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Notes on Trees with Minimal Atom–Bond Connectivity Index

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Abstract

If $G = (\mathbf{V}, \mathbf{E})$ is a molecular graph, and $d(u)$ is the degree of its vertex u, then the atom–bond connectivity index of G is $ABC = \sum_{uv \in \mathbf{E}} \sqrt{[d(u) + d(v) - 2]/[d(u)\,d(v)]}$. This molecular structure descriptor, introduced by Estrada et al. in the late 1990s, found recently interesting applications in the study of the thermodynamic stability of acyclic saturated hydrocarbons, and the strain energy of their cyclic congeners. In connection with this, one needs to know which trees have extremal ABC-values. Whereas it is easy to demonstrate that the star has maximal ABC, characterizing the trees with minimal ABC appears to be a much more difficult task. In this paper we determine a few structural features of the trees with minimal ABC, which brings us a step closer to the complete solution of the problem.

1. Introduction

Until few years ago, the "*atom–bond connectivity index*" (ABC) [1] was just one among the countless molecular–graph based structure descriptors put forward in the chemical literature [2–4]. Initially [1], the ABC-index was shown to be well correlated with the heats of formation of alkanes, and that it thus can serve for predicting their thermodynamic properties. In addition to this, Estrada [5] recently elaborated a novel quantum–theory–like justification for this topological index, showing that it provides a model for taking into account 1,2–, 1,3–, and 1,4-interactions in the carbon–atom skeleton of saturated hydrocarbons, and that it can be used for rationalizing steric effects in such compounds. These results triggered a number of mathematical investigations of the ABC-index [6–14].

When examining a topological index, one of the first questions that needs to be answered is for which graphs this index assumes minimal and maximal values, and what are these extremal values. Usually, one first tries to resolve this problem for trees with a fixed number (n) of vertices. In the case of the ABC-index, finding the tree for which this index is maximal was relatively easy [6]: this is the star. Eventually, also the trees with second–maximal, third–maximal, etc. ABC-index were determined [13].

On the other hand, the problem of characterizing the n-vertex tree(s) for which ABC is minimal, turned out to be much more difficult, and this task has not been completely solved until now.

It was recently shown [14] that by deleting an edge from any graph, the ABC-index decreases. This result implies that among all n-vertex graphs, the complete graph has maximal ABC-value. Further, among all connected n-vertex graphs, minimal ABC is achieved by some tree. Thus the n-vertex tree(s) with minimal ABC-index are also the n-vertex connected graphs with minimal ABC-index.

In what follows, we present the results of our computer–aided quest for trees with minimal ABC, as well as a few mathematical results determining some (but far not all) structural features that such trees must possess.

2. Definitions and notation

The (molecular) graph considered will be denoted by G, and its vertex and edge sets by $\mathbf{V}$ and $\mathbf{E}$, respectively. The number of vertices and edges of G are denoted by n and m, respectively. In the case of trees, $m = n - 1$.

If u and v are two adjacent vertices of G, then the edge connecting them will be denoted by uv.

For $u \in \mathbf{V}$, the degree of the vertex u, denoted by $d(u) = d(u|G)$, is the number of first neighbors of u in the graph G. A vertex of degree one is said to be a pendent. We will distinguish between path-type and of star-type pendent vertices. A path-type (or, shorter: p-type) pendent vertex is adjacent to a vertex of degree two. A star-type (or, shorter: s-type) pendent vertex is adjacent to a vertex of degree three or greater.

The edge whose one end-vertex is of degree one is said to be a pendent edge.

With the above specified notation, the atom–bond connectivity index of the graph G is defined as [1]:

$$ABC = ABC(G) = \sum_{uv \in \mathbf{E}} \sqrt{\frac{d(u) + d(v) - 2}{d(u)\, d(v)}} \,. \tag{1}$$

Let $1 \leq k \leq n-1$ and let $u_0, u_1, \ldots, u_{k-1}, u_k$ be some of the vertices of the graph G. We say that these vertices form a path in G if

(a) u_{i-1} is adjacent to u_i , for $i = 1, 2, \ldots, k$, and

(b) $d(u_i) = 2$ for $1 \leq i \leq k-1$, and

(c) $d(u_0) \geq 3$ and $d(u_k) \neq 2$.

The length of this path is k.

If $d(u_k) \geq 3$, then $u_0, u_1, \ldots, n_{k-1} u_k$ form an *internal path* in the graph G. If, in turn, $d(u_k) = 1$, then $u_0, u_1, \ldots, u_{k-1}, u_k$ form a *pendent path* in the graph G. In addition, if $k = 2$ and $d(u_k) = 1$, we will say that the vertices u_1, u_2 form a 2-branch of the graph G.

3. Trees with up to 30 vertices with minimal ABC-index

In this section we outline the results obtained by an extensive computer quest for trees possessing minimal ABC index. Namely, we determined these trees among all trees up to 30 vertices. Table 1 shows the number of n-vertex trees considered in this in-silico experiment.

n	number of trees	n	number of trees
7	11	19	317955
8	23	20	823065
9	47	21	2144505
10	106	22	5623756
11	235	23	14828074
12	551	24	39299897
13	1301	25	104636890
14	3159	26	279793450
15	7741	27	751065460
16	19320	28	2023443032
17	48629	29	5469566585
18	123867	30	14830871802

Table 1

In Table 2 are depicted the trees having minimal ABC-index among trees with given number n of vertices, $n \in [7, 30]$. For $n \in [4, 6]$, the unique n-vertex tree with minimal ABC-index is the path P_n .

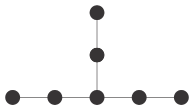
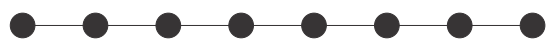
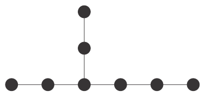
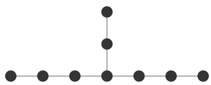
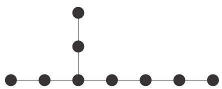
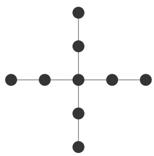
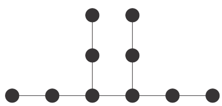
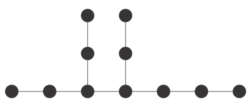
# vertices	Trees with minimal ABC index
7	 
8	 
9	   
10	
11	

Table 2 continues on the next page

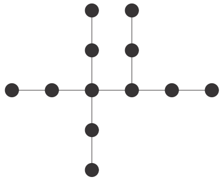
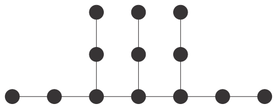
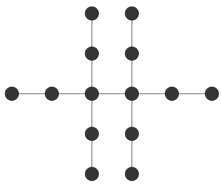
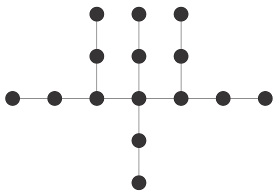
# vertices	Trees with minimal ABC index
12	
13	
14	
15	

Table 2 continues on the next page

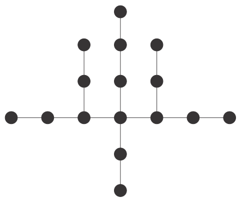
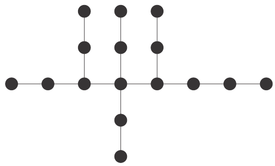
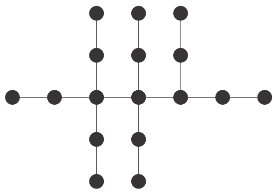
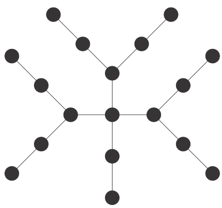
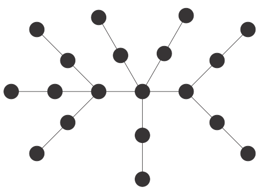
# vertices	Trees with minimal ABC index
16	 
17	
18	
19	

Table 2 continues on the next page

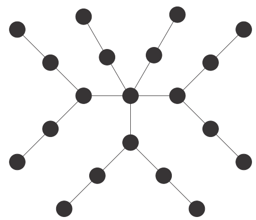
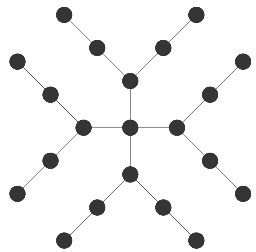
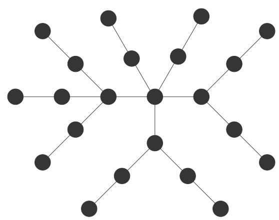
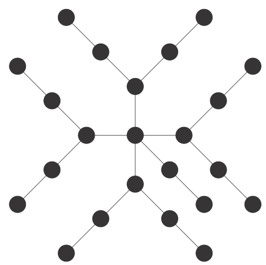
# vertices	Trees with minimal ABC index
20	
21	
22	
23	

Table 2 continues on the next page

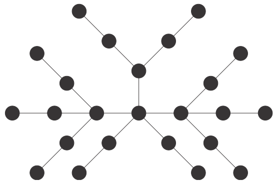
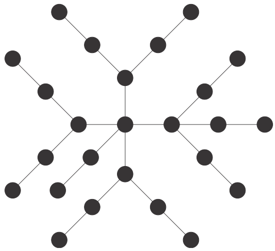
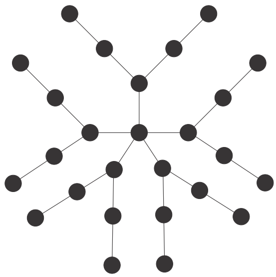
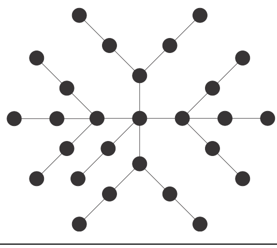
# vertices	Trees with minimal ABC index
24	
25	
26	
27	

Table 2 continues on the next page

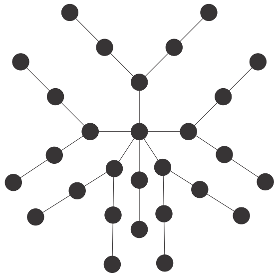
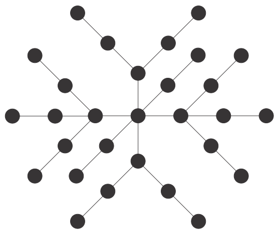
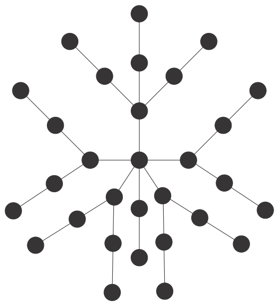
# vertices	Trees with minimal ABC index
28	
29	
30	

Table 2

Based on the data shown in Table 2, the following observations could be deduced:

Observation 1. The n-vertex tree with minimal ABC-index needs not be unique.

Observation 2. For $n \leq 9$ the n-vertex tree (or one of the n-vertex trees) with minimal ABC is the path P_n. For $n \geq 10$ this cannot happen, because it is always possible to construct trees T with $ABC(T) < ABC(P_n)$.

4. Some structural features of trees with minimal ABC-index

The main result of our paper, in addition to the findings of the computer search shown in Table 2, are the following three claims. These shed some light on the structure of the minimal trees, but do not fully characterize their structure. However, the general validity of the below claims could be verified by means of the proofs, given in Section 6.

Proposition 3. If $n \geq 10$, then the n-vertex tree with minimal ABC-index does not contain internal paths of length $k \geq 2$.

Proposition 4. If $n \geq 10$, then the n-vertex tree with minimal ABC-index does not contain pendent paths of length $k \geq 4$.

Proposition 5. If $n \geq 10$, then the n-vertex tree with minimal ABC-index contains at most one pendent path of length $k = 3$.

In order to demonstrate the validity of the above claims, we need some preparation.

5. Preparations: Properties of $[\mathbf{d(u) + d(v) - 2}]/[\mathbf{d(u)\, d(v)}]$

As seen from Eq. (1), the ABC index is equal to the sum over all pairs of adjacent vertices u and v of the increment

$$Q = Q(u,v) = Q(u,v|G) = \sqrt{\frac{d(u)+d(v)-2}{d(u)\,d(v)}}\ .$$

Thus, Q is the contribution to the ABC-value, coming from the edge uv. It is therefore purposeful to establish some properties of this increment.

In what follows, without loss of generality we assume that $d(u) \leq d(v)$. For the sake of simplicity, we write $d(u) = d$ and $d(v) = d + h$

By elementary calculation we establish the following [6]:

Lemma 6.

(a) If $d(u) = 1$, then $Q(u,v) = \sqrt{h/(h+1)}$. Thus, $Q(u,v)$ is a monotonically increasing function of h. Its limit value, for $h \to \infty$, is equal to unity. This means that the value of the increment of a pendent edge belongs to the interval $[\sqrt{1/2}, 1)$, and its minimal value is when u is of p-type (i. e., if $d(v) = 2$).

(b) If $d(u) = 2$, then independently of the value of $d(v)$, $Q(u,v) = \sqrt{1/2}$.

(c) If $d(u) \geq 3$, then

$$Q(u,v) = \sqrt{\frac{2d+h-2}{d(d+h)}}. \tag{2}$$

Considered as a function of the variable h, the expression on the right–hand side of (2) monotonically decreases. Thus its maximal value is $\sqrt{4/9}$, attained in the case $d = 3, h = 0$, i. e., $d(u) = d(v) = 3$. Considered as a function of the variable d, the expression on the right–hand side of (2) is also monotonically decreasing. It is important to note that if $d(u), d(v) \geq 3$, then Q is always less than $\sqrt{1/2}$.

From Lemma 6(b) we get the following noteworthy:

Lemma 7. If an end-vertex of any edge of a graph G is of degree two, then irrespective of any other structural detail, $ABC(G) = m/\sqrt{2}$. If an end-vertex of any edge of a tree T is of degree two, then irrespective of any other structural detail, $ABC(T) = (n-1)/\sqrt{2}$.

From Lemma 6(a) and (c) we see that a tree with minimal value of ABC should possess (α) as few as possible pendent vertices of s-type, (β) as many as possible mutually adjacent vertices of degree greater than two, and (γ) the latter vertices should have degrees as large as possible. The problem of determining the structure of such extremal trees is that the requirements (α), (β), and (γ) contradict to each other, i. e., cannot all three be fully satisfied in the same time.

In the subsequent section, we use Lemma 6 to establish some structural features of the trees with minimal ABC-index.

6. Proofs

In what follows all trees considered are supposed to possess n vertices, and $n \geq 10$. Recall that trees necessarily possess at least two pendent vertices.

Proof of Proposition 3. Suppose that T is a tree, possessing an internal path $u_0, u_1, \ldots, u_k$ of length $k \geq 2$. Thus, u_0 and u_k are the terminal vertices of this internal path, which means that $d(u_0), d(u_k) \geq 3$. Further, let r be a pendent vertex of T, adjacent to the vertex s.

Construct the tree T' by moving the vertex u_{k-1} on the edge rs, and connecting u_{k-2} with u_k. Then T' has an internal path of length $k-1$.

Consider first the case $k > 2$. Then $d(u_{k-2}|T) = 2$ and the transformation $T \to T'$

causes the following change of the ABC-index.

$$\begin{aligned} ABC(T) - ABC(T') &= [Q(u_{k-2}, u_{k-1}|T) + Q(u_{k-1}, u_k|T) + Q(r, s|T)] \\ &- [Q(u_{k-2}, u_k|T') + Q(r, u_{k-1}|T') + Q(s, u_{k-1}|T')] \\ &= \left[\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{d(s|T) - 1}{d(s|T)}}\right] - \left[\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}}\right]. \end{aligned}$$

We see that if r is a pendent vertex of s-type, then $\sqrt{[d(s|T) - 1]/d(s|T)} > \sqrt{1/2}$ and therefore $ABC(T) > ABC(T')$. If r is of p-type, then $\sqrt{[d(s|T) - 1]/d(s|T)} = \sqrt{1/2}$ and $ABC(T) = ABC(T')$. In both cases, the transformation $T \to T'$ either diminishes ABC or leaves it same.

Remains the case $k = 2$. Repeating the above described transformation of the tree T sufficient number of times, we arrive at the tree T_1 in which the vertices u_0, u_1, u_k form an internal path of length 2. Let r^* be a pendent vertex of T_1, adjacent to the vertex s^*.

Construct the tree T_1' by moving the vertex u_1 on the edge r^*s^*, and connecting u_0 with u_k. By this the entire internal path of T has been eliminated. The transformation $T_1 \to T_1'$ causes the following change of the ABC-index:

$$\begin{aligned} ABC(T_1) - ABC(T_1') &= [Q(u_0, u_1|T_1) + Q(u_1, u_k|T_1) + Q(r^*, s^*|T_1)] \\ &- [Q(u_0, u_k|T_1') + Q(r^*, u_1|T_1') + Q(s^*, x_1|T_1')] \\ &= \left[\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{d(s^*) - 1}{d(s^*)}}\right] \\ &- \left[\sqrt{\frac{d(u_0|T) + d(u_k|T) - 2}{d(u_0|T)\, d(u_k|T)}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}}\right]. \end{aligned}$$

Now, as explained in the preceding section,

$$\sqrt{\frac{d(s^*) - 1}{d(s^*)}} \geq \sqrt{\frac{1}{2}} \qquad \text{and} \qquad \sqrt{\frac{d(u_0|T) + d(u_k|T) - 2}{d(u_0|T)\, d(u_k|T)}} \leq \sqrt{\frac{4}{9}} < \sqrt{\frac{1}{2}}\,.$$

Therefore $ABC(T_1')$ is strictly smaller than $ABC(T_1)$ and therefore strictly smaller than $ABC(T)$.

In the step–by–step transformation $T \to T_1'$ the vertices of an internal path were moved into pendent paths, by which the value of ABC strictly diminished. If the tree T has several internal paths, we continue the transformation, until a tree without internal paths is obtained, whose ABC-index is smaller than $ABC(T)$.

Therefore a tree with internal paths of length $k \geq 2$ cannot have minimal ABC index. This completes the proof of Proposition 3. ■

Corollary 8. If T is a tree with minimal ABC-index, then the subgraph induced by the vertices of degree greater than two, is connected (and thus is a tree itself).

In order to deduce Proposition 4, we first need two auxiliary results.

Lemma 9. If T is a tree with star-type pendent vertices and a pendent path of length ≥ 3, then there is either a tree T' without star-type pendent vertices, such that $ABC(T') < ABC(T)$ or there is a tree T'' without pendent paths of length ≥ 3, such that $ABC(T'') < ABC(T)$.

Proof. Suppose that T has a pendent path $u_0, u_1, u_2, \ldots, u_{k-1}, u_k$, $k \geq 3$, and a pendent vertex x of s-type, connected to the vertex y. Construct the tree T_1 by inserting u_{k-1} on the edge xy and by connecting u_{k-2} and u_k. By this the ABC index is changed as:

$$\begin{aligned} ABC(T) - ABC(T_1) &= [Q(u_{k-2}, u_{k-1}|T) + Q(u_{k-1}, u_k|T) + Qx, y|T] \\ &- [Q(u_{k-2}, u_k|T_1) + Q(x, u_{k-1}|T_1) + Q(u_{k-1}, y|T_1)] \\ &= \left[\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{d(y|T)-1}{d(y|T)}}\right] - \left[\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}}\right] \end{aligned}$$

which by Lemma 6(a) is evidently positive–valued. Thus, $ABC(T_1) < ABC(T)$.

By continuing the above described transformation, we shall either eliminate all s-type pendent vertices, arriving at the tree T', or will eliminate all pendent paths of length greater than two, arriving at the tree T''. ■

Lemma 10. If T is a tree without star-type pendent vertices, then there is a tree T' without star-type pendent vertices and without pendent paths of length ≥ 4, such that $ABC(T') < ABC(T)$.

Proof. Suppose that T has a pendent path $u_0, u_1, u_2, \ldots, u_{k-2}, u_{k-1}, u_k$ of length $k \geq 4$. Let r be a vertex of T (not necessarily different from u_0) with maximal degree. Construct the tree T_1 by attaching the vertices u_{k-2} and u_{k-1} to the vertex r, to form a 2-branch, and by connecting the vertices u_{k-3} and u_k. Then,

$$
\begin{aligned}
& ABC(T) - ABC(T_1) \\
= & \left[Q(u_{k-3}, u_{k-2}|T) + Q(u_{k-2}, u_{k-1}|T) + Q(u_{k-1}, u_k|T) + \sum_{r'} Q(r, r'|T) \right] \\
- & \left[Q(u_{k-3}, u_k|T_1) + Q(r, u_{k-2}|T_1) + Q(u_{k-2}, u_{k-1}|T_1) + \sum_{r'} Q(r, r'|T_1) \right] \\
= & \left[\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}} + \sum_{r'} Q(r, r'|T) \right] - \left[\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}} + \sum_{r'} Q(r, r'|T_1) \right] \\
= & \sum_{r'} \left[Q(r, r'|T) - Q(r, r'|T_1) \right]
\end{aligned}
$$

where $\sum\limits_{r'}$ indicates summation over the edges of T whose one end-vertex is r. Since r was chosen to be a vertex with maximal degree, $d(r'|T) \leq d(r|T)$ holds for all vertices r'. Since $d(r|T_1) = d(r|T) + 1$, by Lemma 6(c), the condition $Q(r, r'|T) > Q(r, r'|T_1)$ is satisfied for all r'. Consequently, $\sum\limits_{r'} [Q(r, r'|T) - Q(r, r'|T_1)] > 0$ and therefore $ABC(T') < ABC(T)$.

By repeated application of the above construction we may diminish the lengths of all pendent paths to 2 or 3, introducing a number of new 2-branches. ■

Proof of Proposition 4. Combine Lemmas 9 and 10. ■

Proof of Proposition 5. Suppose that the tree T has no s-type pendent vertices and has two pendent paths of length 3, namely u_0, u_1, u_2, u_3 and v_0, v_1, v_2, v_3. Then by Lemma 6(b), the tree T_1 possessing pendent paths u_0, u_1, u_3 and v_0, v_1, v_2, u_2, v_3 has same ABC index as T. But then Lemma 10 is applicable to T_1, resulting in a tree T' in which the pendent path v_0, v_1, v_2, u_2, v_3 is replaced by two 2-branches. Then $ABC(T') < ABC(T)$. ■

7. Discussion and concluding remarks

Propositions 3-5 provide only a minor step towards the elucidation of the general form of trees with minimal ABC-index. From the structure of such trees with $n \leq 30$, established by a computer–aided search and depicted in a previous section, it is difficult to guess how this general structure might look. However, one detail is evident: all pendent vertices are of path-type.

All our efforts to prove that trees with minimal ABC-index cannot possess star-type pendent vertices were not successful, and this remains a task for the future. Anyway, we believe that the following hypothesis is generally valid:

Conjecture 11. If $n \geq 10$, then each pendent vertex of the n-vertex tree with minimal ABC-index belongs to a pendent path of length k , $2 \leq k \leq 3$.

Concluding this article, we mention one more result that pertains to star-type pendent vertices.

Proposition 12. If a tree T with minimal ABC-index possesses a star-type pendent vertex attached to the vertex r, then pendent paths of length k , $2 \leq k \leq 3$, cannot exist on any vertex of T, whose degree is smaller than the degree of r.

Proof. Let the s-type pendent vertex of T be s. Suppose that contrary to the claim of Proposition 12, T has a 2-path y, u, x, such that $d(x) = 1$, $d(u) = 2$ and $d(r) > d(y) \geq 3$. Then we can construct a tree T' by inserting the vertex u on the edge rs, and by connecting the vertices x and y. The tree T' has smaller ABC-index than T. Indeed,

$$\begin{aligned}
ABC(T) - ABC(T') &= [Q(x,u|T) + Q(u,y|T) + Q(r,s|T)] \\
&- [Q(x,y|T') + Q(r,u|T') + Q(u,s|T')] \\
&= \left[\sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{d(r)-1}{d(r)}}\right] - \left[\sqrt{\frac{d(y)-1}{d(y)}} + \sqrt{\frac{1}{2}} + \sqrt{\frac{1}{2}}\right] \\
&= \sqrt{\frac{d(r)-1}{d(r)}} - \sqrt{\frac{d(y)-1}{d(y)}}
\end{aligned}$$

which is positive–valued sice $d(r) > d(y)$. Therefore, $ABC(T') < ABC(T)$. Therefore, T cannot be the tree with smallest ABC-index.

By this, Proposition 12 is proven for the case $k = 2$. The proof for $k = 3$ is fully analogous. ■

We end the article with one more conjecture, whose validity seems to be less certain than that of Conjecture 11.

Conjecture 13. If $n \geq 17$, then the n-vertex tree with minimal ABC-index is unique.

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