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The ABC Index Conundrum's Complete Solution

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Abstract

The problem of complete characterization of trees with minimal atom-bond-connectivity index (minimal-ABC trees) has a reputation as one of the most challenging and intriguing open problems in mathematical chemistry. Recently, the problem has been completely solved. Here, we provide an overview of the key results that led to its complete solution.

1 Introduction

The evolution of topological indices, defined as numerical values associated with a chemical constitution for correlation of chemical structure with diverse physical properties, chemical reactivity, or biological activity, dates back to the pioneering efforts of applying graph theory to investigate structural phenomena within the molecule [3]. The *atom-bond connectivity index* (*ABC index*), introduced in 1998 by Estrada et al. [32] was a relatively recent addition to the wide list of topological molecular descriptors.

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The ABC index of a simple undirected graph $G = (V, E)$ with vertex set $V = V(G)$ and edge set $E = E(G)$ is defined as

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

where $d(v)$ is the degree of a vertex $v \in V$.

In [32], it was shown that the ABC index has a good correlation with the heat of formation ΔH_f° of alkanes. Later in 2008, Estrada [30] claimed to have provided "*a quantum-chemical explanation for this correlation based on the ratio of* $1,3$-*interactions with respect to the total number of* $1,2$-*,* $1,3$- *and* $1,4$-*interactions in alkanes*", concluding that "*the heat of formation of alkanes can be obtained as a combination of stabilizing effects coming from atoms, bonds and protobranches.*" In a critical evaluation conducted later, Gutman et al. [47] confirmed that the ABC index "*reproduces the heat of formation with an accuracy comparable to that of high-level ab initio and DFT (MP2, B3LYP) quantum chemical calculations*". In light of all this Gutman [43] asserted that "*ABC index happens to be the only topological index for which a theoretical, quantum-theory-based, foundation and justification has been found.*"

After that revelation, interest in the ABC index has grown rapidly. As a well-motivated graph-based invariant, it has received considerable attention within mathematical and chemical research communities. Due to this interest, numerous results, structural properties, and a few variants of the ABC index were established [2, 4, 5, 7, 9–11, 13, 14, 23, 33–35, 37–41, 44, 46, 48, 55, 58, 60, 61, 64–66, 68–70, 72].

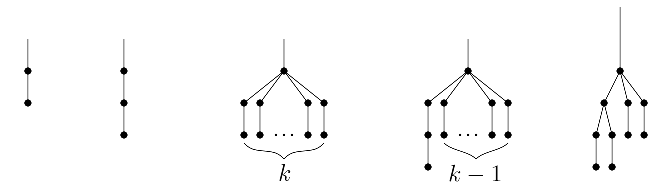
From a mathematical perspective, when a new graph-based structural descriptor is introduced, one of the initial questions to be addressed is which graph attains the maximum or minimum value of the particular descriptor among graphs of the same order. From the fact that deleting an edge in a graph strictly decreases its ABC index [5], or equivalently that adding an edge in a graph strictly increases its ABC index [10], it follows that the complete graph K_n has the maximum ABC index, while a connected graph that has the minimal ABC index must be a tree. To show that the star graph S_n is the unique tree with the maximal ABC index is a fairly easy task [35]. Initially, it appeared that characterizing trees with the minimal ABC index (*minimal-ABC trees*) was not an especially challenging problem, and that standard and routine techniques could solve the problem. However, it turns out that characterizing minimal-ABC trees is a very elusive problem, and despite many attempts, only very recently a full characterization of minimal-ABC trees has been obtained.

1.1 Additional notations

The term *big vertex* refers to a vertex with degree greater than two that is not adjacent to a vertex with degree two.

A path, whose both end-vertices have degrees at least three, and the rest of the vertices have degree two, is called an *internal path*. A *pendant vertex* is a vertex of degree one. A path, whose one end-vertex has degree at least three, the other end-vertex is a pendant vertex, and the rest of the vertices have degree two, is called a *pendant path*.

A path of length two adjacent to a vertex that has at least one child of degree at least three is called a B_1-*branch*. A vertex v with degree $k+1$, $k \geq 2$, together with k pendant paths of length 2 attached to it, comprised a so-called B_k-*branch*. The vertex v is referred to as the *center of the B_k-branch*. By attaching a vertex to a pendant vertex of B_k-branch, one obtains a so-called B_k^*-*branch*. Illustrations of B_k-, B_k^*-, $k \geq 1$, and B_3^{**}-branches are given in Figure 1. We will refer to them in general as *B-branches*.



B_1 B_1^* $B_k (k \geq 2)$ $B_k^* (k \geq 2)$ B_3^{**}

Figure 1. B_k, B_k^*, $k \geq 1$ and B_3^{**} branches.

For a given degree sequence Wang [67] defined greedy trees as follows:

Definition 1. Suppose that the degrees of the non-leaf vertices are given, the greedy tree is achieved by the following 'greedy algorithm':

1. Label the vertex with the largest degree as v (the root);
2. Label the neighbors of v as $v_1, v_2, \ldots$, assign the largest degree available to them such that $d(v_1) \geq d(v_2) \geq \cdots$;
3. Label the neighbors of v_1 (except v) as $v_{11}, v_{12}, \ldots$, such that they take all the largest degrees available and that $d(v_{11}) \geq d(v_{12}) \geq \cdots$, then do the same for $v_2, v_3, \ldots$;
4. Repeat (3) for all newly labeled vertices, always starting with the neighbors of the labeled vertex with largest degree whose neighbors are not labeled yet.

In the rest of the paper, we give an overview of the key results that led to the full characterization of the minimal-ABC trees. As a means of providing a more comprehensive understanding of the milestones during this discovery, we present the results in a logical order - this may not always correspond to the chronological order in which they were published. In Section 2 we present the theoretical results. A separate subsection is dedicated to each important milestone or group of related results. Due to the importance of computational results in indicating and leading the research direction, they are presented in Section 3.

2 Theoretical results

2.1 Some initital results

One of the first mathematical results regarding minimal-ABC trees was that by Furtula et al. [35], where the problem of finding the extremal values of the ABC index was completely solved for chemical trees (trees with maximal degree 4).

Another basic but essential result, already mentioned in the introduction, was presented independently in 2011 in the following two equivalent theorems, obtained by Das et al., and Chen and Guo, respectively.

Theorem 1 ([10]). *Adding an edge in a graph strictly increases its ABC index.*

Theorem 2 ([5]). *Deleting an edge in a graph strictly decreases its ABC index.*

2.2 Greedy tree

The following result by Gan et al. [38] from 2012 characterizes the trees with minimal ABC index with prescribed degree sequences. This characterization was used in many other proofs later.

Theorem 3. *Given the degree sequence, the greedy tree minimizes the ABC index.*

The same result as in Theorem 3, using slightly different notation and approach, was published also in the same year by Xing and Zhou [68].

2.3 Internal and pendent paths

The essential part in characterizing minimal-ABC trees was the earlier results regarding the internal and pendent paths.

Theorem 4 ([46]). *The n-vertex tree with minimal ABC index does not contain internal paths of any length $k \geq 2$.*

The above result by Gutman et al. from 2012 has a very important consequence.

Corollary 1. *Let T be a tree with minimal ABC index. Then the subgraph induced by the vertices of T whose degrees are greater than two is also a tree.*

Lemma 1 ([46, 58]). *If T is a tree with minimal ABC index, then every pendant path in T is of length 2 or 3, and there is at most one pendant path of length 3 in T.*

The next crucial result is the following one published in 2017.

Theorem 5 ([17]). *A minimal-ABC tree of order* $n > 415$ *does not contain a pendant path of length* 3*.*

As a consequence from the results presented in this subsection, it follows that for $n > 415$, a minimal-ABC tree may contain only B_k-branches, and, as it will be shown in Theorem 11 [28], maybe an additional B_3^{**}-branch. In the next section, beside the result about a B_3^{**}-branch, we present results that further reduced the size and the possible number of B_k-branches.

2.4 The size and number of the B-branches

The next group of results has reduced significantly the possible candidates for minimal-ABC trees, by excluding some configurations of B-branches.

Theorem 6 ([14]). *A minimal-ABC tree does not contain a* B_k*-branch,* $k \geq 5$*.*

The last theorem reduced the further investigation only on B_1-, B_2-, B_3-, B_3^{**}-,and B_4-branches. In the sequel, we will mention the most important results regarding each type of the above mentioned B-branches. First we present results that showed some forbidden combinations of B-branches.

Theorem 7 ([22]). *A minimal-ABC tree cannot contain a* B_4*-branch and a* B_1*-branch simultaneously.*

Theorem 8 ([22]). *A minimal-ABC tree cannot contain a* B_4*-branch and a* B_2*-branch simultaneously.*

The following results consider the possible number of B_4-branches contained in the minimal-ABC trees.

Theorem 9 ([14]). *A minimal-ABC tree does not contain more than four* B_4*-branches.*

Theorem 10 ([19]). *A minimal-ABC tree, whose root has degree at least* 1228*, does not contain* B_4*-branches.*

The following two results give the maximum possible numbers of B_1-, B_2- and B_3^{**}-branches, and their correlation.

Theorem 11 ([28]). *A minimal-ABC tree of order larger than* 122 *may contain exactly two B_1-branches, which together with one B_2-branch comprise a B_3^{**}-branch.*

Theorem 12 ([29]). *Let T be a minimal-ABC tree. If T is of order larger than* 39 *and contains B_1-branches, then T contains exactly one B_2-branch. If T is of order larger than* 163 *and contains no B_1-branch, then T contains at most two B_2-branches.*

Proposition 13 ([19]). *Let x and y be vertices of a minimal-ABC tree G that have a common parent vertex z, such that $d(x) \geq d(y) \geq 7$. If x has only B_3-branches as children and y has B_3-branches and one B_2-branch as children, then $d(x) \leq d(y) + 5$. If y has B_3-branches and two B_2-branches as children, then $d(x) \leq d(y) + 9$.*

The next results consider the number of the possible B-branches that may be adjacent to root vertex of a minimal-ABC tree.

Lemma 2 ([19]). *Let G be a minimal-ABC tree. Then all B_4-branches (maximum* 4*) are adjacent to the root vertex of G.*

Lemma 3 ([19]). *A minimal-ABC tree, whose root has degree at least* 1228*, does not contain B_4-branches.*

Lemma 4 ([19]). *The number of B-branches adjacent to the root vertex of a minimal-ABC tree is at most* 919.

Lemma 5 ([19]). *If the root vertex of a minimal-ABC tree has degree at least* 2956*, then there are no B-branches attached to the root.*

2.5 Big vertices and D-branches

Recall that by Corollary 1, it follows that the big vertices induce a tree. The following conjecture was raised by Gutman and Furtula earlier in 2012.

Conjecture 1 ([44]). *A minimal-ABC tree has (at most) one big (central) vertex.*

It was disproved by Ahmadi et al. in 2014 [1], where the correct result was guessed. In this context, it is worth to mention that for a special class of trees, so-called *Kragujevac trees*, that are comprised of a central vertex and B_k-branches, $k \geq 1$, the minimal-ABC trees were fully characterized by Hosseini et al. [49].

Conjecture 2 ([1]). *The subgraph of a minimal-ABC tree induced by its big vertices is a star.*

The above conjecture was proven to be correct several years later independently in [18, 50].

The following conjecture has been arisen also in [1], and was proven later in [19, 50] (see Theorem 17 in the next section).

Conjecture 3 ([1]). *After some enough large n, besides the big vertices, minimal-ABC trees have only B_3-branches.*

Moreover, the structure of the minimal-ABC tree depicted in Figure 2, for enough large trees, was conjectured in [1].

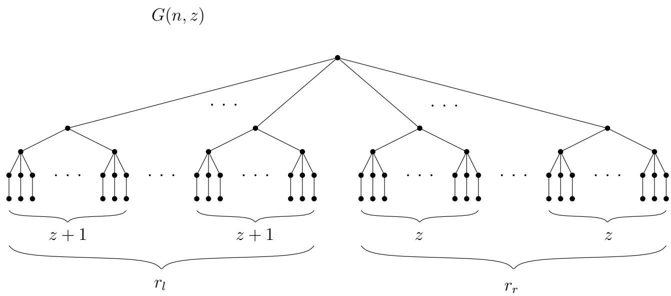


Figure 2. The figure from [1] with the conjectured structure of the minimal-ABC tree.

This prompts the so-called D-branches, introduced in [1], additionally to be considered. Considering the above results on B-branches, few types of D-branches, depicted in Figure 3, were relevant for further consideration.

The vertex of a D-branch to whom the B-branches are attached is referred to as the center of the D-branch.

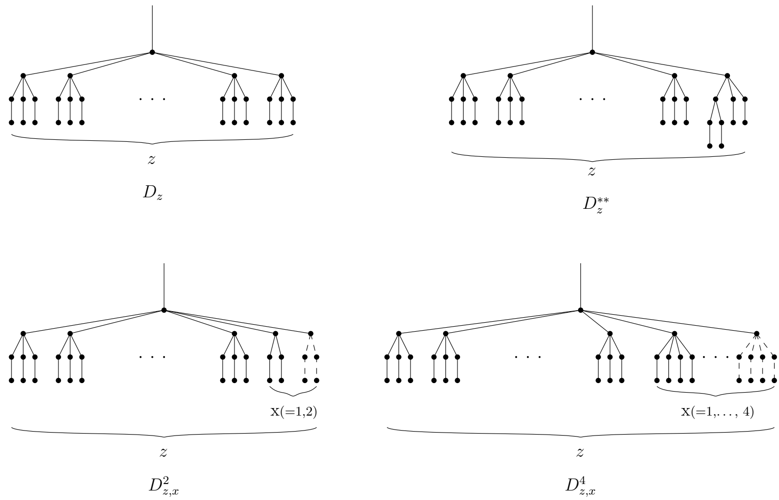


Figure 3. D_z-, D_z^{**}-, $D^2_{z,x}$- ($x = 1, 2$) and $D^4_{z,x}$- ($x = 1, 2, 3, 4$) branches. The dashed line segments are optional.

2.6 Size and number of the D-branches

The following group of results, ones of the last towards the final solution, are about D-branches.

2.6.1 Bounds on the size of the D-branches

Lemma 6 ([18]). *For $z \leq 14$, there is no minimal-ABC tree, which has a D_z- or D_z^{**}-branch.*

Lemma 7 ([18, 19]). *A minimal-ABC tree does not contain a D_z-, D_z^{**}- or $D^2_{z,x}$-branch, $z \geq 132$, for each $x = 1, 2$, if $z \geq 132$.*

Lemma 8 ([19]). *If a minimal-ABC tree contains at least* 261 *D_z-branches, then $z \leq 52$.*

Proposition 14 ([19]). *If a minimal-ABC tree contains a $D^2_{z,2}$-branch, then $25 \leq z \leq 50$. If a minimal-ABC tree contains a $D^2_{z,1}$-branch, then $19 \leq z \leq 97$.*

Proposition 15 ([19]). *If a minimal-ABC tree contains a D^{**}_z-branch, then $47 \leq z \leq 74$.*

2.6.2 The number of the D-branches and some impossible configurations

As a consequence of Lemma 2 we have the following corollary.

Corollary 2. *A minimal-ABC tree does not contain $D^4_{z,x}$-branches, $x = 1, 2, 3, 4$.*

Lemma 9 ([19]). *A minimal-ABC tree with at least 65 D_z-branches and with the root of degree at least 146 does not contain a $D^2_{k,2}$-branch.*

Lemma 10 ([19]). *A minimal-ABC tree with at least 261 D_z-branches and with the root of degree at least 1228 does not contain a $D^2_{k,1}$-branch.*

Lemma 11 ([19]). *If there are at least 56 D_z-branches, then the minimal-ABC tree does not contain a D^{**}_k-branch.*

Theorem 16 ([19]). *A minimal-ABC tree with the root vertex of degree at least 1228 is comprised only of a root and D_z- and D_{z+1}-branches, where $z \in \{50, 51, 52\}$, and maybe of B_3-branches and at most one of $D^2_{t,1}$-branch, $z - 5 \leq t \leq z$, attached to the root.*

Corollary 3 ([19]). *A minimal-ABC tree with the root vertex of degree at least 1441 is comprised only of a root and D_z- and D_{z+1}-branches, where $z \in \{50, 51, 52\}$ and maybe of B_3-branches attached to the root.*

Theorem 17 ([19]). *A minimal-ABC tree with the root vertex of degree at least 2956 is comprised only of a root and D_z- and D_{z+1}-branches, where $z \in \{50, 51, 52\}$.*

A comparable outcome was obtained in [50], albeit with supplementary constraints.

The intuition behind the structure of the minimal-ABC trees, which was already conjectured in 2014 [1], is based on the fact that a B_3–branch has minimal value among all B-branches. Hence, it was anticipated that the B_3-branches would prevail, and the remaining vertices would merely connect the B_3-branches in an optimal manner, thereby minimizing the ABC index. Furthermore, it was expected that for some sufficiently large n, there would be only B_3-branches.

Theorem 18 ([19]). *Let v be the root of a minimal-ABC tree G.*

- *If $2956 \leq d(v) \leq 3241$, then G must contain D_{51}-branches and in addition*
  - *either D_{52}-branches,*
  - *or at most 123 D_{50}-branches.*

  In particular, when $2956 \leq d(v) \leq 3185$, G contains at most 357 D_{52}-branches.

- *If $d(v) \geq 3242$, then G must contain D_{52}-branches and*
  - *either at most 718 D_{51}-branches.*
  - *or at most 178 D_{53}-branches.*

  In particular, when $d(v) \geq 3249$, G contains at most 364 D_{51}-branches.

2.7 The optimization function and determining the parameters of the minimal-ABC trees

According to the results presented in the previous sections, minimal-ABC trees can be described quite closely. A final and exact description, including the parameters of a minimal-ABC tree of order n (the number of particular B-branches/D-branches), can be obtained by solving the following optimization problem:

$min_{T \in \mathcal{T}} ABC(T)$

subject to

(1) $d(v) = n_z + n_{z+1} + b_* + b_1 + b_2 + b_3 \cdot n_3 + b_4 \cdot n_4$

(2) $n = 1 + n_z(7z+1) + n_{z+1}(7(z+1)+1) + b_1(7(k_1-1)+5+1) + b_2(7(k_2-2)+10+1) + b_3 \cdot n_3 \cdot 7 + b_4 \cdot n_4 \cdot 9 + b_* \cdot (7z+4)$

(3) $15 \leq z \leq 131$ (by Lemmas 6 and 7)

(4) $z - 5 \leq k_1 \leq z$ (by Proposition 13)

(5) $z - 9 \leq k_2 \leq z$ (by Proposition 13)

(6) $0 \leq n_4 \leq 4$ (by Theorem 9)

(7) $0 \leq n_3 + n_4 \leq 919$ (by Lemma 4)

(8) $b_*, b_1, b_2, b_3, b_4 \in \{0, 1\}$

(9) at most one of b_*, b_1, b_2, b_4 can be 1 (by Theorems 8 and 12).

In the above optimization function, n_z and n_{z+1} are, respectively, the numbers of D_z- and D_{z+1}-branches, n_3 and n_4 are, respectively, the numbers of B_3- and B_4-branches attached to the root, k_1 is the size of the $D^2_{k,1}$-branch, k_2 is the size of the $D^2_{k,2}$-branch, and parameters $b_*, b_1, b_2, b_3, b_4 \in \{0, 1\}$ are related to the existences of D^{**}_z-, $D^2_{k,1}$-, $D^2_{k,2}$-, B_3- and B_4-branches attached to the root vertex, respectively - for example $b_* = 0/1$ means that T *does not contain/ does contain* D^{**}_z-branch.

With the growth of the order of the trees, the above optimization problem becomes simpler.

When $d(v) \geq 1228$, by Theorem 16, it follows that $n_4 = 0$, $b_* = b_2 = b_4 = 0$, and $50 \leq z \leq 52$. Further, when $d(v) \geq 2956$, by Theorem 17, it follows that $n_3 = n_4 = 0$, $b_* = b_1 = b_2 = b_3 = b_4 = 0$ and $50 \leq z \leq 52$. Moreover, by Theorem 18, when $d(v) \geq 3249$, we have $0 \leq n_{51} \leq 364$ and $0 \leq n_{53} \leq 178$. That allows us to determine the parameters of the minimal-ABC tree for an arbitrary n in a constant time. The minimal-ABC trees and their structures are given in Appendix 4. The minimal-ABC trees of orders up to 1100 were already known [56].

3 Computational results

For complete characterization of the minimal-ABC trees, in addition to the theoretically proven properties, computer supported search has proved extremely helpful in indicating and leading the research direction, as well as in determining the exact number of B-branches in Section 2.7.

The first example of using computer search was done by Furtula et al. [36], where the trees with minimal ABC index of up to size 31 were computed. There, a brute-force approach of generating all trees of a given order, speeded up by using a distributed computing platform, was applied.

A significant advancement towards enhancing computation speed was achieved by focusing solely on the degree sequences of trees and leveraging known structural properties of trees with minimal ABC index [13]. The enumeration of tree degree sequences described in [13] was associated with the enumeration of graph degree sequences, as studied by Ruskey et al. [63], which relied on Havel-Hakimi's recursive characterization of graph degree sequences.

Due to the nature of the recursive relation used in the enumeration of degree sequences in [63], the same degree sequences were generated several times. That disadvantage was improved in [54], where the appropriate degree sequences were enumerated by applying an integer partitioning argument. Subsequently, significant computational improvements were attained by employing a parallelized version of the algorithm based on degree sequences and incorporating additional constraints. These advancements were made possible by leveraging newly obtained theoretical results [25, 56, 59].

An overview of the algorithms, along with some of their performance statistics, can be found in Table 1.

Table 1. The comparison of performance of the existing search algorithms. The abbreviation DS stands for degree sequence.

Algorithm	Range of n	Time (approx.)	Test platform
Brute-force search [36]	$1 \leq n \leq 31$	7 days for $n = 31$	Computer grid 400 CPUs
Original DS algorithm [13]	$1 \leq n \leq 300$	15 days	PC, 2 cores, 2.3 GHz
1. Modified DS algorithm [54]	$1 \leq n \leq 300$	75.5 hours	PC, 2 cores, 2.4 GHz
2. Parallelized modified DS algorithm [59]	$1 \leq n \leq 300$	0.21 hours	Workstation group, 36 cores
	$1 \leq n \leq 400$	23 hours	
3. Modified DS algorithm [25]	$n \leq 300$	13 seconds	PC, 2 cores, 2.3 GHz
	$1 \leq n \leq 400$	3.7 minutes	
	$1 \leq n \leq 700$	20 hours	
	$n = 800$	2.2 hours	
	$1 \leq n \leq 800$	7 days	
4. Modified DS algorithm [56]	$1 \leq n \leq 1100$	7 days	PC, 4 cores, 2.3 GHz
Non-linear opt. problem solver [19]	$n \leq 1329 \cdot 10^{13}$	few seconds	PC, 4 cores, 2.3 GHz

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4 Appendix: Minimal ABC-trees

Case $n \equiv 0 \pmod 7$

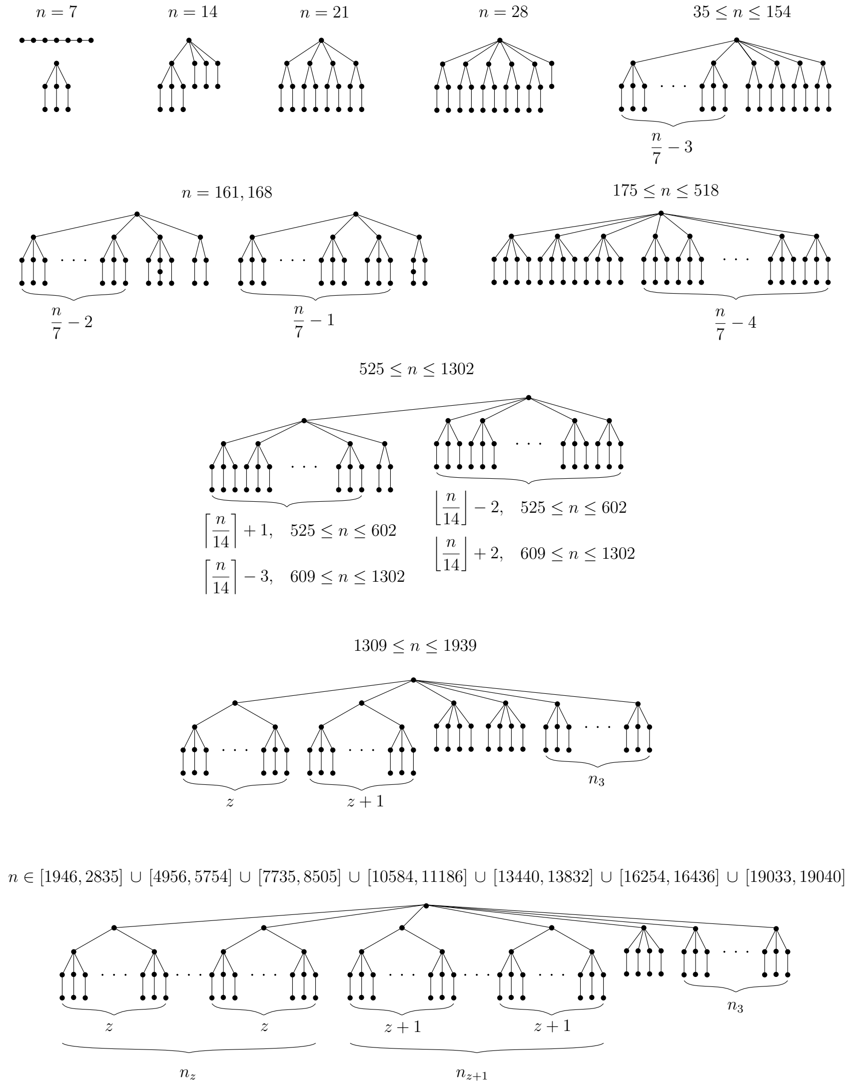
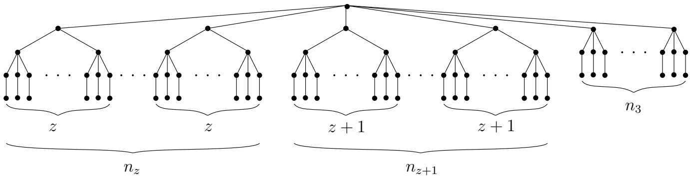


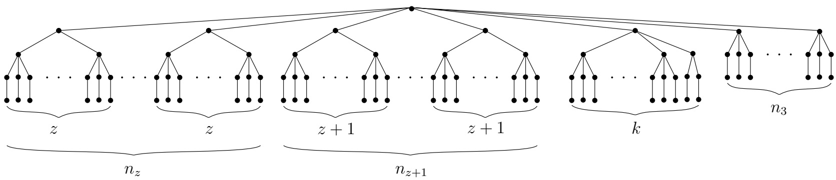
Figure 4. Minimal-ABC trees with n vertices, where $n \equiv 0 \pmod 7$.

Case $n \equiv 0 \pmod 7$

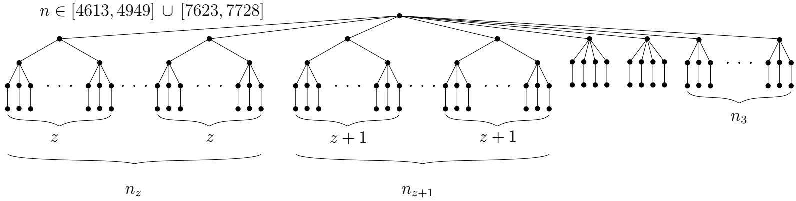
$n \in [2842, 4319] \cup [5761, 7616] \cup [8512, 10577] \cup [11193, 13433] \cup [13839, 16247] \cup [16443, 19026] \cup [19047, 989506]$
$\cup [989520, 991991] \cup [992026, 994476] \cup [994532, 996968] \cup [997038, 999460] \cup [999544, 1001952] \cup [1002050, 1004444]$
$\cup [1004556, 1006943] \cup [1007062, 1009442] \cup [1009568, 1011948] \cup [1012074, 1014447] \cup [1015665, 1016953]$



$4326 \le n \le 4606$



$n \in [4613, 4949] \cup [7623, 7728]$



$n \in \{989513\} \cup [991998, 992019] \cup [994483, 994525] \cup [996975, 997031] \cup [999467, 999537] \cup [1001959, 1002043]$
$\cup [1004451, 1004549] \cup [1006950, 1007055] \cup [1009449, 1009561] \cup [1011955, 1012067] \cup [1014454, 1015658]$
$\cup [1016960, \infty)$

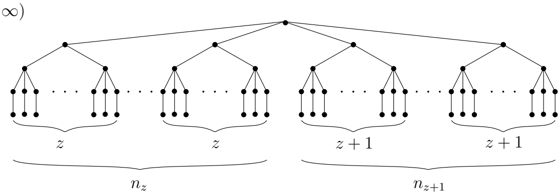


Figure 5. Minimal-ABC trees with n vertices, where $n \equiv 0 \pmod 7$.

Case $n \equiv 1 \pmod 7$

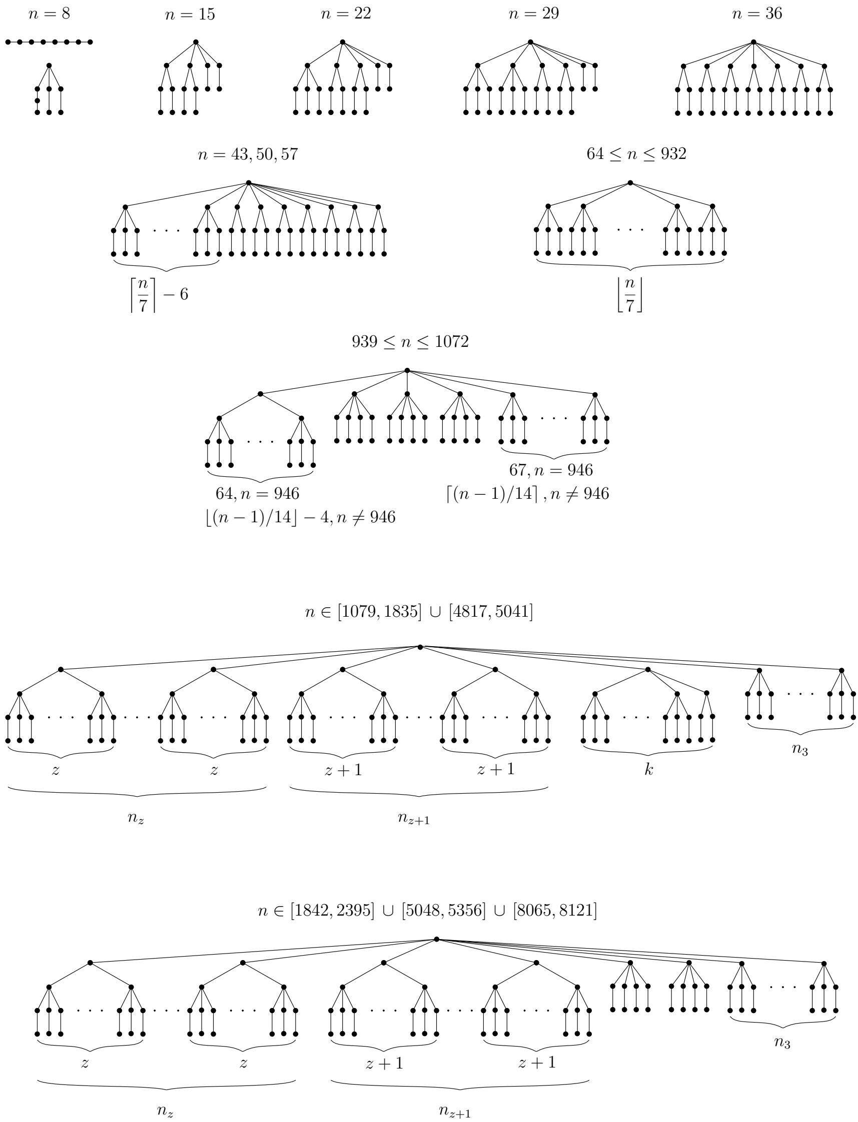
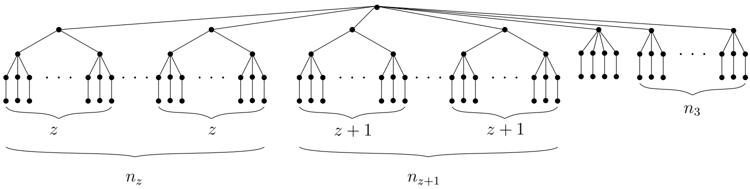


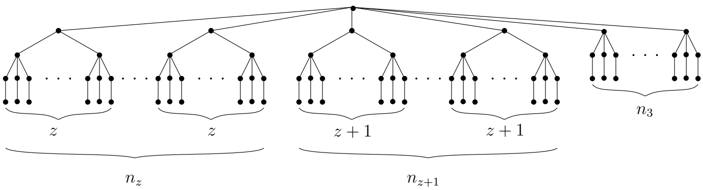
Figure 6. Minimal-ABC trees with n vertices, where $n \equiv 1 \pmod 7$.

Case $n \equiv 1 \pmod 7$

$n \in [2402, 3270] \cup [5363, 6154] \cup [8128, 8891] \cup [10991, 11565] \cup [13840, 14204] \cup [16647, 16808]$



$n \in [3277, 4810] \cup [6161, 8058] \cup [8898, 10984] \cup [11572, 13833] \cup [14211, 16640] \cup [16815, 989864]$
$\cup [989878, 992349] \cup [992384, 994834] \cup [994890, 997326] \cup [997396, 999811] \cup [999902, 1002310]$
$\cup [1002408, 1004802] \cup [1004914, 1007301] \cup [1007420, 1009800] \cup [1009926, 1012306]$
$\cup [1012432, 1014805] \cup [1016611, 1017311]$



$n \in \{989871\} \cup [992356, 992377] \cup [994841, 994883] \cup [997333, 997389] \cup [999818, 999895]$
$\cup [1002317, 1002401] \cup [1004809, 1004907] \cup [1007308, 1007413] \cup [1009807, 1009919]$
$\cup [1012313, 1012425] \cup [1014812, 1016604] \cup [1017318, \infty)$

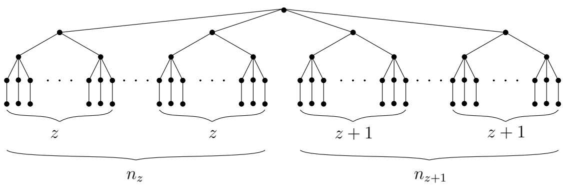


Figure 7. Minimal-ABC trees with n vertices, where $n \equiv 1 \pmod 7$.

Case $n \equiv 2 \pmod 7$

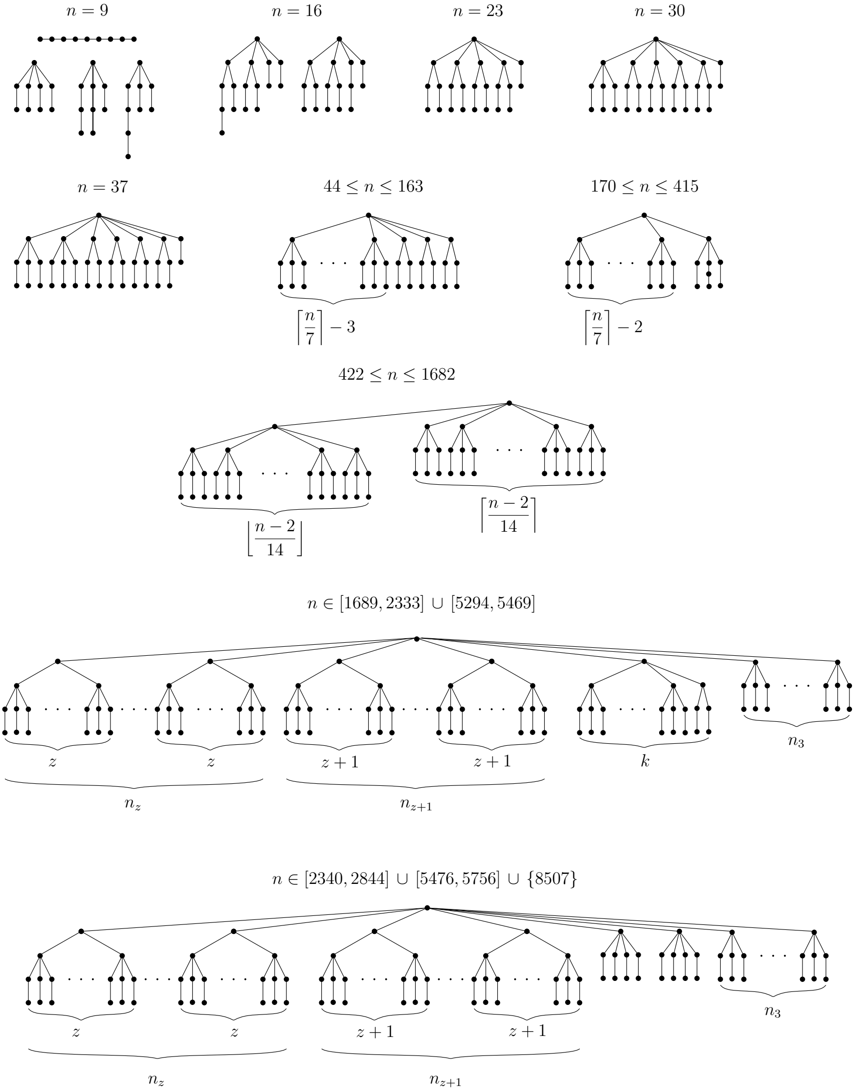
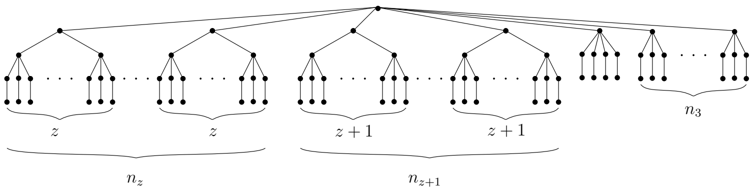


Figure 8. Minimal-ABC trees with n vertices, where $n \equiv 2 \pmod 7$.

Case $n \equiv 2 \pmod 7$

$n \in [2851, 3698] \cup [5763, 6547] \cup [5763, 6547] \cup [8514, 9277] \cup [11405, 11944] \cup [14247, 14576] \cup [17047, 17180]$

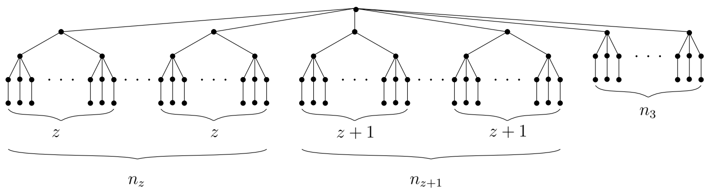


$n \in [3705, 5287] \cup [6554, 8500] \cup [9284, 11398] \cup [11951, 14240] \cup [14583, 17040] \cup [17187, 990215]$

$\cup[990236, 992700] \cup [992742, 995192] \cup [995248, 997677] \cup [997754, 1000169] \cup [1000260, 1002661]$

$\cup[1002766, 1005160] \cup [1005272, 1007659] \cup [1007778, 1010158] \cup [1010284, 1012664] \cup [1012790, 1015163]$

$\cup[1017557, 1017676]$



$n \in [990222, 990229] \cup [992707, 992735] \cup [995199, 995241] \cup [997684, 997747] \cup [1000176, 1000253]$

$\cup[1002668, 1002759] \cup [1005167, 1005265] \cup [1007666, 1007771] \cup [1010165, 1010277]$

$\cup[1012671, 1012783] \cup [1015170, 1017550] \cup [1017683, \infty)$

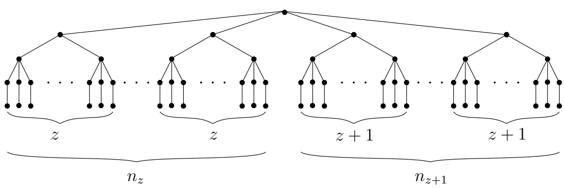
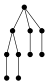


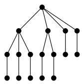
Figure 9. Minimal-ABC trees with n vertices, where $n \equiv 2 \pmod 7$.

Case $n \equiv 3 \pmod 7$

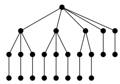
$n = 10$



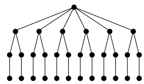
$n = 17$



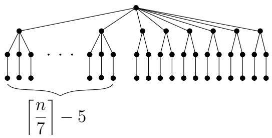
$n = 24$



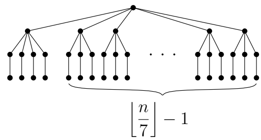
$n = 31$



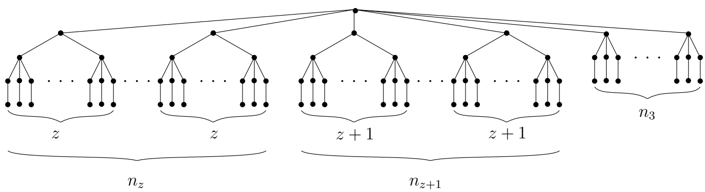
$38 \le n \le 73$



$80 \le n \le 857$



$n \in [864, 2257] \cup [4126, 5764] \cup [6954, 8921] \cup [9670, 11805] \cup [12330, 14640] \cup [14955, 17440] \cup [17559, 990573]$
$\cup [990594, 993058] \cup [993100, 995543] \cup [995606, 998035] \cup [998112, 1000527] \cup [1000618, 1003019]$
$\cup [1003124, 1005518] \cup [1005630, 1008017] \cup [1008136, 1010516] \cup [1010642, 1013015] \cup [1013148, 1015521]$



$n \in [2264, 2810] \cup [5771, 5897]$

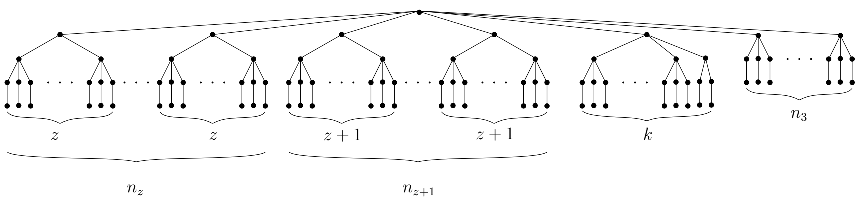
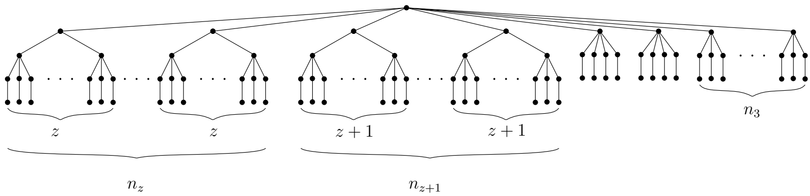


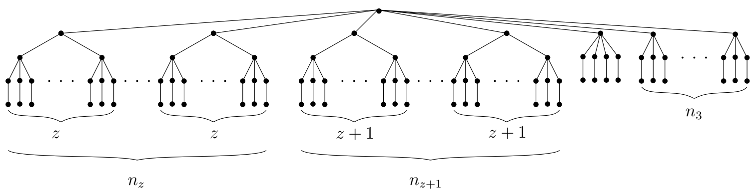
Figure 10. Minimal-ABC trees with n vertices, where $n \equiv 3 \pmod 7$.

Case $n \equiv 3 \pmod 7$

$n \in [2817, 3279] \cup [5904, 6156]$



$n \in [3286, 4119] \cup [6163, 6947] \cup [8928, 9663] \cup [11812, 12323] \cup [14647, 14948] \cup [17447, 17552]$



$$n \in [990580, 990587] \cup [993065, 993093] \cup [995550, 995599] \cup [998042, 998105] \cup [1000534, 1000611]$$
$$\cup [1003026, 1003117] \cup [1005525, 1005623] \cup [1008024, 1008129] \cup [1010523, 1010635]$$
$$\cup [1013022, 1013141] \cup [1015528, \infty)$$

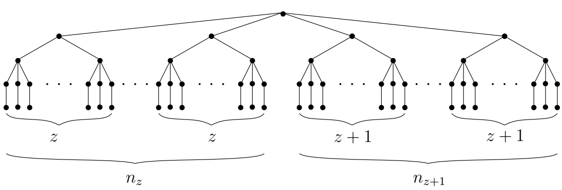


Figure 11. Minimal-ABC trees with n vertices, where $n \equiv 3 \pmod 7$.

Case $n \equiv 4 \pmod 7$

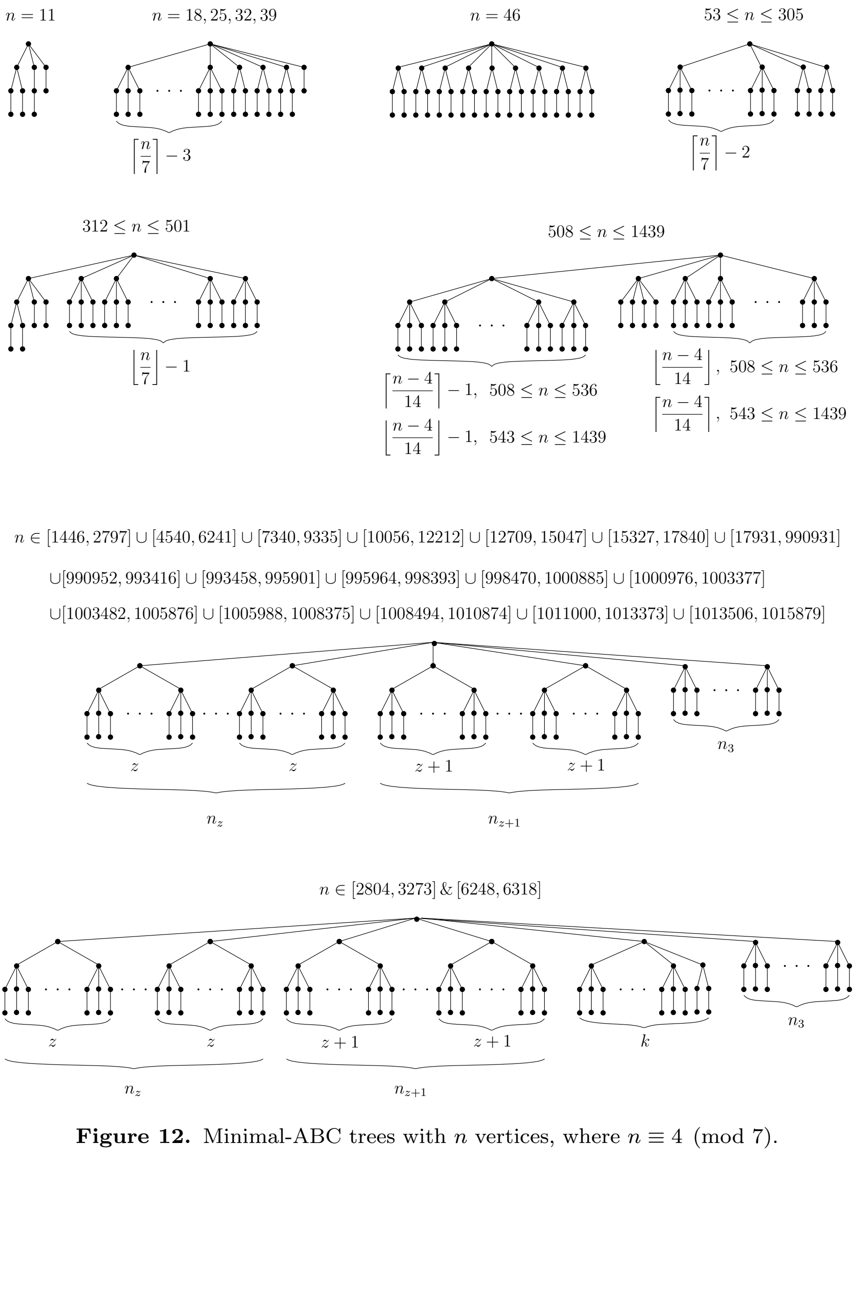
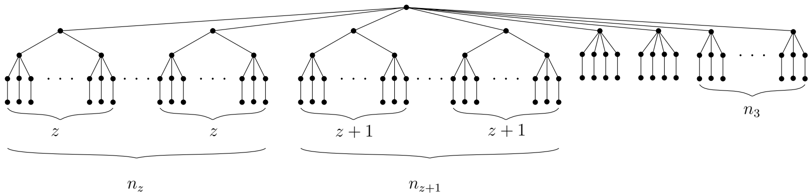


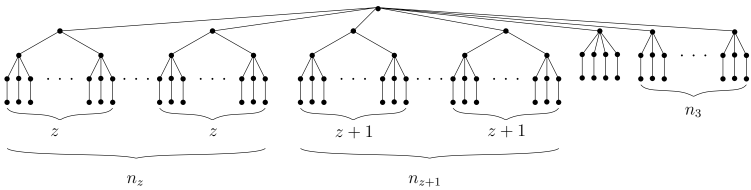
Figure 12. Minimal-ABC trees with n vertices, where $n \equiv 4 \pmod 7$.

Case $n \equiv 4 \pmod 7$

$n \in [3280, 3700] \cup [6325, 6549]$



$n \in [3707, 4533] \cup [6556, 7333] \cup [9342, 10049] \cup [12219, 12702] \cup [15054, 15320] \cup [17847, 17924]$



$n \in [2842, 4319] \cup [5761, 7616] \cup [990938, 990945] \cup [993423, 993451] \cup [995908, 995957] \cup [998400, 998463]$
$\cup [1000892, 1000969] \cup [1003384, 1003475] \cup [1005883, 1005981] \cup [1008382, 1008487] \cup [1010881, 1010993]$
$\cup [1013380, 1013499] \cup [1015886, \infty)$

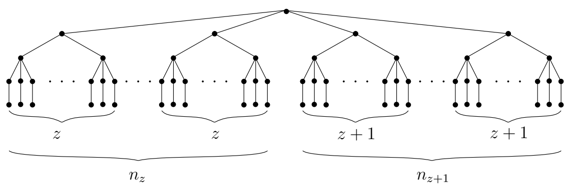
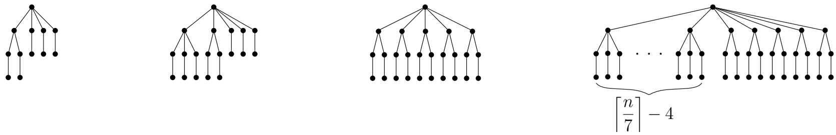


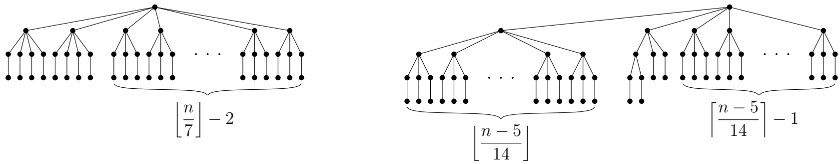
Figure 13. Minimal-ABC trees with n vertices, where $n \equiv 4 \pmod 7$.

Case $n \equiv 5 \pmod 7$

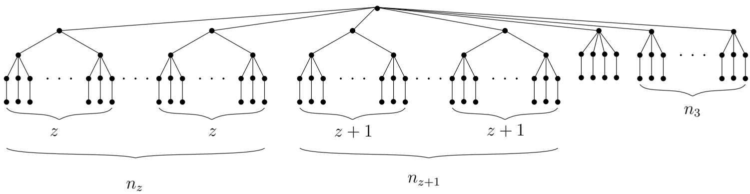
$n = 12$ $n = 19$ $n = 26$ $33 \leq n \leq 110$



$117 \leq n \leq 733$ $740 \leq n \leq 999$



$n \in [1006, 1930] \cup [4128, 4940] \cup [6956, 7726] \cup [9763, 10428] \cup [12626, 13081] \cup [15454, 15692] \cup [18247, 18296]$



$n \in [1937, 3316] \cup [4947, 6711] \cup [7733, 9756] \cup [10435, 12619] \cup [13088, 15447] \cup [15699, 18240] \cup [18303, 991282]$
$\cup [991310, 993767] \cup [993816, 996259] \cup [996322, 998744] \cup [998828, 1001236] \cup [1001334, 1003735]$
$\cup [1003840, 1006227] \cup [1006346, 1008726] \cup [1008852, 1011232] \cup [1011358, 1013731] \cup [1013864, 1016237]$

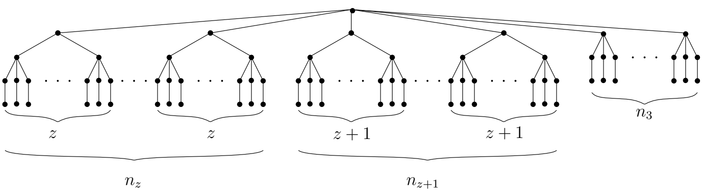
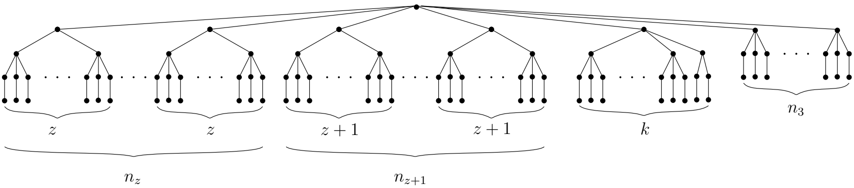


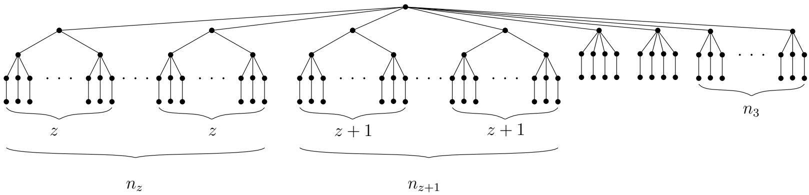
Figure 14. Minimal-ABC trees with n vertices, where $n \equiv 5 \pmod 7$.

Case $n \equiv 5 \pmod 7$

$n \in [3323, 3722] \cup [6718, 6739]$



$n \in [3729, 4121] \cup [6746, 6949]$



$n \in [991289, 991303] \cup [993774, 993809] \cup [996266, 996315] \cup [998751, 998821] \cup [1001243, 1001327]$
$\cup [1003742, 1003833] \cup [1006234, 1006339] \cup [1008733, 1008845] \cup [1011239, 1011351]$
$\cup [1013738, 1013857] \cup [1016244, \infty)$

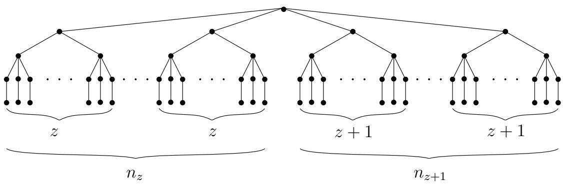


Figure 15. Minimal-ABC trees with n vertices, where $n \equiv 5 \pmod 7$.

Case $n \equiv 6 \pmod 7$

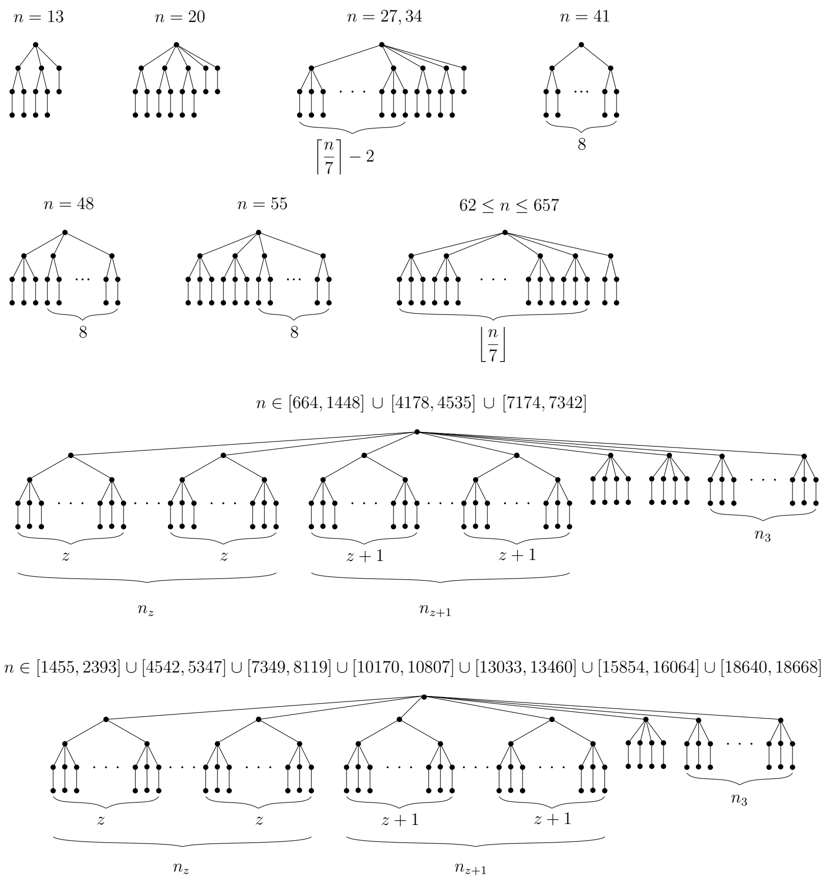
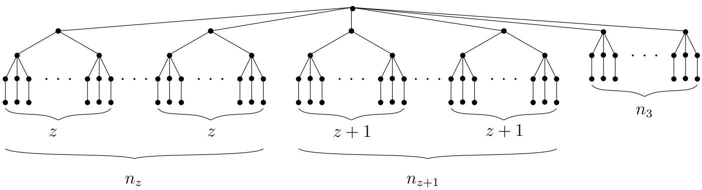


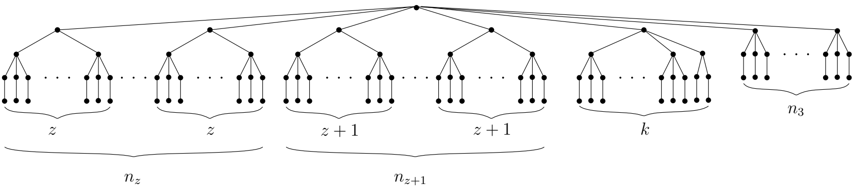
Figure 16. Minimal-ABC trees with n vertices, where $n \equiv 6 \pmod 7$.

Case $n \equiv 6 \pmod 7$

$n \in [2400, 3821] \cup [5354, 7167] \cup [8126, 10163] \cup [10814, 13026] \cup [13467, 15847] \cup [16071, 18633] \cup [18675, 991640]$
$\cup[991668, 994125] \cup [994174, 996610] \cup [996680, 999102] \cup [999186, 1001594] \cup [1001692, 1004086]$
$\cup[1004198, 1006585] \cup [1006704, 1009084] \cup [1009210, 1011590] \cup [1011716, 1014089] \cup [1014712, 1016595]$



$3828 \le n \le 4171$



$n \in [991647, 991661] \cup [994132, 994167] \cup [996617, 996673] \cup [999109, 999179] \cup [1001601, 1001685]$
$\cup[1004093, 1004191] \cup [1006592, 1006697] \cup [1009091, 1009203] \cup [1011597, 1011709]$
$\cup[1014096, 1014705] \cup [1016602, \infty)$

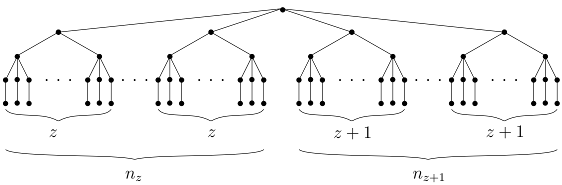


Figure 17. Minimal-ABC trees with n vertices, where $n \equiv 6 \pmod 7$.