

Kragujevac Trees with Minimal Atom–Bond Connectivity Index

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Abstract

In the class of *Kragujevac trees*, the elements having minimal atom–bond connectivity index are determined. By this, an earlier conjecture [*MATCH Commun. Math. Comput. Chem.* **68** (2012) 131–136] is confirmed and slightly corrected.

1 Introduction

The atom–bond connectivity (*ABC*) index is a molecular–graph based structure descriptor, invented by Estrada in the 1990s [2]. Initially, it attracted little attention in mathematical chemistry, but after the publication of Estrada’s second paper [3], the situation has dramatically changed. Nowadays, the chemical applicability of the *ABC* index is reasonably well documented [2–5], and its mathematical properties are studied in due detail.

Let G be a simple graph on n vertices, and let its vertex set be $V(G)$ and edge set $E(G)$. By uv we denote the edge connecting the vertices u and v . The degree of a vertex v is denoted by d_v .

A vertex of degree one is referred to as a *pendent vertex*. An edge whose one end-vertex is pendent is referred to as a *pendent edge*. It is worth noting that in minimal-*ABC* trees all pendent edges connect a pendent vertex with a vertex of degree two [11].

The atom–bond connectivity index of the graph G is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \quad (1)$$

When the mathematical properties of a graph–based structure descriptor are investigated, one of the first questions is for which trees (with a given order n) is this descriptor minimal and maximal. In the case of the *ABC* index it was easily demonstrated [6] that the maximal-*ABC* tree is the star. On the other hand, the other – seemingly equally easy – problem of characterizing the minimal-*ABC* tree has appeared to be a much harder nut to crack. In spite of numerous efforts [1, 7–12] this problem is still unsolved; for review see [13].

In order to possibly envisage the structure of minimal-*ABC* trees, extensive numerical studies have been undertaken [1, 7, 8]. Within these studies, a class of trees emerged, that was believed to contain the minimal-*ABC* tree. Eventually, a conjecture on the actual structure of the minimal-*ABC* tree was formulated [1] (see below). Later studies [9, 10] revealed that the conjecture was false, and that the true structure of the minimal-*ABC* tree is more complex than the computer–aided studies indicated.

The trees that were considered as candidates for having minimal *ABS*-value, have an interesting structure and are worth of further investigation. Since all the researches [1, 7, 8] were done at the University of Kragujevac, we propose that these trees be named *Kragujevac trees* or, if pronunciation is difficult, *Krag trees*. These are defined as follows.

Let $B_1, B_2, B_3, \dots$ be branches whose structure is depicted in Fig. 1.

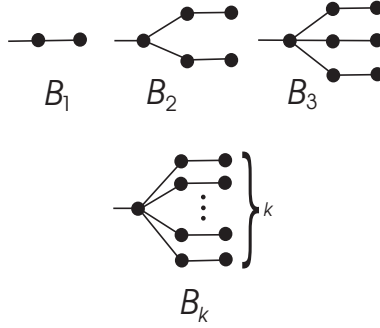


Fig. 1. The branches of proper Kragujevac trees.

Definition 1. A proper Kragujevac tree is a tree possessing a central vertex of degree at least 3, to which branches of the form B_1 and/or B_2 and/or B_3 and/or $\dots$ are attached. The set of all proper Kragujevac trees of order n will be denoted by $\mathbf{Kg}_n$.

Definition 2. An improper Kragujevac tree is a tree obtained by inserting a new vertex (of degree 2) on a pendent edge of a proper Kragujevac tree. The set of all improper Kragujevac trees of order n will be denoted by $\mathbf{Kg}_n^*$.

In the subsequent section we show that the value of the ABC index of an improper Kragujevac tree does not depend on the position of the inserted degree-two vertex (cf. Lemma 5). In view of this, we will assume that this vertex is inserted into a B_3 branch, and such a branch (with 8 vertices) will be denoted by B_3^* , see Fig. 2.

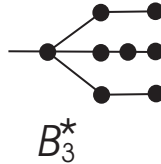


Fig. 2. A branch of improper Kragujevac trees.

In the work [1] the computer-aided search for minimal- ABC tree was (implicitly) restricted to Kragujevac trees. The results obtained there could this be understood as a conjecture on minimal- ABC (proper and improper) Kragujevac trees. Assuming

that n is sufficiently large (which values are specified in [1]), this modulo 7 conjecture reads as follows:

Conjecture 3. *Let $T_{\min}$ be the minimal-ABC index tree in the set $\mathbf{Kg}_n \cup \mathbf{Kg}_n^*$.*

- (a) *If $n \equiv 0 \pmod{7}$, then $T_{\min}$ possesses three B_4 -branches, whereas all other branches are of B_3 -type.*
- (b) *If $n \equiv 1 \pmod{7}$, then all branches of $T_{\min}$ are of B_3 -type.*
- (c) *If $n \equiv 2 \pmod{7}$, then $T_{\min}$ possesses a single B_3^* -branch, whereas all other branches are of B_3 -type.*
- (d) *If $n \equiv 3 \pmod{7}$, then $T_{\min}$ possesses a single B_4 -branch, whereas all other branches are of B_3 -type.*
- (e) *If $n \equiv 4 \pmod{7}$, then $T_{\min}$ possesses two B_2 -branches, whereas all other branches are of B_3 -type.*
- (f) *If $n \equiv 5 \pmod{7}$, then $T_{\min}$ possesses two B_4 -branches, whereas all other branches are of B_3 -type.*
- (g) *If $n \equiv 6 \pmod{7}$, then $T_{\min}$ possesses a single B_2 -branch, whereas all other branches are of B_3 -type.*

In this paper we provide a mathematical proof of the above conjecture for $n \equiv k \pmod{7}$, $k = 0, 1, 3, 5, 6$, and show how it needs to be amended for $n \equiv k \pmod{7}$, $k = 2, 4$. To do this we need some preparations.

2 Preparatory considerations

Bearing in mind Eq. (1), define the function f as

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

Evidently, $f(x, y) = f(y, x)$. In addition, if $x = 2$ then irrespective of the value of the variable y ,

$$f(x, y) = \frac{1}{\sqrt{2}}. \quad (3)$$

This observation implies the following auxiliary results:

Lemma 4. [8] *If at least one end-vertex of every edge of a tree T is of degree two, then irrespective of any other structural detail of this tree, $ABC(T) = (n - 1)/\sqrt{2}$.*

Lemma 5. *Let $X \in \mathbf{Kg}_{n-1}$ and let the Kragujevac tree $Y \in \mathbf{Kg}_n^*$ be obtained by inserting a new vertex (of degree two) on a pendent edge of X . Then $ABC(Y) = ABC(X) + 1/\sqrt{2}$. Consequently, the ABC index of an improper Kragujevac tree is independent of the actual position of the inserted vertex.*

In what follows, the degree of the central vertex of a Kragujevac tree will be denoted by m . (Recall that by Definition 1, $m \geq 3$). Some branches attached to a Kragujevac tree will not be directly involved in our considerations. In order to reduce the amount of computation (which anyway is complicated) we proceed as follows.

The degrees of vertices attached to the central vertex, which are not involved in our computations will be denoted by $p_1, p_2, \dots, p_i, \dots$. These vertices, as well as the branches to which they belong will not be presented in the diagrams that follow. To make this point clear, look at Fig. 3.

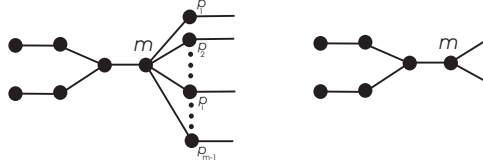


Fig. 3. An example showing how some structural details of a Kragujevac tree (left), irrelevant for the present considerations, are represented by a simplified diagram (right); for details see text.

3 Main results

Theorem 6. *A minimal-ABC Kragujevac tree does not contain branches B_h with $h > 5$.*

Proof. Let X be a Kragujevac tree containing a branch B_h , $h > 5$ (that is, let the parameter k in Fig. 4 be greater than 6). Let Y be the tree obtained from X as indicated in Fig. 4. Recall that the structure of the branch B_3^* is depicted in Fig. 2. We show that $ABC(X) > ABC(Y)$.

Consider the difference $\Delta = ABC(X) - ABC(Y)$. We need to demonstrate that $\Delta > 0$.

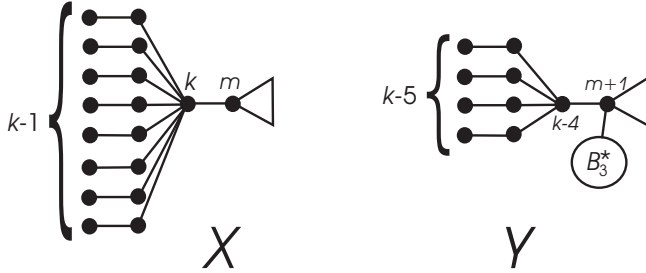


Fig. 4. The trees used in the proof of Theorem 6.

From the definition of the ABC index, bearing in mind Eq. (2), Fig. 3, and the structure of the trees X and Y shown in Fig. 4, we obtain:

$$\begin{aligned} \Delta &= \left[\sum_{i=1}^{m-1} f(m, p_i) + f(m, k) + (k-1)f(k, 2) + (k-1)f(2, 1) \right] \\ &- \left[\sum_{i=1}^{m-1} f(m+1, p_i) + f(m+1, k-4) + (k-5)f(k-4, 2) \right. \\ &\quad \left. + (k-5)f(2, 1) + f(m+1, 4) + 3f(4, 2) + f(2, 2) + 3f(2, 1) \right] \end{aligned}$$

which in view of Eq. (3) yields

$$\Delta = \sum_{i=1}^{m-1} [f(m, p_i) - f(m+1, p_i)] + f(m, k) - f(m+1, k-4) + f(2, 1) - f(m+1, 4). \quad (4)$$

The right-hand side of the above expression is increasing with respect to p_i (which has been proven in [12]). In view of this, we may set $p_i = 2$ (the lowest value) to construct the worst case. Then Eq. (4) is simplified as

$$\Delta = f(m, k) - f(m+1, k-4) + f(2, 1) - f(m+1, 4) \quad (5)$$

It is known [12] that $f(x, y) - f(x-1, y)$ strictly decreases with respect to $y \geq 1$ and strictly increases with respect to x for fixed $y \geq 2$. Bearing this in mind, we rewrite Eq. (5) as

$$\begin{aligned} \Delta &= [f(m, k) - f(m+1, k)] + [f(m+1, k) - f(m+1, k-1)] \\ &+ [f(m+1, k-1) - f(m+1, k-2)] + [f(m+1, k-2) - f(m+1, k-3)] \end{aligned}$$

$$+ [f(m+1, k-3) - f(m+1, k-4)] + f(2, 1) - f(m+1, 4) .$$

It is easy to see that Δ increases as k increases. So, we should select the lowest value of k to have the worst case. As claimed in the theorem, we have to show that if $h \geq 6$ i.e., $k \geq 7$, then the tree X is not minimal. Noting that for $k \leq 6$, Δ in Eq. (5) is negative-valued, we put $k = 7$. This yields

$$\Delta = \sqrt{\frac{m+5}{7m}} + \frac{1}{\sqrt{2}} - \sqrt{\frac{m+2}{3(m+1)}} - \sqrt{\frac{m+3}{4(m+1)}} \quad (6)$$

By means of a mathematical software like MATLAB, it can be checked that the right-hand side of Eq. (6) is increasing with respect to $m \geq 3$ and is positive-valued for $m = 3$. Therefore, $\Delta > 0$ and we have shown that the transformation $X \rightarrow Y$ decreases ABC .

If X is a proper Kragujevac tree, then Y is an improper Kragujevac tree and we are done. If, however, X is an improper Kragujevac tree, then according to Definition 2, Y is not a Kragujevac tree, since it possesses two pendent paths of length 3. If so, then by a result from [8], the tree Y can be transformed into another three Y' , replacing the two pendent paths of length 3 by three pendent paths of length 2, which makes Y' a proper Kragujevac tree. For instance, if Y possess two B_3^* -branches, then Y' is obtained by replacing then by a B_3 -branch and a B_4 -branch.

As shown in [6], $ABC(Y') < ABC(Y)$, and, then $ABC(Y') < ABC(X)$. In other words, if there is a Kragujevac tree with a B_h -branch, $h > 5$, then one can construct another Kragujevac tree (of the same order) without such a B_h -branch, and with smaller ABC -index.

The proof of Theorem 6 is thus completed. $\square$

Theorem 7. *A minimal-ABC Kragujevac tree does not contain B_5 -branches.*

Proof. We show that is there is a B_5 -branch in a Kragujevac tree, then another Kragujevac tree can be constructed, having smaller ABC -value. We have to distinguish between five cases.

Case 1. Let $X \in \mathbf{Kg}_n \cup \mathbf{Kg}_n^*$, and X has two B_5 -branches, see Fig. 5. Then a tree Y of order n can be constructed, also depicted in Fig. 5, such that $ABC(Y) < ABC(X)$.

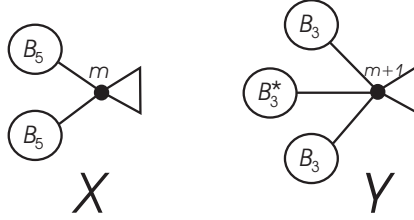


Fig. 5. The trees considered in Case 1 of the proof of Theorem 7.

Indeed, $\Delta = ABC(X) - ABC(Y)$ can be calculated in an analogous manner as in the proof of Theorem 6. Then, by setting $p_i = 2$ (pertaining to the lowest value of Δ), we get

$$\Delta = 2f(m, 6) + f(2, 1) - 3f(m + 1, 4)$$

which is positive-valued for $m \geq 3$, implying $ABC(Y) < ABC(X)$.

If $X \in \mathbf{Kg}_n$, then $Y \in \mathbf{Kg}_n^*$ and we are done. If, however, $X \in \mathbf{Kg}_n^*$, then Y has two pendent paths of length 3 and is thus not a Kragujevac tree. Then, as explained in the proof of Theorem 6, a tree Y' can be constructed, such that $Y' \in \mathbf{Kg}_n$ and $ABC(Y') < ABC(Y) < ABC(X)$.

Case 2. Let $X \in \mathbf{Kg}_n \cup \mathbf{Kg}_n^*$, and X has a B_5 -branch and a B_3 -branch, see Fig. 6. Then a tree Y of order n can be constructed, also depicted in Fig. 6, such that $ABC(Y) < ABC(X)$.

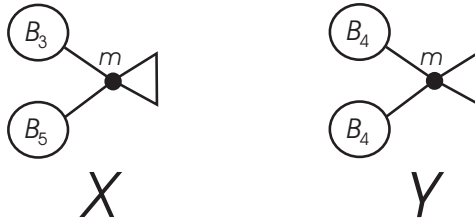


Fig. 6. The trees considered in Case 2 of the proof of Theorem 7.

An argument analogous to what was used in Case 1 yields,

$$\Delta = f(m, 6) + f(m, 4) - 2f(m, 5) > 0$$

and $\Delta > 0$ for all $m \geq 3$. This time Y is necessarily a Kragujevac tree.

Cases 3 & 4, namely when X has, respectively, a B_5 -branch and a B_2 -branch, and a B_5 -branch and a B_1 -branch, are fully analogous. The details of the transformation $X \rightarrow Y$ are seen from Figs. 7 and 8.

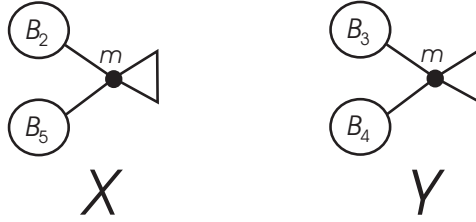


Fig. 7. The trees considered in Case 3 of the proof of Theorem 7.

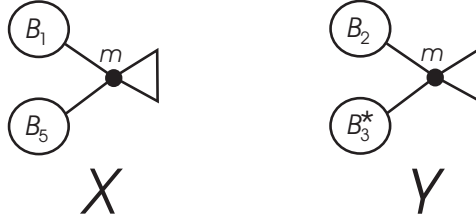


Fig. 8. The trees considered in Case 4 of the proof of Theorem 7.

Case 5. From Cases 1-4 we see that the minimal- ABC Kragujevac tree could only possess a single B_5 -branch and additional B_4 -branches. Because $m \geq 3$, there must be at least two B_4 -branches. Then the transformation $X \rightarrow Y$, indicated in Fig. 9, could be applied, resulting in a Kragujevac tree (either Y or Y') without a B_5 -branch and with ABC -value lower than $ABC(X)$.

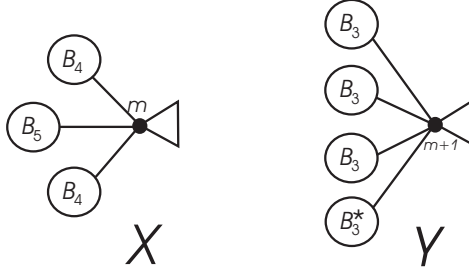


Fig. 9. The trees considered in Case 5 of the proof of Theorem 7.

The proof of Theorem 7 is thus completed. $\square$

Theorem 8. *A minimal-ABC Kragujevac tree has at most five B_4 -branches.*

Proof. Consider the trees X and Y depicted in Fig. 10. In the worst case, when all $p_i = 2$, we get

$$\Delta = 6f(m, 5) + 2f(2, 1) - 7f(m + 2, 4) - f(m + 2, 3)$$

which is positive-valued for all $m \geq 3$. $\square$

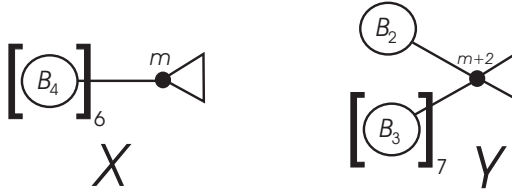


Fig. 10. The trees used in the proof of Theorem 8.

Theorem 9. *In minimal-ABC Kragujevac trees, B_2 - and B_4 -branches cannot simultaneously occur.*

Proof. Consider the trees X and Y depicted in Fig. 11. Then

$$\Delta = f(m, 5) + f(m, 3) - 2f(m, 4)$$

which is positive-valued for all $m \geq 3$. $\square$

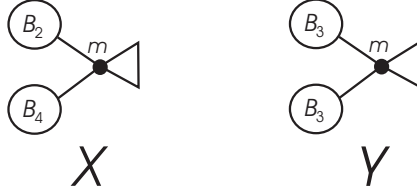


Fig. 11. The trees used in the proof of Theorem 9.

Theorem 10. *If $m \geq 25$, then in minimal-ABC Kragujevac trees, there are at most two B_2 -branches.*

Proof. Consider the trees X and Y depicted in Fig. 12. Then

$$\Delta = \sum_{i=1}^{m-3} [f(m, p_i) - f(m-1, p_i)] + 3f(m, 3) - 2f(m-1, 4) - f(2, 1)$$

The value of Δ is decreasing with respect to p_i . Therefore, since we intend to show that $\Delta > 0$, we have to examine the case when Δ is minimal. For this, we choose p_i as large as possible. Based on Theorems 6, 7, and 9, we have $p_i \leq 4$. Setting $p_i = 4$, by direct calculation we show that $\Delta > 0$ if $m \geq 25$.

The case when $X \in \mathbf{Kg}_n^*$ and therefore $Y \notin \mathbf{Kg}_n \cup \mathbf{Kg}_n^*$, is treated in the same way as in Theorem 6. $\square$

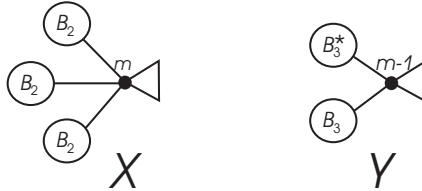


Fig. 12. The trees used in the proof of Theorem 10.

Theorem 11. *If $m \geq 19$, then in minimal-ABC Kragujevac trees, there are no B_1 -branches.*

Proof. In the previous theorems we have already shown that in minimal- ABC Kragujevac trees only branches B_i , $i = 1, 2, 3, 4$ may occur. Therefore, in order that also B_1 -branches must be absent, we have to separately consider four cases.

Case 1: B_1 - and B_2 -branches are simultaneously present. Then by the transformation $X \rightarrow Y$, indicated in Fig. 13, a Kragujevac tree Y without B_1 -branch is obtained, having smaller ABC index than X . For this transformation, choosing the worst case $p_i = 4$, we get

$$\Delta = f(m, 3) + (m - 2)f(m, 4) - (m - 1)f(m - 1, 4)$$

which is positive-valued if $m \geq 9$.

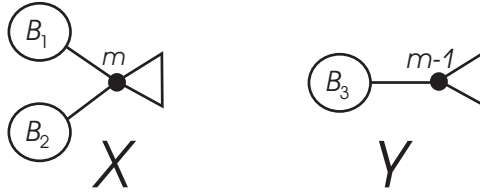


Fig. 13. The trees considered in Case 1 of the proof of Theorem 11.

Case 2: B_1 - and B_3 -branches are simultaneously present. Then the transformation $X \rightarrow Y$, indicated in Fig. 14 is applicable, which for the worst case $p_i = 5$ yields

$$\Delta = f(m, 4) + (m - 2)f(m, 5) - (m - 1)f(m, 5)$$

which is positive-valued if $m \geq 15$.

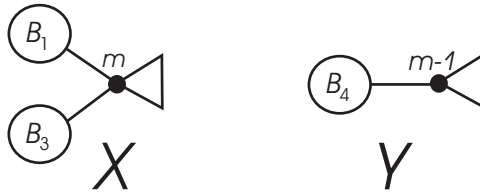


Fig. 14. The trees considered in Case 2 of the proof of Theorem 11.

Case 3: B_1 - and B_4 -branches are simultaneously present. Then the transformation $X \rightarrow Y$, indicated in Fig. 15 is applicable, which for the worst case $p_i = 5$ yields

$$\Delta = (m-1)f(m, 5) - (m-2)f(m, 5) - f(m-1, 6)$$

which is positive-valued if $m \geq 19$.

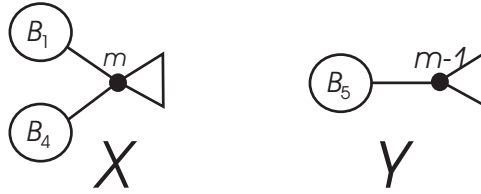


Fig. 15. The trees considered in Case 3 of the proof of Theorem 11.

Case 4: All branches are of B_1 -type. Let X be such a Kragujevac tree. All edges of X are incident to a vertex of degree two. Then by Lemma 4, the $ABC(X)$ is equal to the ABC index of the path with equal number of vertices. It is known [8] that paths of order greater than 9 are not minimal- ABC trees. Therefore, also Case 4 is impossible, and Theorem 11 follows. $\square$

Theorem 12. *If a minimal- ABC Kragujevac tree possesses a B_3^* -branch, then (a) it does not possess B_2 -branches, and (b) it has at most one B_4 -branch.*

Proof. (a) Consider a Kragujevac tree X possessing a B_2 - and a B_3^* -branch. If the order of X is sufficiently large, then X will possess more than three B_3 -branches. Then by the transformation $X \rightarrow Y$, see Fig. 16, the ABC index will be diminished. Calculation analogous to what was used in the proofs of previous theorems, shown that $ABC(Y) < ABC(X)$ will happen if $m \geq 25$.

(b) Perform the transformation $X \rightarrow Y$, indicated in Fig. 17. $\square$

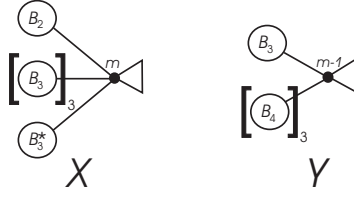


Fig. 16. The trees used in the proof of part (a) of Theorem 12.

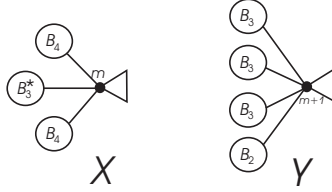


Fig. 17. The trees used in the proof of part (b) of Theorem 12.

By means of Theorems 6–12 it was shown that most combinations of branches B_i , $i = 1, 2, 3, \dots$ must not occur in minimal- ABC Kragujevac trees. Only 10 combinations remain, depicted in Fig. 18.

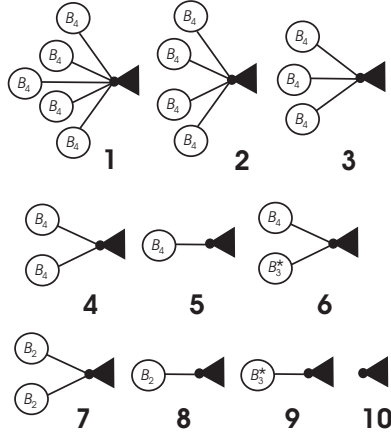


Fig. 18. Types of Kragujevac trees not eliminated by means of Theorems 6–12. The black triangles indicate an arbitrary number of B_3 -branches attached to the central vertex.

4 Verifying and amending Conjecture 3

A B_3 -branch has 7 vertices. Therefore, all trees of a given type, as depicted in Fig. 18, have number of vertices (n) congruent modulo 7.

The only trees from Fig. 18 for which $n \equiv 0 \pmod{7}$ are those of type **3**. By this, Conjecture 3(a) is confirmed.

The only trees from Fig. 18 for which $n \equiv 1 \pmod{7}$ are those of type **10**. By this, Conjecture 3(b) is confirmed.

The only trees from Fig. 18 for which $n \equiv 3 \pmod{7}$ are those of type **5**. By this, Conjecture 3(d) is confirmed.

The only trees from Fig. 18 for which $n \equiv 5 \pmod{7}$ are those of type **4**. By this, Conjecture 3(f) is confirmed.

The only trees from Fig. 18 for which $n \equiv 6 \pmod{7}$ are those of type **8**. By this, Conjecture 3(g) is confirmed.

In Fig. 18 there are two types of trees for which $n \equiv 2 \pmod{7}$, namely **2** and **9**. By direct calculation it can be shown that for $n = 7k + 2$, $k \leq 168$ (i.e., for $n \leq 1178$), the minimal- ABC Kragujevac tree is **9**, which agrees with Conjecture 3(c). However, for $k \geq 169$ (i.e., for $n \geq 1185$), the minimal- ABC Kragujevac tree is **2**. Thus, Conjecture 3(c) does not hold for trees with more than 1178 vertices, and needs to be amended as:

(c) If $n \equiv 2 \pmod{7}$, then T_{min} possesses four B_4 -branches, whereas all other branches are of B_3 -type.

In Fig. 18 there are three types of trees for which $n \equiv 4 \pmod{7}$, namely **1**, **6**, and **7**. By direct calculation it can be shown that for $n = 7k + 4$, $k \leq 287$ (i.e., for $n \leq 2013$), the minimal- ABC Kragujevac tree is **7**, which agrees with Conjecture 3(e). However, for $k \geq 288$ (i.e., for $n \geq 2020$), the minimal- ABC Kragujevac tree is **1**. Thus, Conjecture 3(e) does not hold for trees with more than 2013 vertices, and needs to be amended as:

(e) If $n \equiv 4 \pmod{7}$, then T_{min} possesses five B_4 -branches, whereas all other branches are of B_3 -type.

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