## Article

# Extremal Trees with Respect to the Difference between Atom-Bond Connectivity Index and Randić Index 

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#### Abstract

Let $G$ be a simple, connected and undirected graph. The atom-bond connectivity index $(A B C(G))$ and Randić index $(R(G))$ are the two most well known topological indices. Recently, Ali and Du (2017) introduced the difference between atom-bond connectivity and Randić indices, denoted as $A B C-R$ index. In this paper, we determine the fourth, the fifth and the sixth maximum chemical trees values of $A B C-R$ for chemical trees, and characterize the corresponding extremal graphs. We also obtain an upper bound for $A B C-R$ index of such trees with given number of pendant vertices. The role of symmetry has great importance in different areas of graph theory especially in chemical graph theory.


Keywords: Randić index; Atom-bond connectivity index; tree

## 1. Introduction

Let $G$ be a simple, connected and undirected graph. having $V(G)$ and $E(G)$ as the set of vertices and edges respectively. The number of vertices and edges in $G$ are denoted by $n m$, respectively. Let $d_{u}$ denotes the degree of vertex $u$ in $G$, while $\triangle(G)$ and $\delta(G)$ are used to denote the maximum and minimum degree of $G$. The distance $d_{G}(x, y)$ between vertices $x$ and $y$ is defined as the length of any shortest path in $G$ connecting $x$ and $y$. The eccentricity of $v_{i}$ in $G$ is defined as $e_{i}=\max _{v_{j} \in V(G)} d_{G}\left(v_{i}, v_{j}\right)$. For more concepts and terminologies in Graph Theory, we refer to [1].

Topological indices is one of the useful tools of graph theory [2]. Molecular compounds are often modeled by molecular graphs are used to represent the molecules and molecular compounds with the help of lines and dots. In study of QSPR/QSAR, topological indices are considered as one of the useful topics [3].

In 1975, Randić [4] defined the Randić index as follows:

$$
R(G)=\sum_{u v \in E(G)} \frac{1}{\sqrt{d_{u} d_{v}}}
$$

Details about Randić index and most of its mathematical properties can be found in [5-10].

Estrada et al. [11] proposed the atom-bond connectivity ( $A B C$ for short) for a molecular graph as

$$
A B C(G)=\sum_{u v \in E(G)} \sqrt{\frac{d_{u}+d_{v}-2}{d_{u} d_{v}}} .
$$

This index became popular only ten years later, when the paper [12] was published. For the details, see the surveys [13], the recent papers [14-19] and the references cited therein.

Nowadays, studying the relationship or comparison between topological indices, see [20-23], is becoming popular. Recently, Ali and Du [24] investigated extremal binary and chemical trees results for the difference between $A B C$ and $R$ indices. A tree with maximum degree at most three or four called a binary and chemical tree, respectively.

For a connected graph $G$ of order at least 3 , the difference between $A B C$ and $R$ is represented as (see [24])

$$
(A B C-R)(G)=\sum_{u v \in E(G)} \frac{\sqrt{d_{u}+d_{v}-2}-1}{\sqrt{d_{u} d_{v}}}
$$

Note that $(A B C-R)(G) \geq 0$ and equality holds if and only if $G=P_{3}$. So in our discussion we consider $n \geq 4$.

In this paper, motivated by the results in [24], we further investigated the extremal chemical trees for $A B C-R$. Moreover, maximal trees with fixed number of pendant vertices are also investigated for $A B C-R$ index. The techniques used in this paper are very similar to that of Refs. [19,24,25].

## 2. Preliminary Results

Let the number of edges connecting the vertices of degree $p$ and $q$ is denoted by $x_{p, q}$. In term of $p, q$ and $x_{p, q} A B C-R$ can be rewritten as follows [24]:

$$
\begin{equation*}
(A B C-R)(G)=\sum_{\delta \leq p \leq q \leq \Delta} \frac{\sqrt{p+q-2}-1}{\sqrt{p q}} x_{p, q} . \tag{1}
\end{equation*}
$$

Let $n_{p}$ be the number of vertices of degree $p$ in $G$, where $1 \leq p \leq 4$. Then for any $n$-vertex chemical tree the following system of equations holds (see [19,24]):

$$
\begin{gather*}
n_{1}+n_{2}+n_{3}+n_{4}=n  \tag{2}\\
n_{1}+2 n_{2}+3 n_{3}+4 n_{4}=2(n-1)  \tag{3}\\
x_{1,2}+x_{1,3}+x_{1,4}=n_{1}  \tag{4}\\
x_{1,2}+2 x_{2,2}+x_{2,3}+x_{2,4}=2 n_{2}  \tag{5}\\
x_{1,3}+x_{2,3}+2 x_{3,3}+x_{3,4}=3 n_{3}  \tag{6}\\
x_{1,4}+x_{2,4}+x_{3,4}+2 x_{4,4}=4 n_{4} \tag{7}
\end{gather*}
$$

From Equations (2) and (3), it follows that

$$
n_{2}+2 n_{3}+3 n_{4}=n-2
$$

and thus,

$$
\begin{equation*}
n \equiv n_{2}+2 n_{3}+2(\bmod 3) \tag{8}
\end{equation*}
$$

By solving the sysmtem of Equations (2)-(7), the values of $x_{1,4}$ and $x_{4,4}$ are, respectively, given as below (see also Refs. [24,26]):

$$
\begin{gathered}
x_{1,4}=\frac{2 n+2}{3}-\frac{4}{3} x_{1,2}-\frac{10}{9} x_{1,3}-\frac{2}{3} x_{2,2}-\frac{4}{9} x_{2,3}-\frac{1}{3} x_{2,4}-\frac{2}{9} x_{3,3}-\frac{1}{9} x_{3,4} \\
x_{4,4}=\frac{n-5}{3}+\frac{1}{3} x_{1,2}+\frac{1}{9} x_{1,3}-\frac{1}{3} x_{2,2}-\frac{5}{9} x_{2,3}-\frac{2}{3} x_{2,4}-\frac{7}{9} x_{3,3}-\frac{8}{9} x_{3,4}
\end{gathered}
$$

Note that the detailed calculation of obtaining the values for $x_{1,4}$ and $x_{4,4}$ can be referred in [26]. By substituting these values of $x_{1,4}$ and $x_{4,4}$ in Equation (1), one has:

$$
\begin{align*}
(A B C-R)(G)= & \frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{4 \sqrt{3}-5 \sqrt{6}+1}{12}-\frac{8 \sqrt{3}-\sqrt{6}-7}{12} x_{1,2} \\
& -\frac{32 \sqrt{3}-13 \sqrt{6}-19}{36} x_{1,3}-\frac{4 \sqrt{3}+\sqrt{6}-6 \sqrt{2}+1}{12} x_{2,2} \\
& -\frac{8 \sqrt{3}+11 \sqrt{6}-18 \sqrt{2}-13}{36} x_{2,3}-\frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12} x_{2,4} \\
& -\frac{4 \sqrt{3}+7 \sqrt{6}-23}{36} x_{3,3}-\frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} x_{3,4} . \tag{9}
\end{align*}
$$

Let

$$
\begin{align*}
\theta= & \frac{8 \sqrt{3}-\sqrt{6}-7}{12} x_{1,2}+\frac{32 \sqrt{3}-13 \sqrt{6}-19}{36} x_{1,3}+\frac{4 \sqrt{3}+\sqrt{6}-6 \sqrt{2}+1}{12} x_{2,2} \\
& +\frac{8 \sqrt{3}+11 \sqrt{6}-18 \sqrt{2}-13}{36} x_{2,3}+\frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12} x_{2,4} \\
& +\frac{4 \sqrt{3}+7 \sqrt{6}-23}{36} x_{3,3}+\frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} x_{3,4} . \tag{10}
\end{align*}
$$

Then Equation (9) can be rewritten as

$$
\begin{equation*}
(A B C-R)(G)=\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{4 \sqrt{3}-5 \sqrt{6}+1}{12}-\theta \tag{11}
\end{equation*}
$$

since

$$
\begin{align*}
\theta \approx & 0.367243 x_{1,2}+0.127285 x_{1,3}+0.157701 x_{2,2}+0.0651375 x_{2,3} \\
& +0.0100367 x_{2,4}+0.0298509 x_{3,3}+0.00595623 x_{3,4} . \tag{12}
\end{align*}
$$

From Equation (12) we have $\theta \geq 0$. Moreover Equation (11) implies that a chemical tree which gives the minimum value of $\theta$ will produce the maximum of $(A B C-R)$.

Theorem 1 ([24]). Consider the set of all n-vertex chemical trees.
(1) Suppose that $n \equiv 0(\bmod 3)$.
(1.1) For $n \geq 9$, the maximum $A B C-R$ value is

$$
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{3+2 \sqrt{2}-3 \sqrt{6}}{4}
$$

which is uniquely attained by those trees that contain a unique vertex of degree 2 and no vertex of degree 3 , that is, $n_{2}=1$ and $n_{3}=0$, such that the unique vertex of degree 2 is adjacent to two vertices of degree 4 , that is, $x_{1,2}=0$ and $x_{2,4}=2$.
(1.2) For $n \geq 21$, the second maximum $A B C-R$ value is

$$
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{4 \sqrt{15}-7 \sqrt{6}-4 \sqrt{3}+7}{4}
$$

which is uniquely attained by those trees that contain no vertex of degree 2 and exactly two vertices of degree 3 , that is, $n_{2}=0$ and $n_{3}=2$, such that each vertex of degree 3 is adjacent to three vertices of degree 4 , that is, $x_{1,3}=x_{3,3}=0$ and $x_{3,4}=6$.
(1.3) For $n \geq 21$, the third maximum $A B C-R$ value is

$$
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{4 \sqrt{15}-4 \sqrt{3}-9 \sqrt{6}+11}{6}
$$

which is uniquely attained by those trees that contain no vertex of degree 2 and exactly two vertices of degree 3 , which are adjacent, that is, $n_{2}=0, n_{3}=2$, and $x_{3,3}=1$ such that each vertex of degree 3 is adjacent to exactly two vertices of degree 4 , that is, $x_{1,3}=0$ and $x_{3,4}=4$.
(2) Suppose that $n \equiv 1(\bmod 3)$.
(2.1) For $n \geq 13$, the maximum $A B C-R$ value is

$$
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{11+6 \sqrt{15}-4 \sqrt{3}-13 \sqrt{6}}{12}
$$

and the equality holds if and only if $n_{2}=0$ and $n_{3}=1$ such that $x_{1,3}=0$ and $x_{3,4}=3$.
For $n \geq 13$, the second maximum $A B C-R$ value is

$$
\begin{equation*}
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{12 \sqrt{2}-13 \sqrt{6}-4 \sqrt{3}+17}{12} \tag{2.2}
\end{equation*}
$$

which is uniquely attained by those trees that contain exactly two vertices of degree 2 and no vertex of degree 3 , that is, $n_{2}=2$ and $n_{3}=0$, such that either vertex of degree 2 is adjacent to two vertices of degree 4 , that is, $x_{1,2}=x_{2,2}=0$ and $x_{2,4}=4$.
For $n \geq 25$, the third maximum $A B C-R$ value is

$$
\begin{equation*}
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{12 \sqrt{15}-6 \sqrt{2}-25 \sqrt{6}-16 \sqrt{3}+29}{12} \tag{2.3}
\end{equation*}
$$

which is uniquely attained by those trees that contain a unique vertex of degree 2 and exactly two vertices of degree 3 , that is, $n_{2}=1$ and $n_{3}=2$, such that each vertex of degree 2 and 3 is adjacent to only vertices of degree 4 , that is, $x_{1,2}=x_{1,3}=x_{2,3}=x_{3,3}=0, x_{2,4}=2$, and $x_{3,4}=6$.
(3) Suppose that $n \equiv 2(\bmod 3)$.

For $n \geq 5$, the maximum $A B C-R$ value is

$$
\begin{equation*}
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{4 \sqrt{3}-5 \sqrt{6}+1}{12} \tag{3.1}
\end{equation*}
$$

which is uniquely attained by those trees that contain no vertex of degree 2 or 3 , that is, $n_{2}=$ $n_{3}=0$.
For $n \geq 17$, the second maximum $A B C-R$ value is

$$
\begin{equation*}
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{6 \sqrt{15}+6 \sqrt{2}-17 \sqrt{6}-8 \sqrt{3}+19}{12} \tag{3.2}
\end{equation*}
$$

which is uniquely attained by those trees that contain a unique vertex of degree 2 and a unique vertex of degree 3 , that is, $n_{2}=n_{3}=1$, such that each vertex of degree 2 and 3 is adjacent to only vertices of degree 4 , that is, $x_{1,2}=x_{1,3}=x_{2,3}=0, x_{2,4}=2$, and $x_{3,4}=3$.
(3.3) For $n \geq 29$, the third maximum $A B C-R$ value is

$$
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{18 \sqrt{15}-29 \sqrt{6}-20 \sqrt{3}+31}{12}
$$

which is uniquely attained by those trees that contain no vertex of degree 2 and exactly three vertices of degree 3 , that is, $n_{2}=0$ and $n_{3}=3$, such that each vertex of degree 3 is adjacent to three vertices of degree 4 , that is, $x_{1,3}=x_{3,3}=0$, and $x_{3,4}=9$.

## 3. Maximum $A B C-R$ Index for Chemical Trees

In this section, we present a main result which deals with the maximal chemical trees for $A B C-R$ index.

Theorem 2. Consider the set of all n-vertex chemical trees.
(1) Suppose that $n \equiv 0(\bmod 3)$.
(1.1) For $n \geq 21$, the fourth maximum $A B C-R$ value is

$$
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{18 \sqrt{15}+36 \sqrt{2}-36 \sqrt{3}-63 \sqrt{6}+81}{36}
$$

and the equality holds if and only if $n_{2}=2$ and $n_{3}=1$ such that $x_{1,2}=x_{1,3}=x_{2,2}=x_{2,3}=0$, $x_{2,4}=4$ and $x_{3,4}=3$.
(1.2) For $n \geq 33$, the fifth maximum $A B C-R$ value is

$$
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{54 \sqrt{15}+18 \sqrt{2}-72 \sqrt{3}-99 \sqrt{6}+117}{36}
$$

and the equality holds if and only if $n_{2}=1$ and $n_{3}=3$ such that $x_{1,2}=x_{1,3}=x_{2,3}=x_{3,3}=0$, $x_{2,4}=2$ and $x_{3,4}=9$.
For $n \geq 33$, the sixth maximum $A B C-R$ value is

$$
\begin{equation*}
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{24 \sqrt{2}-12 \sqrt{3}-21 \sqrt{6}+33}{12} \tag{1.3}
\end{equation*}
$$

and the equality holds if and only if $n_{2}=4, n_{3}=0$ such that $x_{1,2}=x_{2,2}=0$ and $x_{2,4}=8$.
(2) Suppose that $n \equiv 1(\bmod 3)$.
(2.1) For $n \geq 37$, the fourth maximum $A B C-R$ value is

$$
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{72 \sqrt{15}-84 \sqrt{3}-111 \sqrt{6}+123}{36}
$$

and the equality holds if and only if $n_{2}=0$ and $n_{3}=4$ such that $x_{1,3}=x_{3,3}=0$ and $x_{3,4}=12$.
(2.2) For $n \geq 37$, the fifth maximum $A B C-R$ value is

$$
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{24 \sqrt{15}+18 \sqrt{2}-36 \sqrt{3}-66 \sqrt{6}+90}{36}
$$

and the equality holds if and only if $n_{2}=1, n_{3}=2$ such that $x_{3,3}=1, x_{1,2}=x_{1,3}=x_{2,3}=0$, $x_{2,4}=2$, and $x_{3,4}=4$.
(2.3) For $n \geq 37$, the sixth maximum $A B C-R$ value is

$$
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{18 \sqrt{15}+54 \sqrt{2}-48 \sqrt{3}-75 \sqrt{6}+105}{36}
$$

and the equality holds if and only if $n_{2}=3$ and $n_{3}=1$ such that $x_{1,2}=x_{1,3}=x_{2,2}=x_{2,3}=0$, $x_{2,4}=6$, and $x_{3,4}=3$.
(3) Suppose that $n \equiv 2(\bmod 3)$.
(3.1) For $n \geq 29$, the fourth maximum $A B C-R$ value is

$$
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{18 \sqrt{2}-8 \sqrt{3}-17 \sqrt{6}+25}{12}
$$

and the equality holds if and only if $n_{2}=3$ and $n_{3}=0$ such that $x_{1,2}=x_{2,2}=0$ and $x_{2,4}=6$.
For $n \geq 29$, the fifth maximum $A B C-R$ value is

$$
\begin{equation*}
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{42 \sqrt{15}-78 \sqrt{6}-48 \sqrt{3}+96}{36} \tag{3.2}
\end{equation*}
$$

and the equality holds if and only if $n_{2}=0$ and $n_{3}=3$ such that $x_{1,3}=0, x_{3,3}=1$ and $x_{3,4}=7$.
For $n \geq 29$, the sixth maximum $A B C-R$ value is

$$
\begin{equation*}
\frac{4 \sqrt{3}+\sqrt{6}-5}{12} n+\frac{36 \sqrt{15}+36 \sqrt{2}-60 \sqrt{3}-87 \sqrt{6}+111}{36} \tag{3.3}
\end{equation*}
$$

and the equality holds if and only if $n_{2}=2$ and $n_{3}=2$ such that $x_{1,2}=x_{1,3}=x_{2,2}=x_{2,3}=$ $x_{3,3}=0, x_{2,4}=4$ and $x_{3,4}=6$.

Proof. First, we claim that $\theta>0.080294$ when $x_{1,2}+x_{1,3}+x_{2,2} \geq 1$ or $x_{2,3} \geq 2$. More precisely, from Equation (12),

- when $x_{1,2} \geq 1$,

$$
\theta \geq \frac{8 \sqrt{3}-\sqrt{6}-7}{12} \approx 0.367243>0.080294
$$

- when $x_{1,3} \geq 1$,

$$
\theta \geq \frac{32 \sqrt{3}-13 \sqrt{6}-19}{36} \approx 0.127285>0.080294
$$

- when $x_{2,2} \geq 1$,

$$
\theta \geq \frac{4 \sqrt{3}+\sqrt{6}-6 \sqrt{2}+1}{12} \approx 0.157701>0.080294
$$

- when $x_{2,3} \geq 2$,

$$
\theta \geq 2 \cdot \frac{8 \sqrt{3}+11 \sqrt{6}-18 \sqrt{2}-13}{36} \approx 0.130275>0.080294
$$

So we may assume that $x_{1,2}=x_{1,3}=x_{2,2}=0$, and $x_{2,3}=0$ or 1 . It follows from Equations (5) and (6) that

$$
\begin{equation*}
x_{2,4}=2 n_{2}-x_{2,3} \tag{13}
\end{equation*}
$$

and

$$
\begin{equation*}
2 x_{3,3}+x_{3,4}=3 n_{3}-x_{2,3} \tag{14}
\end{equation*}
$$

Case 1. $x_{2,3}=1$.
Observe that $n_{2} \geq 1, n_{3} \geq 1$, and thus $x_{2,4} \geq 1$ from Equation (13).
If $x_{2,4} \geq 2$, then by the Equation (12),

$$
\theta \geq \frac{8 \sqrt{3}+11 \sqrt{6}-18 \sqrt{2}-13}{36}+2 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12} \approx 0.0852109>0.080294
$$

Suppose now that $x_{2,4}=1$. If $x_{3,3}=0$, then by Equation (14), $x_{3,4} \geq 2$, together with Equation (12), it leads to

$$
\begin{align*}
\theta \geq & \frac{8 \sqrt{3}+11 \sqrt{6}-18 \sqrt{2}-13}{36}+\frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12} \\
& +2 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \\
\approx & 0.08708666>0.080294 \tag{15}
\end{align*}
$$

If $x_{3,3} \geq 1$, then by Equation (12),

$$
\begin{align*}
\theta \geq & \frac{8 \sqrt{3}+11 \sqrt{6}-18 \sqrt{2}-13}{36}+\frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12} \\
& +\frac{4 \sqrt{3}+7 \sqrt{6}-23}{36} \\
\approx & 0.1050251>0.080294 \tag{16}
\end{align*}
$$

Case 2. $x_{2,3}=0$.
From Equations (13) and (14), it follows that

$$
\begin{equation*}
x_{2,4}=2 n_{2} \tag{17}
\end{equation*}
$$

and

$$
\begin{equation*}
2 x_{3,3}+x_{3,4}=3 n_{3} \tag{18}
\end{equation*}
$$

If $x_{3,3} \geq 3$, then by Equation (12),

$$
\theta \geq 3 \cdot \frac{4 \sqrt{3}+7 \sqrt{6}-23}{36} \approx 0.0895526>0.0802936
$$

If $x_{3,3}=2$, then $n_{3} \geq 3$, and $x_{3,4} \geq 5$ from Equation (14), and thus by Equation (12),

$$
\theta \geq 2 \cdot \frac{4 \sqrt{3}+7 \sqrt{6}-23}{36}+5 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \approx 0.0894829>0.0802936
$$

Now, we consider the two cases: $x_{3,3}=1$ and $x_{3,3}=0$.
Subcase 2.1. $x_{3,3}=1$.
Clearly, $n_{3} \geq 2$. The proofs will be partitioned into several parts according to the value of $n_{3}$ : $n_{3}=2, n_{3}=3, n_{3} \geq 4$.

Firstly suppose that $n_{3}=2$, then, $x_{3,4}=4$ from Equation (14). Note that the case $n_{2}=0$ is known to belong to one of the first three minimum $\theta$ values, see Theorem 1-(1.3). If $n_{2}=1$, then $n \equiv 1(\bmod 3)$ from Equation (8), $x_{2,4}=2$ from Equation (17), and by Equation (12),

$$
\begin{aligned}
\theta & =2 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12}+\frac{4 \sqrt{3}+7 \sqrt{6}-23}{36}+4 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \\
& \approx 0.0737492
\end{aligned}
$$

If $n_{2} \geq 2$, then, $x_{2,4} \geq 4$ from Equation (17), and by Equation (12),

$$
\begin{aligned}
\theta & \geq 4 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12}+\frac{4 \sqrt{3}+7 \sqrt{6}-23}{36}+4 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \\
& \approx 0.09382262>0.0802936
\end{aligned}
$$

Next, suppose that $n_{3}=3$, then $x_{3,4}=7$ from Equation (14). If $n_{2}=0$, then $n \equiv 2(\bmod 3)$ from Equation (8), $x_{2,4}=0$ from Equation (17), and by Equation (12),

$$
\theta=\frac{4 \sqrt{3}+7 \sqrt{6}-23}{36}+7 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \approx 0.0715445
$$

If $n_{2} \geq 1$, then $x_{2,4} \geq 2$ from Equation (17), and by Equation (12),

$$
\begin{aligned}
\theta & \geq 2 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12}+\frac{4 \sqrt{3}+7 \sqrt{6}-23}{36}+7 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \\
& \approx 0.0916179>0.0802936
\end{aligned}
$$

Finally, if $n_{3} \geq 4$, then $x_{3,4} \geq 10$ from Equation (16), and by Equation (12),

$$
\begin{aligned}
\theta & \geq \frac{4 \sqrt{3}+7 \sqrt{6}-23}{36}+10 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \\
& \approx 0.0894132>0.0802936
\end{aligned}
$$

Subcase 2.2. $x_{3,3}=0$.
In this case, $x_{3,4}=3 n_{3}$ from Equation (18). This time, we partition the proofs according to the value of $n_{2}: n_{2}=0, n_{2}=1, n_{2}=2, n_{2}=3, n_{2}=4, n_{2} \geq 5$.

Firstly suppose that $n_{2}=0$, that is, $x_{2,4}=0$ from Equation (17). Note that the cases $n_{3}=0,1,2,3$ were known to belong to the first three minimum $\theta$ value, see Theorem 1 . If $n_{3}=4$, then $n \equiv 1(\bmod 3)$ from Equation (8), $x_{3,4}=12$, and by Equation (12),

$$
\theta=12 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \approx 0.0714748
$$

If $n_{3} \geq 5$, then $x_{3,4} \geq 15$, and by Equation (12),

$$
\theta \geq 15 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \approx 0.08934345>0.0802936
$$

Next, suppose that $n_{2}=1$, that is, $x_{2,4}=2$ from Equation (17). Note that the cases $n_{3}=0,1,2$ were known to belong to the first three minimum $\theta$ values, see Theorem 1. If $n_{3}=3$, then $n \equiv 0(\bmod 3)$ from Equation (8), $x_{3,4}=9$, and by Equation (12),

$$
\theta=2 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12}+9 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \approx 0.0736795
$$

If $n_{3} \geq 4$, then $x_{3,4} \geq 12$, and by Equation (12),

$$
\begin{aligned}
\theta & \geq 2 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12}+12 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \\
& \approx 0.091548>0.0802936
\end{aligned}
$$

Now, suppose that $n_{2}=2$, that is, $x_{2,4}=4$ from Equation (17). The case $n_{3}=0$ was known to belong to one of the first three minimum $\theta$ values, see Theorem 1-(2.2). If $n_{3}=1$, then $n \equiv 0(\bmod 3)$ from Equation (8), $x_{3,4}=3$, and by Equation (12),

$$
\theta=4 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12}+3 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \approx 0.0580155 .
$$

If $n_{3}=2$, then $n \equiv 2(\bmod 3)$ from Equation $(8), x_{3,4}=6$, and by Equation (12),

$$
\theta=4 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12}+6 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \approx 0.07588419
$$

If $n_{3} \geq 3$, then $x_{3,4} \geq 9$, and by Equation (12),

$$
\begin{aligned}
\theta & \geq 4 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12}+9 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \\
& \approx 0.09375289>0.0802936
\end{aligned}
$$

Suppose that $n_{2}=3$, that is, $x_{2,4}=6$ from Equation (17). If $n_{3}=0$, then $n \equiv 2(\bmod 3)$ from Equation (8), $x_{3,4}=0$, and by Equation (12),

$$
\theta=6 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12} \approx 0.0602202
$$

If $n_{3}=1$, then $n \equiv 1(\bmod 3)$ from Equation $(8), x_{3,4}=3$, and by Equation (12),

$$
\theta=6 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12}+3 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \approx 0.0780889 .
$$

If $n_{3} \geq 2$, then $x_{3,4} \geq 6$, and by Equation (12),

$$
\begin{aligned}
\theta & \geq 6 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12}+6 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \\
& \approx 0.0959576>0.0802936
\end{aligned}
$$

Suppose that $n_{2}=4$, that is, $x_{2,4}=8$ from Equation (17). If $n_{3}=0$, then $n \equiv 0(\bmod 3)$ from Equation (8), $x_{3,4}=0$, and by Equation (12),

$$
\theta=8 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12} \approx 0.0802936
$$

If $n_{3} \geq 1$, then $x_{3,4} \geq 3$, and by Equation (12),

$$
\begin{aligned}
\theta & \geq 8 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12}+3 \cdot \frac{4 \sqrt{3}+4 \sqrt{6}-3 \sqrt{15}-5}{18} \\
& \approx 0.0981623>0.0802936
\end{aligned}
$$

Finally, if $n_{2} \geq 5$, then $x_{2,4} \geq 10$ from Equation (17), and by Equation (12),

$$
\theta \geq 10 \cdot \frac{2 \sqrt{3}+2 \sqrt{6}-3 \sqrt{2}-4}{12} \approx 0.100367>0.0802936
$$

In conclusion, we obtain the following
(i) If $n \equiv 0(\bmod 3)$, then the fourth, fifth and sixth minimum $\theta$ values are $0.0580155,0.0736795$ and 0.0802936 , respectively.
(ii) If $n \equiv 1(\bmod 3)$, then the fourth, fifth and sixth minimum $\theta$ values are $0.0714748,0.0737492$ and 0.0780889 , respectively.
(iii) If $n \equiv 2(\bmod 3)$, then the fourth, fifth and sixth minimum $\theta$ values are $0.0602202,0.0715445$ and 0.07588419 , respectively.

Now, the Equation (11) implies the fourth, fifth and sixth maximum $A B C-R$.
In Figures 1-3, the chemical trees with the smallest numbers of vertices in Theorem 2 are listed.


Figure 1. Chemical trees with the fourth (A), the fifth (B) and the sixth (C) maximum $A B C-R$ values in Theorem 2-(1).

(D)

(E)

(F)

Figure 2. Chemical trees with the fourth (D), the fifth (E) and the sixth (F) maximum $A B C-R$ values in Theorem 2-(2).

(G)

(H)

(I)

Figure 3. Chemical trees with the fourth (G), the fifth (H) and the sixth (I) maximum $A B C-R$ values in Theorem 2-(3).

## 4. Upper Bound for $A B C-R$ Index of Molecular Trees

In this section, we consider the class of molecular tress and investigated the sharp bound on $A B C-R$ for this class of graphs.

Let $\mathcal{T}_{n, n_{1}}$ be the set of molecular trees satisfying

$$
\begin{gathered}
x_{1,4}=n_{1} \\
x_{2,2}=n-2 n_{1}+3-\frac{1}{3} x_{2,3}
\end{gathered}
$$

and

$$
x_{2,4}=n_{1}-4-\frac{2}{3} x_{2,3}
$$

Theorem 3 ([19]). Let $T$ be a molecular tree with $n$ vertices, $n_{1} \geq 5$ of which are pendant vertices. Then

$$
(A B C)(T) \leq \frac{\sqrt{2}}{2} n+\frac{\sqrt{3}-\sqrt{2}}{2} n_{1}-\frac{\sqrt{2}}{2}
$$

with equality holds if and only if $T \in \mathcal{T}_{n, n_{1}}$.
Obviously, from Equation (1) we obtain

$$
\begin{align*}
(A B C-R)(T)= & \frac{\sqrt{2}-1}{\sqrt{3}} x_{1,3}+\frac{\sqrt{3}-1}{2} x_{1,4}+\frac{\sqrt{2}-1}{2} x_{2,2}+\frac{\sqrt{3}-1}{\sqrt{6}} x_{2,3}+ \\
& \frac{1}{\sqrt{8}} x_{2,4}+\frac{1}{3} x_{3,3}+\frac{\sqrt{5}-1}{\sqrt{12}} x_{3,4}+\frac{\sqrt{6}-1}{4} x_{4,4} \tag{19}
\end{align*}
$$

Now let $\mathcal{T}_{n, n_{1}}^{\prime}$ be the set of molecular trees satisfying

$$
\begin{gathered}
x_{1,4}=n_{1} \\
x_{2,2}=n-2 n_{1}+3
\end{gathered}
$$

and

$$
x_{2,4}=n_{1}-4
$$

Theorem 4. Let $T$ be a molecular tree of order $n$ and $n_{1} \geq 5$ pendant vertices, then

$$
(A B C-R)(T) \leq \frac{\sqrt{2}-1}{2} n+\frac{2-3 \sqrt{2}+2 \sqrt{3}}{4} n_{1}+\frac{1}{\sqrt{2}}-\frac{3}{2}
$$

with equality holds if and only if $T \in \mathcal{T}_{n, n_{1}}^{\prime}$.
Proof. Since $T$ is a molecular tree, we have Equations (2)-(7). Suppose that

$$
\begin{aligned}
f_{1} & =x_{1,2}+x_{1,3}+x_{1,4} \\
f_{2} & =x_{1,2}+x_{2,3} \\
f_{3} & =x_{1,3}+x_{2,3}+2 x_{3,3}+x_{3,4} \\
f_{4} & =x_{1,4}+x_{3,4}+2 x_{4,4}
\end{aligned}
$$

that is,

$$
\begin{aligned}
& f_{1}=n_{1} \\
& f_{2}=2 n_{2}-2 x_{2,2}-x_{2,4} \\
& f_{3}=3 n_{3} \\
& f_{4}=4 n_{4}-x_{2,4}
\end{aligned}
$$

we have

$$
\begin{aligned}
\sum_{i=1}^{4} f_{i} & =2(n-1)-2\left(x_{2,2}+x_{2,4}\right) \\
\sum_{i=1}^{4} \frac{1}{i} f_{i} & =n-\left(x_{2,2}+\frac{3}{4} x_{2,4}\right)
\end{aligned}
$$

implying that

$$
\begin{aligned}
& x_{2,2}=\frac{3}{2} \sum_{i=1}^{4} f_{i}-4 \sum_{i=1}^{4} \frac{1}{i} f_{i}+n+3 \\
& x_{2,4}=-2 \sum_{i=1}^{4} f_{i}+4 \sum_{i=1}^{4} \frac{1}{i} f_{i}-4 .
\end{aligned}
$$

Thus we have

$$
\begin{aligned}
& x_{1,4}=n_{1}-x_{1,2}-x_{1,3} \\
& x_{2,2}=n-2 n_{1}+3-x_{1,2}-\frac{1}{3} x_{1,3}-\frac{1}{3} x_{2,3}+\frac{1}{3} x_{3,3}+\frac{2}{3} x_{3,4}+x_{4,4} \\
& x_{2,4}=n_{1}-4+x_{1,2}+\frac{1}{3} x_{1,3}-\frac{2}{3} x_{2,3}-\frac{4}{3} x_{3,3}-\frac{5}{3} x_{3,4}-2 x_{4,4} .
\end{aligned}
$$

Substituting them back into Equation (19), we have

$$
\begin{aligned}
(A B C-R)(T)= & \frac{\sqrt{2}-1}{2} n+\frac{2-3 \sqrt{2}+2 \sqrt{3}}{4} n_{1}+\frac{1}{\sqrt{2}}-\frac{3}{2} \\
& +\frac{4-\sqrt{2}-2 \sqrt{3}}{4} x_{1,2}+\frac{8-\sqrt{2}-10 \sqrt{3}+4 \sqrt{6}}{12} x_{1,3} \\
& +\frac{1+\sqrt{2}-\sqrt{6}}{6} x_{2,3}+\frac{1-\sqrt{2}}{6} x_{3,3} \\
& +\frac{2 \sqrt{15}-4-\sqrt{2}-2 \sqrt{3}}{12} x_{3,4}+\frac{\sqrt{6}-3}{4} x_{4,4} \\
\approx & \frac{\sqrt{2}-1}{2} n+\frac{2-3 \sqrt{2}+2 \sqrt{3}}{4} n_{1}+\frac{1}{\sqrt{2}}-\frac{3}{2} \\
& -0.219579 x_{1,2}-0.078064 x_{1,3}-0.005879 x_{2,3} \\
& -0.069036 x_{3,3}-0.094362 x_{3,4}-0.137628 x_{4,4}
\end{aligned}
$$

with negative coefficients $x_{1,2}, x_{1,3}, x_{2,3}, x_{3,3}, x_{3,4}$ and $x_{4,4}$. Thus

$$
(A B C-R)(T) \leq \frac{\sqrt{2}-1}{2} n+\frac{2-3 \sqrt{2}+2 \sqrt{3}}{4} n_{1}+\frac{1}{\sqrt{2}}-\frac{3}{2}
$$

and equality in above holds if and only if $x_{1,2}=x_{1,3}=x_{2,3}=x_{3,3}=x_{3,4}=x_{4,4}=0$, or equivalently, $x_{1,4}=n_{1}, x_{2,2}=n-2 n_{1}+3, x_{2,4}=n_{1}-4$, i.e., $T \in \mathcal{T}_{n, n_{1}}^{\prime}$.

## 5. Conclusions

In this paper, we considered more maximum values of the difference $A B C-R$, where $A B C$ and $R$ are the atom-bond connectivity index and Randić index, respectively. In particular, we characterized the fourth, the fifth and the sixth maximum chemical trees with respect to the invariant $A B C-R$, and thus extended the result by Ali and Du [24] in 2017. It is very challenging to find more maximum values of $A B C-R$ invariant unless new efficient method is introduced. By using the technique from [19], we also obtained a sharp upper bound for the $A B C-R$ index of molecular (or chemical) trees with fixed number of pendant vertices. The work on bounds for the $A B C-R$ index of general graphs and trees is widely open and one can consider many directions.

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