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Trees with Smallest Atom–Bond Connectivity Index

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Abstract

The structure of trees with a single high-degree vertex and smallest ABC index is determined.

1. Introduction

The atom–bond connectivity (ABC) index is a vertex–degree-based graph invariant, that found chemical applications [1, 2]. Recently a long series of mathematical investigations of the ABC index was communicated [3–9, 11–14]. It could be easily shown [3, 10, 12] that the n-vertex graph and the n-vertex tree with maximal ABC index are, respectively, the complete graph and the star. On the other hand, the structure of the n-vertex tree with minimal ABC (which also is the connected n-vertex graph with minimal ABC [10, 12]) remained obscure.

In a recent work [13] a combination of computer search and mathematical analysis was undertaken, aimed at elucidating the structure of the minimum-ABC trees. In [13] the n-vertex minimum-ABC tree(s) were determined up to $n = 30$. By inspecting the structure of these trees it could be seen that these consist of a central, high-degree vertex to which branches of the type B_1, B_2, and B_3 are attached, see Fig. 1. It was also proven [13] that a minimum-ABC tree may possess at most one external path with (exactly) three vertices of degree two.

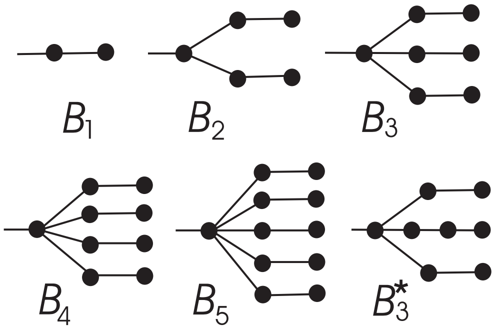

Fig. 1. Branches taken into account in the search for the the minimum-ABC trees.

It is imaginable that for $n > 30$ also branches similar to B_2 and B_3 could occur in the minimum-ABC trees. Therefore we have considered also the branches B_4 and B_5 depicted in Fig. 1.

Let x_i be the numbers of branches of the type B_i, $i = 1, 2, 3, 4, 5$, attached to the central vertex, possessing 2, 5, 7, 9, and 11 vertices, respectively.

Then the minimum-ABC tree has

$$n = 1 + 2\,x_1 + 5\,x_2 + 7\,x_3 + 9\,x_4 + 11\,x_5 + x_6 \qquad (1)$$

vertices, where $x_6 \in \{0, 1\}$ counts the external paths with three vertices of degree 2.

The parameters $n, x_1, x_2, x_3, x_4, x_5, x_6$ in Eq. (1) are non-negative integers. Therefore, for a given value of n, formula (1) can be viewed as a Diophantine equation in the unknowns x_i , $i = 1, 2, \ldots, 6$. The solutions of this equation are not too numerous, and could be easily determined. Then the respective ABC-values were calculated and the tree(s) with smallest ABC identified. That our guess was reasonable is seen from the fact that for all examined values of n we found $x_5 = 0$, i. e., the branch B_5 was never present.

Calculations were done until $n = 700$, and the respective minimum-ABC tree(s) identified. It was found that initially the structures of the so determined minimum-ABC trees are quite irregular, but after n becoming sufficiently large, the following simple regularities emerge.

If $n \equiv 0$ $(mod\ 7)$, $k \geq 21$, and $n = 7k + 28$, then the minimum-ABC tree has the structure shown in Fig. 2.

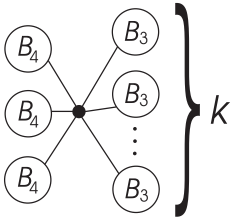

Fig. 2. Minimum-ABC trees with $7k + 28$ vertices, for $k \geq 21$. The smallest such tree has $n = 175$ vertices. The form of the branches B_3 and B_4 is shown in Fig. 1.

If $n \equiv 1$ $(mod\ 7)$, $k \geq 9$, and $n = 7k + 1$, then the minimum-ABC tree has the structure shown in Fig. 3.

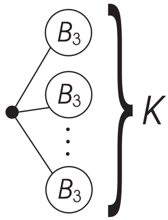

Fig. 3. Minimum-ABC trees with $7k + 1$ vertices, for $k \geq 9$. The smallest such tree has $n = 64$ vertices. The form of the branch B_3 is shown in Fig. 1.

If $n \equiv 2$ $(mod\ 7)$, $k \geq 23$, and $n = 7k + 9$, then the minimum-ABC tree has the structure shown in Fig. 4.

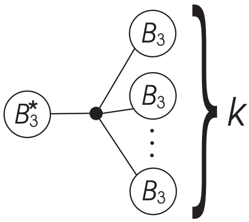

Fig. 4. Minimum-ABC trees with $7k + 9$ vertices, for $k \geq 23$. The smallest such tree has $n = 170$ vertices. The form of the branches B_3 and B_3^* is shown in Fig. 1.

If $n \equiv 3$ $(mod\ 7)$, $k \geq 10$, and $n = 7k + 10$, then the minimum-ABC tree has the structure shown in Fig. 5.

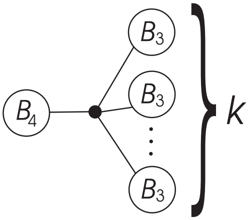

Fig. 5. Minimum-ABC trees with $7k + 10$ vertices, for $k \geq 10$. The smallest such tree has $n = 80$ vertices. The form of the branches B_3 and B_4 is shown in Fig. 1.

If $n \equiv 4$ $(mod\ 7)$, $k \geq 6$, and $n = 7k + 11$, then the minimum-ABC tree has the structure shown in Fig. 6.

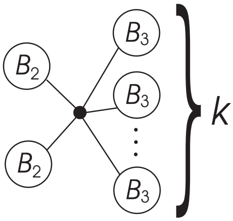

Fig. 6. Minimum-ABC trees with $7k + 11$ vertices, for $k \geq 6$. The smallest such tree has $n = 53$ vertices. The form of the branches B_2 and B_3 is shown in Fig. 1.

If $n \equiv 5$ $(mod\ 7)$, $k \geq 14$, and $n = 7k + 19$, then the minimum-ABC tree has the structure shown in Fig. 7.

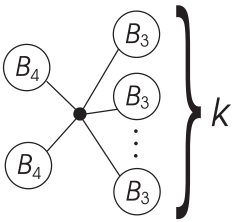

Fig. 7. Minimum-ABC trees with $7k + 19$ vertices, for $k \geq 14$. The smallest such tree has $n = 117$ vertices. The form of the branches B_3 and B_4 is shown in Fig. 1.

If $n \equiv 6$ $(mod\ 7)$, $k \geq 8$, and $n = 7k + 6$, then the minimum-ABC tree has the structure shown in Fig. 8.

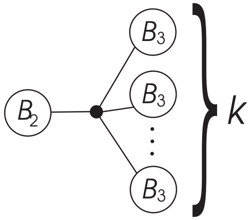

Fig. 8. Minimum-ABC trees with $7k+6$ vertices, for $k \geq 8$. The smallest such tree has $n = 62$ vertices. The form of the branches B_2 and B_3 is shown in Fig. 1.

The above results are valid under the assumption that the central vertex of the minimum-ABC tree is unique.

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