of vertices of degree 2 in G is zero, then

*Proof.* Define a function f of two variables x and y as

$$f(x,y) = \sqrt{\frac{x+y-2}{x+y}} - \sqrt{\frac{x+y-2}{xy}}$$

where  $y \ge x \ge 1$  and  $y \ge 3$ . Note that the function f is strictly increasing (in both x and y). Also, if x and y are integers satisfying the inequalities  $y \ge x \ge 1$  and  $y \ge 3$ , then the inequality f(x, y) < 0 holds if and only if x = 1. Thus,

$$-0.10939 \approx \frac{1}{\sqrt{2}} - \sqrt{\frac{2}{3}} = f(1,3) \le f(1,y) < 0$$

for every  $y \ge 3$ . Also,

$$f(x,y) \ge f(3,3) = \sqrt{\frac{2}{3}} - \frac{2}{3} \approx 0.14983$$

for  $y \ge x \ge 3$ . Let p denote the number of pendent vertices of G. Then,  $m - p \ge p$ . Now, by keeping in mind these observations, we have

$$\begin{split} ABS(G) - ABC(G) &= \sum_{uv \in \mathbf{E}(G)} \left( \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}} - \sqrt{\frac{d_u + d_v - 2}{d_u \, d_v}} \right) \\ &= \sum_{uv \in \mathbf{E}(G); \, d_u = 1} \left( \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}} - \sqrt{\frac{d_u + d_v - 2}{d_u \, d_v}} \right) \\ &+ \sum_{uv \in \mathbf{E}(G); \, \min\{d_u, d_v\} \geq 3} \left( \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}} - \sqrt{\frac{d_u + d_v - 2}{d_u \, d_v}} \right) \\ &\geq \sum_{uv \in \mathbf{E}(G); \, d_u = 1} \left( \frac{1}{\sqrt{2}} - \sqrt{\frac{2}{3}} \right) \\ &+ \sum_{uv \in \mathbf{E}(G); \, \min\{d_u, d_v\} \geq 3} \left( \sqrt{\frac{2}{3}} - \frac{2}{3} \right) \\ &= p \left( \frac{1}{\sqrt{2}} - \sqrt{\frac{2}{3}} \right) + (m - p) \left( \sqrt{\frac{2}{3}} - \frac{2}{3} \right) \\ &\geq p \left( \frac{1}{\sqrt{2}} - \sqrt{\frac{2}{3}} \right) + p \left( \sqrt{\frac{2}{3}} - \frac{2}{3} \right) > 0 \; . \end{split}$$

**Theorem 2.8.** Let G be a connected graph of size m such that if  $v \in V(G)$ is a vertex of degree 2 then v has no neighbor of either of the degrees 2, 3, 4. If the number of pendent vertices of G is at most  $\lfloor m/2 \rfloor$ , then ABS(G) > ABC(G).

*Proof.* Consider the function f of two variables x and y defined in the proof of Theorem 2.7 with the constraints  $y \ge x \ge 1$  and  $y \ge 2$ . Note that the function f is strictly increasing (in both x and y). Also, if x and y are integers satisfying the inequalities  $y \ge x \ge 1$  and  $y \ge 2$ , then the

inequality f(x, y) < 0 holds if and only if x = 1. Thus,

$$-0.129757 \approx \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} = f(1,2) \le f(1,y) < 0$$

for every  $y \ge 2$ . Also,

$$f(x,y) \ge f(2,5) = \sqrt{\frac{5}{7}} - \frac{1}{\sqrt{2}} \approx 0.138047$$

for  $y \ge x \ge 2$  with  $y \ge 5$  and

$$f(x,y) \ge f(3,3) > f(2,5)$$

for  $y \geq x \geq 3.$  Let P denote the set of pendent edges of G. Then,

$$|\mathbf{E}(G) \setminus P| \ge |P|.$$

Now, by keeping in mind the above observations, we have

$$\begin{split} ABS(G) - ABC(G) &= \sum_{uv \in \mathbf{E}(G) \setminus P} \left( \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}} - \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \right) \\ &+ \sum_{uv \in P} \left( \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}} - \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \right) \\ &\geq \sum_{uv \in \mathbf{E}(G) \setminus P} \left( \sqrt{\frac{5}{7}} - \frac{1}{\sqrt{2}} \right) + \sum_{uv \in P} \left( \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \right) \\ &= |\mathbf{E}(G) \setminus P| \left( \sqrt{\frac{5}{7}} - \frac{1}{\sqrt{2}} \right) + |P| \left( \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \right) \\ &\geq |P| \left( \sqrt{\frac{5}{7}} - \frac{1}{\sqrt{2}} \right) + |P| \left( \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{2}} \right) > 0. \end{split}$$

## 3 Conclusion and Some Open Problems

In this paper, we established a few relations between the atom-bond connectivity (ABC) and atom-bond sum-connectivity (ABS) vertex-degreebased topological indices. In the case of graphs without pendent vertices, this relation is trivially easy (see Proposition 2.1). On the other hand, in the case of graphs possessing pendent vertices, especially for trees, this relation becomes perplexed and the complete solution of the problem awaits additional studies.

Denote the difference ABC - ABS by  $\Theta$ . By means of computer search we found that for trees with  $n \leq 15$  vertices (except in the trivial cases n = 1, 2),  $\Theta = 0$  never happens. It would be of some interest to extend this finding to higher values of n, or to discover a tree (or a graph with minimum degree 1) for which  $\Theta = 0$ .

Let  $T_n$  be the number of trees of order n, and  $t_n$  the number of trees of order n for which  $\Theta < 0$ . We know that  $t_n/T_n > 0$  for  $n \ge 11$ . It is an open problem what the value of  $\lim_{n\to\infty} t_n/T_n$  is, especially whether it is equal to zero or to unity.

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