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

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Received: 23 July 2020; Accepted: 23 August 2020; Published: 25 September 2020



**Abstract:** Let *G* be a simple, connected and undirected graph. The atom-bond connectivity index (ABC(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 ABC - R index. In this paper, we determine the fourth, the fifth and the sixth maximum chemical trees values of ABC - R for chemical trees, and characterize the corresponding extremal graphs. We also obtain an upper bound for ABC - 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  $e_i = \max_{v_j \in V(G)} d_G(v_i, v_j)$ . 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:

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}.$$

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 (ABC for short) for a molecular graph as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

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 *ABC* 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 *ABC* and *R* is represented as (see [24])

$$(ABC - R)(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u + d_v - 2} - 1}{\sqrt{d_u d_v}}$$

Note that  $(ABC - R)(G) \ge 0$  and equality holds if and only if  $G = P_3$ . So in our discussion we consider  $n \ge 4$ .

In this paper, motivated by the results in [24], we further investigated the extremal chemical trees for ABC - R. Moreover, maximal trees with fixed number of pendant vertices are also investigated for ABC - 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  $x_{p,q} ABC - R$  can be rewritten as follows [24]:

$$(ABC - R)(G) = \sum_{\delta \le p \le q \le \Delta} \frac{\sqrt{p + q - 2} - 1}{\sqrt{pq}} x_{p,q}.$$
(1)

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

$$n_1 + n_2 + n_3 + n_4 = n, (2)$$

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n-1), \tag{3}$$

$$x_{1,2} + x_{1,3} + x_{1,4} = n_1, (4)$$

$$x_{1,2} + 2x_{2,2} + x_{2,3} + x_{2,4} = 2n_2, (5)$$

$$x_{1,3} + x_{2,3} + 2x_{3,3} + x_{3,4} = 3n_3, (6)$$

$$x_{1,4} + x_{2,4} + x_{3,4} + 2x_{4,4} = 4n_4.$$
<sup>(7)</sup>

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

$$n_2 + 2n_3 + 3n_4 = n - 2$$

and thus,

$$n \equiv n_2 + 2n_3 + 2 \pmod{3}.$$
 (8)

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

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

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:

$$(ABC - R)(G) = \frac{4\sqrt{3} + \sqrt{6} - 5}{12}n + \frac{4\sqrt{3} - 5\sqrt{6} + 1}{12} - \frac{8\sqrt{3} - \sqrt{6} - 7}{12}x_{1,2} - \frac{32\sqrt{3} - 13\sqrt{6} - 19}{36}x_{1,3} - \frac{4\sqrt{3} + \sqrt{6} - 6\sqrt{2} + 1}{12}x_{2,2} - \frac{8\sqrt{3} + 11\sqrt{6} - 18\sqrt{2} - 13}{36}x_{2,3} - \frac{2\sqrt{3} + 2\sqrt{6} - 3\sqrt{2} - 4}{12}x_{2,4} - \frac{4\sqrt{3} + 7\sqrt{6} - 23}{36}x_{3,3} - \frac{4\sqrt{3} + 4\sqrt{6} - 3\sqrt{15} - 5}{18}x_{3,4}.$$
(9)

Let

$$\theta = \frac{8\sqrt{3} - \sqrt{6} - 7}{12}x_{1,2} + \frac{32\sqrt{3} - 13\sqrt{6} - 19}{36}x_{1,3} + \frac{4\sqrt{3} + \sqrt{6} - 6\sqrt{2} + 1}{12}x_{2,2} + \frac{8\sqrt{3} + 11\sqrt{6} - 18\sqrt{2} - 13}{36}x_{2,3} + \frac{2\sqrt{3} + 2\sqrt{6} - 3\sqrt{2} - 4}{12}x_{2,4} + \frac{4\sqrt{3} + 7\sqrt{6} - 23}{36}x_{3,3} + \frac{4\sqrt{3} + 4\sqrt{6} - 3\sqrt{15} - 5}{18}x_{3,4}.$$
(10)

Then Equation (9) can be rewritten as

$$(ABC - R)(G) = \frac{4\sqrt{3} + \sqrt{6} - 5}{12}n + \frac{4\sqrt{3} - 5\sqrt{6} + 1}{12} - \theta.$$
 (11)

since

$$\theta \approx 0.367243x_{1,2} + 0.127285x_{1,3} + 0.157701x_{2,2} + 0.0651375x_{2,3} + 0.0100367x_{2,4} + 0.0298509x_{3,3} + 0.00595623x_{3,4}.$$
(12)

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

**Theorem 1** ([24]). Consider the set of all *n*-vertex chemical trees.

- (1) Suppose that  $n \equiv 0 \pmod{3}$ .
  - (1.1) For  $n \ge 9$ , the maximum ABC 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  $n \ge 21$ , the second maximum ABC - 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  $n \ge 21$ , the third maximum ABC - 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  $n \equiv 1 \pmod{3}$ .
  - (2.1) For  $n \ge 13$ , the maximum ABC 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  $x_{3,4} = 3$ . (2.2) For  $n \ge 13$ , the second maximum ABC – R value is

$$\frac{4\sqrt{3}+\sqrt{6}-5}{12}n+\frac{12\sqrt{2}-13\sqrt{6}-4\sqrt{3}+17}{12},$$

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  $x_{2,4} = 4$ .

(2.3) For  $n \ge 25$ , the third maximum ABC - R value is

$$\frac{4\sqrt{3}+\sqrt{6}-5}{12}n+\frac{12\sqrt{15}-6\sqrt{2}-25\sqrt{6}-16\sqrt{3}+29}{12}$$

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  $n \equiv 2 \pmod{3}$ .
  - (3.1) For  $n \ge 5$ , the maximum ABC R value is

$$\frac{4\sqrt{3}+\sqrt{6}-5}{12}n+\frac{4\sqrt{3}-5\sqrt{6}+1}{12},$$

which is uniquely attained by those trees that contain no vertex of degree 2 or 3, that is,  $n_2 = n_3 = 0$ .

(3.2) For  $n \ge 17$ , the second maximum ABC - R value is

$$\frac{4\sqrt{3}+\sqrt{6}-5}{12}n+\frac{6\sqrt{15}+6\sqrt{2}-17\sqrt{6}-8\sqrt{3}+19}{12},$$

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  $n \ge 29$ , the third maximum ABC - 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 ABC – R Index for Chemical Trees

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

**Theorem 2.** Consider the set of all *n*-vertex chemical trees.

- (1) Suppose that  $n \equiv 0 \pmod{3}$ .
  - (1.1) For  $n \ge 21$ , the fourth maximum ABC 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  $n \ge 33$ , the fifth maximum ABC – 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  $x_{3,4} = 9$ .

(1.3) For  $n \ge 33$ , the sixth maximum ABC – R value is

$$\frac{4\sqrt{3}+\sqrt{6}-5}{12}n+\frac{24\sqrt{2}-12\sqrt{3}-21\sqrt{6}+33}{12}$$

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  $n \equiv 1 \pmod{3}$ .
  - (2.1) For  $n \ge 37$ , the fourth maximum ABC 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  $n \ge 37$ , the fifth maximum ABC – 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  $n \ge 37$ , the sixth maximum ABC - 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  $n \equiv 2 \pmod{3}$ .
  - (3.1) For  $n \ge 29$ , the fourth maximum ABC 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  $x_{2,4} = 6$ . (3.2) For  $n \ge 29$ , the fifth maximum ABC – R value is

$$\frac{4\sqrt{3}+\sqrt{6}-5}{12}n+\frac{42\sqrt{15}-78\sqrt{6}-48\sqrt{3}+96}{36},$$

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  $x_{3,4} = 7$ . (3.3) For  $n \ge 29$ , the sixth maximum ABC – R value is

$$\frac{4\sqrt{3}+\sqrt{6}-5}{12}n+\frac{36\sqrt{15}+36\sqrt{2}-60\sqrt{3}-87\sqrt{6}+111}{36}$$

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  $x_{1,2} + x_{1,3} + x_{2,2} \ge 1$  or  $x_{2,3} \ge 2$ . More precisely, from Equation (12),

• when  $x_{1,2} \ge 1$ ,

$$heta \geq rac{8\sqrt{3}-\sqrt{6}-7}{12} pprox 0.367243 > 0.080294,$$

• when  $x_{1,3} \ge 1$ ,

$$heta \geq rac{32\sqrt{3} - 13\sqrt{6} - 19}{36} pprox 0.127285 > 0.080294,$$

• when  $x_{2,2} \ge 1$ ,

$$heta \geq rac{4\sqrt{3} + \sqrt{6} - 6\sqrt{2} + 1}{12} pprox 0.157701 > 0.080294,$$

• when  $x_{2,3} \ge 2$ ,

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

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

$$x_{2,4} = 2n_2 - x_{2,3} \tag{13}$$

and

$$2x_{3,3} + x_{3,4} = 3n_3 - x_{2,3}.$$
 (14)

**Case 1.** *x*<sub>2,3</sub> = 1.

Observe that  $n_2 \ge 1$ ,  $n_3 \ge 1$ , and thus  $x_{2,4} \ge 1$  from Equation (13). If  $x_{2,4} \ge 2$ , 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),  $x_{3,4} \ge 2$ , together with Equation (12), it leads to

$$\theta \geq \frac{8\sqrt{3} + 11\sqrt{6} - 18\sqrt{2} - 13}{36} + \frac{2\sqrt{3} + 2\sqrt{6} - 3\sqrt{2} - 4}{12} \\ + 2 \cdot \frac{4\sqrt{3} + 4\sqrt{6} - 3\sqrt{15} - 5}{18} \\ \approx 0.08708666 > 0.080294.$$
 (15)

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

$$\theta \geq \frac{8\sqrt{3} + 11\sqrt{6} - 18\sqrt{2} - 13}{36} + \frac{2\sqrt{3} + 2\sqrt{6} - 3\sqrt{2} - 4}{12} + \frac{4\sqrt{3} + 7\sqrt{6} - 23}{36} \approx 0.1050251 > 0.080294.$$
(16)

**Case 2.**  $x_{2,3} = 0$ .

From Equations (13) and (14), it follows that

$$x_{2,4} = 2n_2$$
 (17)

and

$$2x_{3,3} + x_{3,4} = 3n_3. (18)$$

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

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

If  $x_{3,3} = 2$ , then  $n_3 \ge 3$ , and  $x_{3,4} \ge 5$  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,  $n_3 \ge 2$ . The proofs will be partitioned into several parts according to the value of  $n_3$ :  $n_3 = 2$ ,  $n_3 = 3$ ,  $n_3 \ge 4$ .

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  $n \equiv 1 \pmod{3}$  from Equation (8),  $x_{2,4} = 2$  from Equation (17), and by Equation (12),

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

If  $n_2 \ge 2$ , then,  $x_{2,4} \ge 4$  from Equation (17), and by Equation (12),

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

Next, suppose that  $n_3 = 3$ , then  $x_{3,4} = 7$  from Equation (14). If  $n_2 = 0$ , then  $n \equiv 2 \pmod{3}$  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  $n_2 \ge 1$ , then  $x_{2,4} \ge 2$  from Equation (17), and by Equation (12),

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

Finally, if  $n_3 \ge 4$ , then  $x_{3,4} \ge 10$  from Equation (16), and by Equation (12),

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

**Subcase 2.2.**  $x_{3,3} = 0$ .

In this case,  $x_{3,4} = 3n_3$  from Equation (18). This time, we partition the proofs according to the value of  $n_2$ :  $n_2 = 0$ ,  $n_2 = 1$ ,  $n_2 = 2$ ,  $n_2 = 3$ ,  $n_2 = 4$ ,  $n_2 \ge 5$ .

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  $n \equiv 1 \pmod{3}$  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  $n_3 \ge 5$ , then  $x_{3,4} \ge 15$ , and by Equation (12),

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

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  $n \equiv 0 \pmod{3}$  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  $n_3 \ge 4$ , then  $x_{3,4} \ge 12$ , and by Equation (12),

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

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  $n \equiv 0 \pmod{3}$  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  $n \equiv 2 \pmod{3}$  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  $n_3 \ge 3$ , then  $x_{3,4} \ge 9$ , and by Equation (12),

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

Suppose that  $n_2 = 3$ , that is,  $x_{2,4} = 6$  from Equation (17). If  $n_3 = 0$ , then  $n \equiv 2 \pmod{3}$  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  $n \equiv 1 \pmod{3}$  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  $n_3 \ge 2$ , then  $x_{3,4} \ge 6$ , and by Equation (12),

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

Suppose that  $n_2 = 4$ , that is,  $x_{2,4} = 8$  from Equation (17). If  $n_3 = 0$ , then  $n \equiv 0 \pmod{3}$  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  $n_3 \ge 1$ , then  $x_{3,4} \ge 3$ , and by Equation (12),

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

Finally, if  $n_2 \ge 5$ , then  $x_{2,4} \ge 10$  from Equation (17), and by Equation (12),

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

In conclusion, we obtain the following

- (i) If  $n \equiv 0 \pmod{3}$ , then the fourth, fifth and sixth minimum  $\theta$  values are 0.0580155, 0.0736795 and 0.0802936, respectively.
- (ii) If  $n \equiv 1 \pmod{3}$ , then the fourth, fifth and sixth minimum  $\theta$  values are 0.0714748, 0.0737492 and 0.0780889, respectively.
- (iii) If  $n \equiv 2 \pmod{3}$ , 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 ABC - 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 ABC - R values in Theorem 2-(1).



**Figure 2.** Chemical trees with the fourth (D), the fifth (E) and the sixth (F) maximum ABC - R values in Theorem 2-(2).



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

## 4. Upper Bound for *ABC* – *R* Index of Molecular Trees

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

Let  $T_{n,n_1}$  be the set of molecular trees satisfying

$$x_{1,4} = n_1,$$
  
$$x_{2,2} = n - 2n_1 + 3 - \frac{1}{3}x_{2,3},$$
  
$$x_{2,4} = n_1 - 4 - \frac{2}{3}x_{2,3}.$$

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,  $n_1 \ge 5$  of which are pendant vertices. Then

$$(ABC)(T) \le \frac{\sqrt{2}}{2}n + \frac{\sqrt{3} - \sqrt{2}}{2}n_1 - \frac{\sqrt{2}}{2}$$

with equality holds if and only if  $T \in \mathcal{T}_{n,n_1}$ .

Obviously, from Equation (1) we obtain

$$(ABC - R)(T) = \frac{\sqrt{2} - 1}{\sqrt{3}} x_{1,3} + \frac{\sqrt{3} - 1}{2} x_{1,4} + \frac{\sqrt{2} - 1}{2} x_{2,2} + \frac{\sqrt{3} - 1}{\sqrt{6}} x_{2,3} + \frac{1}{\sqrt{8}} x_{2,4} + \frac{1}{3} x_{3,3} + \frac{\sqrt{5} - 1}{\sqrt{12}} x_{3,4} + \frac{\sqrt{6} - 1}{4} x_{4,4}$$
(19)

Now let  $\mathcal{T}'_{n,n_1}$  be the set of molecular trees satisfying

$$x_{1,4} = n_1,$$
  
$$x_{2,2} = n - 2n_1 + 3,$$
  
$$x_{2,4} = n_1 - 4$$

and

$$x_{2,4} = n_1 - 4.$$

**Theorem 4.** Let *T* be a molecular tree of order *n* and  $n_1 \ge 5$  pendant vertices, then

$$(ABC - R)(T) \le \frac{\sqrt{2} - 1}{2}n + \frac{2 - 3\sqrt{2} + 2\sqrt{3}}{4}n_1 + \frac{1}{\sqrt{2}} - \frac{3}{2}$$

with equality holds if and only if  $T \in \mathcal{T}'_{n,n_1}$ .

**Proof.** Since *T* is a molecular tree, we have Equations (2)–(7). Suppose that

$$f_{1} = x_{1,2} + x_{1,3} + x_{1,4}$$

$$f_{2} = x_{1,2} + x_{2,3}$$

$$f_{3} = x_{1,3} + x_{2,3} + 2x_{3,3} + x_{3,4}$$

$$f_{4} = x_{1,4} + x_{3,4} + 2x_{4,4},$$

that is,

$$f_1 = n_1$$
  

$$f_2 = 2n_2 - 2x_{2,2} - x_{2,4}$$
  

$$f_3 = 3n_3$$
  

$$f_4 = 4n_4 - x_{2,4}$$

we have

$$\sum_{i=1}^{4} f_i = 2(n-1) - 2(x_{2,2} + x_{2,4})$$
$$\sum_{i=1}^{4} \frac{1}{i} f_i = n - (x_{2,2} + \frac{3}{4}x_{2,4}),$$

implying that

$$x_{2,2} = \frac{3}{2} \sum_{i=1}^{4} f_i - 4 \sum_{i=1}^{4} \frac{1}{i} f_i + n + 3$$
  
$$x_{2,4} = -2 \sum_{i=1}^{4} f_i + 4 \sum_{i=1}^{4} \frac{1}{i} f_i - 4.$$

Thus we have

$$\begin{aligned} x_{1,4} &= n_1 - x_{1,2} - x_{1,3} \\ x_{2,2} &= n - 2n_1 + 3 - x_{1,2} - \frac{1}{3}x_{1,3} - \frac{1}{3}x_{2,3} + \frac{1}{3}x_{3,3} + \frac{2}{3}x_{3,4} + x_{4,4} \\ x_{2,4} &= n_1 - 4 + x_{1,2} + \frac{1}{3}x_{1,3} - \frac{2}{3}x_{2,3} - \frac{4}{3}x_{3,3} - \frac{5}{3}x_{3,4} - 2x_{4,4}. \end{aligned}$$

Substituting them back into Equation (19), we have

$$(ABC - R)(T) = \frac{\sqrt{2} - 1}{2}n + \frac{2 - 3\sqrt{2} + 2\sqrt{3}}{4}n_1 + \frac{1}{\sqrt{2}} - \frac{3}{2} \\ + \frac{4 - \sqrt{2} - 2\sqrt{3}}{4}x_{1,2} + \frac{8 - \sqrt{2} - 10\sqrt{3} + 4\sqrt{6}}{12}x_{1,3} \\ + \frac{1 + \sqrt{2} - \sqrt{6}}{6}x_{2,3} + \frac{1 - \sqrt{2}}{6}x_{3,3} \\ + \frac{2\sqrt{15} - 4 - \sqrt{2} - 2\sqrt{3}}{12}x_{3,4} + \frac{\sqrt{6} - 3}{4}x_{4,4} \\ \approx \frac{\sqrt{2} - 1}{2}n + \frac{2 - 3\sqrt{2} + 2\sqrt{3}}{4}n_1 + \frac{1}{\sqrt{2}} - \frac{3}{2} \\ - 0.219579x_{1,2} - 0.078064x_{1,3} - 0.005879x_{2,3} \\ - 0.069036x_{3,3} - 0.094362x_{3,4} - 0.137628x_{4,4} \end{aligned}$$

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

$$(ABC - R)(T) \le \frac{\sqrt{2} - 1}{2}n + \frac{2 - 3\sqrt{2} + 2\sqrt{3}}{4}n_1 + \frac{1}{\sqrt{2}} - \frac{3}{2}$$

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,  $x_{1,4} = n_1, x_{2,2} = n - 2n_1 + 3, x_{2,4} = n_1 - 4$ , i.e.,  $T \in \mathcal{T}'_{n,n_1}$ .  $\Box$ 

#### 5. Conclusions

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

Author Contributions: Conceptualization, R.H. and Z.D.; methodology, W.N.N.N.W.Z.; validation, R.H., Z.D. and M.K.J.; formal analysis, W.N.N.N.W.Z.; investigation, W.N.N.N.W.Z., R.H. and Z.D.; resources, R.H.; writing—original draft preparation, R.H.; writing—review and editing, R.H., Z.D. and M.K.J.; supervision, R.H. and Z.D.; project administration, R.H.; funding acquisition, R.H. All authors have read and agreed to the published version of the manuscript

Funding: This research received no external funding.

Acknowledgments: This research is supported by the Research Intensified Grant Scheme (RIGS), Phase 1/2019, Universiti Malaysia Terengganu, Malaysia with Grant Vot. 55192/6. The authors would like to thanks the referees for the constructive and valuable comments that improved the paper.

Conflicts of Interest: The authors declare no conflict of interest.

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