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Disproving a Conjecture on Trees with Minimal Atom–Bond Connectivity Index

Mohammad Bagher Ahmadi[a], **Darko Dimitrov**[b1], **Ivan Gutman**[c], **Seyyed Aliasghar Hosseini**[d]

[a]*Department of Mathematics, College of Sciences, Shiraz University 71454, Shiraz, Iran*
mbahmadi@shirazu.ac.ir

[b]*Institute of Computer Science, Freie Universität Berlin, Takustraße 9, D–14195 Berlin, Germany*
darko@mi.fu-berlin.de

[c]*Faculty of Science, University of Kragujevac, P. O. Box 60, 34000 Kragujevac, Serbia*
gutman@kg.ac.rs

[d]*Department of Mathematics, Simon Fraser University, 8888 University Drive, Burnaby, B.C., Canada V5A 1S6*
sahossei@sfu.ca

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Abstract

The problem of complete characterization of trees with minimal *atom-bond connectivity (ABC)* index is still an open problem. In [21], a conjecture on the structure of the trees with minimal ABC index, based on the assumption of existence of a central vertex, was posed. This conjecture was partially disproved in [1, 2], and subsequently in [12], which led to its modification. Here, we show that for sufficiently large trees, also the modified version of the conjecture fails in all of its cases. Presented counterexamples and their analysis suggest new conjectures.

[1]Corresponding author

1 Introduction

Let $G = (V, E)$ be a simple undirected graph of order $n = |V|$ and size $m = |E|$. For $v \in V(G)$, the degree of v, denoted by $d(v)$, is the number of edges incident to v. Then the *atom-bond connectivity (ABC) index* of G is defined as

$$\mathrm{ABC}(G) = \sum_{uv \in E(G)} f(u, v),$$

where $f(u, v) = \sqrt{(d(u) + d(v) - 2)/(d(u)d(v))}$. This vertex-degree-based graph topological index was proposed in 1998 by Estrada et al. [15], who showed that the ABC index can be a valuable predictive tool in the study of the heat of formation in alkanes. Later, the physico-chemical applicability of the ABC index was confirmed and extended in several studies [14, 24].

The ABC index has attracted a lot of interest in the last several years both in mathematical and chemical research communities and numerous results and structural properties of ABC index were established [3–10, 13, 16, 17, 19–23, 26, 27, 29–33].

In [9] it was shown that adding an edge in a graph strictly increases its ABC index (equivalently, in [4] it was shown that deleting an edge in a graph strictly decreases its ABC index). From this result, two immediate consequences follow: Firstly, among all connected graphs with n vertices, the complete graph K_n has maximal value of ABC index, and secondly, among all connected graphs with n vertices, the graph with minimal ABC index is a tree.

To show that the star graph S_n is a tree with maximal ABC index is fairly easy [17], while the complete characterization of trees with minimal ABC index (also refereed as minimal-ABC trees) is still an open problem. To accomplish that task, besides the theoretically proven properties of the trees with minimal ABC index, computer supported search can be of help [12, 18]. The plausible structural computational model and its refined version presented in [18] is based on the main assumption that the minimal-ABC tree posses a single *central vertex*, or said with other words, it is based on the assumption that the vertices of a minimal-ABC tree of degree ≥ 3 induce a star graph. Related to this concept, we introduce a notation of a big vertex, that will be used later in the paper. A vertex is *big*, if its degree is at least 3 and it is not adjacent to a vertex of degree 2. The assumption of a central vertex raised a conjecture of the structural properties of trees with minimal ABC index was proposed [21].

Also based on the central vertex assumption and some known properties of minimal ABC trees, a new class of trees, so-called *Kragujevac trees*, was introduced [25]. A Kragujevac tree is a tree that is comprised of a central vertex and B_k-branches, $k \geq 1$ (see Figure 1 for an illustration of B_k-branches). For Kragujevac trees the conjecture from [21] was answer in affirmative.

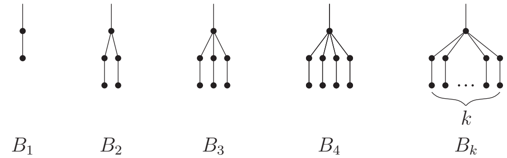

Figure 1: B_k-branches. The vertex of a B_k-branch with degree $k+1$ is considered as the root of the branch.

In [1, 2], and sequentially in [12], counterexamples for the cases $n \equiv 2 \pmod 7$ and $n \equiv 4 \pmod 7$ to the conjecture in [21] were found (see graphs T_2 and T_4 in Figure 2 in this paper). As result of those counterexamples the modified conjecture was obtained [12]:

Conjecture 1.1. *Let G be a tree with minimal ABC index among all trees of size n.*

(i) If $n \equiv 0 \pmod 7$ and $n \geq 175$, then G has the structure T_0 depicted in Figure 2.

(ii) If $n \equiv 1 \pmod 7$ and $n \geq 64$, then G has the structure T_1 depicted in Figure 2.

(iii) If $n \equiv 2 \pmod 7$ and $n \geq 1185$, then G has the structure T_2 depicted in Figure 2.

(iv) If $n \equiv 3 \pmod 7$ and $n \geq 80$, then G has the structure T_3 depicted in Figure 2.

(v) If $n \equiv 4 \pmod 7$ and $n \geq 312$, then G has the structure T_4 depicted in Figure 2.

(vi) If $n \equiv 5 \pmod 7$ and $n \geq 117$, then G has the structure T_5 depicted in Figure 2.

(vii) If $n \equiv 6 \pmod 7$ and $n \geq 62$, then G has the structure T_6 depicted in Figure 2.

Note that except for $n \equiv 4 \pmod 7$, in all other cases of Conjecture 1.1 the assumption of the existence of a central vertex is supported. In the next section, we present counterexamples for all cases of Conjecture 1.1 with more than one central vertex.

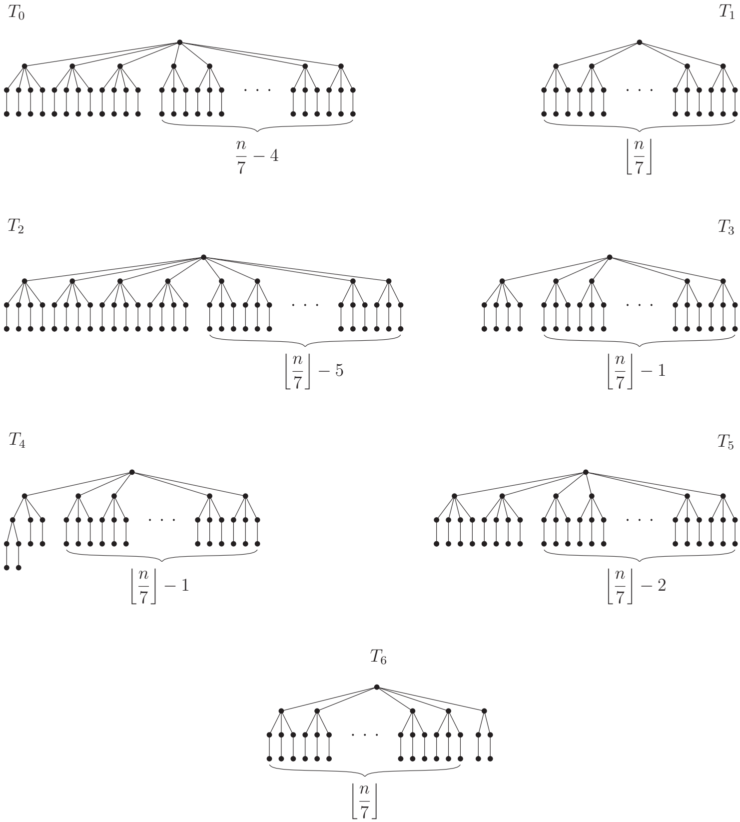

Figure 2: Types of trees with minimal ABC index that correspond to Conjecture 1.1.

2 Counterexamples to Conjecture 1.1

The counterexamples presented in this section (see Figure 3) not only shattered the conjecture of existence of a central vertex, as it did the example in [1, 12], but they also show that the minimal-ABC trees may have more than two central vertices. We would like to stress that, the second central vertex from the counterexample from [1, 12], graph T_4 in Figure 2, is of degree 4, while here we present trees with smaller values of ABC-index than in Conjecture 1.1 with degrees of central vertices of order $O(n)$. Also, we present counterexamples that have smaller ABC-index than the

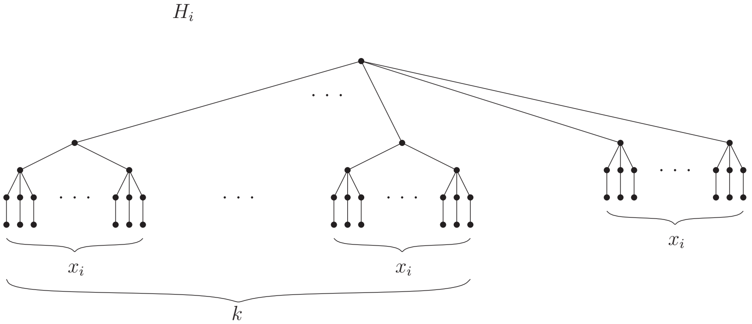

Figure 3: Graph H_i, $i = 0, 1, \ldots, 6$ that have smaller ABC-index than its corresponding graph T_i from Conjecture 1.1. For $i = 0, 2, 3, 4, 5, 6$, $k = (i + 6) \mod 7$, and $k = 7$, for $i = 1$.

two counterexamples for cases $n \equiv 2 \pmod 7$ and $n \equiv 4 \pmod 7$ proposed in [1,2,12] (graphs T_2 and T_4 in Figure 2). A brief comparison analysis between the examples from Conjecture 1.1 and the corresponding counterexamples in Figure 3 follows.

Case $n \equiv 0 \pmod 7$**.** Let $n/7 - 4 = 7x_0 - 3$. Then, T_0 and H_0 have same number of vertices. For $x_0 \geq 4$, T_0 and H_0 satisfy the requirements of Conjecture 1.1(i). We show that H_0 has smaller ABC-index than T_0, for $x \geq 42$. Indeed, the ABC-index of T_0 is

$$\begin{aligned} \mathrm{ABC}(T_0) &= 3f(7x_0, 5) + (7x_0 - 3)f(7x_0, 4) + 3 \cdot 4 \cdot f(5, 2) + 3 \cdot 4 \cdot f(2, 1) \\ &\quad +3(7x_0 - 3)f(4, 2) + 3(7x_0 - 3)f(2, 1), \end{aligned}$$

while the ABC-index of H_0 is

$$\begin{aligned} \mathrm{ABC}(H_0) &= 6f(x_0 + 6, x_0 + 1) + x_0 f(x_0 + 6, 4) + 6x_0 f(x_0 + 1, 4) \\ &\quad +3 \cdot 7x_0 \cdot f(4, 2) + 3 \cdot 7x_0 \cdot f(2, 1). \end{aligned}$$

Evaluating and simplifying the difference of the last two expressions, we obtain

$$\begin{aligned} \mathrm{ABC}(T_0) - \mathrm{ABC}(H_0) &= 3\sqrt{2} - \frac{3}{2}\sqrt{1 + \frac{2}{7x}} + \frac{3}{\sqrt{35}}\sqrt{7 + \frac{3}{x}} - 6\sqrt{\frac{5 + 2x}{6 + 7x + x^2}} \\ &\quad -\frac{1}{2}x\left(-\sqrt{7}\sqrt{7 + \frac{2}{x}} + 6\sqrt{\frac{3 + x}{1 + x}} + \sqrt{\frac{8 + x}{6 + x}}\right). \end{aligned}$$

The graph of the function $\mathrm{ABC}(T_0) - \mathrm{ABC}(H_0)$ is depicted in Figure 4. For $x_0 \geq 2$ the function is monotonically increasing, with $\lim_{x_0 \to \infty}(\mathrm{ABC}(T_0) - \mathrm{ABC}(H_0)) = 1.08428$ and it is positive for every integer at least 42. From here it follows that ever graph of type H_0 is a counterexample to the graph T_0 if both are of equal order $n \geq 2065$.

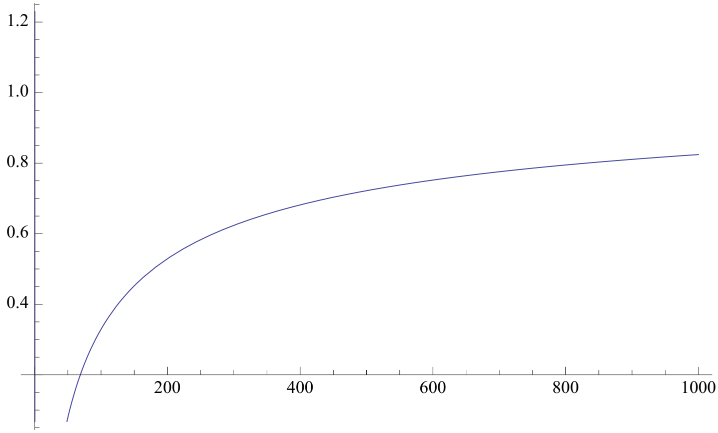

Figure 4: Graph of the function $\mathrm{ABC}(G_0(x_0)) - \mathrm{ABC}(H_0(x_0))$.

Next, we consider the cases $n \equiv 1, 2, \ldots, 6 \pmod 7$. Since the explanations for them are similar with that in the case $n \equiv 0 \pmod 7$, we will omit the complete analysis and just state the final conclusions.

Case $n \equiv 1 \pmod 7$**.** In this case consider the graphs T_1 and H_1. When $x_1 \geq 1$ and $\lfloor n/7 \rfloor = 8x_1 + 1$, the graphs satisfy Conjecture 1.1(ii). For $x_1 \geq 46$ $(n \geq 2584)$, it follows that $\mathrm{ABC}(T_1) > \mathrm{ABC}(H_1)$.

Case $n \equiv 2 \pmod 7$**.** Consider the graphs T_2 and H_2. When $x_2 \geq 85$ and $\lfloor n/7 \rfloor - 5 = 2x_2 - 5$, the graphs satisfy Conjecture 1.1(iii). We obtain that $\mathrm{ABC}(T_2) > \mathrm{ABC}(H_2)$, for $x_2 \geq 49$, which corresponds to $n \geq 688$.

Case $n \equiv 3 \pmod 7$**.** The graphs T_3 and H_3 satisfy Conjecture 1.1(iv), for $x_3 \geq 4$ and $\lfloor n/7 \rfloor - 1 = 3x_2 - 1$. For $x_3 \geq 43$ $(n \geq 906)$, the relation $\mathrm{ABC}(T_3) > \mathrm{ABC}(H_3)$ holds.

Case $n \equiv 4 \pmod 7$**.** In this case consider the graphs T_4 and H_4. When $x_4 \geq 11$ and $\lfloor n/7 \rfloor - 1 = x_4 - 1$, the graphs satisfy Conjecture 1.1(v). For $x_4 \geq 40$ $(n \geq 1124)$, it holds that $\mathrm{ABC}(T_4) > \mathrm{ABC}(H_4)$.

Case $n \equiv 5 \pmod 7$**.** Consider now the graphs T_5 and H_5. When $x_5 \geq 4$ and $\lfloor n/7 \rfloor - 2 = x_5 - 2$, the graphs satisfy Conjecture 1.1(vi). We obtain that $\mathrm{ABC}(T_5) > \mathrm{ABC}(H_5)$, for $x_5 \geq 42$ ($n \geq 1475$).

Case $n \equiv 6 \pmod 7$**.** The graphs T_6 and H_6 satisfy Conjecture 1.1(vii), for $x_6 \geq 2$ and $\lfloor n/7 \rfloor = x_6$. Graph H_6 is a counterexample to the graph T_6, since for $x_6 \geq 42$ ($n \geq 1770$), the relation $\mathrm{ABC}(T_6) > \mathrm{ABC}(H_6)$, holds.

3 Further counterexamples

In this section we present trees that for large n have smaller ABC than those presented in the previous section. Consider the example depicted in Figure 5.

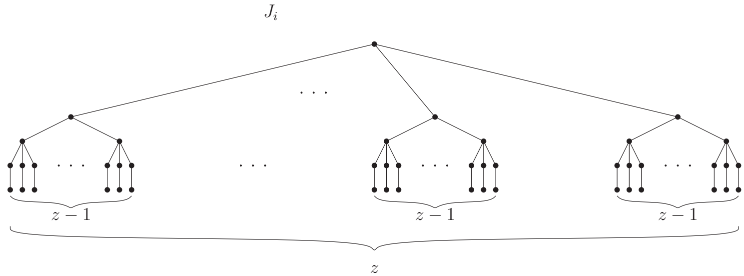

Figure 5: Graph J_i, $i = 0, 1, \ldots, 6$ that for enough big n has smaller ABC-index than its corresponding graph H_i in Figure 3. The root vertex of J_i has z children vertices, each of degree z.

It holds that

$$\mathrm{ABC}(J_i) = zf(z,z) + z(z-1)f(z,4) + 6z(z-1)f(2,1), \tag{1}$$

for $i = 0, 1, \ldots, 6$. On the other hand,

$$\begin{aligned}\mathrm{ABC}(H_i) &= kf(x_i+k,z) + x_i f(x_i+k,4) + kx_i f(x_i+1,4) \\ &\quad +3kx_i f(4,2) + 3kx_i f(4,2) + 3x_i f(4,2) + 3x_i f(2,1).\end{aligned} \tag{2}$$

Since we consider graphs of same order n,

$$n = 7kx_i + k + 1 + 7x_i = 1 + z + 7z(z-1), \tag{3}$$

and

$$i = (z+1) \mod 7 = (k+1) \mod 7, \tag{4}$$

must hold. From (1) and (2), after a simplification, we obtain

$$\begin{aligned} \mathrm{ABC}(H_i) - \mathrm{ABC}(J_i) &= 3\sqrt{2}(1+k)x_i + \frac{1}{2}kx_i\sqrt{\frac{3+x}{1+x_i}} + k\sqrt{\frac{-1+k+2x}{(1+x_i)(k+x_i)}} \\ &\quad + \frac{1}{2}x_i\sqrt{1+\frac{2}{k+x_i}} - 3\sqrt{2}(-1+z)z - \frac{1}{2}(-1+z)z\sqrt{\frac{2+z}{z}} \\ &\quad - z\sqrt{\frac{-2+2z}{z^2}}. \end{aligned} \tag{5}$$

Considering the constrains (3) and (4), it is easy to determine when the difference (5) is positive. In the sequel, we summarize those results for each of the seven cases with respect to $n \equiv i \pmod 7$.

Case $n \equiv 0 \pmod 7$**.** In this case $k = 6$ and the difference $\mathrm{ABC}(H_0) - \mathrm{ABC}(J_0)$ is positive for $x_0 > 541$, which corresponds to $n \geq 26537$.

Case $n \equiv 1 \pmod 7$**.** In this $k = 7$ and the difference $\mathrm{ABC}(H_1) - \mathrm{ABC}(J_1)$ is positive for $x_1 > 489$, which corresponds to $n \geq 27406$.

Case $n \equiv 2 \pmod 7$**.** In this case $k = 1$ and the difference $\mathrm{ABC}(H_2) - \mathrm{ABC}(J_2)$ is positive for $x_2 > 1228$, which corresponds to $n \geq 17201$.

Case $n \equiv 3 \pmod 7$**.** In this case $k = 2$ and the difference $\mathrm{ABC}(H_3) - \mathrm{ABC}(J_3)$ is positive for $x_3 > 852$, which corresponds to $n \geq 17902$.

Case $n \equiv 4 \pmod 7$**.** In this case $k = 3$ and the difference $\mathrm{ABC}(H_4) - \mathrm{ABC}(J_4)$ is positive for $x_4 > 857$, which corresponds to $n \geq 24014$.

Case $n \equiv 5 \pmod 7$**.** In this case $k = 4$ and the difference $\mathrm{ABC}(H_5) - \mathrm{ABC}(J_5)$ is positive for $x_5 > 709$, which corresponds to $n \geq 24841$.

Case $n \equiv 6 \pmod 7$**.** In this case $k = 5$ and the difference $\mathrm{ABC}(H_6) - \mathrm{ABC}(J_6)$ is positive for $x_6 > 611$, which corresponds to $n \geq 25682$.

From the examples in Figures 3 and 5, one can deduce the following conjectures.

Conjecture 3.1. *The big vertices of the minimal ABC-tree induce a star graph.*

Conjecture 3.2. *After some enough big n beside the big vertices, minimal ABC-trees have only B_3-branches.*

4 A generalization of the example in Figure 5

Note that the counterexamples presented in Figures 3 and 5 are not feasible for every n. However, those counterexamples can be easily extended for trees of any order. Such an extension of the construction in Figure 5 is the graph $G(n, z)$ depicted in Figure 6. For that purpose, in this construction, the B_3 branches are divided in two groups: r_l subgraphs of $z + 1$ B_3-branches with common parent vertex, and r_r subgraphs of z B_3-branches with common parent vertex.

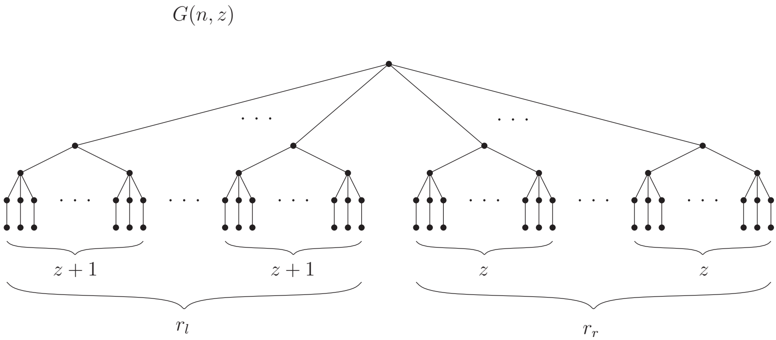

Figure 6: A generalization of the construction in Figure 5.

The ABC index of $G(n, z)$ depends on two variables n and z. Determining the parameter z for a fixed n, such that $G(n, z)$ has minimal ABC index is done in the next section.

4.1 Determining the optimal parameters

For a fixed number of vertices n, the so-called D_z*-branch* (depicted in Figure 7) plays the main role in the construction of a tree in Figure 6. Using D_z-branches we can construct only trees with specific number of vertices, $n = N_z*(1+z*7)+1$, where N_z is the number of used D_z-branches. So, to construct a tree with an arbitrary number of vertices we should use other kinds of branches. Our observations show that, in addition to D_z, we should use only D_{z-1} or D_{z+1}.

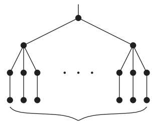

Figure 7: Main branch in the structure of minimal ABC-trees, D_z, comprised of z B_3-branches and their common parent vertex.

We can model the structure of trees with minimum ABC-index as below:

$$\begin{aligned} \text{minimize} \quad & N_{z-1} * (ABC(c,z) + (z-1) * ABC(z,4) + (z-1) * 6 * ABC(2,1)) \\ & + N_z * (ABC(c,z+1) + z * ABC(z+1,4) + z * 6 * ABC(2,1)) \\ & + N_{z+1} * (ABC(c,z+2) + (z+1) * ABC(z+2,4) \\ & + (z+1) * 6 * ABC(2,1)) \\ \text{subject to} \quad & n = N_{z-1} * (1 + (z-1) * 7) + N_z * (1 + z * 7) \\ & + N_{z+1} * (1 + (z+1) * 7) + 1 \\ & c = N_z + N_{z-1} + N_{z+1} \\ & N_{z-1} * N_{z+1} = 0 \\ & z, c, N_z, N_{z-1}, N_{z+1} \in \mathbb{Z}^{\geq 0}. \end{aligned}$$

In this model c is the degree of the central vertex and other variables are as discussed above. The third constraint shows that D_{z+1} and D_{z-1} should not occur simultaneously and this condition will be satisfied since it has been proved that two D_z branches will always be better than one D_{z-1} and one D_{z+1}, so D_{z-1} and D_{z+1} do not occur simultaneously in the minimum structure. It is necessary to mention that the first two conditions can be substituted to the objective function, therefore we can substitute c and N_z easily without lose of generality. So we have to minimize a function with three non-negative integer variables (z, N_{z-1} and N_{z+1}) and with no extra condition.

Now, let's consider the integer conditions. Since D_z is the main branch in an interval so number of D_{z-1} and D_{z+1} branches will be as small as possible. For a fixed z we can find N_{z-1} by using the following optimization program:

$$\begin{aligned} \text{minimize} \quad & N_{z-1} \\ \text{subject to} \quad & N_z = \frac{n - N_{z-1}(1 + 7(z-1))}{1 + 7z} \in \mathbb{Z}^{\geq 0}. \end{aligned}$$

This program indicates that we should use the smallest number of D_{z-1} branch such that N_z (that has been calculated from the first condition in the main program) become an integer. Since D_{z-1} and D_{z+1} can not occur simultaneously, here we suppose that $N_{z+1} = 0$.

Similarly, we can use the following program to find the optimized value for N_{z+1}:

$$\begin{array}{ll} \text{minimize} & N_{z+1} \\ \text{subject to} & N_z = \dfrac{(n - N_{z+1}(1 + 7(z+1))}{1 + 7z} \in \mathbb{Z}^{\geq 0}. \end{array}$$

It is easy to show that we can use $7z + 3$ of D_z instead of $7z + 1$ of D_{z+1} and we can use $7z - 1$ of D_z instead of $7z + 1$ of D_{z-1} with smaller ABC-index. So, for a fixed z we can conclude that $0 \leq N_{z-1}, N_{z+1} \leq 7z$. Therefore, each of the above programs can be easily solved by a simple loop.

In the first program we have considered that $N_{z+1} = 0$ and in the second one we have $N_{z+1} = 0$ and we have constructed two different structures. So, after solving each of the above programs we should compare these two structures and figure out which one is better and use that one to solve the main program. Since for a fixed z we can find N_z^*, N_{z+1}^* and N_{z-1}^*, we have to solve a minimization program with only one variable, z.

The optimum value of z in this program, z^*, increases with respect to n and when we solve this minimization program without considering the integer conditions for infinitely large n, we have $z^* = 51.89$. So we can conclude that $z^* \leq 52$ by considering the integer conditions.

Therefore, the three variables of the main program are bounded and the program can be solved by three simple loops in $O(1)$ time for every n. A pseudocode for solving this program is given next.

Alg. 1 OptimalParameters(n). An algorithm for calculating the optimal parameters, with respect to the minimal ABC index, of trees of the type depicted in Figure 6.

Input: An order n of a tree
Output: The optimal parameters with respect to the minimal ABC index

1: min-ABC $:= \infty$
2: **for** $z \leq 52$ **do**
3:     **for** $N_{z-1} \leq 7z$ **do**
4:         $N_z := \dfrac{n - N_{z-1}(1 + 7(z-1))}{1 + 7z}$
5   **if** N_z is an integer **then**
6:             **goto** 9
7   **end if**
8   **end for**
9:     ABC1 := ABC-index of the structure with z, N_z, N_{z-1} and $N_{z+1} = 0$
10:     **for** $N_{z+1} \leq 7z$ **do**
11:         $N_z := \dfrac{(n - N_{z+1}(1 + 7(z+1))}{1 + 7z}$
12:         **if** N_z is an integer **then**
13:             **goto** 16
14:         **end if**
15   **end for**
16:     ABC2 := ABC-index of the structure with z, N_z, N_{z+1} and $N_{z-1} = 0$
17:     **if** ABC1 or ABC2 is less than min-ABC **then**
18:         Update min-ABC, z^*, N_z^*, N_{z-1}^* and N_{z+1}^*
19:     **end if**
20: **end for**

References

[1] M. B. Ahmadi, S. A. Hosseini, P. Salehi Nowbandegani, On trees with minimal atom bond connectivity index, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 559–563.

[2] M. B. Ahmadi, S. A. Hosseini, M. Zarrinderakht, On large trees with minimal atom–bond connectivity index, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 565–569.

[3] M. B. Ahmadi, M. Sadeghimehr, Atom bond connectivity index of an infinite class $NS_1[n]$ of dendrimer nanostars, *Optoelectron. Adv. Mat.* **4** (2010) 1040–1042.

[4] J. Chen, X. Guo, Extreme atom–bond connectivity index of graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 713–722.

[5] J. Chen, X. Guo, The atom–bond connectivity index of chemical bicyclic graphs, *Appl. Math. J. Chinese Univ.* **27** (2012) 243–252.

[6] J. Chen, J. Liu, X. Guo, Some upper bounds for the atom-bond connectivity index of graphs, *Appl. Math. Lett.* **25** (2012) 1077–1081.

[7] J. Chen, J. Liu, Q. Li, The atom–bond connectivity index of catacondensed polyomino graphs, *Discr. Dyn. Nat. Soc.* **2013** (2013) ID 598517.

[8] K. C. Das, Atom–bond connectivity index of graphs, *Discr. Appl. Math.* **158** (2010) 1181–1188.

[9] K. C. Das, I. Gutman, B. Furtula, On atom–bond connectivity index, *Chem. Phys. Lett.* **511** (2011) 452–454.

[10] K. C. Das, I. Gutman, B. Furtula, On atom–bond connectivity index, *Filomat* **26** (2012) 733–738.

[11] J. Devillers, A T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon and Breach, Amsterdam, 1999.

[12] D. Dimitrov, Efficient computation of trees with minimal atom–bond connectivity index, *Appl. Math. Comput.* **224** (2013) 663–670.

[13] D. Dimitrov, On structural properties of trees with minimal atom–bond connectivity index, *Discr. Appl. Math.* **172** (2014) 28–44.

[14] E. Estrada, Atom–bond connectivity and the energetic of branched alkanes, *Chem. Phys. Lett.* **463** (2008) 422–425.

[15] E. Estrada, L. Torres, L. Rodríguez, I. Gutman, An atom–bond connectivity index: Modelling the enthalpy of formation of alkanes, *Indian J. Chem.* **37A** (1998) 849–855.

[16] G. H. Fath-Tabar, B Vaez-Zadeh, A. R. Ashrafi, A. Graovac, Some inequalities for the atom–bond connectivity index of graph operations, *Discr. Appl. Math.* **159** (2011) 1323–1330.

[17] B. Furtula, A. Graovac, D. Vukičević, Atom–bond connectivity index of trees, *Discr. Appl. Math.* **157** (2009) 2828–2835.

[18] B. Furtula, I. Gutman, M. Ivanović, D. Vukičević, Computer search for trees with minimal ABC index, *Appl. Math. Comput.* **219** (2012) 767–772.

[19] L. Gan, H. Hou, B. Liu, Some results on atom–bond connectivity index of graphs, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 669–680.

[20] L. Gan, B. Liu, Z. You, The ABC index of trees with given degree sequence, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 137–145.

[21] I. Gutman, B. Furtula, Trees with smallest atom–bond connectivity index, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 131–136.

[22] I. Gutman, B. Furtula, M. B. Ahmadi, S. A. Hosseini, P. Salehi Nowbandegani, M. Zarrinderakht, The ABC index conundrum, *Filomat* **27** (2013) 1075–1083.

[23] I. Gutman, B. Furtula, M. Ivanović, Notes on trees with minimal atom–bond connectivity index, *MATCH Commun. Math. Comput. Chem.* **67** (2012) 467–482.

[24] I. Gutman, J. Tošović, S. Radenković, S. Marković, On atom–bond connectivity index and its chemical applicability, *Indian J. Chem.* **51A** (2012) 690–694.

[25] S. A. Hosseini, M. B. Ahmadi, I. Gutman, Kragujevac trees with minimal atom–bond connectivity index, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 5–20.

[26] X. Ke, Atom–bond connectivity index of benzenoid systems and fluoranthene congeners, *Polycyc. Aromat. Comp.* **32** (2012) 27–35.

[27] W. Lin, X. Lin, T. Gao, X. Wu, Proving a conjecture of Gutman concerning trees with minimal ABC index, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 549–557.

[28] R. Todeschini, V. Consonni, *Molecular Descriptors for Chemoinformatics*, Wiley–VCH, Weinheim, 2009.

[29] T. S. Vassilev, L. J. Huntington, On the minimum ABC index of chemical trees, *Appl. Math.* **2** (2012) 8–16.

[30] R. Xing, B. Zhou, Extremal trees with fixed degree sequence for atom–bond connectivity index, *Filomat* **26** (2012) 683–688.

[31] R. Xing, B. Zhou, F. Dong, On atom–bond connectivity index of connected graphs, *Discr. Appl. Math.* **159** (2011) 1617–1630.

[32] R. Xing, B. Zhou, Z. Du, Further results on atom–bond connectivity index of trees, *Discr. Appl. Math.* **158** (2011) 1536–1545.

[33] J. Yang, F. Xia, H. Cheng, The atom–bond connectivity index of benzenoid systems and phenylenes, *Int. Math. Forum* **6** (2011) 2001–2005.