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On Chemical Trees That Maximize Atom–Bond Connectivity Index, Its Exponential Version, and Minimize Exponential Geometric–Arithmetic Index

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Abstract

A chemical tree is a tree that has no vertex of degree greater than 4. We denote the set of chemical trees with n vertices as $\mathcal{C}_n$. The $\mathcal{ABC}$ index of a chemical tree T is defined as

$$\mathcal{ABC}(T) = \sum_{1 \leq i \leq j \leq 4} m_{i,j}(T) \sqrt{\frac{i+j-2}{ij}},$$

where $m_{i,j}(T)$ is the number of edges in T joining vertices of degree i and j. Furtula, Graovac and Vukičević in 2009 found trees with maximal $\mathcal{ABC}$ index among all trees in $\mathcal{C}_n$, when $n \equiv 1 \mod 4$. In this paper we find the trees with maximal $\mathcal{ABC}$ index in $\mathcal{C}_n$ for all n. Using the same technique, we find the trees with maximal $e^{\mathcal{ABC}}$ and minimal $e^{\mathcal{GA}}$ over $\mathcal{C}_n$ for all n, where

$$e^{\mathcal{ABC}}(T) = \sum_{1 \leq i \leq j \leq 4} m_{i,j}(T)\, e^{\sqrt{\frac{i+j-2}{ij}}}$$

and

$$e^{\mathcal{GA}}(T) = \sum_{1 \leq i \leq j \leq 4} m_{i,j}(T)\, e^{\frac{2\sqrt{ij}}{i+j}}.$$

1 Introduction

Let T be a tree with n vertices. We denote by $n_j = n_j(T)$ the number of vertices in T of degree j, and by $m_{i,j} = m_{i,j}(T)$ the number of edges in T joining vertices of degree i and j. A chemical tree is a tree that has no vertex of degree greater than 4. We denote the set of chemical trees with n vertices as $\mathcal{C}_n$. The following relations are well known for a chemical tree $T \in \mathcal{C}_n$.

$$\begin{array}{r} 2m_{1,1} + m_{1,2} + m_{1,3} + m_{1,4} = n_1 \\ m_{1,2} + 2m_{2,2} + m_{2,3} + m_{2,4} = 2n_2 \\ m_{1,3} + m_{2,3} + 2m_{3,3} + m_{3,4} = 3n_3 \\ m_{1,4} + m_{2,4} + m_{3,4} + 2m_{4,4} = 4n_4 \end{array}, \tag{1}$$

$$n_1 + n_2 + n_3 + n_4 = n, \tag{2}$$

and

$$\sum_{1 \leq i \leq j \leq 4} m_{i,j} = n - 1. \tag{3}$$

A vertex-degree-based (VDB) topological index defined over $\mathcal{C}_n$ is a function $\varphi : \mathcal{C}_n \longrightarrow \mathbb{R}$ induced by numbers $\{\varphi(i,j)\}_{(i,j) \in K}$, where

$$K = \{(i,j) \in \mathbb{N} \times \mathbb{N} : 1 \leq i \leq j \leq 4\},$$

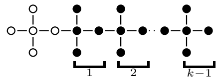
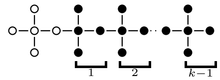
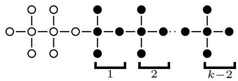
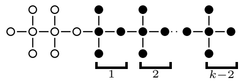
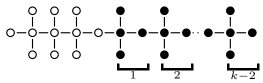
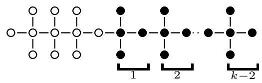
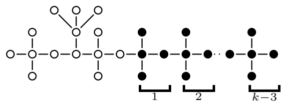
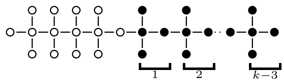
defined for every $T \in \mathcal{C}_n$ as

$$\varphi(T) = \sum_{(i,j) \in K} m_{i,j}(T)\, \varphi(i,j). \tag{4}$$

In the particular case when $\varphi(i,j) = \frac{1}{\sqrt{ij}}$ we obtain the connectivity index χ, introduced by Randić in 1975 [27], one of the best known and widely used molecular descriptor in QSPR/QSAR studies [32, 33]. However, in this paper our main concern is the atom-bond connectivity index ($\mathcal{ABC}$) proposed by Estrada et al. in [14], a valuable predictive molecular descriptor in the study of heat formation in alkanes [14, 15]. It is defined as in (4), where $\varphi(i,j) = \sqrt{\frac{i+j-2}{ij}}$. Also we will study $e^{\mathcal{ABC}}$, the exponential of $\mathcal{ABC}$ induced by the numbers $\varphi(i,j) = e^{\sqrt{\frac{i+j-2}{ij}}}$ [26]. For recent results on $\mathcal{ABC}$ and $e^{\mathcal{ABC}}$ we refer to [3, 4, 6, 7, 11, 13, 16, 19, 30, 35, 36].

Furtula, Graovac and Vukičević considered in 2009 [17] the problem of finding the trees with maximal $\mathcal{ABC}$ among all trees in $\mathcal{C}_n$. They showed that when $n = 4k + 1$ $(k \geq 1)$, the tree T_k shown in Table 1 has maximal $\mathcal{ABC}$ index over $\mathcal{C}_n$. In this paper we give the complete solution for all n to the maximal $\mathcal{ABC}$ and $e^{\mathcal{ABC}}$ over $\mathcal{C}_n$. The results are shown

Table 1. Maximal trees with respect to $\mathcal{ABC}$ and $e^{\mathcal{ABC}}$ indices over $\mathcal{C}_n$

	Maximal $\mathcal{ABC}$	Maximal $e^{\mathcal{ABC}}$
$n = 4k+1$ $(k \geqslant 1)$	T_k 	T_k 
$n = 4k$ $(k \geqslant 2)$	P_k 	P_k 
$n = 4k+3$ $(k \geqslant 2)$	Q_k 	Q_k 
$n = 4k+2$ $(k \geqslant 3)$	T'_k 	R_k 

in Table 1. As you can see, when $n = 4k + 2$ $(k \geq 3)$, the maximal value of $\mathcal{ABC}$ and the maximal value of $e^{\mathcal{ABC}}$ are attained in different trees.

Another important VDB topological index is the geometric-arithmetic index $\mathcal{GA}$, introduced by Vukičević and Furtula in 2009 [34], defined for a chemical tree T as in (4), with $\varphi(i, j) = \frac{2\sqrt{ij}}{i+j}$. For recent results in $\mathcal{GA}$ see ([1, 2, 5, 18, 20–25, 28, 29, 31]) and the survey [10]. The minimal value of $\mathcal{GA}$ over $\mathcal{C}_n$ was solved in [34] for all n. In this paper we consider the exponential of $\mathcal{GA}$ [26], denoted by $e^{\mathcal{GA}}$, and induced by the numbers $\varphi(i, j) = e^{\frac{2\sqrt{ij}}{i+j}}$ in (4). We solve the minimal value of $e^{\mathcal{GA}}$ over $\mathcal{C}_n$, for all n. The results are shown in Table 2. We note in this case that when $n = 3k + 1$, the minimal value of $\mathcal{GA}$ and the minimal value of $e^{\mathcal{GA}}$ are attained in different trees.

The maximal value of $e^{\mathcal{ABC}}$ and the minimal value of $e^{\mathcal{GA}}$ over $\mathcal{C}_n$ were both open problems proposed in [9].

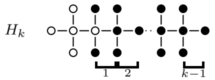
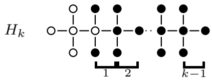
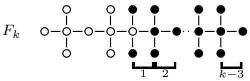
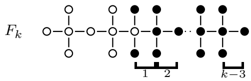
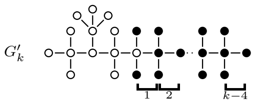
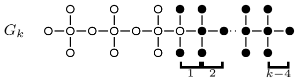
2 Operations in chemical trees

There are three functions which play an important role in the variation of a VDB topological index φ, when operations are performed in chemical trees:

$$f(p, q) = [\varphi(2, p) - \varphi(3, p)] + [\varphi(2, q) - \varphi(3, q)], \tag{5}$$

$$\begin{aligned} g(p, q, r) &= [\varphi(2, p) - \varphi(4, p)] + [\varphi(3, q) - \varphi(4, q)] \\ &\quad + [\varphi(3, r) - \varphi(4, r)], \end{aligned} \tag{6}$$

Table 2. Minimal trees with respect to $\mathcal{GA}$ and $e^{\mathcal{GA}}$ indices over $\mathcal{C}_n$

	Minimal $\mathcal{GA}$	Minimal $e^{\mathcal{GA}}$
$n = 3k+2$ $(k \geqslant 1)$		
$n = 3k$ $(k \geqslant 3)$		
$n = 3k+1$ $(k \geqslant 4)$		

and

$$h(p,q,r,s) = [\varphi(3,p) - \varphi(4,p)] + [\varphi(3,q) - \varphi(2,q)] + [\varphi(3,r) - \varphi(4,r)] + [\varphi(3,s) - \varphi(4,s)], \quad (7)$$

where p, q, r, s are integers such that $1 \leq p, q, r, s \leq 4$. In fact, these functions appear when we perform the operations described below.

Proposition 2.1. *(Operation 1) Let φ be a VDB topological index. Let xy be an edge of T such that $d_x = d_y = 2$ and $\widehat{T}$ as in Figure 1. Then*

$$\varphi(T) - \varphi(\widehat{T}) = f(d_a, d_b) + \varphi(2,2) - \varphi(1,3). \quad (8)$$

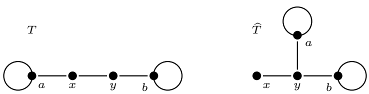


Figure 1. Operation 1 on T.

Proof. Note that

$$\begin{aligned}\varphi(T) - \varphi(\widehat{T}) &= \varphi(2,d_a) + \varphi(2,2) + \varphi(2,d_b) \\ &\quad - \varphi(1,3) - \varphi(3,d_a) - \varphi(3,d_b) \\ &= f(d_a,d_b) + \varphi(2,2) - \varphi(1,3).\end{aligned}$$

∎

Proposition 2.2. *(Operation 2) Let φ be a VDB topological index. Let xy be an edge of T such that $d_x = 2, d_y = 3$ and $\widehat{T}$ as in Figure 2. Then*

$$\varphi(T) - \varphi(\widehat{T}) = g(d_a, d_b, d_c) + \varphi(2,3) - \varphi(1,4). \tag{9}$$

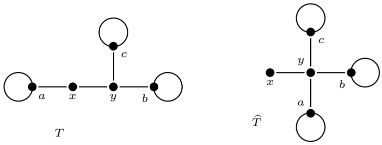


Figure 2. Operation 2 on T.

Proof. In fact,

$$\begin{aligned}\varphi(T) - \varphi(\widehat{T}) &= \varphi(2,d_a) + \varphi(2,3) + \varphi(3,d_b) + \varphi(3,d_c) \\ &\quad -\varphi(1,4) - \varphi(4,d_a) - \varphi(4,d_b) - \varphi(4,d_c) \\ &= g(d_a, d_b, d_c) + \varphi(2,3) - \varphi(1,4).\end{aligned}$$

■

Proposition 2.3. *(Operation 3) Let φ be a VDB topological index. Let xy be an edge of T such that $d_x = d_y = 3$ and $\widehat{T}$ as in Figure 3. Then*

$$\varphi(T) - \varphi(\widehat{T}) = h(d_a, d_b, d_c, d_e) + \varphi(3,3) - \varphi(2,4). \tag{10}$$

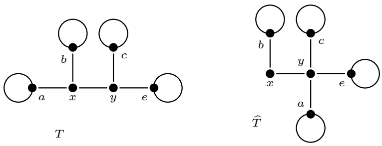


Figure 3. Operation 3 on T.

Proof. Note that

$$\begin{aligned}\varphi(T) - \varphi(\widehat{T}) &= \varphi(3,d_a) + \varphi(3,d_b) + \varphi(3,3) + \varphi(3,d_c) + \varphi(3,d_e) \\ &\quad -\varphi(2,d_b) - \varphi(2,4) - \varphi(4,d_a) - \varphi(4,d_c) - \varphi(4,d_e) \\ &= h(d_a, d_b, d_c, d_e) + \varphi(3,3) - \varphi(2,4).\end{aligned}$$

■

It is of great interest to us to determine the sign of $\varphi(T) - \varphi(\widehat{T})$, because this information indicates whether φ increases or decreases when the correspondent operation is carried out. We will do this for the topological indices $\mathcal{ABC}$, $e^{\mathcal{ABC}}$ and $e^{\mathcal{GA}}$.

We begin with Operation 1. Let us denote by $p = d_a(T)$ and $q = d_b(T)$ in Figure 1. Without loosing generality, we may assume that $1 \leq p \leq q \leq 4$. The values of $\varphi(T) - \varphi(\widehat{T})$ are given in Table 3.

Table 3. Values of $\varphi(T) - \varphi(\widehat{T})$ in Operation 1 for $\mathcal{ABC}$, $e^{\mathcal{ABC}}$ and $e^{\mathcal{GA}}$ indices

p	q	$\mathcal{ABC}$	$e^{\mathcal{ABC}}$	$e^{\mathcal{GA}}$	p	q	$\mathcal{ABC}$	$e^{\mathcal{ABC}}$	$e^{\mathcal{GA}}$
1	1	-0.328	-0.703	0.720	2	3	-0.069	-0.154	0.341
1	2	-0.219	-0.469	0.585	2	4	-0.048	-0.113	0.272
1	3	-0.178	-0.389	0.476	3	3	-0.029	-0.074	0.232
1	4	-0.157	-0.348	0.407	3	4	-0.007	-0.033	0.163
2	2	-0.109	-0.234	0.450	4	4	0.014	0.008	0.094

Now we consider Operation 2. Assume that $p = d_a(T)$ and $q = d_b(T), r = d_c(T)$ in Figure 2. Clearly $1 \leq p \leq 4$ and we may assume that $1 \leq q \leq r \leq 4$. Then the values of $\varphi(T) - \varphi(\widehat{T})$ are given in Table 4.

Table 4. Values of $\varphi(T) - \varphi(\widehat{T})$ in Operation 2 for $\mathcal{ABC}$, $e^{\mathcal{ABC}}$ and $e^{\mathcal{GA}}$ indices

p	q	r	$\mathcal{ABC}$	$e^{\mathcal{ABC}}$	$e^{\mathcal{GA}}$	p	q	r	$\mathcal{ABC}$	$e^{\mathcal{ABC}}$	$e^{\mathcal{GA}}$
1	1	1	-0.417	-0.928	1.084	3	1	1	-0.196	-0.458	0.716
1	1	2	-0.367	-0.814	1.029	3	1	2	-0.147	-0.343	0.660
1	1	3	-0.346	-0.773	0.960	3	1	3	-0.126	-0.302	0.591
1	1	4	-0.334	-0.751	0.904	3	1	4	-0.114	-0.281	0.536
1	2	2	-0.318	-0.699	0.973	3	2	2	-0.097	-0.228	0.605
1	2	3	-0.297	-0.658	0.904	3	2	3	-0.076	-0.187	0.536
1	2	4	-0.285	-0.637	0.849	3	2	4	-0.064	-0.166	0.481
1	3	3	-0.275	-0.617	0.835	3	3	3	-0.055	-0.147	0.467
1	3	4	-0.264	-0.596	0.780	3	3	4	-0.043	-0.125	0.412
1	4	4	-0.252	-0.574	0.725	3	4	4	-0.031	-0.104	0.356
2	1	1	-0.258	-0.579	0.893	4	1	1	-0.163	-0.396	0.591
2	1	2	-0.208	-0.464	0.838	4	1	2	-0.114	-0.281	0.536
2	1	3	-0.187	-0.423	0.769	4	1	3	-0.093	-0.240	0.467
2	1	4	-0.175	-0.402	0.714	4	1	4	-0.081	-0.219	0.411
2	2	2	-0.159	-0.349	0.783	4	2	2	-0.064	-0.166	0.481
2	2	3	-0.138	-0.309	0.714	4	2	3	-0.043	-0.125	0.412
2	2	4	-0.126	-0.287	0.658	4	2	4	-0.031	-0.104	0.356
2	3	3	-0.117	-0.268	0.645	4	3	3	-0.022	-0.084	0.343
2	3	4	-0.105	-0.246	0.589	4	3	4	-0.010	-0.063	0.287
2	4	4	-0.093	-0.225	0.534	4	4	4	0.002	-0.042	0.232

Finally, let us consider Operation 3. Set $p = d_a(T), q = d_b(T)$ and $r = d_c(T), s = d_e(T)$ in Figure 3. We may assume that $1 \leq p \leq q \leq 4$, in other words, we perform Operation 3 by moving the vertex adjacent to x (different from y) with the least degree. We also assume that $1 \leq r \leq s \leq 4$. Moreover, we will apply Operation 3 when $p \neq 2, q \neq 2, r \neq 2$, and $s \neq 2$. Then under these conditions, the values of $\varphi(T) - \varphi(\widehat{T})$ are given in Table 5.

Table 5. Values of $\varphi(T) - \varphi(\widehat{T})$ in Operation 3 for $\mathcal{ABC}$, $e^{\mathcal{ABC}}$ and $e^{\mathcal{GA}}$ indices

p	q	r	s	$\mathcal{ABC}$	$e^{\mathcal{ABC}}$	$e^{\mathcal{GA}}$	p	q	r	s	$\mathcal{ABC}$	$e^{\mathcal{ABC}}$	$e^{\mathcal{GA}}$
1	1	1	1	-0.080	-0.191	0.417	3	4	1	1	-0.180	-0.391	0.606
1	1	1	3	-0.009	-0.035	0.293	3	4	1	3	-0.109	-0.235	0.482
1	1	1	4	0.003	-0.014	0.237	3	4	1	4	-0.097	-0.214	0.426
1	3	1	3	-0.159	-0.350	0.537	3	4	3	3	-0.039	-0.079	0.358
1	3	1	4	-0.147	-0.328	0.482	3	4	3	4	-0.027	-0.058	0.302
1	4	1	4	-0.168	-0.369	0.551	3	4	4	4	-0.015	-0.036	0.247
3	3	1	1	-0.159	-0.350	0.537	4	4	1	1	-0.168	-0.369	0.551
3	3	1	3	-0.088	-0.194	0.413	4	4	1	3	-0.097	-0.214	0.426
3	3	1	4	-0.076	-0.173	0.357	4	4	1	4	-0.085	-0.192	0.371
3	3	3	3	-0.017	-0.038	0.289	4	4	3	3	-0.027	-0.058	0.302
3	3	3	4	-0.005	-0.017	0.233	4	4	3	4	-0.015	-0.036	0.247
3	3	4	4	0.007	0.004	0.178	4	4	4	4	-0.003	-0.015	0.191

3 Maximal value of the $\mathcal{ABC}$ index among chemical trees

The following lemmas are useful in the sequel.

Lemma 3.1. *Suppose that xy is an edge of $T \in \mathcal{C}_n$ such that $d_x = d_y = 2$ as in Figure 1. If $(d_a, d_b) \neq (4,4)$ then we can find a tree $\widehat{T} \in \mathcal{C}_n$ such that $\mathcal{ABC}(T) < \mathcal{ABC}(\widehat{T})$.*

Proof. This is a consequence of Proposition 2.1 and Table 3. ■

Lemma 3.2. *Suppose that xy is an edge of $T \in \mathcal{C}_n$ such that $d_x = 2$ and $d_y = 3$ as in Figure 2. If $d_a \neq 4$ or $(d_b, d_c) \neq (4,4)$ then we can find a tree $\widehat{T} \in \mathcal{C}_n$ such that $\mathcal{ABC}(T) < \mathcal{ABC}(\widehat{T})$.*

Proof. This is a consequence of Proposition 2.2 and Table 4. ■

Lemma 3.3. *Suppose that xy is an edge of $T \in \mathcal{C}_n$ such that $d_x = d_y = 3$ as in Figure 3. If $d_z = 2$ for some $z \in \{a, b, c, e\}$, then we can find a tree $\widehat{T} \in \mathcal{C}_n$ such that $\mathcal{ABC}(T) < \mathcal{ABC}(\widehat{T})$.*

Proof. Assume that $d_a = 2$. Then ax is an edge of T such that $d_a = 2$ and $d_x = 3$. Moreover, $(d_b, d_y) \neq (4,4)$. It follows from Lemma 3.2 that there exists a tree $\widehat{T} \in \mathcal{C}_n$ such that $\mathcal{ABC}(T) < \mathcal{ABC}(\widehat{T})$. ■

From now on we will say that a tree $T \in \mathcal{C}_n$ is maximal with respect to $\mathcal{ABC}$ over $\mathcal{C}_n$ if

$$\mathcal{ABC}(S) \leq \mathcal{ABC}(T),$$

for all $S \in \mathcal{C}_n$.

Proposition 3.4. *Let $n \geq 10$. If T is maximal with respect to $\mathcal{ABC}$ over $\mathcal{C}_n$, then $m_{1,3}(T) = 0$.*

Proof. Assume that $m_{1,3}(T) > 0$. Then T is of the form depicted in Figure 4, where we may assume $1 \leq d_c \leq d_x \leq 4$. We consider four cases:

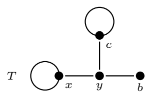


Figure 4. Form of $T \in \mathcal{C}_n$ when $m_{1,3}(T) > 0$.

1. $d_x = 1$. Then $d_c = 1$ which implies $n = 4$, a contradiction.

2. $d_x = 2$. Then xy is an edge of T such that $d_x = 2, d_y = 3$. Moreover, $(d_b, d_c) = (1, d_c) \neq (4,4)$. By Lemma 3.2 we arrive at a contradiction.

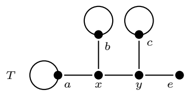


Figure 5. Form of $T \in \mathcal{C}_n$ when $m_{1,3}(T) > 0$ and $d_x = 3$.

3. $d_x = 3$. Then T has the form depicted in Figure 5. By Lemma 3.3, $d_a \neq 2, d_b \neq 2$, and $d_c \neq 2$. Now, since xy is an edge of T such that $d_x = d_y = 3$, we apply Proposition 2.3 and Table 5 to deduce that $d_c = 4, d_a = d_b = 1$. In this case, we construct the tree T' in Figure 6. Then

$$\begin{aligned} \mathcal{ABC}(T) - \mathcal{ABC}(T') &= 3\sqrt{\frac{2}{3}} + \sqrt{\frac{4}{9}} + \sqrt{\frac{5}{12}} + \sqrt{\frac{d_w+2}{4d_w}} \\ &\quad -2\sqrt{\frac{1}{2}} - 3\sqrt{\frac{3}{4}} - \sqrt{\frac{6}{16}} \qquad (11) \\ &< 0, \end{aligned}$$

for all $2 \leq d_w \leq 4$. A contradiction. So the only case left is when $d_u = d_v = d_w = 1$, but in this case $n = 9$, a contradiction.

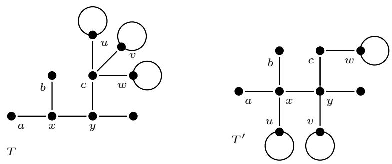


Figure 6. Operation on $T \in \mathcal{C}_n$ when $m_{1,3}(T) > 0$, $d_x = 3$, $d_a = d_b = 1$ and $d_c = 4$.

4. $d_x = 4$. Then T has the form depicted in Figure 7. Let T'' be the tree shown in Figure 7. It follows that

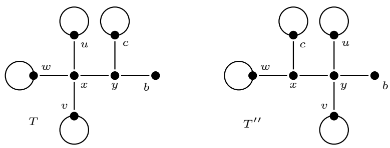


Figure 7. Operation on $T \in \mathcal{C}_n$ when $m_{1,3}(T) > 0$, $d_x = 4$ and $2 \leq d_w \leq 4$.

$$\mathcal{ABC}\,(T) - \mathcal{ABC}\,(T'') \;=\; \sqrt{\frac{d_w+2}{4d_w}} + \sqrt{\frac{2}{3}} - \sqrt{\frac{d_w+1}{3d_w}} - \sqrt{\frac{3}{4}} < 0, \qquad (12)$$

for all $2 \leq d_w \leq 4$. A contradiction. So we may assume that $d_u = d_v = d_w = 1$,

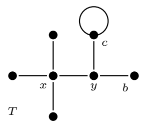


Figure 8. Form of $T \in \mathcal{C}_n$ when $m_{1,3}(T) > 0$, $d_x = 4$ and $d_u = d_v = d_w = 1$.

as shown in Figure 8. If $d_c = 1$ then $n = 7$, a contradiction. If $d_c = 2$ then we get a contradiction by Lemma 3.2. If $d_c = 3$, then we repeat the argument of case 3. So we may assume that $d_c = 4$. In this case we again apply the same operation considered in Figure 7, to conclude that all three vertices adjacent to c (different from y) have degree 1, and so $n = 10$, a contradiction. ■

Proposition 3.5. *Let $n \geq 7$. If T is maximal with respect to $\mathcal{ABC}$ over $\mathcal{C}_n$, then $m_{1,2}(T) = 0$.*

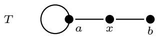


Figure 9. Form of $T \in \mathcal{C}_n$ when $m_{1,2}(T) > 0$.

Proof. Assume that $m_{1,2}(T) > 0$ so T has the form depicted in Figure 9. If $d_a = 1$, then $n = 3$, a contradiction. If $d_a = 2$ then ax is an edge of T such that $d_a = d_x = 2$. Then we get a contradiction by Lemma 3.1. If $d_a = 3$, then xa is an edge of T such that $d_x = 2$ and $d_a = 3$. So we get a contradiction using Lemma 3.2. So we may assume that $d_a = 4$. Then we construct the tree T' shown in Figure 10. Therefore

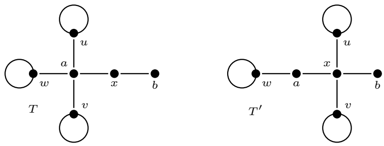


Figure 10. Operation on $T \in \mathcal{C}_n$ when $m_{1,2}(T) > 0$ and $d_a = 4$.

$$\mathcal{ABC}(T) - \mathcal{ABC}(T') = \sqrt{\frac{d_w + 2}{4d_w}} - \sqrt{\frac{3}{4}} < 0, \tag{13}$$

for all $2 \leq d_w \leq 4$. Hence we may assume that $d_u = d_v = d_w = 1$, but in this case $n = 6$, a contradiction. Consequently, $m_{1,2}(T) = 0$. ■

Proposition 3.6. *Let $n \geq 11$. If T is maximal with respect to $\mathcal{ABC}$ over $\mathcal{C}_n$, then $m_{2,2}(T) = 0$.*

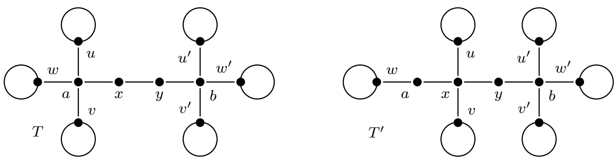


Figure 11. Operation on $T \in \mathcal{C}_n$ when $m_{2,2}(T) > 0$ and $d_a = d_b = 4$.

Proof. If $m_{2,2}(T) > 0$ then T has the form depicted in Figure 1. Then by Lemma 3.1, $d_a = d_b = 4$. Let T' be the tree in Figure 11. Then

$$\mathcal{ABC}(T) - \mathcal{ABC}(T') = \sqrt{\frac{d_w + 2}{4d_w}} - \sqrt{\frac{1}{2}} < 0, \tag{14}$$

for all $3 \le d_w \le 4$. So we may assume that all vertices u, v, w, u', v', w' have degree ≤ 2. If they are all 1's, then $n = 10$, a contradiction. So one of them has degree 2, say $d_w = 2$. Then we define the tree T'' in Figure 12. Hence

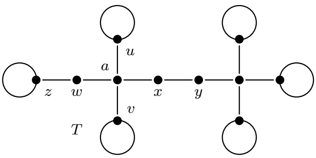


Figure 12. Operation on $T \in \mathcal{C}_n$ when $m_{2,2}(T) > 0$, $d_a = d_b = 4$ and $d_w = 2$.

$$\mathcal{ABC}(T) - \mathcal{ABC}(T'') = 3\sqrt{\frac{1}{2}} - \sqrt{\frac{3}{4}} - \sqrt{\frac{5}{12}} - \sqrt{\frac{d_z + 1}{3d_z}} < 0, \tag{15}$$

for all $1 \le d_z \le 4$. This is a contradiction. In conclusion, $m_{2,2}(T) = 0$. ■

Proposition 3.7. *If T is maximal with respect to $\mathcal{ABC}$ over $\mathcal{C}_n$, then $m_{3,3}(T) = 0$.*

Proof. If $m_{3,3}(T) > 0$ then T has the form depicted in Figure 3. By Lemma 3.3, $d_a \ne 2$, $d_b \ne 2, d_c \ne 2$, and $d_e \ne 2$. We also know by Proposition 3.4 that $d_a \ne 1, d_b \ne 1, d_c \ne 1$, and $d_e \ne 1$. Now we apply Proposition 2.3 and Table 5 to deduce that $d_a = d_b = 3$ and $d_c = d_e = 4$. Then T has the form shown in Figure 13. Since $d_b = d_x = d_a = 3$, we repeat the same argument to the edges bx and ax of T to conclude that $d_u = d_v = d_{b'} = d_z = 4$. Now we define T' as in Figure 13. Then

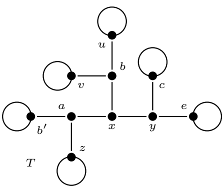


Figure 13. Operation on $T \in \mathcal{C}_n$ when $m_{3,3}(T) > 0$, $d_a = d_b = 3$ and $d_c = d_e = 4$.

$$\mathcal{ABC}(T) - \mathcal{ABC}(T') = 3\sqrt{\frac{4}{9}} - 2\sqrt{\frac{1}{2}} - \sqrt{\frac{6}{16}} < 0. \tag{16}$$

This is a contradiction. Hence $m_{3,3}(T) = 0$. ■

Proposition 3.8. *If T is maximal with respect to $\mathcal{ABC}$ over $\mathcal{C}_n$, then $m_{2,3}(T) \leq 1$.*

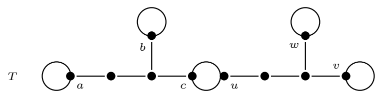


Figure 14. Form of $T \in \mathcal{C}_n$ when $m_{2,3}(T) \geq 2$.

Proof. Assume that $m_{2,3}(T) \geq 2$. By Lemma 3.2, T is of the form depicted in Figure 14, where $d_a = d_b = d_c = d_u = d_v = d_w = 4$ ($u = c$ is possible). Define T' as in Figure 15. Then

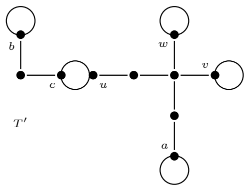


Figure 15. Operation on $T \in \mathcal{C}_n$ when $m_{2,3}(T) \geq 2$.

$$\mathcal{ABC}(T) - \mathcal{ABC}(T') = 4\sqrt{\frac{5}{12}} - 2\sqrt{\frac{1}{2}} - 2\sqrt{\frac{6}{16}} < 0, \tag{17}$$

this is a contradiction. Hence, $m_{2,3}(T) \leq 1$. ■

Proposition 3.9. *Let T be maximal with respect to $\mathcal{ABC}$ over $\mathcal{C}_n$.*

1. *If $m_{2,3}(T) = 0$ then $n_3(T) = 0$;*

2. *If $m_{2,3}(T) = 1$ then $n_3(T) = 1$.*

Proof.
1. Suppose that $m_{2,3}(T) = 0$ and $n_3(T) > 0$. Consider the tree T' defined from T as indicated in Figure 16. From the Propositions 3.4, 3.7 and the fact that $m_{2,3}(T) = 0$, we deduce that $d_a = d_b = d_c = d_e = 4$. Hence

$$\mathcal{ABC}(T) - \mathcal{ABC}(T') = 3\sqrt{\frac{5}{12}} + \sqrt{\frac{3}{4}} - 4\sqrt{\frac{1}{2}} < 0, \tag{18}$$

a contradiction. Consequently, $n_3(T) = 0$.

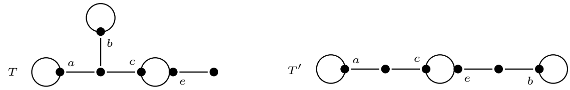


Figure 16. Operation on $T \in \mathcal{C}_n$ when $m_{2,3}(T) = 0$ and $n_3(T) > 0$.

2. Assume that $m_{2,3}(T) = 1$. Then $n_3(T) \geq 1$ and T has the form depicted in Figure 17. As in part 1., it is clear that $d_a = d_b = d_c = 4$ is not possible. Then by Propositions 3.4 and 3.7, $d_z = 2$ for some $z \in \{a, b, c\}$. In other words, every vertex of degree 3 has at least one neighbor of degree 2. Consequently, if $n_3(T) \geq 2$, then $m_{2,3}(T) \geq 2$, a contradiction. In conclusion, $n_3(T) = 1$. ■

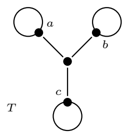


Figure 17. Form of $T \in \mathcal{C}_n$ when $m_{2,3}(T) = 1$ and $n_3(T) \geq 1$.

Corollary 3.10. *If T is maximal with respect to $\mathcal{ABC}$ over $\mathcal{C}_n$ then $T \in \mathcal{U}$ or $T \in \mathcal{V}$, where*

$$\mathcal{U} = \{T \in \mathcal{C}_n : m_{1,2} = m_{2,2} = n_3 = 0\}$$

or

$$\mathcal{V} = \{T \in \mathcal{C}_n : m_{1,3} = m_{1,2} = m_{2,2} = 0, m_{2,3} = n_3 = 1\}.$$

Proof. If T is maximal with respect to $\mathcal{ABC}$ over $\mathcal{C}_n$, then by Propositions 3.4, 3.5, 3.6, 3.7

$$m_{1,3} = m_{1,2} = m_{2,2} = m_{3,3} = 0.$$

By Proposition 3.8, $m_{2,3} \leq 1$. If $m_{2,3} = 0$ then by Proposition 3.9, $n_3 = 0$. Hence $T \in \mathcal{U}$. If $m_{2,3} = 1$, then $n_3 = 1$ again by Proposition 3.9 and $T \in \mathcal{V}$. ■

Next we compute the $\mathcal{ABC}$ index of the trees in $\mathcal{U}$ and in $\mathcal{V}$. From now on we use the following notation:

$$\begin{aligned}
\alpha &= \frac{1}{2}\left(\sqrt{\frac{3}{4}} + \sqrt{\frac{1}{2}}\right), \beta = \frac{1}{2}\left(\sqrt{\frac{3}{4}} - 3\sqrt{\frac{1}{2}} + 2\sqrt{\frac{6}{16}}\right), \\
\gamma &= \frac{1}{2}\left(3\sqrt{\frac{3}{4}} - 5\sqrt{\frac{1}{2}}\right), \delta = \left(2\sqrt{\frac{3}{4}} - 5\sqrt{\frac{1}{2}} + 2\sqrt{\frac{5}{12}}\right).
\end{aligned}$$

Proposition 3.11. *Let $T \in \mathcal{C}_n$.*

1. *If $T \in \mathcal{U}$ then*

$$\mathcal{ABC}(T) = \alpha n + \beta m_{4,4} + \gamma;$$

2. *If $T \in \mathcal{V}$ then*

$$\mathcal{ABC}(T) = \alpha n + \beta m_{4,4} + \delta.$$

Proof. 1. If $T \in \mathcal{U}$ then by relations (1)

$$\begin{array}{c} m_{1,4} = n_1 \\ m_{2,4} = 2n_2 \\ m_{1,4} + m_{2,4} + 2m_{4,4} = 4n_4 \end{array}.$$

It follows from relation (2) that

$$\begin{aligned} n &= n_1 + n_2 + n_4 \\ &= m_{1,4} + \frac{1}{2}m_{2,4} + \frac{1}{4}\left(m_{1,4} + m_{2,4} + 2m_{4,4}\right), \end{aligned}$$

and from relation (3),

$$n - 1 = m_{1,4} + m_{2,4} + m_{4,4}.$$

In other words, we have the relations

$$\begin{array}{c} 4n = 5m_{1,4} + 3m_{2,4} + 2m_{4,4} \\ n = m_{1,4} + m_{2,4} + m_{4,4} + 1 \end{array}.$$

As a consequence, we can express both $m_{1,4}$ and $m_{2,4}$ in terms of n and $m_{4,4}$:

$$2m_{1,4} = n + 3 + m_{4,4} \tag{19}$$

$$2m_{2,4} = n - 5 - 3m_{4,4}. \tag{20}$$

Hence,

$$\begin{aligned} 2\mathcal{ABC}(T) &= 2m_{1,4}\sqrt{\frac{3}{4}} + 2m_{2,4}\sqrt{\frac{1}{2}} + 2m_{4,4}\sqrt{\frac{6}{16}} \\ &= \left(n + 3 + m_{4,4}\right)\sqrt{\frac{3}{4}} + \left(n - 5 - 3m_{4,4}\right)\sqrt{\frac{1}{2}} + 2m_{4,4}\sqrt{\frac{6}{16}} \\ &= \left(\sqrt{\frac{3}{4}} + \sqrt{\frac{1}{2}}\right)n + \left(\sqrt{\frac{3}{4}} - 3\sqrt{\frac{1}{2}} + 2\sqrt{\frac{6}{16}}\right)m_{4,4} \\ &\quad + \left(3\sqrt{\frac{3}{4}} - 5\sqrt{\frac{1}{2}}\right). \end{aligned}$$

2. If $T \in \mathcal{V}$ then by relations (1)

$$\begin{array}{c} m_{1,4} = n_1 \\ 1 + m_{2,4} = 2n_2 \\ 1 + m_{3,4} = 3 \\ m_{1,4} + m_{2,4} + 2 + 2m_{4,4} = 4n_4 \end{array}.$$

In particular, $m_{3,4} = 2$. It follows from relation (2) that

$$\begin{aligned} n &= n_1 + n_2 + 1 + n_4 \\ &= m_{1,4} + \frac{1}{2}\left(1 + m_{2,4}\right) + 1 + \frac{1}{4}\left(m_{1,4} + m_{2,4} + 2 + 2m_{4,4}\right), \end{aligned}$$

and from relation (3),

$$n - 1 = m_{1,4} + 1 + m_{2,4} + 2 + m_{4,4}.$$

In other words, we have the relations

$$\begin{array}{c} 4n = 5m_{1,4} + 3m_{2,4} + 2m_{4,4} + 8 \\ n = m_{1,4} + m_{2,4} + m_{4,4} + 4. \end{array}.$$

From here we deduce that

$$\begin{array}{c} 2m_{1,4} = n + 4 + m_{4,4} \\ 2m_{2,4} = n - 12 - 3m_{4,4} \end{array}.$$

Hence,

$$\begin{aligned} 2\mathcal{ABC}(T) &= 2m_{1,4}\sqrt{\frac{3}{4}} + 2m_{2,3}\sqrt{\frac{1}{2}} + 2m_{2,4}\sqrt{\frac{1}{2}} + 2m_{3,4}\sqrt{\frac{5}{12}} + 2m_{4,4}\sqrt{\frac{6}{16}} \\ &= \left(n + 4 + m_{4,4}\right)\sqrt{\frac{3}{4}} + 2\sqrt{\frac{1}{2}} + \left(n - 12 - 3m_{4,4}\right)\sqrt{\frac{1}{2}} + 4\sqrt{\frac{5}{12}} + 2m_{4,4}\sqrt{\frac{6}{16}} \\ &= \left(\sqrt{\frac{3}{4}} + \sqrt{\frac{1}{2}}\right)n + \left(\sqrt{\frac{3}{4}} - 3\sqrt{\frac{1}{2}} + 2\sqrt{\frac{6}{16}}\right)m_{4,4} \\ &\quad + \left(4\sqrt{\frac{3}{4}} - 10\sqrt{\frac{1}{2}} + 4\sqrt{\frac{5}{12}}\right). \end{aligned}$$

■

Remark 3.12. *The coefficient β that appears with $m_{4,4}$ in the expression for $\mathcal{ABC}(T)$ when $T \in \mathcal{U}$ or $T \in \mathcal{V}$ in Proposition 3.11 is $\beta \approx -1.5275 \times 10^{-2} < 0$. Hence, the $\mathcal{ABC}$ index is strictly decreasing on $m_{4,4}$ over $\mathcal{U}$ and over $\mathcal{V}$.*

By Corollary 3.10 we know that if T is maximal with respect to $\mathcal{ABC}$ over $\mathcal{C}_n$, then $T \in \mathcal{U}$ or $T \in \mathcal{V}$. Furthermore, based on the Remark 3.12, we next show that T belongs to

$$\mathcal{U}_i = \{T \in \mathcal{U} : m_{4,4} = i\}$$

or

$$\mathcal{V}_i = \{T \in \mathcal{V} : m_{4,4} = i\},$$

for some $i = 0, 1, 2, 3$.

Proposition 3.13. *Let n be a positive integer. Then:*

1. *$\mathcal{U}_0 \neq \emptyset$ if and only if $n \equiv 1 \mod 4$ ($n \geq 5$);*
2. *$\mathcal{U}_1 \neq \emptyset$ if and only if $n \equiv 0 \mod 4$ ($n \geq 8$);*
3. *$\mathcal{U}_2 \neq \emptyset$ if and only if $n \equiv 3 \mod 4$ ($n \geq 11$);*
4. *$\mathcal{U}_3 \neq \emptyset$ if and only if $n \equiv 2 \mod 4$ ($n \geq 14$).*

Proof. 1. If $n \equiv 1 \mod 4$, say $n = 4k+1$ with $k \geq 1$, then the tree T_k defined in Table 1 satisfies

$$n(T_k) = 5 + 4(k-1) = 4k + 1 = n,$$

and $T_k \in \mathcal{U}_0$.

Conversely, assume that $T \in \mathcal{U}_0$. Then by (1) and (3),

$$\begin{aligned} m_{1,4} + m_{2,4} &= 4n_4 \\ m_{1,4} + m_{2,4} &= n - 1. \end{aligned}$$

Consequently, $n = 4n_4 + 1$ and so $n \equiv 1 \mod 4$.

2. If $n \equiv 0 \mod 4$, say $n = 4k$ with $k \geq 2$, then the tree P_k defined in Table 1 satisfies

$$n(P_k) = 8 + 4(k-2) = 4k = n,$$

and $P_k \in \mathcal{U}_1$.

Conversely, assume that $P \in \mathcal{U}_1$. Then by (1) and (3),

$$\begin{aligned} m_{1,4} + m_{2,4} + 2 &= 4n_4 \\ m_{1,4} + m_{2,4} + 1 &= n - 1. \end{aligned}$$

Consequently, $n = 4n_4$ and so $n \equiv 0 \mod 4$.

3. If $n \equiv 3 \mod 4$, say $n = 4k+3$ with $k \geq 2$, then the tree Q_k defined in Table 1 satisfies

$$n(Q_k) = 11 + 4(k-2) = 4k + 3 = n$$

and $Q_k \in \mathcal{U}_2$.

Conversely, assume that $Q \in \mathcal{U}_2$. Then by (1) and (3),

$$\begin{aligned} m_{1,4} + m_{2,4} + 4 &= 4n_4 \\ m_{1,4} + m_{2,4} + 2 &= n - 1. \end{aligned}$$

Consequently, $n = 4(n_4 - 1) + 3$ and so $n \equiv 3 \mod 4$.

4. If $n \equiv 2 \mod 4$, say $n = 4k + 2$ with $k \geq 3$, then the tree R_k defined in Table 1 satisfies

$$n(R_k) = 14 + 4(k - 3) = 4k + 2 = n$$

and $R_k \in \mathcal{U}_3$.

Conversely, assume that $R \in \mathcal{U}_3$. Then by (1) and (3),

$$\begin{aligned} m_{1,4} + m_{2,4} + 6 &= 4n_4 \\ m_{1,4} + m_{2,4} + 3 &= n - 1. \end{aligned}$$

Consequently, $n = 4(n_4 - 1) + 2$ and so $n \equiv 2 \mod 4$. ■

We also have a similar result to Proposition 3.13 relative to the sets $\mathcal{V}_i$.

Proposition 3.14. *Let n be a positive integer.*

1. *$\mathcal{V}_0 \neq \emptyset$ if and only if $n \equiv 2 \mod 4$ ($n \geq 14$);*
2. *$\mathcal{V}_1 \neq \emptyset$ if and only if $n \equiv 1 \mod 4$ ($n \geq 17$);*
3. *$\mathcal{V}_2 \neq \emptyset$ if and only if $n \equiv 0 \mod 4$ ($n \geq 20$);*
4. *$\mathcal{V}_3 \neq \emptyset$ if and only if $n \equiv 3 \mod 4$ ($n \geq 23$).*

Proof. 1. If $n \equiv 2 \mod 4$, say $n = 4k + 2$ with $k \geq 3$, then the tree T'_k defined in Table 1 satisfies

$$n(T'_k) = 14 + 4(k - 3) = 4k + 2 = n$$

and $T'_k \in \mathcal{V}_0$.

Conversely, assume that $T' \in \mathcal{V}_0$. Then by (1) and (3), $m_{3,4} = 2$ and so

$$\begin{aligned} m_{1,4} + m_{2,4} + 2 &= 4n_4 \\ m_{1,4} + m_{2,4} + 3 &= n - 1. \end{aligned}$$

Consequently, $n = 4n_4 + 2$ and so $n \equiv 2 \mod 4$.

2. If $n \equiv 1 \mod 4$, say $n = 4k+1$ with $k \geq 4$, then the tree P'_k defined in Figure 18 satisfies

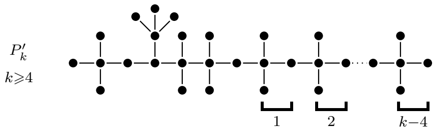


Figure 18. Tree $P'_k \in \mathcal{V}_1$.

$$n\left(P'_k\right) = 17 + 4\left(k-4\right) = 4k+1 = n,$$

and $P'_k \in \mathcal{V}_1$.

Conversely, assume that $P' \in \mathcal{V}_1$. Then by (1) and (3), $m_{3,4} = 2$ and

$$\begin{aligned} m_{1,4} + m_{2,4} + 4 &= 4n_4 \\ m_{1,4} + m_{2,4} + 4 &= n - 1. \end{aligned}$$

Consequently, $n = 4n_4 + 1$ and so $n \equiv 1 \mod 4$.

3. If $n \equiv 0 \mod 4$, say $n = 4k$ with $k \geq 5$, then the tree Q'_k defined in Figure 19 satisfies

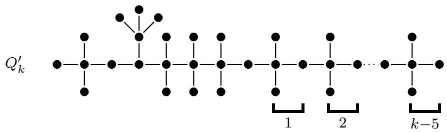


Figure 19. Tree $Q'_k \in \mathcal{V}_2$.

$$n\left(Q'_k\right) = 20 + 4\left(k-5\right) = 4k = n,$$

and $Q'_k \in \mathcal{V}_2$.

Conversely, assume that $Q' \in \mathcal{V}_2$. Then by (1) and (3), $m_{3,4} = 2$ and

$$\begin{aligned} m_{1,4} + m_{2,4} + 6 &= 4n_4 \\ m_{1,4} + m_{2,4} + 5 &= n - 1. \end{aligned}$$

Hence $n = 4n_4$ and so $n \equiv 0 \mod 4$.

4. If $n \equiv 3 \mod 4$, say $n = 4k + 3$ with $k \geq 5$, then the tree R'_k defined in Figure 20 satisfies

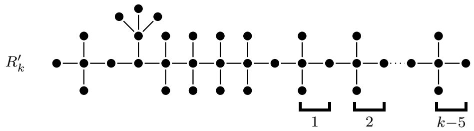


Figure 20. Tree $R'_k \in \mathcal{V}_3$.

$$n\left(R'_k\right) = 23 + 4\left(k - 5\right) = 4k + 3 = n$$

and $R'_k \in \mathcal{V}_3$.

Conversely, assume that $R' \in \mathcal{V}_3$. Then by (1) and (3), $m_{3,4} = 2$ and

$$\begin{aligned} m_{1,4} + m_{2,4} + 8 &= 4n_4 \\ m_{1,4} + m_{2,4} + 6 &= n - 1. \end{aligned}$$

Consequently, $n = 4\left(n_4 - 1\right) + 3$ and so $n \equiv 3 \mod 4$. ■

Corollary 3.15. *Let T be maximal with respect to $\mathcal{ABC}$ over $\mathcal{C}_n$.*

1. *If $n \equiv 0 \mod 4$ then $T \in \mathcal{U}_1$ or $T \in \mathcal{V}_2$;*
2. *If $n \equiv 1 \mod 4$ then $T \in \mathcal{U}_0$ or $T \in \mathcal{V}_1$;*
3. *If $n \equiv 2 \mod 4$ then $T \in \mathcal{U}_3$ or $T \in \mathcal{V}_0$;*
4. *If $n \equiv 3 \mod 4$ then $T \in \mathcal{U}_2$ or $T \in \mathcal{V}_3$.*

Proof. By Corollary 3.10, $T \in \mathcal{U}$ or $T \in \mathcal{V}$. If $T \in \mathcal{U}$ then by Proposition 3.11,

$$\mathcal{ABC}\left(T\right) = \alpha n + \beta m_{4,4}\left(T\right) + \gamma.$$

Consider the following cases:

1. $n \equiv 0 \mod 4$. Then by Proposition 3.13, there exists $U \in \mathcal{U}_1$ and $m_{4,4}\left(T\right) \neq 0, m_{4,4}\left(T\right) \neq 2$ and $m_{4,4}\left(T\right) \neq 3$. If $T \notin \mathcal{U}_1$ then $m_{4,4}\left(T\right) \neq 1$ and since $\beta < 0$, we conclude that

$$\mathcal{ABC}\left(T\right) - \mathcal{ABC}\left(U\right) = \beta\left(m_{4,4}\left(T\right) - 1\right) < 0,$$

a contradiction. Hence $T \in \mathcal{U}_1$.

2. $n \equiv 1 \mod 4$. Then by Proposition 3.13, there exists $U \in \mathcal{U}_0$ and $m_{4,4}(T) \neq 1, m_{4,4}(T) \neq 2$ and $m_{4,4}(T) \neq 3$. If $T \notin \mathcal{U}_0$ then $m_{4,4}(T) \neq 0$ and since $\beta < 0$, we conclude that

$$\mathcal{ABC}(T) - \mathcal{ABC}(U) = \beta m_{4,4}(T) < 0,$$

a contradiction. Hence $T \in \mathcal{U}_0$.

3. $n \equiv 2 \mod 4$. Then by Proposition 3.13, there exists $U \in \mathcal{U}_3$ and $m_{4,4}(T) \neq 0, m_{4,4}(T) \neq 1$ and $m_{4,4}(T) \neq 2$. If $T \notin \mathcal{U}_3$ then $m_{4,4}(T) \neq 3$ and since $\beta < 0$, we conclude that

$$\mathcal{ABC}(T) - \mathcal{ABC}(U) = \beta(m_{4,4}(T) - 3) < 0,$$

a contradiction. Hence $T \in \mathcal{U}_3$.

4. $n \equiv 3 \mod 4$. Then by Proposition 3.13, there exists $U \in \mathcal{U}_2$ and $m_{4,4}(T) \neq 0, m_{4,4}(T) \neq 1$ and $m_{4,4}(T) \neq 3$. If $T \notin \mathcal{U}_2$ then $m_{4,4}(T) \neq 2$ and since $\beta < 0$, we conclude that

$$\mathcal{ABC}(T) - \mathcal{ABC}(U) = \beta(m_{4,4}(T) - 2) < 0,$$

a contradiction. Hence $T \in \mathcal{U}_2$.

If $T \in \mathcal{V}$ then by Proposition 3.11,

$$\mathcal{ABC}(T) = \alpha n + \beta m_{4,4}(T) + \delta,$$

where $\delta = \left(2\sqrt{\frac{3}{4}} - 5\sqrt{\frac{1}{2}} + 2\sqrt{\frac{5}{12}}\right)$. A similar argument based on Proposition 3.14 shows that $T \in \mathcal{V}_2$ if $n \equiv 0$; $T \in \mathcal{V}_1$ if $n \equiv 1 \mod 4$; $T \in \mathcal{V}_0$ if $n \equiv 2 \mod 4$; and $T \in \mathcal{V}_3$ if $n \equiv 3 \mod 4$. ■

Theorem 3.16. *Let n be a positive integer. The maximal value of $\mathcal{ABC}$ over $\mathcal{C}_n$ is attained in*

1. *$\mathcal{U}_1$ if $n \equiv 0 \mod 4$ $(n \geq 8)$, with maximal value*

$$\frac{1}{2}\left(\sqrt{\frac{3}{4}} + \sqrt{\frac{1}{2}}\right)n + \sqrt{\frac{6}{16}} + 2\sqrt{\frac{3}{4}} - 4\sqrt{\frac{1}{2}}.$$

2. *$\mathcal{U}_0$ if $n \equiv 1 \mod 4$ $(n \geq 5)$, with maximal value*

$$\frac{1}{2}\left(\sqrt{\frac{3}{4}} + \sqrt{\frac{1}{2}}\right)n + \frac{3}{2}\sqrt{\frac{3}{4}} - \frac{5}{2}\sqrt{\frac{1}{2}}.$$

3. *$\mathcal{V}_0$ if $n \equiv 2 \mod 4$ $(n \geq 14)$, with maximal value*

$$\frac{1}{2}\left(\sqrt{\frac{3}{4}} + \sqrt{\frac{1}{2}}\right)n + 2\sqrt{\frac{3}{4}} - 5\sqrt{\frac{1}{2}} + 2\sqrt{\frac{5}{12}}.$$

4. $\mathcal{U}_2$ *if* $n \equiv 3 \mod 4$ *(*$n \geq 11$*), with maximal value*

$$\frac{1}{2}\left(\sqrt{\frac{3}{4}}+\sqrt{\frac{1}{2}}\right)n+2\sqrt{\frac{6}{16}}+\frac{5}{2}\sqrt{\frac{3}{4}}-\frac{11}{2}\sqrt{\frac{1}{2}}.$$

Proof. Let T be maximal with respect to $\mathcal{ABC}$ over $\mathcal{C}_n$.

1. If $n \equiv 0 \mod 4$ then by Corollary 3.15, $T \in \mathcal{U}_1$ or $T \in \mathcal{V}_2$. By Proposition 3.11, $\mathcal{ABC}$ is constant in $\mathcal{U}_1$ with value

$$\alpha n+\beta+\gamma,$$

and is constant in $\mathcal{V}_2$ with value

$$\alpha n+2\beta+\delta.$$

Now the value of $\mathcal{ABC}$ is larger in $\mathcal{U}_1$ than in $\mathcal{V}_2$ since

$$(\alpha n+\beta+\gamma)-(\alpha n+2\beta+\delta)=\gamma-\beta-\delta\approx 0.06>0.$$

Hence $T \in \mathcal{U}_1$.

2. If $n \equiv 1 \mod 4$ then by Corollary 3.15, $T \in \mathcal{U}_0$ or $T \in \mathcal{V}_1$. By Proposition 3.11, $\mathcal{ABC}$ is constant in $\mathcal{U}_0$ with value

$$\alpha n+\gamma,$$

and is constant in $\mathcal{V}_1$ with value

$$\alpha n+\beta+\delta.$$

Since

$$(\alpha n+\gamma)-(\alpha n+\beta+\delta)=\gamma-\beta-\delta\approx 0.06>0,$$

we conclude that $T \in \mathcal{U}_0$.

3. If $n \equiv 2 \mod 4$ then by Corollary 3.15, $T \in \mathcal{U}_3$ or $T \in \mathcal{V}_0$. By Proposition 3.11, $\mathcal{ABC}$ is constant in $\mathcal{U}_3$ with value

$$\alpha n+3\beta+\gamma,$$

and is constant in $\mathcal{V}_0$ with value

$$\alpha n+\delta.$$

Since

$$(\alpha n+3\beta+\gamma)-(\alpha n+\delta)=3\beta+\gamma-\delta\approx -2.0653\times 10^{-3}<0.$$

it follows that $T \in \mathcal{V}_0$.

4. If $n \equiv 3 \mod 4$ then by Corollary 3.15, $T \in \mathcal{U}_2$ or $T \in \mathcal{V}_3$. By Proposition 3.11, $\mathcal{ABC}$ is constant in $\mathcal{U}_2$ with value

$$\alpha n + 2\beta + \gamma,$$

and is constant in $\mathcal{V}_3$ with value

$$\alpha n + 3\beta + \delta.$$

Since

$$(\alpha n + 2\beta + \gamma) - (\alpha n + 3\beta + \delta) = \gamma - \beta - \delta \approx 0.06 > 0.$$

we deduce that $T \in \mathcal{U}_2$. ■

4 Maximal value of $e^{\mathcal{ABC}}$ among chemical trees

Recall that the exponential of $\mathcal{ABC}$ is denoted by $e^{\mathcal{ABC}}$ and defined for a tree $T \in \mathcal{C}_n$ as

$$e^{\mathcal{ABC}}(T) = \sum_{(i,j)\in K} m_{i,j}(T)\, e^{\sqrt{\frac{i+j-2}{ij}}}.$$

We will find in this section the maximal value of $e^{\mathcal{ABC}}$ over $\mathcal{C}_n$. The arguments in the previous section work for $e^{\mathcal{ABC}}$, mainly because the behaviour of $e^{\mathcal{ABC}}$ in Tables 3-5 is similar to the behaviour of $\mathcal{ABC}$, in other words, the increasing properties of $\mathcal{ABC}$ and $e^{\mathcal{ABC}}$ are similar when the operations 1-3 are performed. Also, the signs in relations (11), (12), (13), (14), (15), (16), (17), and (18) hold when $\mathcal{ABC}$ is changed to $e^{\mathcal{ABC}}$.

The only difference appears in Table 4, where $e^{\mathcal{ABC}}$ increases even when $p = 4$ and $(q, r) = (4, 4)$. This situation has important implications which simplify the analysis of the study of the maximal value of $e^{\mathcal{ABC}}$ in $\mathcal{C}_n$. In fact, by Proposition 2.2 and Table 4 we deduce immediately that if T is maximal with respect to $e^{\mathcal{ABC}}$ over $\mathcal{C}_n$, then $m_{2,3}(T) = 0$. Hence, we have

Corollary 4.1. *If T is maximal with respect to $e^{\mathcal{ABC}}$ over $\mathcal{C}_n$ then $T \in \mathcal{U}$.*

As in Proposition 3.11:

Proposition 4.2. *If $T \in \mathcal{U}$, then*

$$\begin{aligned} e^{\mathcal{ABC}}(T) &= \frac{1}{2}\left(e^{\sqrt{\frac{3}{4}}} + e^{\sqrt{\frac{1}{2}}}\right) n + \frac{1}{2}\left(e^{\sqrt{\frac{3}{4}}} - 3e^{\sqrt{\frac{1}{2}}} + 2e^{\sqrt{\frac{6}{16}}}\right) m_{4,4} \\ &+ \frac{1}{2}\left(3e^{\sqrt{\frac{3}{4}}} - 5e^{\sqrt{\frac{1}{2}}}\right). \end{aligned}$$

It is important to note that the companion coefficient of $m_{4,4}$ in this expression is

$$\frac{1}{2}\left(e^{\sqrt{\frac{3}{4}}} - 3e^{\sqrt{\frac{1}{2}}} + 2e^{\sqrt{\frac{6}{16}}}\right) \approx -8.648\,2 \times 10^{-3} < 0,$$

so again $e^{\mathcal{ABC}}$ is decreasing on $m_{4,4}$ over $\mathcal{U}$. Consequently, as in Corollary 3.15, we have

Corollary 4.3. *Let T be maximal with respect to $e^{\mathcal{ABC}}$ over $\mathcal{C}_n$.*

1. *If $n \equiv 0 \mod 4$ then $T \in \mathcal{U}_1$;*
2. *If $n \equiv 1 \mod 4$ then $T \in \mathcal{U}_0$;*
3. *If $n \equiv 2 \mod 4$ then $T \in \mathcal{U}_3$;*
4. *If $n \equiv 3 \mod 4$ then $T \in \mathcal{U}_2$.*

Following the proof of Theorem 3.16 we deduce the maximal value of $e^{\mathcal{ABC}}$ over $\mathcal{C}_n$.

Theorem 4.4. *Let n be a positive integer. The maximal value of $e^{\mathcal{ABC}}$ over $\mathcal{C}_n$ is attained in*

1. *$\mathcal{U}_1$ if $n \equiv 0 \mod 4$ $(n \geq 8)$, with maximal value*

$$\frac{1}{2}\left(e^{\sqrt{\frac{3}{4}}} + e^{\sqrt{\frac{1}{2}}}\right) n + 2e^{\sqrt{\frac{3}{4}}} + e^{\sqrt{\frac{6}{16}}} - 4e^{\sqrt{\frac{1}{2}}};$$

2. *$\mathcal{U}_0$ if $n \equiv 1 \mod 4$ $(n \geq 5)$, with maximal value*

$$\frac{1}{2}\left(e^{\sqrt{\frac{3}{4}}} + e^{\sqrt{\frac{1}{2}}}\right) n + \frac{3}{2}e^{\sqrt{\frac{3}{4}}} - \frac{5}{2}e^{\sqrt{\frac{1}{2}}};$$

3. *$\mathcal{U}_3$ if $n \equiv 2 \mod 4$ $(n \geq 14)$, with maximal value*

$$\frac{1}{2}\left(e^{\sqrt{\frac{3}{4}}} + e^{\sqrt{\frac{1}{2}}}\right) n + 3e^{\sqrt{\frac{3}{4}}} + 3e^{\sqrt{\frac{6}{16}}} - 7e^{\sqrt{\frac{1}{2}}};$$

4. *$\mathcal{U}_2$ if $n \equiv 3 \mod 4$ $(n \geq 11)$, with maximal value*

$$\frac{1}{2}\left(e^{\sqrt{\frac{3}{4}}} + e^{\sqrt{\frac{1}{2}}}\right) n + \frac{5}{2}e^{\sqrt{\frac{3}{4}}} - \frac{11}{2}e^{\sqrt{\frac{1}{2}}} + 2e^{\sqrt{\frac{6}{16}}}.$$

In conclusion, the maximal value of $e^{\mathcal{ABC}}$ and $\mathcal{ABC}$ are attained in the same trees except when $n \equiv 2 \mod 4$. When $n \equiv 2 \mod 4$ the $\mathcal{ABC}$ index attains its maximal value in $\mathcal{V}_0$ and $e^{\mathcal{ABC}}$ attains its maximal value in $\mathcal{U}_3$.

5 Minimal value of $e^{\mathcal{GA}}$ among chemical trees

$e^{\mathcal{GA}}$ is defined for a chemical tree T as

$$e^{\mathcal{GA}}(T) = \sum_{(i,j)\in K} m_{i,j}(T)\, e^{\frac{2\sqrt{ij}}{i+j}}.$$

If we look at Tables 3-5 we note that the behavior of $e^{\mathcal{GA}}$ is even more favorable than the previous ones but with opposite signs. So when the operations 1-3 are performed, $e^{\mathcal{GA}}$ decreases and the minimal value of $e^{\mathcal{GA}}$ over $\mathcal{C}_n$ is obtained. In fact, the version of Lemmas 3.1, 3.2, and 3.3 for $e^{\mathcal{GA}}$ are as follows:

Lemma 5.1. *Let xy be an edge of $T \in \mathcal{C}_n$ such that $d_x = d_y = 2$ as in Figure 1. Then we can find a tree $\widehat{T} \in \mathcal{C}_n$ such that $e^{\mathcal{GA}}(T) > e^{\mathcal{GA}}(\widehat{T})$.*

Lemma 5.2. *Let xy be an edge of $T \in \mathcal{C}_n$ such that $d_x = 2$ and $d_y = 3$ as in Figure 2. Then we can find a tree $\widehat{T} \in \mathcal{C}_n$ such that $e^{\mathcal{GA}}(T) > e^{\mathcal{GA}}(\widehat{T})$.*

Lemma 5.3. *Let xy be an edge of $T \in \mathcal{C}_n$ such that $d_x = d_y = 3$ as in Figure 3. If $d_z = 2$ for some $z \in \{a, b, c, e\}$, then we can find a tree $\widehat{T} \in \mathcal{C}_n$ such that $e^{\mathcal{GA}}(T) > e^{\mathcal{GA}}(\widehat{T})$.*

Note that Lemmas 5.1 and 5.2 already imply that $m_{2,2}(T) = m_{2,3}(T) = 0$ when T is minimal with respect to $e^{\mathcal{GA}}$ over $\mathcal{C}_n$. Moreover, following the results in Section 3, one proves:

Corollary 5.4. *If T is minimal with respect to $e^{\mathcal{GA}}$ over $\mathcal{C}_n$ then $T \in \mathcal{U}$.*

We also can compute $e^{\mathcal{GA}}$ for trees in $\mathcal{U}$ as in the previous sections.

Proposition 5.5. *If $T \in \mathcal{U}$, then*

$$\begin{aligned} e^{\mathcal{GA}}(T) &= \frac{1}{2}\left(e^{\frac{2\sqrt{4}}{5}} + e^{\frac{2\sqrt{8}}{6}}\right) n + \frac{1}{2}\left(e^{\frac{2\sqrt{4}}{5}} - 3e^{\frac{2\sqrt{8}}{6}} + 2e^{\frac{2\sqrt{16}}{8}}\right) m_{4,4} \\ &\quad + \frac{1}{2}\left(3e^{\frac{2\sqrt{4}}{5}} - 5e^{\frac{2\sqrt{8}}{6}}\right). \end{aligned}$$

Since the companion coefficient of $m_{4,4}$ in this expression is

$$\frac{1}{2}\left(e^{\frac{2\sqrt{4}}{5}} - 3e^{\frac{2\sqrt{8}}{6}} + 2e^{\frac{2\sqrt{16}}{8}}\right) \approx -1.9722 \times 10^{-2} < 0,$$

it follows that $e^{\mathcal{GA}}$ is decreasing on $m_{4,4}$ over $\mathcal{U}$. From now on everything changes, because we are searching for the minimal value of $e^{\mathcal{GA}}$ over $\mathcal{U}$. In other words, we now have to consider subsets of $\mathcal{U}$ with large $m_{4,4}$. From equation (20), it is clear that the maximal number of $m_{4,4}$ in $\mathcal{U}$ occur in the trees F_k, G_k, and H_k shown in Table 2, depending on the congruence of n modulo 3. So let us define

$$\begin{aligned} \mathcal{U}_{\frac{n-9}{3}} &= \left\{T \in \mathcal{U} : m_{4,4} = \frac{n-9}{3}\right\}; \\ \mathcal{U}_{\frac{n-13}{3}} &= \left\{T \in \mathcal{U} : m_{4,4} = \frac{n-13}{3}\right\}; \\ \mathcal{U}_{\frac{n-5}{3}} &= \left\{T \in \mathcal{U} : m_{4,4} = \frac{n-5}{3}\right\}. \end{aligned}$$

Clearly, $F_k \in \mathcal{U}_{\frac{n-9}{3}}, G_k \in \mathcal{U}_{\frac{n-13}{3}}$, and $H_k \in \mathcal{U}_{\frac{n-5}{3}}$. It is easy to see that

Proposition 5.6. *Let n be a positive integer. Then:*

1. $\mathcal{U}_{\frac{n-9}{3}} \neq \emptyset$ *if and only if* $n \equiv 0 \mod 3$ *(*$n \geq 9$*);*
2. $\mathcal{U}_{\frac{n-13}{3}} \neq \emptyset$ *if and only if* $n \equiv 1 \mod 3$ *(*$n \geq 13$*);*
3. $\mathcal{U}_{\frac{n-5}{3}} \neq \emptyset$ *if and only if* $n \equiv 2 \mod 3$ *(*$n \geq 5$*).*

So we conclude the following:

Corollary 5.7. *Let T be minimal with respect to $e^{\mathcal{GA}}$ over $\mathcal{C}_n$.*

1. *If* $n \equiv 0 \mod 3$ *(*$n \geq 9$*) then* $T \in \mathcal{U}_{\frac{n-9}{3}}$;
2. *If* $n \equiv 1 \mod 3$ *(*$n \geq 13$*) then* $T \in \mathcal{U}_{\frac{n-13}{3}}$;
3. *If* $n \equiv 2 \mod 3$ *(*$n \geq 5$*) then* $T \in \mathcal{U}_{\frac{n-5}{3}}$.

Finally we obtain:

Theorem 5.8. *Let n be a positive integer. The minimal value of $e^{\mathcal{GA}}$ over $\mathcal{C}_n$ is attained in*

1. $\mathcal{U}_{\frac{n-9}{3}}$ *if* $n \equiv 0 \mod 3$ *(*$n \geq 9$*) with minimal value*

$$\frac{1}{3}\left(2e^{\frac{2\sqrt{4}}{5}} + e^{\frac{2\sqrt{16}}{8}}\right)n + 2e^{\frac{2\sqrt{8}}{6}} - 3e^{\frac{2\sqrt{16}}{8}};$$

2. $\mathcal{U}_{\frac{n-13}{3}}$ *if* $n \equiv 1 \mod 3$ *(*$n \geq 13$*), with minimal value*

$$\frac{1}{3}\left(2e^{\frac{2\sqrt{4}}{5}} + e^{\frac{2\sqrt{16}}{8}}\right)n + 4e^{\frac{2\sqrt{8}}{6}} - \frac{2}{3}e^{\frac{2\sqrt{4}}{5}} - \frac{13}{3}e^{\frac{2\sqrt{16}}{8}};$$

3. $\mathcal{U}_{\frac{n-5}{3}}$ *if* $n \equiv 2 \mod 3$ *(*$n \geq 5$*) with minimal value*

$$\frac{1}{3}\left(2e^{\frac{2\sqrt{4}}{5}} + e^{\frac{2\sqrt{16}}{8}}\right)n + \frac{2}{3}e^{\frac{2\sqrt{4}}{5}} - \frac{5}{3}e^{\frac{2\sqrt{16}}{8}}.$$

Note that when $n = 3k+1$, the minimal value of $\mathcal{GA}$ and the minimal value of $e^{\mathcal{GA}}$ are attained in different trees (see Table 2).

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