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On the Maximum ABS Index of Fixed-Order Trees with a Given Maximum Degree

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Abstract: The ABS (atom-bond sum-connectivity) index of a graph G is denoted by $ABS(G)$ and is defined as $\sum_{xy\in E(G)} \sqrt{(d_x+d_y)^{-1}(d_x+d_y-2)}$, where d_x represents the degree of the vertex x in G. In this paper, we derive the best possible upper bounds on the ABS index for fixed-order trees possessing a given maximum degree, which provides a solution to the open problem proposed quite recently by Hussain, Liu and Hua.

Keywords: topological index; atom-bond sum-connectivity index; tree graph; maximum degree

MSC: 05C05; 05C07; 05C09

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1. Introduction

For terminology and notions concerning graph theory or chemical graph theory, we refer the reader to books [1,2] or [3,4], respectively.

A property of graphs that remains the same under graph isomorphism is referred to as a graph invariant [5]. The graph invariants that take only numerical quantities are commonly known as topological indices in chemical graph theory [4]. It is important to note that the choice of topological index depends on the specific application and the structural features of interest.

Various topological indices capture different aspects of molecular structure and properties to aid in the prediction of molecular characteristics, and they are often used in QSPR (quantitative structure–property relationship) studies and cheminformatics to correlate the structure of chemical compounds with their properties or activities [6].

A common tool in mathematical chemistry to predict the physico-chemical characteristics of chemical compounds is the connectivity index [7], which is a topological index introduced in the mid-1970s. For a graph G, this index is represented by $R(G)$ and is defined as

$$R(G) = \sum_{xy\in E(G)} (d_x\, d_y)^{-1/2},$$

where $E(G)$ is used for representing the edge set of G, and d_x is used for representing the degree of the vertex x in G. (If two or more graphs are under consideration at once, then we use $d_G(x)$ instead of d_x to represent the degree of x in G.) To discover more about the connectivity index, see the books [8–10] and survey papers [11,12].

The atom-bond connectivity index (ABC index) [13,14] as well as the sum-connectivity (SC) index [15] are variants of the connectivity index, which were introduced with the aim of improving QSAR studies involving topological indices. These two indices for a graph G are defined as

$$ABC(G) = \sum_{xy \in E(G)} \sqrt{(d_x d_y)^{-1}(d_x + d_y - 2)} \quad \text{and} \quad SC(G) = \sum_{xy \in E(G)} (d_x + d_y)^{-1/2}.$$

We remark here that both the SC index and the connectivity index take into account only the degrees of atoms in a molecular graph, while the ABC index takes into account the degrees of both atoms and bonds in a molecular graph, providing a more detailed characterization compared to some indices that focus only on atoms or bonds individually. To discover more about the ABC index, see the surveys [16–20] and the related papers cited therein. Particularly, the reader can consult [21,22] for the solution of a well-researched problem on this index. Moreover, the surveys [19,23] and the related papers cited therein can be consulted for additional information about the SC index.

The atom-bond sum-connectivity index (ABS index) [24] can be considered as a variant of each of the ABC, connectivity and SC indices. For a graph G, this index is defined as

$$ABS(G) = \sum_{xy \in E(G)} \sqrt{(d_x + d_y)^{-1}(d_x + d_y - 2)}.$$

We remark that the ABS is a particular form of a more general index studied in [25].

Although the ABS index has been introduced quite recently, a considerable number of publications on this index have already appeared. In [26–28], this index was not only examined for its chemical applications but its mathematical aspects were also investigated. Some results regarding the extremum values of the ABS index of trees having a fixed number of degree-one and fixed-order vertices can be found in [29,30]. The ABS index was directly compared with the SC index in [31]; see also [32], where several relationships between the ABS index and some other connectivity indices were derived; see [33] for the general case. The greatest values of this index over certain families of graphs with given parameters were studied in [34]. The study on the extremum values of this index of fixed-order chemical trees, chemical unicyclic graphs, chemical bicyclic graphs and chemical tricyclic graphs was carried out in [35]. The ABS index of line graphs was studied in [36]. Some other extremal problems regarding the ABS index of trees were addressed in [37,38].

For a graph G and $x \in V(G)$, we define $N_G(x) = \{\alpha : \alpha x \in E(G)\}$; particularly, every element of this set is referred to as a neighbor of x. Also, x is a pendent vertex if $d_G(x) = 1$, and x is branching if $d_G(x) > 2$. Moreover, x is referred to as a claw if $d_G(x) - 1$ of its neighbors are pendent. Let $V_0(G)$ represent the set of pendent vertices of G. Define $V_1(G) = \{y \in V(G) : N_G(y) \cap V_0(G) \neq \emptyset\}$. The maximum degree of G is represented as $\Delta = \Delta(G)$. The graph that results from G by removing $x \in V(G)$ is represented by $G - x$. Also, the graph that results from G by deleting $xy \in E(G)$ is represented as $G - xy$. Similarly, if $xy \notin E(G)$, then $G + xy$ represents the graph that is constructed from G after inserting the edge xy. A pendent path $P = v_0 v_1 \cdots v_r$ in a graph G is a nontrivial path such that $d_G(v_0) = 1$, $d_G(v_r) \geq 3$, and $d_G(v_i) = 2$ whenever $2 \leq i \leq r - 1$. We call the vertices v_0 and v_r as the end vertices of P. The number r is called the length of the pendent path P. When r equals 1, P represents a pendent edge. Consider T as a tree with $n = |V(T)|$ and $\Delta = \Delta(T)$. When Δ equals 2, then $T = P_n$. Also, when Δ equals $n - 1$, then $T = K_{1,n-1}$. Thus, for the subsequent discussion, we assume that Δ lies between 3 and $n - 2$.

We are interested in the following problem, posed recently in [39]:

Problem 1. *Let $\mathbb{T}(n, \Delta)$ denote the class of all n-order trees with a maximum degree of Δ. Find the tree(s) possessing the largest ABS index over $\mathbb{T}(n, \Delta)$.*

The next section gives a solution to Problem 1 when $\Delta \in \{3, 4\}$. In Section 3, a solution to Problem 1 is provided when $3 \leq \lceil n/2 \rceil \leq \Delta \leq n - 2$. Finally, Problem 1 with the constraints $5 \leq \Delta < \lceil n/2 \rceil$ is addressed in Section 4, where we utilize computer software to determine trees possessing the largest ABS index over $\mathbb{T}(n, \Delta)$ for every pair (n, Δ) satisfying $5 \leq \Delta < \lceil n/2 \rceil$ and $11 \leq n \leq 16$. Based on the structures of the obtained extremal trees, we pose two conjectures.

2. Trees with Maximum Degree 3 or 4

This section is concerned with a solution to Problem 1 when $\Delta \in \{3, 4\}$. The solution to Problem 1 for $\Delta = 4$ and $n \geq 11$ follows from Theorem 12 of [24] because the trees possessing the largest ABS index over $\mathbb{T}(n, 2) \cup \mathbb{T}(n, 3) \cup \mathbb{T}(n, 4)$ have a maximum degree of 4 for $n \geq 11$ (see Theorem 12 in [24]). Also, $\mathbb{T}(6, 4)$ consists of exactly one graph. The graphs with the greatest ABS index in $\mathbb{T}(n, 4)$ with $7 \leq n \leq 10$ are given in Figure 1; these trees are found by utilizing computer software. In what follows, we provide a solution to Problem 1 when $\Delta = 3$.

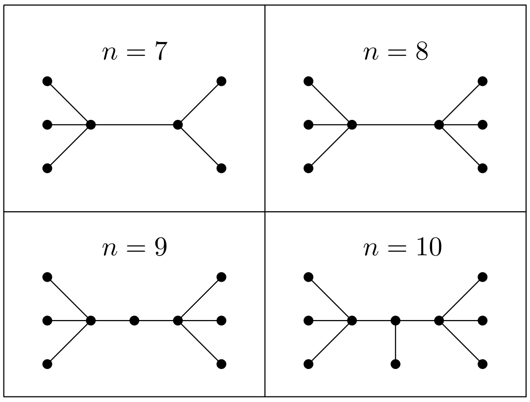

Figure 1. The trees possessing the greatest ABS index in $\mathbb{T}(n, 4)$ with $7 \leq n \leq 10$.

The number of edges in an n-order tree T with a maximum degree of 3 that join the vertices of degrees α and β is denoted by $m_{\alpha,\beta}$. The ABS index can therefore be expressed in terms of $m_{\alpha,\beta}$, as given below:

$$ABS(T) = \sum_{1 \leq \alpha \leq \beta \leq 3} \sqrt{1 - \frac{2}{\alpha + \beta}}\, m_{\alpha,\beta}, \tag{1}$$

Let n_α represent the number of degree α vertices in tree T. Then,

$$\sum_{\alpha=1}^{3} n_\alpha = n, \tag{2}$$

$$\sum_{\alpha=1}^{3} \alpha \cdot n_\alpha = 2(n-1), \tag{3}$$

$$\sum_{\substack{1 \leq \alpha \leq 3 \\ \alpha \neq \beta}} m_{\beta,\alpha} + 2m_{\beta,\beta} = \beta \cdot n_\beta, \quad \beta = 1, 2, 3. \tag{4}$$

Theorem 1. *Let $\mathbb{T}(n, 3)$ denote the class of all n-order trees such that $\Delta = 3$.*

(a). *If n is even and $n \geq 4$, then the largest ABS index in $\mathbb{T}(n, 3)$ is*

$$\left(\frac{3\sqrt{2} + 2\sqrt{6}}{12}\right) n + \frac{3\sqrt{2} - 4\sqrt{6}}{6},$$

which is possessed by only those trees that consist of vertices of degrees 1 and 3; for an example, see Figure 2.

(b). *If n is odd and $n \geq 7$, then the largest ABS index in $\mathbb{T}(n,3)$ is*

$$\left(\frac{3\sqrt{2}+2\sqrt{6}}{12}\right)n + \frac{15\sqrt{2}-70\sqrt{6}+24\sqrt{15}}{60},$$

which is possessed by only those trees that have only one vertex with a degree of 2, whose both neighbors have degree 3; for an example, see Figure 3.

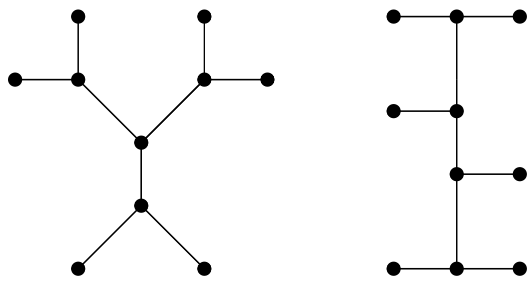

Figure 2. Examples of trees possessing the greatest ABS index in the class $\mathbb{T}(10,3)$.

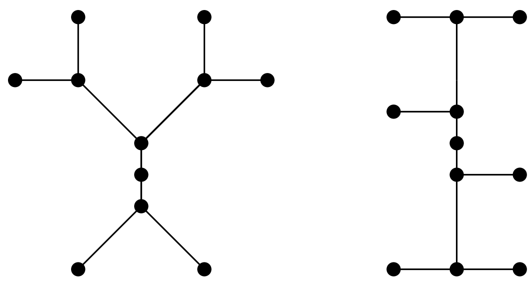

Figure 3. Examples of trees possessing the greatest ABS index in the class $\mathbb{T}(11,3)$.

Proof. For the unknowns $m_{1,3}, m_{3,3}, n_3, n_2$ and n_1, we solve Equations (2)–(4). The values of $m_{1,3}$ and $m_{3,3}$ are provided below:

$$m_{1,3} = \frac{1}{4}(2n + 4 - m_{2,3} - 2m_{2,2} - 5m_{1,2}), \tag{5}$$

$$m_{3,3} = \frac{1}{4}(2n - 8 - 3m_{2,3} - 2m_{2,2} + m_{1,2}). \tag{6}$$

By utilizing Equations (5) and (6) in Equation (1), we arrive at the following equation:

$$\begin{aligned} ABS(T) &= \left(\frac{3\sqrt{2}+2\sqrt{6}}{12}\right)n + \frac{3\sqrt{2}-4\sqrt{6}}{6} + \left(\frac{2\sqrt{6}-15\sqrt{2}+8\sqrt{3}}{24}\right)m_{1,2} \\ &\quad + \left(\frac{3\sqrt{2}-2\sqrt{6}}{12}\right)m_{2,2} + \left(\frac{8\sqrt{15}-5\sqrt{2}-10\sqrt{6}}{40}\right)m_{2,3}. \end{aligned} \tag{7}$$

Let

$$\begin{aligned} \Gamma_{ABS}(T) = \left(\frac{2\sqrt{6}-15\sqrt{2}+8\sqrt{3}}{24}\right)m_{1,2} + \left(\frac{3\sqrt{2}-2\sqrt{6}}{12}\right)m_{2,2} \\ + \left(\frac{8\sqrt{15}-5\sqrt{2}-10\sqrt{6}}{40}\right)m_{2,3}. \end{aligned} \tag{8}$$

Thus, Equation (7) can be rewritten as follows:

$$ABS(T) = \left(\frac{3\sqrt{2}+2\sqrt{6}}{12}\right)n + \frac{3\sqrt{2}-4\sqrt{6}}{6} + \Gamma_{ABS}(T). \tag{9}$$

Observe that

$$\Gamma_{ABS}(T) \approx -0.10240\, m_{1,2} - 0.05469\, m_{2,2} - 0.01455\, m_{2,3} \leq 0, \tag{10}$$

which means that it suffices to search tree T for which $\Gamma_{ABS}(T)$ is maximum in order to achieve the greatest values of the ABS index of T.

(a). Suppose that n is even and $n \geq 4$. Let T_4 be the star graph of order 4. Let T_{n+2} denote the tree formed by attaching two new pendent vertices at a pendent vertex of T_n. Thus, it is always possible to construct an n-order tree consisting of only vertices of degrees 1 and 3 when n is even and $n \geq 4$; for such a tree, the value of Γ_{ABS} is 0. Thus, part (a) now follows from (8) and (10).

(b). Suppose that n is odd and $n \geq 7$. Then, every n-order tree T with a maximum degree of 3 possesses at least one vertex of degree 2. However, (8) or (10) imply that

$$\Gamma_{ABS}(T) \leq \frac{8\sqrt{15}-5\sqrt{2}-10\sqrt{6}}{20} \tag{11}$$

with equality if and only if $n_2 = 1$, $m_{2,3} = 2$ and $m_{1,2} = m_{2,2} = 0$. Let T_7^* denote the tree with 7 vertices depicted in Figure 4. Denote the constructed tree by T_{n+2}^* by attaching two new pendent vertices at a pendent vertex of T_n^* for odd $n \geq 7$. Thus, it is always possible to construct an n-order tree such that $\Delta = 3$ and where it only has a single vertex with a degree of 2, whenever n is odd and $n \geq 7$; for such a tree, the value of Γ_{ABS} is $\frac{8\sqrt{15}-5\sqrt{2}-10\sqrt{6}}{20}$. Thus, part (b) now follows from (8) and (11).

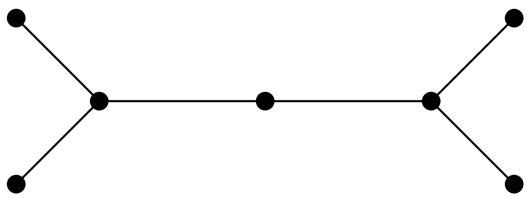

Figure 4. The tree T_7^* used in the proof of Theorem 1.

□

3. On *n*-Order Trees of Maximum Degree at Least $\lceil n/2 \rceil$

This section is devoted to finding a solution to Problem 1 when $\Delta \geq \lceil n/2 \rceil$. Before proving the main result of the present section, we prove a crucial lemma.

Lemma 1. *For a tree T, take $x, y \in V(T)$, satisfying $d_T(x) > d_T(y) \geq 2$. Also, take $xx_0, yy_0 \in E(T)$, where y_0 is pendent and x_0 does not lie on the unique path connecting x and y. Let $N_T(x_0) \setminus \{x\} = \{x_1, x_2, \cdots, x_{r-1}\}$ with $r \geq 2$. Assume that T' is the tree formed from T by removing the edges $x_0x_1, x_0x_2, \cdots, x_0x_{r-1}$ and inserting the edges $y_0x_1, y_0x_2, \cdots, y_0x_{r-1}$. Then,*

$$ABS(T') > ABS(T).$$

Proof. Observe that

$$
\begin{aligned}
ABS(T') - ABS(T) &= \sqrt{1 - \frac{2}{d_T(y) + r}} + \sqrt{1 - \frac{2}{d_T(x) + 1}} \\
&\quad - \sqrt{1 - \frac{2}{d_T(x) + r}} - \sqrt{1 - \frac{2}{d_T(y) + 1}} \\
&= \left(\sqrt{1 - \frac{2}{d_T(y) + r}} - \sqrt{1 - \frac{2}{d_T(x) + r}} \right) \\
&\quad + \left(\sqrt{1 - \frac{2}{d_T(x) + 1}} - \sqrt{1 - \frac{2}{d_T(y) + 1}} \right).
\end{aligned} \tag{12}
$$

The derivative of the function Ψ defined by

$$
\Psi(\alpha) = \left(\sqrt{1 - \frac{2}{d_T(y) + \alpha}} - \sqrt{1 - \frac{2}{d_T(x) + \alpha}} \right) \quad \text{with } \alpha \geq 2,
$$

is

$$
\Psi'(\alpha) = \Phi(d_T(y) + \alpha) - \Phi(d_T(x) + \alpha),
$$

where $d_T(x)$ and $d_T(y)$ are fixed integers satisfying $d_T(x) > d_T(y) \geq 2$, and

$$
\Phi(\beta) = \frac{1}{\beta^2} \sqrt{\frac{\beta}{\beta - 2}}.
$$

Certainly, the function Φ is strictly decreasing for $\beta > 2$; thus, $\Psi'(\alpha) > 0$ for $\alpha \geq 2$. Hence, $\Psi(\alpha) \geq \Psi(2)$; thus, (12) yields

$$
\begin{aligned}
ABS(T') - ABS(T) &\geq \left(\sqrt{1 - \frac{2}{d_T(y) + 2}} - \sqrt{1 - \frac{2}{d_T(x) + 2}} \right) \\
&\quad + \left(\sqrt{1 - \frac{2}{d_T(x) + 1}} - \sqrt{1 - \frac{2}{d_T(y) + 1}} \right) \\
&= \left(\sqrt{1 - \frac{2}{d_T(y) + 2}} - \sqrt{1 - \frac{2}{d_T(y) + 1}} \right) \\
&\quad - \left(\sqrt{1 - \frac{2}{d_T(x) + 2}} - \sqrt{1 - \frac{2}{d_T(x) + 1}} \right).
\end{aligned} \tag{13}
$$

As the function Υ defined by

$$
\Upsilon(\gamma) = \left(\sqrt{1 - \frac{2}{\gamma + 2}} - \sqrt{1 - \frac{2}{\gamma + 1}} \right) \quad \text{with } \gamma \geq 2,
$$

is strictly decreasing, one gets $ABS(T') > ABS(T)$ from (13). □

Now, we prove the main result of this section.

Theorem 2. *If T is an n-order tree of maximum degree Δ satisfying the condition $3 \leq \left\lceil \frac{n}{2} \right\rceil \leq \Delta \leq n-2$, then*

$$ABS(T) \leq (\Delta-1)\sqrt{1-\frac{2}{\Delta+1}} + (n-\Delta-1)\sqrt{1-\frac{2}{n-\Delta+1}} + \sqrt{1-\frac{2}{n}}. \tag{14}$$

The sufficient and necessary condition for the equality in (14) is $T \cong \mathcal{W}_{n,\Delta}$, where $\mathcal{W}_{n,\Delta}$ is the graph constructed by attaching $n-\Delta-1$ pendent vertices to one pendent vertex of $K_{1,\Delta}$ (see Figure 5).

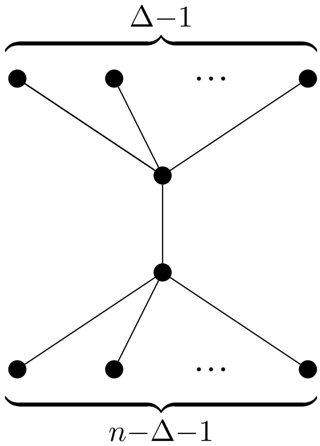

Figure 5. The tree $\mathcal{W}_{n,\Delta}$ defined in Theorem 2.

Proof. If T is isomorphic to $\mathcal{W}_{n,\Delta}$, then

$$ABS(T) = (\Delta-1)\sqrt{1-\frac{2}{\Delta+1}} + (n-\Delta-1)\sqrt{1-\frac{2}{n-\Delta+1}} + \sqrt{1-\frac{2}{n}}.$$

Next, we establish (14).

Among all n-order trees of maximum degree Δ satisfying the given condition, we assume that T is the one for which $ABS(T)$ is maximum. Suppose that there exists $z \in V(T)$, provided that $d_T(z) = \Delta$, where $\Delta \geq 3$. Given that Δ is greater than or equal to $\left\lceil \frac{n}{2} \right\rceil$, it follows that $N_T(z) \cap V_0(T)$ is not an empty set. Now, let us choose a vertex x_0 from $V_0(T)$, such that zx_0 forms an edge in $E(T)$. Our primary goal is to illustrate two crucial facts.

Fact 1. *The vertex z is a claw.*

Proof of Fact 1. Suppose that z does not exhibit a claw-like structure. Let us consider a vertex y from $V_1(T)$ excluding z, such that there exists an edge yy_0 within $E(T)$, where y_0 belongs to $V_0(T)$. Under this condition, we can identify a vertex x within $N_T(z)$ that is not a part of $V_0(T)$ and does not lie on the unique path connecting z and y. Let us take $N_T(x) \setminus \{z\} = \{x_1, x_2, \dots, x_r\}$, where $r \geq 1$. Given that Δ is greater than or equal to $\left\lceil \frac{n}{2} \right\rceil$ and y is distinct from z, we can deduce that

$$d_T(y) \leq n-\Delta-1 \leq \left\lfloor \frac{n}{2} - 1 \right\rfloor \leq \Delta - 1 < d_T(z).$$

Set

$$\mathcal{T}' = T - xx_1 - \cdots - xx_r + y_0x_1 + \cdots + y_0x_r.$$

Note that $\mathcal{T}'$ has maximum degree Δ and that $V(\mathcal{T}') = V(T)$. By utilizing Lemma 1, we conclude that

$$ABS(\mathcal{T}') \geq ABS(T),$$

which contradicts the choice we made regarding T. □

According to Fact 1, we have the option to designate a vertex x such that it is the unique vertex with an edge zx in $E(T)$, and $d_T(x)$ is greater than or equal to 2. Now, consider the sub-tree T_x which includes the vertex x in the graph obtained by removing vertex z from graph T.

Fact 2. $T_x \cong K_{1,n-\Delta-1}$.

Proof of Fact 2. Let us assume that T_x is not isomorphic to $K_{1,n-\Delta-1}$. In this case, there must be an edge $y'y$ in the sub-tree where neither y nor y' is a pendent vertex. Additionally, let us denote the degrees of y' and y as s and t, respectively, where both s and t are greater than or equal to 2. We select edge $y'y$ in such a way that the distance between z and y is maximized. Consequently, y takes the form of a claw with its neighbors in the set $N_T(y) \cap V_0(T)$ denoted as $y_1, y_2, \ldots, y_{t-1}$. Now, we define $\mathcal{T}'$ as the result of removing the edges $yy_1, yy_2, \ldots, yy_{t-1}$ and adding the edges $y'y_1, y'y_2, \ldots, y'y_{t-1}$ to the original graph T. Then,

$$
\begin{aligned}
ABS(T) - ABS(\mathcal{T}') &< (t-1)\sqrt{1-\frac{2}{1+t}} + \sqrt{1-\frac{2}{s+t}} - t\sqrt{1-\frac{2}{s+t}} \\
&= (t-1)\sqrt{1-\frac{2}{1+t}} - (t-1)\sqrt{1-\frac{2}{s+t}} \\
&= (t-1)\left[\sqrt{1-\frac{2}{1+t}} - \sqrt{1-\frac{2}{s+t}}\right] \\
&< 0,
\end{aligned}
$$

which contradicts the choice we made regarding T. □

Now, in view of Facts 1 and 2, the proof of Theorem 2 is completed. □

4. On n-Order Trees of Maximum Degree Less than $\lceil n/2 \rceil$

In this section, we consider Problem 1 when $5 \leq \Delta < \lceil n/2 \rceil$. We use a computer program to find a tree possessing the largest ABS index over $\mathbb{T}(n, \Delta)$ for every pair (n, Δ) satisfying $5 \leq \Delta < \lceil n/2 \rceil$ and $11 \leq n \leq 16$; these trees with the largest ABS index are depicted in Figure 6 (The authors would like to thank Tariq Alraqad for helping in obtaining the trees shown in Figure 6). Based on the structures of these trees, we pose the following conjectures.

Conjecture 1. *If T is a graph possessing the largest ABS index over $\mathbb{T}(n, \Delta)$ with $5 \leq \Delta < \lceil n/2 \rceil$, then T has at most a single vertex of degree t, where $2 \leq t \leq \Delta - 1$.*

Conjecture 2. *Let T denote a graph possessing the largest ABS index over $\mathbb{T}(n, \Delta)$ with $5 \leq \Delta < \lceil n/2 \rceil$. If T contains a vertex u with a degree of t, with $2 \leq t \leq \Delta - 1$, and if Δ is fixed, then there exists an integer n_0, provided that for every $n \geq n_0$, all the neighbors of u have degree Δ.*

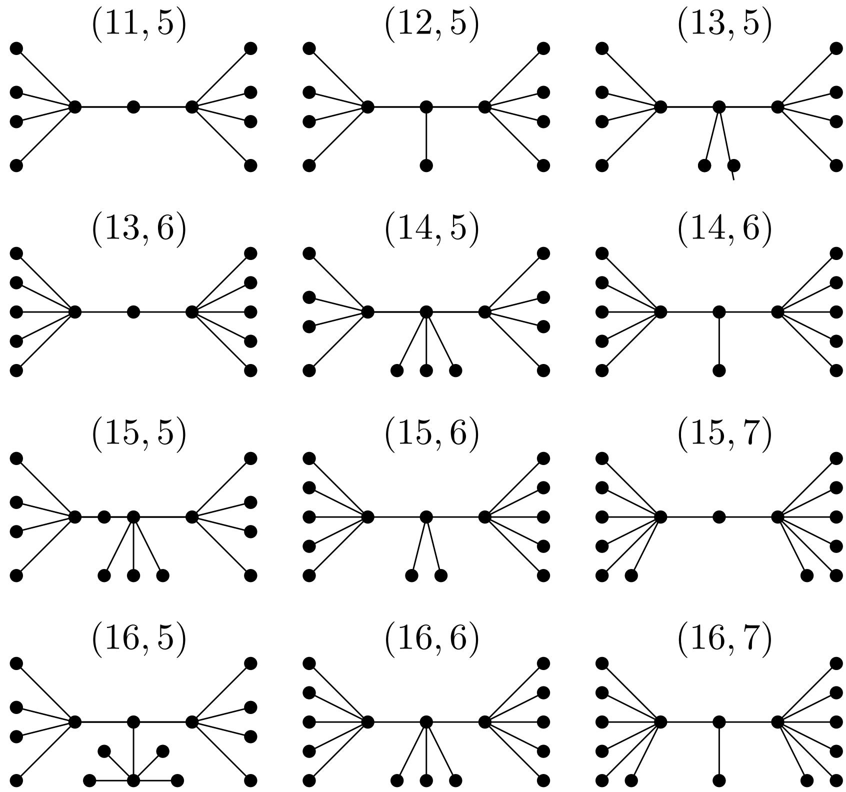

Figure 6. The trees that have the greatest ABS indices in $\mathbb{T}(n, \Delta)$ for every pair (n, Δ) satisfying $5 \le \Delta < \lceil n/2 \rceil$ and $11 \le n \le 16$.

5. Concluding Remarks

In this paper, the best possible upper bounds on the *ABS* index for fixed-order trees possessing a given maximum degree under certain constraints are derived. In particular, a solution to Problem 1 (that was posed quite recently by Hussain, Liu and Hua in [39]) is provided when $3 \le \lceil n/2 \rceil \le \Delta \le n-2$. Problem 1 with the constraints $5 \le \Delta < \lceil n/2 \rceil$ is also addressed by utilizing computer software to determine trees possessing the largest ABS indices over the class $\mathbb{T}(n, \Delta)$ for every pair (n, Δ) satisfying $5 \le \Delta < \lceil n/2 \rceil$ and $11 \le n \le 16$. Based on the structures of the obtained extremal trees for $5 \le \Delta < \lceil n/2 \rceil$, we posed two conjectures, namely Conjectures 1 and 2. Consequently, Problem 1 with the constraints $5 \le \Delta < \lceil n/2 \rceil$ is generally open for further research. Also, the present study can be extended towards the fixed-order and fixed-size graphs containing cycles with a given maximum degree; for instance, fixed-order unicyclic graphs, bicyclic graphs, and tricyclic graphs, with a given maximum degree.

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