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Minimum Augmented Zagreb Index on Chemical Trees with Given Number of Pendent Vertices

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Abstract: **Given a graph G, the augmented Zagreb index (AZI) is defined to be $AZI(G)=\sum_{uv\in E(G)}(\frac{d_u d_v}{d_u+d_v-2})^3$ where u and v are vertices of G, d_u denotes the degree of the vertex u. In this paper, we consider chemical trees with a given number of pendent vertices and derive sharp lower bounds for the AZI index among this class of trees. We also characterize the extremal chemical trees with a fixed number of pendent vertices.**

Keywords: **Chemical trees, Augmented Zagreb index, Topological indices, Extremal graphs.**

I. INTRODUCTION

Let G be a simple, finite and undirected graph with vertex set $V(G)$ and edge set $E(G)$. For $v\in V(G)$, the degree of v, denoted by d_v, is the number of vertices incident to v in G. A vertex of degree one is said to be a pendent vertex. If u and v are two adjacent vertices of G, then the edge connecting then will be denoted by uv.

A description of the structure or shape of molecules is very helpful in predicting the activity and properties of molecules in complex experiments. Among them, so-called topological indices [1] play an important role. Nowadays, there exists a legion of topological indices that have been found some applications in chemistry [2,13]. Here, we consider a relatively new topological index. In 2010, B. Furtula *et al.* [3] proposed a new vertex-degree-based graph topological index called the augmented Zagreb index (AZI), defined as

$$AZI(G)=\sum_{uv\in E(G)}(\frac{d_u d_v}{d_u+d_v-2})^3,$$

and showed that it is a valuable predictive index in the study of the heat of formation in heptanes and octanes. Moreover, I. Gutman and J. Tašovič [5] recently tested the correlation abilities of 20 vertex-degree-based topological indices for the case of standard heats of formation and normal boiling points of octane isomers. They found that the AZI index yields the best results. Consequently, the AZI index should be preferred in designing quantitative, structure-property relations.

Since then, many authors have investigated the AZI index. B. Furtula *et al.* [3] obtained some tight upper and lower bounds of the AZI index of a chemical tree, and showed that among all trees the star graph has the minimal AZI value. Y. Huang *et al.* [6] and D. Wang *et al.* [7] gave some bounds on the AZI indices of connected graphs and characterized the corresponding extremal graphs. A. Ali *et al.* [14] established inequalities between AZI and several other vertex-degree-based topological indices. A. Ali *et al.* [4] proposed tight upper bounds for the AZI index of chemical bicyclic and unicyclic graphs, and gave a Nordhaus-Gaddum-type result for AZI index.

A chemical tree T is a tree with maximum degree at most 4. Also of interest is to maximize and minimize chemically relevant. degree-based indices on trees (or chemical trees) with a given number of pendent vertices. In [8], M. Goubko and I. Gutman employ dynamic programming to characterize optimal trees of the first and second Zagreb index, and the atom-bond connectivity index among trees, but not to the AZI index. In this paper, we derive sharp lower bounds for the augmented Zagreb index (AZI) for chemical treeswith the given number of pendent vertices and characterize optimal trees.

II. PRELIMINARIES

For convenience, let $A(x,y)=\left(\frac{xy}{x+y-2}\right)^3$ for $x,y\geq 1$ with $x+y>2$. Obviously, $A(x,y)=A(y,x)$.

Lemma 1 ([9]): (i) $A(1,y)$ is decreasing for $y\geq 2$; (ii) $A(2,y)=8$; (iii) If $y\geq 3$ is fixed, then $A(x,y)$ is increasing for $x\geq 3$.

Lemma 2 ([9]): $A(1,\Delta)\leq A(1,i)\leq A(1,2)=A(2,j)<A(3,3)\leq A(k,l)\leq A(\Delta,\Delta)$, where $2\leq i,j\leq\Delta$ and $3\leq k\leq l\leq\Delta$.

Let $\mathrm{T}(n)$ be the set of all chemical tree with $n(\geq 5)$ pendent vertices and $\mathrm{T}^*(n)$ be the set of all AZI-minimizers in $\mathrm{T}(n)$.

Lemma 3 If $T\in\mathrm{T}^*(n)$, then $d_u\geq 3$ or $d_v\geq 3$ for any edge $uv\in E(T)$.

Proof Assume the opposite, i.e., that $d_u\leq 2$ and $d_v\leq 2$. If $d_u=d_v=1$, then $T\cong K_2$, the chemical tree T cannot have $n(\geq 5)$ pendent vertices. With no loss of generality suppose that $d_u=2$ and $d_v\leq d_u$. Thus, u would have exactly two neighbors (say, v and v') in T. Construct a chemical tree T' by deleting the vertex u and its incident edges and adding an edge vv' instead. The tree T and T' have the same number of pendent vertices. So, $T'\in\mathrm{T}(n)$. Consider the difference $AZI(T')-AZI(T)=A(d_v,d_{v'})-16$.

- If $d_v=2$, by Lemma 1, then $AZI(T')-AZI(T)=-8<0$, which is a contradiction.
- If $d_v=1$, by Lemma 2, then $AZI(T')-AZI(T)=A(1,d_{v'})-16<0$, which is a contradiction.

This completes the proof.

Lemma 4 If $T\in\mathrm{T}^*(n)$, then $(d_u,d_v)=(4,4)\notin E(T)$ for any edge $uv\in E(T)$.

Proof Assume the opposite, and consider chemical tree T has an edge uv with $d_u=d_v=4$. We construct a tree T' by splitting edge uv in the path of length 2. Then T' is still a chemical tree with n pendent vertices. By simple calculations, we have

$$\begin{aligned}AZI(T')-AZI(T)&=A(2,d_u)+A(2,d_v)-A(d_u,d_v)\\&=2A(2,4)-A(4,4)<0.\end{aligned}$$

So, $AZI(T')<AZI(T)$. This contradiction completes the proof.

III. MAIN RESULTS

In this section we employ the notion of the attached tree from [10].

Definition 1 Any edge $uv\in E(T)$ of a chemical tree T divides T into two connected components, T_u containing the vertex u, and T_v containing the vertex v. The rooted tree $T_{uv}=T_v\bigcup uv$ with the root u is referred to as the attached chemical tree and is denoted with T_{uv}. The vertex v incident to the root u is called a sub-root.

Definition 2 The cost of an attached chemical tree T_{uv} with the root u of degree p and a sub-root v of degree d is defined as

$$B(T_{uv}, p) = A(p, d) + \sum_{xy \in E(T_{uv})} A(d_x, d_y).$$

Below any tree minimizing AZI index over the set of all chemical trees with n pendent vertices is called optimal for short.

For any $k, p \in \mathbb{N}$, denote by $B^*(k, p)$ the minimum cost of an attached chemical tree with k pendent vertices and degree p of the root. Let $\mathrm{T}^*(k, p)$ be the set of all optimal attached chemical tree with k pendent vertices and degree p of the root.

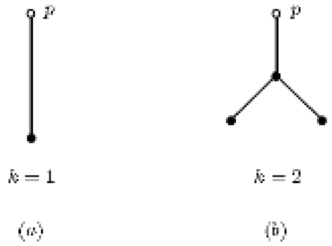
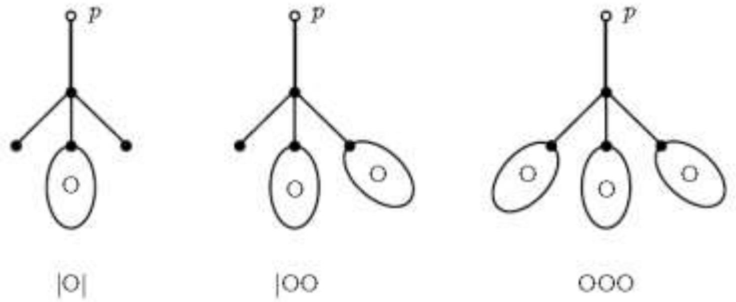


Fig. 1 AZI **-minimal attached chemical trees**

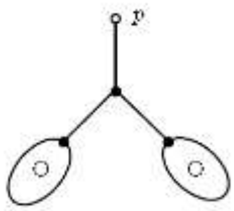
Next let us evaluate $B^*(k, p)$.

If $k = 1$, then the only AZI -minimal attached chemical tree is K_2, see Fig. 1(a). So $B^*(1, p) = A(1, p)$ $(p = 2, 3, 4)$. If $k = 2$, then the only AZI -minimal attached chemical tree is $K_{1,3}$, see Fig. 1(b). So $B^*(2, p) = A(p, 3) + 2A(1, 3)$ $(p = 1, 2, 3, 4)$.

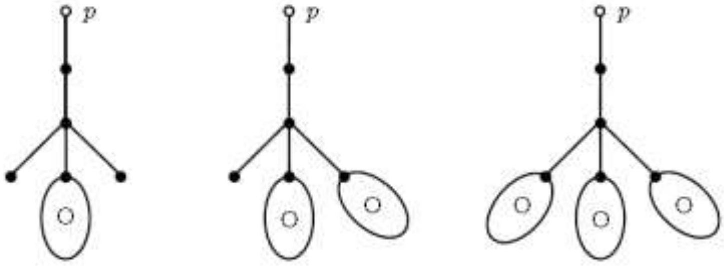
In order to evaluate $B^*(k, p)$ for $k \geq 3$, we first introduce a shorthand notation for typical attached chemical trees. In order to refer to optimal sub-trees we will denote the one for $k = 1$ with the symbol $"|"$, the one for $k = 2$ with the symbol $"\wedge"$, $"\mathrm{E}"$ will stand for the optimal attached sub-tree with even number of pendent vertices, while $"\mathrm{O}"$ for that with odd number of pendent vertices.



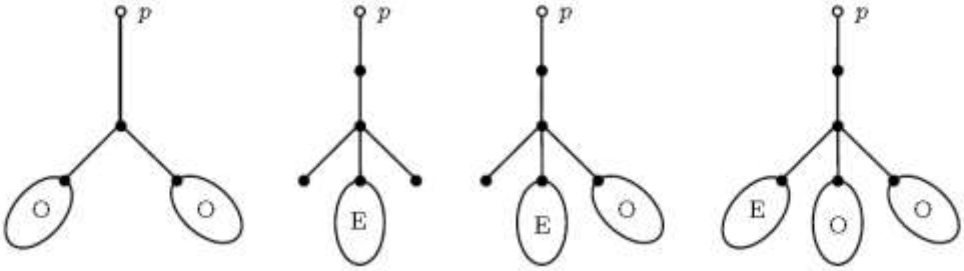
(a) The optimal attached chemical trees for $p = 3$ **and odd** k **.**



(b) The optimal attached chemical trees for $p = 3$ **and even** k **.**



(c) The optimal attached chemical trees for $p = 4$ and odd k .



(d) The optimal attached chemical trees for $p = 4$ and even k .

Fig. 2 The optimal attached chemical trees for $p = 3,4$

Lemma 5 For $k \geq 3$, we have

$$B^*(k,3) = \begin{cases} kA(1,4) + 8(k-3) + A(3,4) & k \text{ is odd} \\ kA(1,4) + 8(k-6) + A(3,3) + 2A(3,4) & k \text{ is even} \end{cases}$$

and

$$B^*(k,4) = \begin{cases} k\mathrm{A}(1,4) + 8(k-1) & k \text{ is odd} \\ k\mathrm{A}(1,4) + 8(k-6) + 3\mathrm{A}(3,4) & k \text{ is even} \end{cases}$$

Moreover, all the optimal attached chemical trees are depicted in Fig. 2.

Proof We use induction on k to prove the Lemma. Suppose the conclusion is true for smaller values of k . Below we prove the results holds for k . From Lemma 3, if degree p of the root is no more than 3 , then the sub-root must have some degree $d \in \{1,2,3,4\}$. Since $k \geq 3$, we have $d \neq 1$. If $p = 4$, then $d \neq 4$ by Lemma 4. We divide our discussion into two cases according to parameters k .

Case 1 When k is odd, there are three subcases in the following:

Subcase 1.1 If $d = 3$. In this case, all possible classes of attached chemical trees have the following three types, see Fig. 3.

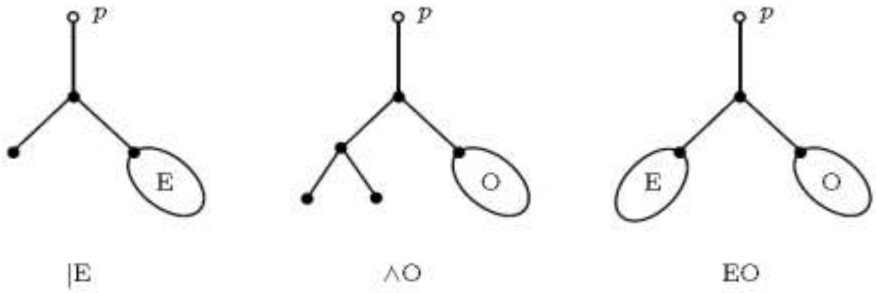


Fig. 3 The attached chemical trees when k is odd and $d = 3$

By the inductive assumption, we have

$B(|\text{E}, p) = A(p,3) + A(1,3) + (k-1)A(1,4) + 8(k-7) + A(3,3) + 2A(3,4),$

$B(\wedge\text{O}, p) = A(p,3) + A(3,3) + 2A(1,3) + (k-2)A(1,4) + 8(k-5) + A(3,4),$

$B(\text{EO}, p) = A(p,3) + kA(1,4) + 8(k-9) + A(3,3) + 3A(3,4).$

- For $p = 3$, we have

$B(|\text{E},3) = kA(1,4) + 8(k-3) + A(3,4) + 5.61 > B^*(k,3),$

$B(\wedge\text{O},3) = kA(1,4) + 8(k-3) + A(3,4) + 8.79 > B^*(k,3),$

$B(\text{EO},3) = kA(1,4) + 8(k-3) + A(3,4) + 2.43 > B^*(k,3).$

- For $p = 4$, we have

$B(|\text{E},4) = kA(1,4) + 8(k-1) + 5.868 > B^*(k,4),$

$B(\wedge\text{O},4) = kA(1,4) + 8(k-1) + 9.05 > B^*(k,4),$

$B(\text{EO},4) = kA(1,4) + 8(k-1) + 2.69 > B^*(k,4).$

Subcase 1.2 If $d = 4$. In this case, all possible classes of attached chemical trees are depicted in Fig. 4.

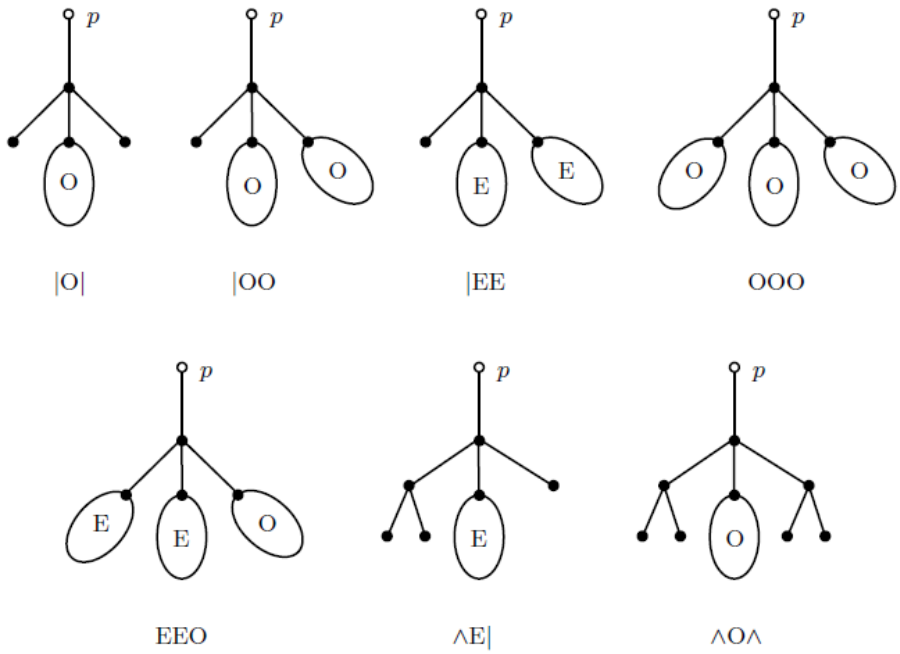


Fig. 4 The attached chemical trees when k is odd and $d = 4$

Note that by Lemma 4 we know $p \neq 4$. By the inductive assumption, we have

$B(|\text{O}|, p) = A(p,4) + 2A(1,4) + (k-2)A(1,4) + 8(k-3),$

$B(|\text{OO}, p) = A(p,4) + kA(1,4) + 8(k-3),$

$B(|\text{EE}, p) = A(p,4) + kA(1,4) + 8(k-13) + 6A(3,4),$

$B(\text{OOO}, p) = A(p,4) + kA(1,4) + 8(k-3),$

$B(\text{EEO}, p) = A(p,4) + kA(1,4) + 8(k-13) + 6A(3,4),$

$B(\wedge\text{E}|, p) = A(p,4) + (k-2)A(1,4) + 8(k-9) + 2A(1,3) + 4A(3,4),$

$B(\wedge\text{O}\wedge, p) = A(p,4) + 2A(3,4) + 4A(1,3) + (k-4)A(1,4) + 8(k-5).$

By some calculation, we have

$B(|\text{O}|, 4) = B(|\text{OO}, 4) = B(\text{OOO}, 4) = B^*(k,4),$

$B(|\text{EE}, 4) = kA(1,4) + 8(k-3) + A(3,4) + 2.944 > B^*(k,4),$

$B(\text{EEO}, 4) = kA(1,4) + 8(k-3) + A(3,4) + 2.944 > B^*(k,4),$

$B(\wedge\text{E}|, 4) = kA(p,4) + 8(k-3) + A(3,4) + 9.3 > B^*(k,4),$

$B(\wedge\text{O}\wedge, 4) = kA(p,4) + 8(k-3) + A(3,4) + 15.668 > B^*(k,4).$

Subcase 1.3 If $d = 2$. In this case, all possible classes of attached chemical trees are depicted in Fig. 5.

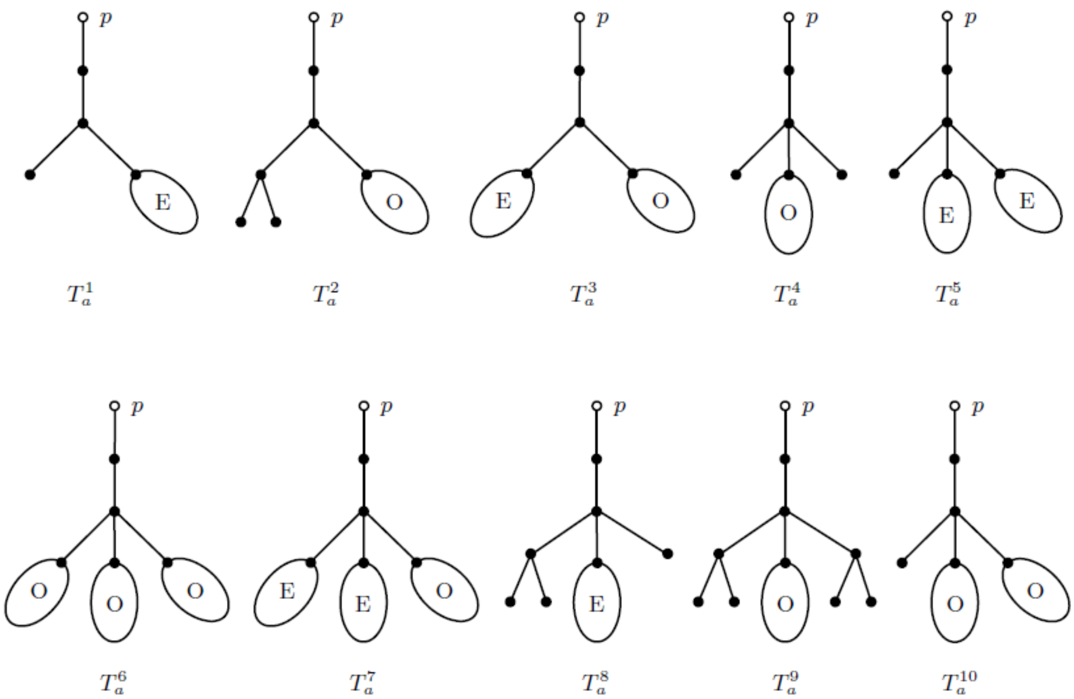


Fig. 5 The attached chemical trees when k is even and $d = 2$

- For $p = 3$, by Lemma 2, we have $A(2, p) = 8$ and $A(3,3) < A(3,4) < 16$. Similar to the discuss of subcase 1.1 and subcase 1.2, we conclude that $B(k,3) > B^*(k,3)$.

- For $p = 4$, we have

$B(T_a^1, 4) = kA(1,4) + 8(k-1) + 8.044 > B^*(k,4),$

$B(T_a^2, 4) = kA(1,4) + 8(k-1) + 11.225 > B^*(k,4),$

$B(T_a^3, 4) = kA(1,4) + 8(k-1) + 20.863 > B^*(k,4),$

$B(T_a^4, 4) = B(T_a^6, 4) = B(T_a^{10}, 4) = kA(1,4) + 8(k-1) = B^*(k,4),$

$B(T_a^5, 4) = kA(1,4) + 8(k-1) + 2.944 > B^*(k,4),$

$B(T_a^7, 4) = kA(1,4) + 8(k-1) + 2.944 > B^*(k,4),$

$B(T_a^8, 4) = kA(1,4) + 8(k-1) + 9.306 > B^*(k,4),$

$B(T_a^9, 4) = kA(1,4) + 8(k-1) + 15.668 > B^*(k,4).$

From subcase 1.1--subcase 1.3, when k is odd we obtain that attached chemical trees "|O|", "|OO", "OOO" (see Fig. 4) have the minimum-cost for $p=3$ and attached chemical trees "T_a^4", "T_a^6", "T_a^{10}" (see Fig. 5) have the minimum-cost for $p=4$.

Case 2 When k is even, there are three subcases in the following:

Subcase 2.1 If $d=3$. In this case, all possible classes of attached chemical trees are depicted in Fig. 6.

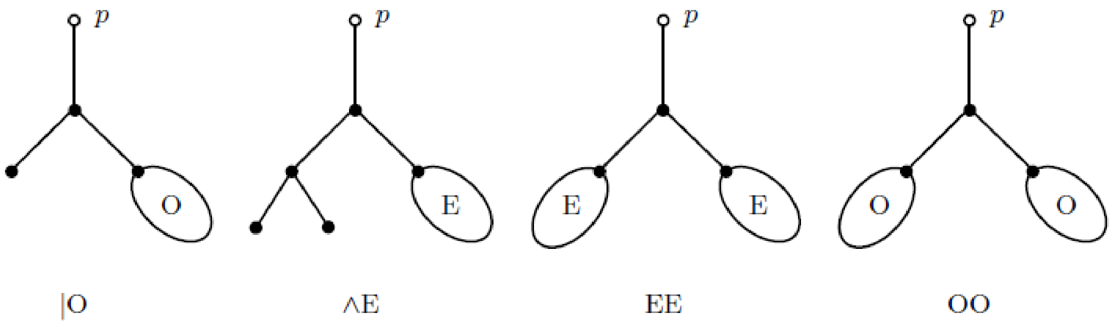


Fig. 6 The attached chemical trees when k is even and $d=3$

By the inductive assumption, we have

$B(|\mathrm{O}, p) = A(p,3) + A(1,3) + (k-1)A(1,4) + 8(k-4) + A(3,4),$

$B(\wedge\mathrm{E}, p) = A(p,3) + (k-2)A(1,4) + 8(k-8) + 2A(1,3) + 2A(3,3) + 2A(3,4),$

$B(\mathrm{EE}, p) = A(p,3) + kA(1,4) + 8(k-12) + 2A(3,3) + 4A(3,4),$

$B(\mathrm{OO}, p) = A(p,3) + kA(1,4) + 8(k-6) + 2A(3,4).$

By some calculation, we conclude that $B(\mathrm{OO},3) = B^*(k,3)$, $B(\mathrm{OO},4) = B^*(k,4)$, $\{B(|\mathrm{O},3), B(\wedge\mathrm{E},3),$

$B(\mathrm{EE},3)\} > B^*(k,3)$ and $\{B(|\mathrm{O},4), B(\wedge\mathrm{E},4), \ B(\mathrm{EE},4)\} > B^*(k,4)$\$.

$B(\mathrm{EE},3) = kA(1,4) + 8(k-6) + A(3,3) + 2A(3,4) + 2.43 > B^*(k,3),$

$B(\mathrm{OO},3) = kA(1,4) + 8(k-6) + A(3,3) + 2A(3,4).$

For $p=4$, we have

$B(|\mathrm{O},4) = kA(1,4) + 8(k-6) + 3A(3,4) + 3.181 > B^*(k,4),$

$B(\wedge\mathrm{E},4) = kA(1,4) + 8(k-6) + 3A(3,4) + 8.791 > B^*(k,4),$

$B(\mathrm{EE},4) = kA(1,4) + 8(k-6) + 3A(3,4) + 2.43 > B^*(k,4),$

$B(\mathrm{OO},4) = kA(1,4) + 8(k-6) + 3A(3,4) = B^*(k,4).$

Subcase 2.2 If $d = 4$, then all possible classes of attached chemical trees are depicted in Fig. 7.

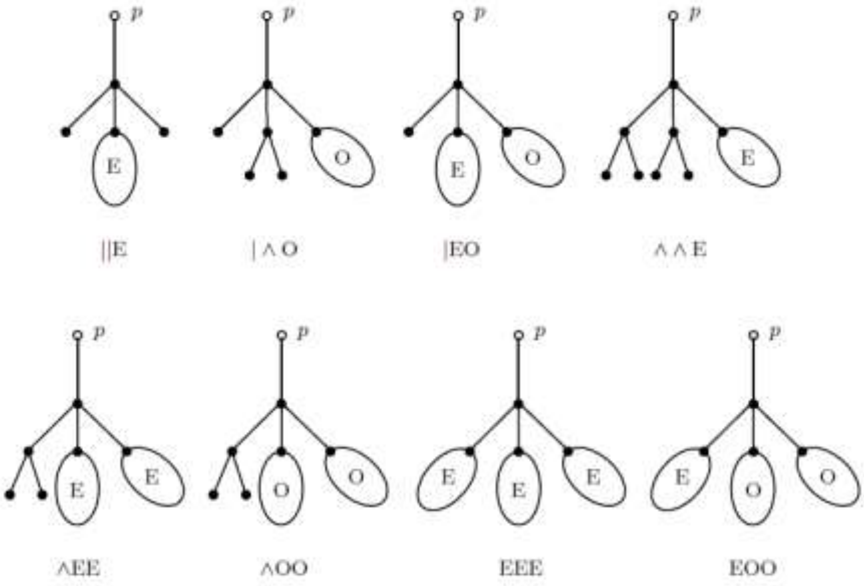


Fig. 7 The attached chemical trees when k is even and $d = 4$

By the inductive assumption and some calculation, we have

$B(\|\,\mathrm{E}, p) = A(p,4) + kA(1,4) + 8(k-8) + 3A(3,4),$

$B(|\wedge\mathrm{O}, p) = A(p,4) + A(3,4) + 2A(1,3) + 8(k-4) + (k-2)A(1,4),$

$B(|\,\mathrm{EO}, p) = A(p,4) + 8(k-8) + kA(1,4) + 3A(3,4),$

$B(\wedge\wedge\mathrm{E}, p) = A(p,4) + 4A(1,3) + (k-4)A(1,4) + 8(k-10) + 5A(3,4),$

$B(\wedge\mathrm{EE}, p) = A(p,4) + (k-2)A(1,4) + 8(k-14) + 7A(3,4) + 2A(1,3),$

$B(\wedge\mathrm{OO}, p) = A(p,4) + (k-2)A(1,4) + 8(k-4) + A(3,4) + 2A(1,3),$

$B(\mathrm{EEE}, p) = A(p,4) + kA(1,4) + 8(k-18) + 9A(3,4),$

$B(\mathrm{EOO}, p) = A(p,4) + kA(1,4) + 8(k-8) + 3A(3,4).$

For $p = 3$, we have

$B(\|\,\mathrm{E},3) = kA(1,4) + 8(k-6) + A(3,3) + 2A(3,4) + 0.257 > B^*(k,3),$

$B(|\wedge\mathrm{O},3) = kA(1,4) + 8(k-6) + A(3,3) + 2A(3,4) + 6.619 > B^*(k,3),$

$B(|\,\mathrm{EO},3) = kA(1,4) + 8(k-6) + A(3,3) + 2A(3,4) + 0.257 > B^*(k,3),$

$B(\wedge\wedge\mathrm{E},3) = kA(1,4) + 8(k-6) + A(3,3) + 2A(3,4) + 15.925 > B^*(k,3),$

$B(\wedge\mathrm{EE},3) = kA(1,4) + 8(k-6) + A(3,3) + 2A(3,4) + 9.563 > B^*(k,3),$

$B(\wedge\mathrm{OO},3) = kA(1,4) + 8(k-6) + A(3,3) + 2A(3,4) + 6.619 > B^*(k,3),$

$B(\mathrm{EEE},3) = kA(1,4) + 8(k-6) + A(3,3) + 2A(3,4) + 3.201 > B^*(k,3),$

$B(\mathrm{EOO},3) = kA(1,4) + 8(k-6) + A(3,3) + 2A(3,4) + 0.257 > B^*(k,3).$

Subcase 2.3 If $d = 2$, then all possible classes of attached chemical trees are depicted in Fig. 8.

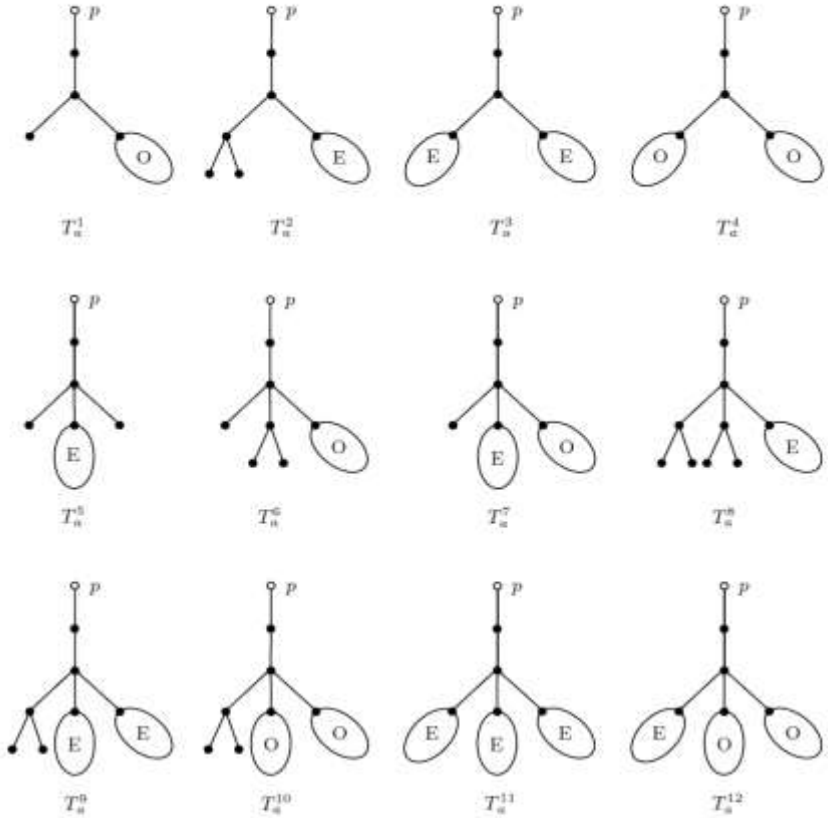


Fig. 8 The attached chemical trees for k is even and $d = 2$

- For $p = 3$, from Lemma 2, we have $A(3,3) < A(3,4) < 2A(2,p) = 16$. Thus, $B(k,3) > B^*(k,3)$.
- For $p = 4$, we have

$B(T_a^1,4) > B^*(T_a^{11},4)$, $B(T_a^2,4) > B^*(T_a^{11},4)$, $B(T_a^3,4) > B^*(T_a^{11},4)$, $B(T_a^4,4) > B^*(T_a^{11},4)$.

$$B(T_a^5,4) = 16 + kA(1,4) + 8(k-8) + 3A(3,4) = B^*(k,4),$$

$$\begin{aligned} B(T_a^6,4) &= 16 + A(3,4) + 2A(1,3) + 8(k-4) + (k-2)A(1,4) \\ &= kA(1,4) + 8(k-6) + 3A(3,4) + 6.362 > B^*(k,4), \end{aligned}$$

$$B(T_a^7,4) = 16 + kA(1,4) + 8(k-8) + 3A(3,4) = B^*(k,4),$$

$$\begin{aligned} B(T_a^8,4) &= 16 + 5A(3,4) + 4A(1,3) + 8(k-10) + (k-4)A(1,4) \\ &= kA(1,4) + 8(k-6) + 3A(3,4) + 15.668 > B^*(k,4), \end{aligned}$$

$$\begin{aligned} B(T_a^9,4) &= 16 + 7A(3,4) + 2A(1,3) + 8(k-14) + (k-2)A(1,4) \\ &= kA(1,4) + 8(k-6) + 3A(3,4) + 9.306 > B^*(k,4), \end{aligned}$$

$$\begin{aligned} B(T_a^{10},4) &= 16 + A(3,4) + 2A(1,3) + 8(k-4) + (k-2)A(1,4) \\ &= kA(1,4) + 8(k-6) + 3A(3,4) + 6.362 > B^*(k,4), \end{aligned}$$

$$\begin{aligned} B(T_a^{11},4) &= 16 + 9A(3,4) + 8(k-18) + kA(1,4) \\ &= kA(1,4) + 8(k-6) + 3A(3,4) + 2.944 > B^*(k,4), \end{aligned}$$

$B(T_a^{12},4)=16+3A(3,4)+8(k-8)+kA(1,4)=B^*(k,4).$

From subcase 2.1-subcase 2.2, when k is even we obtain that attached chemical trees "OO" (see Fig. 6) have the minimum-cost for $p=3$ and attached chemical trees "T_a^5", "T_a^7", "T_a^{12}" (see Fig. 8) have the minimum-cost for $p=4$. The proof is complete.

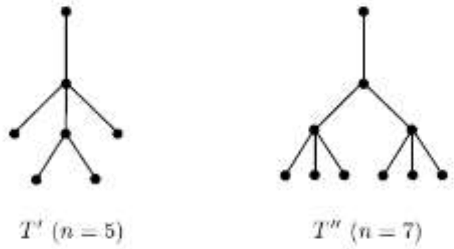


Fig. 9 The AZI -minimal chemical trees for $n=5,7$

Theorem 1 Let $T \in \mathrm{T}(n)$, we obtain:

(i) if n is even, then $AZI(T) \geq nA(1,4)+8(n-4)=\frac{280}{27}n-32$, with equality holding if and only if each non-pendent vertex in T has degree 4 or 2 and $e \in \{(1,4),(2,4)\}$ for all $e \in E(T)$;

(ii) if $n \geq 9$ is odd, then $AZI(T) \geq \frac{280}{27}n-\frac{3816}{125}$ with equality holding if and only if each non-pendent vertex in T has degree 4 or 2 except one vertex of degree 3 and $e \in \{(1,4),(2,4),(3,4)\}$ for all $e \in E(T)$;

(iii) if $n=5$, then $AZI(T) \geq \frac{124583}{4500}$ with equality holding if and only if $T=T'$; if $n=7$, then $AZI(T) \geq \frac{218791}{4500}$ with equality holding if and only if $T=T''$ (see Fig. 9).

Proof Let us employ again the idea of an attached tree from Lemma 5. We will consider the root as a pendent vertex only when its degree $p=1$. Note that $AZI(T)=B(T,1)$ for attached chemical tree T. Therefore, the problem of minimization of AZI over the set of all trees with n pendent vertices is equivalent to the problem of minimization of the cost of an attached chemical tree with $n-1$ pendent vertices and the root of degree 1, that is, min- $AZI(T)=B^*(T,1)$.

By Lemma 3, we obtain that the sub-root w have degree $d=3$ or 4. Below we distinguish two case:

Case 1 If n is even, then the possible classes of attached chemical trees with $n-1$ pendent vertices are "$|$E", "$\wedge$O", "EO", "$|$O$|$", "$|$OO", "$|$EE", "OOO", "EEO", "$\wedge$E$|$", "$\wedge$O$\wedge$"(see Fig. 6 and Fig. 7). By Lemma 5, we have

$B(|\mathrm{E},1)=2A(1,3)+(n-2)A(1,4)+8(n-8)+A(3,3)+2A(3,4)=nA(1,4)+8(n-4)+9.049,$

$B(\wedge\mathrm{O},1)=3A(1,3)+(n-3)A(1,4)+8(n-6)+A(3,3)+A(3,4)=nA(1,4)+8(n-4)+12.230,$

$B(\mathrm{EO},1)=A(1,3)+(n-1)A(1,4)+8(n-10)+A(3,3)+3A(3,4)=nA(1,4)+8(n-4)+5.868,$

$B(|\mathrm{O}|,1)=nA(1,4)+8(n-4),$

$B(|\mathrm{OO},1)=nA(1,4)+8(n-4),$

$B(|\mathrm{EE},1)=nA(1,4)+8(n-14)+6A(3,4)=nA(1,4)+8(n-4)+2.944,$

$B(\mathrm{OOO},1)=nA(1,4)+8(n-4),$

$B(\mathrm{EEO},1)=nA(1,4)+8(n-14)+6A(3,4)=nA(1,4)+8(n-4)+2.944,$

$B(\wedge \mathrm{E}|,1) = 2A(1,3) + (n-2)A(1,4) + 8(n-10) + 4A(3,4) = nA(1,4) + 8(n-4) + 9.306,$

$B(\wedge \mathrm{O} \wedge,1) = 4A(1,3) + (n-4)A(1,4) + 8(n-6) + 2A(3,4) = nA(1,4) + 8(n-4) + 15.668.$

Thus, we conclude that if n is even, then $B^*(n-1,1) = B(|\mathrm{O}|,1) = B(|\mathrm{OO},1) = B(\mathrm{OOO},1) = nA(1,4) +$ $8(n-4)$. Combining this with Lemma 5, Lemma 3 and Lemma 4, equality holding if and only if each non-pendent vertex in $\mathrm{T}^*(n)$ has degree 4 or 2 and $e \in \{(1,4),(2,4)\}$ for each edge e.

Case 2 If n is odd, then the possible classes of attached chemical trees with $n-1$ pendent vertices are "$|\mathrm{O}$", "$\wedge \mathrm{E}$", "EE", "O", "$\|\mathrm{E}$", "$|\wedge \mathrm{O}$", "$|\mathrm{EO}$", "$\wedge\wedge \mathrm{E}$", "$\wedge \mathrm{EE}$", "$\wedge \mathrm{OO}$", "EEE", "EOO" (see Fig. 3 and Fig. 4). By the Lemma 5, we have

$B(|\mathrm{O},1) = 2A(1,3) + (n-2)A(1,4) + 8(n-5) + A(3,4) = nA(1,4) + 8(n-9) + 3A(3,4) + 6.362,$

$B(\wedge \mathrm{E},1) = 3A(1,3) + (n-3)A(1,4) + 8(n-9) + 2A(3,3) + 2A(3,4) = nA(1,4) + 8(n-9) + 3A(3,4) + 11.972,$

$B(\mathrm{EE},1) = A(1,3) + (n-1)A(1,4) + 8(n-139) + 2A(3,3) + 4A(3,4) = nA(1,4) + 8(n-9) + 3A(3,4) + 5.610,$

$B(\mathrm{OO},1) = A(1,3) + (n-1)A(1,4) + 8(n-7) + 2A(3,4) = nA(1,4) + 8(n-9) + 3A(3,4) + 3.181,$

$B(\|\mathrm{E},1) = A(1,4) + (n-1)A(1,4) + 8(n-9) + 3A(3,4) = nA(1,4) + 8(n-9) + 3A(3,4),$

$B(|\wedge \mathrm{O},1) = 2A(1,3) + (n-2)A(1,4) + 8(n-5) + A(3,4) = nA(1,4) + 8(n-9) + 3A(3,4) + 6.362,$

$B(|\mathrm{EO},1) = nA(1,4) + 8(n-9) + 3A(3,4),$

$B(\wedge\wedge \mathrm{E},1) = 4A(1,3) + (n-4)A(1,4) + 8(n-11) + 5A(3,4) = nA(1,4) + 8(n-9) + 3A(3,4) + 15.668,$

$B(\wedge \mathrm{EE},1) = 2A(1,3) + (n-2)A(1,4) + 8(n-15) + 7A(3,4) = nA(1,4) + 8(n-9) + 3A(3,4) + 9.306,$

$B(\wedge \mathrm{OO},1) = 2A(1,3) + (n-2)A(1,4) + 8(n-5) + A(3,4) = nA(1,4) + 8(n-9) + 3A(3,4) + 6.362,$

$B(\mathrm{EEE},1) = nA(1,4) + 8(n-19) + 9A(3,4) = nA(1,4) + 8(n-9) + 3A(3,4) + 2.944,$

$B(\mathrm{EOO},1) = nA(1,4) + 8(n-9) + 3A(3,4).$

Thus, $B(\|\mathrm{E},1) = B(|\mathrm{EO},1) = B(\mathrm{EOO},1) = nA(1,4) + 8(n-9) + 3A(3,4)$. Therefore, we conclude that if n is odd, then $B^*(n-1,1) = B(\|\mathrm{E},1) = B(|\mathrm{EO},1) = B(\mathrm{EOO},1) = nA(1,4) + 8(n-9) + 3A(3,4)$. Combining this with Lemma 3, Lemma 4 and Lemma 5, equality holding if and only if only one non-pendent vertex in $\mathrm{T}^*(n)$ has degree 3, while other non-pendent vertices having degree 4 or 2, and $e \in \{(1,4),(2,4),(3,4)\}$ for each edge e. In particular, for $n = 5,7$, by simple calculation, the optimal chemical trees is shown in Fig. 9.

This completes the proof.

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