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On Extremum Geometric–Arithmetic Indices of (Molecular) Trees

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Abstract

The geometric-arithmetic index (GA index for short) is a newly proposed graph invariant, based on the end-vertex degrees of all edges of a graph, in mathematical chemistry. Du *et al.* [On geometric arithmetic indices of (molecular) trees, unicyclic graphs and bicyclic graphs, MATCH Commun. Math. Comput. Chem. 66 (2011), 681–697] determined the first six maximum values for the GA indices of trees. In this paper, we will present a further ordering for the GA indices of trees, and determine the first fourteen maximum values. In particular, the trees with the first fourteen maximum GA indices are all molecular trees.

1 Introduction

Molecular descriptors play a significant role in mathematical chemistry, especially in the QSPR/QSAR investigations. Among them, special place is reserved for the so-called topological indices [2]. Nowadays, there exists a legion of topological indices that found some applications in chemistry [6].

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The Randić connectivity index [5] is one of the most well-known topological indices, which is based on the end-vertex degrees of all edges in a graph. Motivated by Randić connectivity index, Vukičević and Furtula [7] proposed another topological index based on the end-vertex degrees of all edges in a graph, which is named geometric-arithmetic index (GA index for short).

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. For $u \in V(G)$, let d_u denote the degree of vertex u in G. The GA index of the graph G is defined as [7]

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v},$$

where the summation extends over all edges uv in G.

It is noted in [7] that the predictive power of GA index for physico-chemical properties (e.g., boiling point, entropy, enthalpy and standard enthalpy of vaporization, enthalpy of formation, acentric factor) is somewhat better that the one of Randić connectivity index.

In [7], Vukičević and Furtula established some lower and upper bounds for the GA index of graphs, and identified the trees with the minimum and the maximum GA indices, which are the star and the path, respectively. In [8], Yuan *et al.* gave the lower and upper bounds for the GA index of molecular graphs in terms of the numbers of vertices and edges, they also determined the n-vertex molecular trees with the minimum, the second minimum and the third minimum, as well as the second maximum and the third maximum GA indices.

Since then, the GA index received considerable attention of mathematicians also, but there are few papers about it dedicated to molecular graphs [3, 4]. In [1], the authors collected all hitherto obtained results on the GA index of graphs.

Recently, Du *et al.* [3] determined the trees with the first six maximum GA indices. In this paper, we will extend this ordering, and determine the trees with the first fourteen maximum GA indices.

2 Preliminary Results

Note that for an edge uv of a graph G,

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v} \leq 1$$

with equality if and only if $d_u = d_v$. This fact will be used frequently in our proof.

A pendant vertex is a vertex of degree one. A pendant edge is an edge incident with a pendant vertex. A path $u_1 u_2 \cdots u_r$ in a graph G is said to be a pendant path at u_1 if $d_{u_1} \geq 3$, $d_{u_i} = 2$ for $2, \ldots, r-1$ and $d_{u_r} = 1$.

Lemma 1 *[3] If there are k pendant paths in an n-vertex tree G, then*

$$GA(G) \leq \left(\frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} \right) k + n - 1 - 2k \ .$$

Among the n-vertex trees with $n \geq 4$, the path P_n is the unique tree with the maximum GA index, which is equal to $n - 3 + \frac{4\sqrt{2}}{3}$, see [7].

The following results were obtained in [3].

Theorem A *[3] Among the set of n-vertex trees,*

(*i*) *for $n \geq 7$, the trees with a single vertex of maximum degree three, adjacent to three vertices of degree two, are the unique trees with the second maximum GA index, which is equal to $n - 7 + \frac{6\sqrt{6}}{5} + 2\sqrt{2}$,*

(*ii*) *for $n \geq 7$, the trees with a single vertex of maximum degree three, adjacent to one vertex of degree one and two vertices of degree two, are the unique trees with the third maximum GA index, which is equal to $n - 6 + \frac{4\sqrt{6}}{5} + \frac{\sqrt{3}}{2} + \frac{4\sqrt{2}}{3}$,*

(*iii*) *for $n \geq 10$, the trees with exactly two adjacent vertices of maximum degree three, each adjacent to two vertices of degree two, are the unique trees with the fourth maximum GA index, which is equal to $n - 9 + \frac{8\sqrt{6}}{5} + \frac{8\sqrt{2}}{3}$,*

(*iv*) *for $n \geq 10$, the tree with a single vertex of maximum degree three, adjacent to two vertices of degree one and one vertex of degree two, is the unique tree with the fifth maximum GA index, which is equal to $n - 5 + \frac{2\sqrt{6}}{5} + \sqrt{3} + \frac{2\sqrt{2}}{3}$,*

(*v*) *for $n \geq 11$, the trees with exactly two vertices of maximum degree three, each adjacent to three vertices of degree two, are the unique trees with the sixth maximum GA index, which is equal to $n - 11 + \frac{12\sqrt{6}}{5} + \frac{8\sqrt{2}}{3}$.*

3 Main Results

In this section, we present our main theorem.

Theorem 1 *Among the set of n-vertex trees,*

(*i*) *for $n \geq 11$, the trees with exactly two adjacent vertices of maximum degree three, one is adjacent to two vertices of degree two, and the other is adjacent to one vertex of degree two and one vertex of degree one, are the unique trees with the seventh maximum GA index, which is equal to $n - 8 + \frac{6\sqrt{6}}{5} + \frac{\sqrt{3}}{2} + 2\sqrt{2}$,*

(*ii*) *for $n \geq 13$, the trees with exactly three vertices of maximum degree three, say u, v, w, where both u and v, and v and w are adjacent, each of u, w is adjacent to two vertices of degree two, and v is adjacent to one vertex of degree two, are the unique trees with the eighth maximum GA index, which is equal to $n - 11 + 2\sqrt{6} + \frac{10\sqrt{2}}{3}$,*

(*iii*) *for $n \geq 13$, the trees with exactly two non-adjacent vertices of maximum degree three, one is adjacent to three vertices of degree two, and the other is adjacent to two vertices of degree two and one vertex of degree one, are the unique trees with the ninth maximum GA index, which is equal to $n - 10 + 2\sqrt{6} + \frac{\sqrt{3}}{2} + 2\sqrt{2}$,*

(*iv*) *for $n \geq 13$, the trees with exactly two adjacent vertices of maximum degree three, each adjacent to one vertex of degree two and one vertex of degree one, or one is adjacent to two vertices of degree two, and the other is adjacent to two vertices of degree one, are the unique trees with the tenth maximum GA index, which is equal to $n - 7 + \frac{4\sqrt{6}}{5} + \sqrt{3} + \frac{4\sqrt{2}}{3}$,*

(*v*) *for $n \geq 14$, the trees with exactly three vertices of maximum degree three, say u, v, w, where u and v are not adjacent, and v and w are adjacent, u is adjacent to three vertices of degree two, each of v, w is adjacent to two vertices of degree two, are the unique trees with the eleventh maximum GA index, which is equal to $n - 13 + \frac{14\sqrt{6}}{5} + \frac{10\sqrt{2}}{3}$,*

(*vi*) *for $n \geq 14$, the trees with exactly three vertices of maximum degree three, say u, v, w, where both u and v, and v and w are adjacent, each of u, w is adjacent to two vertices of degree two, and v is adjacent to one vertex of degree one, or u is adjacent to two vertices of degree two, v is adjacent to one vertex of degree two, and w is adjacent* *to one vertex of degree two and one vertex of degree one, are the unique trees with the twelfth maximum GA index, which is equal to* $n - 10 + \frac{8\sqrt{6}}{5} + \frac{\sqrt{3}}{2} + \frac{8\sqrt{2}}{3}$,

(*vii*) *for* $n \geq 14$, *the trees with a single vertex of maximum degree four, adjacent to four vertices of degree two, and without vertices of degree three, are the unique trees with the thirteenth maximum GA index, which is equal to* $n - 9 + \frac{16\sqrt{2}}{3}$,

(*viii*) *for* $n \geq 14$, *the trees with exactly two non-adjacent vertices of maximum degree three, each adjacent to two vertices of degree two and one vertex of degree one, or one is adjacent to three vertices of degree two, and the other is adjacent to two vertices of degree one and one vertex of degree two, are the unique trees with the fourteenth maximum GA index, which is equal to* $n - 9 + \frac{8\sqrt{6}}{5} + \sqrt{3} + \frac{4\sqrt{2}}{3}$,

Proof: Let G be an n-vertex tree different from the six types of trees mentioned in Theorem A with the first six maximum GA indices, where $n \geq 11$. Obviously, there are at least four pendant paths in G.

If there are $k \geq 6$ pendant paths in G, then by Lemma 1, we have

$$\begin{aligned} GA(G) &\leq \left(\frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} \right) k + n - 1 - 2k \\ &\leq \left(\frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} \right) \cdot 6 + n - 1 - 2 \cdot 6 \\ &< n - 9 + \frac{8\sqrt{6}}{5} + \sqrt{3} + \frac{4\sqrt{2}}{3}. \end{aligned}$$

Case 1. There are exactly four pendant paths in G.

In the following, there are still two subcases need to be considered.

Subcase 1.1. There are exactly two vertices of maximum degree three in G, and other vertices are of degree one or two.

Subcase 1.2. There is a single vertex of maximum degree four in G, and other vertices are of degree one or two.

Suppose that **Subcase 1.1** holds. Denote by u and v the two vertices of maximum degree three in G.

First suppose that there is exactly one pendant path of length one in G. If u and v are adjacent in G, then we have

$$GA(G) = n - 8 + \frac{6\sqrt{6}}{5} + \frac{\sqrt{3}}{2} + 2\sqrt{2}\ .$$

If u and v are non-adjacent, then we have

$$GA(G) = n - 10 + 2\sqrt{6} + \frac{\sqrt{3}}{2} + 2\sqrt{2}\,.$$

Next suppose that there are exactly two pendant paths of length one in G. If u and v are adjacent in G, then we have

$$GA(G) = n - 7 + \frac{4\sqrt{6}}{5} + \sqrt{3} + \frac{4\sqrt{2}}{3}\,.$$

If u and v are non-adjacent, then we have

$$GA(G) = n - 9 + \frac{8\sqrt{6}}{5} + \sqrt{3} + \frac{4\sqrt{2}}{3}\,.$$

Suppose that there are exactly three or four pendant paths of length one in G. Denote by k the number of pendant paths of length one in G. Clearly, $k = 3, 4$. Then

$$\begin{aligned}
GA(G) &\leq k \cdot \frac{2\sqrt{1\cdot 3}}{1+3} + (4-k)\left(\frac{2\sqrt{1\cdot 2}}{1+2} + \frac{2\sqrt{2\cdot 3}}{2+3}\right) \\
&\quad + (n-1) - (8-k) \\
&= \left(\frac{\sqrt{3}}{2} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{6}}{5} + 1\right) k + n - 9 + \frac{8\sqrt{6}}{5} + \frac{8\sqrt{2}}{3} \\
&\leq \left(\frac{\sqrt{3}}{2} - \frac{2\sqrt{2}}{3} - \frac{2\sqrt{6}}{5} + 1\right) 3 + n - 9 + \frac{8\sqrt{6}}{5} + \frac{8\sqrt{2}}{3} \\
&< n - 9 + \frac{8\sqrt{6}}{5} + \sqrt{3} + \frac{4\sqrt{2}}{3}\,.
\end{aligned}$$

Now suppose that **Subcase 1.2** holds. Denote by k the number of pendant paths of length one in G. Clearly, $k = 0, 1, 2, 3$. Then

$$\begin{aligned}
GA(G) &= k \cdot \frac{2\sqrt{1\cdot 4}}{1+4} + (4-k)\left(\frac{2\sqrt{1\cdot 2}}{1+2} + \frac{2\sqrt{2\cdot 4}}{2+4}\right) \\
&\quad + (n-1) - (8-k) \\
&= \left(\frac{9}{5} - \frac{4\sqrt{2}}{3}\right) k + n - 9 + \frac{16\sqrt{2}}{3}\,.
\end{aligned}$$

If $k = 0$, i.e., all the four pendant paths in G are of length at least two, then

$$GA(G) = n - 9 + \frac{16\sqrt{2}}{3}\,.$$

If $k = 1, 2, 3$, then

$$GA(G) = \left(\frac{9}{5} - \frac{4\sqrt{2}}{3}\right) k + n - 9 + \frac{16\sqrt{2}}{3}$$

$$
\begin{aligned}
&\le \left(\frac{9}{5}-\frac{4\sqrt{2}}{3}\right)1+n-9+\frac{16\sqrt{2}}{3}\\
&< n-9+\frac{8\sqrt{6}}{5}+\sqrt{3}+\frac{4\sqrt{2}}{3}\,.
\end{aligned}
$$

Case 2. Suppose that there are exactly five pendant paths in G.

In this case, there are three subcases need to be considered.

Subcase 2.1. There are exactly three vertices of maximum degree three, and other vertices are of degree one or two.

Subcase 2.2. There is a single vertex of maximum degree five in G, and other vertices are of degree one or two.

Subcase 2.3. There is exactly one vertex of degree three, one vertex of maximum degree four, and other vertices are of degree one or two.

Suppose that **Subcase 2.1** holds. Note that there are at most two pairs of adjacent vertices both of maximum degree three.

First suppose that there are exactly two pairs of adjacent vertices both of maximum degree three. Denote by k the number of pendant paths of length one in G. Clearly, $0 \le k \le 5$. Then

$$
\begin{aligned}
GA(G) &= k\cdot\frac{2\sqrt{1\cdot 3}}{1+3}+(5-k)\left(\frac{2\sqrt{1\cdot 2}}{1+2}+\frac{2\sqrt{2\cdot 3}}{2+3}\right)\\
&\quad +(n-1)-(10-k)\\
&= \left(\frac{\sqrt{3}}{2}-\frac{2\sqrt{2}}{3}-\frac{2\sqrt{6}}{5}+1\right)k+n-11+2\sqrt{6}+\frac{10\sqrt{2}}{3}\,.
\end{aligned}
$$

If $k=0$, i.e., all the five pendant paths in G are of length at least two, then

$$GA(G)=n-11+2\sqrt{6}+\frac{10\sqrt{2}}{3}\,.$$

If $k=1$, i.e., there is exactly one pendant path of length one in G, then

$$GA(G)=n-10+\frac{8\sqrt{6}}{5}+\frac{\sqrt{3}}{2}+\frac{8\sqrt{2}}{3}\,.$$

If $k=2,3,4,5$, then

$$
\begin{aligned}
GA(G) &= \left(\frac{\sqrt{3}}{2}-\frac{2\sqrt{2}}{3}-\frac{2\sqrt{6}}{5}+1\right)k+n-11+2\sqrt{6}+\frac{10\sqrt{2}}{3}\\
&\le \left(\frac{\sqrt{3}}{2}-\frac{2\sqrt{2}}{3}-\frac{2\sqrt{6}}{5}+1\right)2+n-11+2\sqrt{6}+\frac{10\sqrt{2}}{3}
\end{aligned}
$$

$$< \quad n-9+\frac{8\sqrt{6}}{5}+\sqrt{3}+\frac{4\sqrt{2}}{3}\ .$$

Next suppose that any two vertices of maximum degree three are not adjacent. Denote by k the number of pendant paths of length one in G. Clearly, $0 \le k \le 5$. Then

$$\begin{aligned}
GA(G) &= k\cdot\frac{2\sqrt{1\cdot 3}}{1+3}+(5-k)\left(\frac{2\sqrt{1\cdot 2}}{1+2}+\frac{2\sqrt{2\cdot 3}}{2+3}\right)\\
&\quad +4\cdot\frac{2\sqrt{2\cdot 3}}{2+3}+(n-1)-(14-k)\\
&= \left(\frac{\sqrt{3}}{2}-\frac{2\sqrt{2}}{3}-\frac{2\sqrt{6}}{5}+1\right)k+n-15+\frac{18\sqrt{6}}{5}+\frac{10\sqrt{2}}{3}\\
&\le n-15+\frac{18\sqrt{6}}{5}+\frac{10\sqrt{2}}{3}<n-9+\frac{8\sqrt{6}}{5}+\sqrt{3}+\frac{4\sqrt{2}}{3}\ .
\end{aligned}$$

Now suppose that there is exactly one pair of adjacent vertices both of maximum degree three. Denote by k the number of pendant paths of length one in G. Clearly, $0 \le k \le 5$. Then

$$\begin{aligned}
GA(G) &= k\cdot\frac{2\sqrt{1\cdot 3}}{1+3}+(5-k)\left(\frac{2\sqrt{1\cdot 2}}{1+2}+\frac{2\sqrt{2\cdot 3}}{2+3}\right)\\
&\quad +2\cdot\frac{2\sqrt{2\cdot 3}}{2+3}+(n-1)-(12-k)\\
&= \left(\frac{\sqrt{3}}{2}-\frac{2\sqrt{2}}{3}-\frac{2\sqrt{6}}{5}+1\right)k+n-13+\frac{14\sqrt{6}}{5}+\frac{10\sqrt{2}}{3}\ .
\end{aligned}$$

If $k=0$, i.e., all the five pendant paths in G are of length at least two, then

$$GA(G)=n-13+\frac{14\sqrt{6}}{5}+\frac{10\sqrt{2}}{3}\ .$$

If $k=1,2,3,4,5$, then

$$\begin{aligned}
GA(G) &= \left(\frac{\sqrt{3}}{2}-\frac{2\sqrt{2}}{3}-\frac{2\sqrt{6}}{5}+1\right)k+n-13+\frac{14\sqrt{6}}{5}+\frac{10\sqrt{2}}{3}\\
&\le \left(\frac{\sqrt{3}}{2}-\frac{2\sqrt{2}}{3}-\frac{2\sqrt{6}}{5}+1\right)1+n-13+\frac{14\sqrt{6}}{5}+\frac{10\sqrt{2}}{3}\\
&< n-9+\frac{8\sqrt{6}}{5}+\sqrt{3}+\frac{4\sqrt{2}}{3}\ .
\end{aligned}$$

Suppose that **Subcase 2.2** holds. Denote by k the number of pendant paths of length one in G. Then

$$GA(G) = k\cdot\frac{2\sqrt{1\cdot 5}}{1+5}+(5-k)\left(\frac{2\sqrt{1\cdot 2}}{1+2}+\frac{2\sqrt{2\cdot 5}}{2+5}\right)+(n-1)-(10-k)$$

$$
\begin{aligned}
&= \left(\frac{\sqrt{5}}{3}-\frac{2\sqrt{2}}{3}-\frac{2\sqrt{10}}{7}+1\right)k+n-11+\frac{10\sqrt{10}}{7}+\frac{10\sqrt{2}}{3}\\
&\le n-11+\frac{10\sqrt{10}}{7}+\frac{10\sqrt{2}}{3}<n-9+\frac{8\sqrt{6}}{5}+\sqrt{3}+\frac{4\sqrt{2}}{3}\ .
\end{aligned}
$$

Now we suppose that **Subcase 2.3** holds. Denote by k_1 (k_2, respectively) the number of pendant paths of length one attached to the unique vertex of degree three (four, respectively) in G. Clearly, $k_1 = 0, 1, 2$ and $k_2 = 0, 1, 2, 3$. Then

$$
\begin{aligned}
GA(G) \ &\le\ k_1\cdot\frac{2\sqrt{1\cdot 3}}{1+3}+(2-k_1)\left(\frac{2\sqrt{1\cdot 2}}{1+2}+\frac{2\sqrt{2\cdot 3}}{2+3}\right)\\
&\quad k_2\cdot\frac{2\sqrt{1\cdot 4}}{1+4}+(3-k_2)\left(\frac{2\sqrt{1\cdot 2}}{1+2}+\frac{2\sqrt{2\cdot 4}}{2+4}\right)\\
&\quad +(n-1)-(10-k_1-k_2)\\
&= \left(\frac{\sqrt{3}}{2}-\frac{2\sqrt{2}}{3}-\frac{2\sqrt{6}}{5}+1\right)k_1+\left(\frac{9}{5}-\frac{4\sqrt{2}}{3}\right)k_2\\
&\quad +n-11+\frac{4\sqrt{6}}{5}+\frac{16\sqrt{2}}{3}\\
&\le n-11+\frac{4\sqrt{6}}{5}+\frac{16\sqrt{2}}{3}<n-9+\frac{8\sqrt{6}}{5}+\sqrt{3}+\frac{4\sqrt{2}}{3}\ .
\end{aligned}
$$

Finally, it is easy to check that

$$
\begin{aligned}
&n-9+\frac{8\sqrt{6}}{5}+\sqrt{3}+\frac{4\sqrt{2}}{3}<n-9+\frac{16\sqrt{2}}{3}\\
&<n-10+\frac{8\sqrt{6}}{5}+\frac{\sqrt{3}}{2}+\frac{8\sqrt{2}}{3}<n-13+\frac{14\sqrt{6}}{5}+\frac{10\sqrt{2}}{3}\\
&<n-7+\frac{4\sqrt{6}}{5}+\sqrt{3}+\frac{4\sqrt{2}}{3}<n-10+2\sqrt{6}+\frac{\sqrt{3}}{2}+2\sqrt{2}\\
&<n-11+2\sqrt{6}+\frac{10\sqrt{2}}{3}<n-8+\frac{6\sqrt{6}}{5}+\frac{\sqrt{3}}{2}+2\sqrt{2}\ .
\end{aligned}
$$

From the above arguments, if $GA(G)$ is not equal to one of these eight values, then

$$GA(G)<n-9+\frac{8\sqrt{6}}{5}+\sqrt{3}+\frac{4\sqrt{2}}{3}\ .$$

Now the result follows easily. ■

The trees with the smallest number of vertices in Theorem 1 are listed in Appendix.

4 Conclusions

In this paper, we presented a further ordering for the GA indices of trees, and determined the first fourteen maximum GA indices of trees. In particular, in our proof, we mainly investigated the GA indices of trees with exactly four or five pendant paths. If one want to order more trees with large GA indices, it need only to consider the trees with more pendant paths (e.g., the trees with exactly six or seven pendant paths).

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5 Appendix

In the following, the trees with the smallest number of vertices in Theorem 1 are listed.

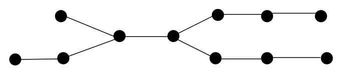

Figure 1: The tree in Theorem 1 (i) with $n = 11$.

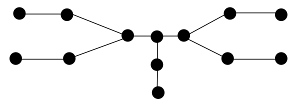

Figure 2: The tree in Theorem 1 (ii) with $n = 13$.

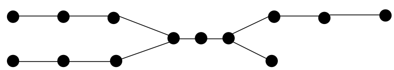

Figure 3: The tree in Theorem 1 (iii) with $n = 13$.

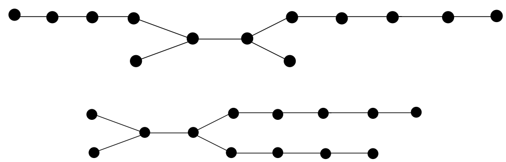

Figure 4: The tree in Theorem 1 (iv) with $n = 13$.

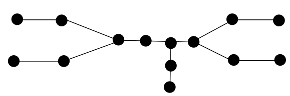

Figure 5: The tree in Theorem 1 (v) with $n = 14$.

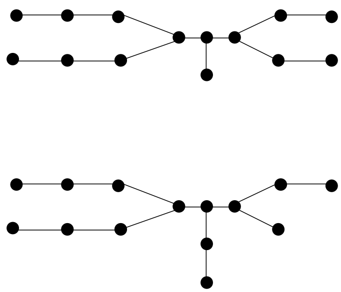

Figure 6: The tree in Theorem 1 (vi) with $n = 14$.

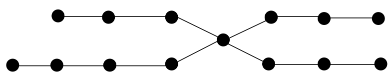

Figure 7: The tree in Theorem 1 (vii) with $n = 14$.

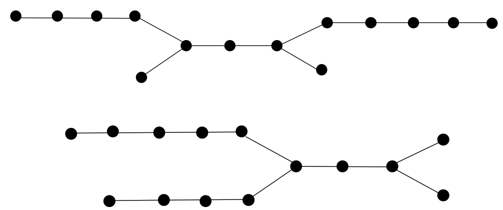

Figure 8: The tree in Theorem 1 (viii) with $n = 14$.