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Research Article

On chemical trees with minimum augmented Zagreb index

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Abstract

Let G be a simple connected graph with order at least 3, vertex set $V(G)$, and edge set $E(G)$. For a vertex $v \in V(G)$, denote by $d_G(v)$ the degree of v. The augmented Zagreb index of the graph G is denoted by $\mathcal{AZ}(G)$ and is defined as $\mathcal{AZ}(G) = \sum_{uv\in E(G)} \big(d_G(u)d_G(v)/\big(d_G(u)+d_G(v)-2\big)\big)^3$. In this paper, the minimum augmented Zagreb index of chemical trees of order n is determined. The extremal chemical trees of order n with the minimum augmented Zagreb index are also characterized.

Keywords: chemical tree; augmented Zagreb index; extremal tree.

2020 Mathematics Subject Classification: 05C05, 05C09, 05C92.

1. Introduction

All graphs considered in this paper are simple connected of order at least 3. Let G be a such graph with vertex set $V(G)$ and edge set $E(G)$. For $v \in V(G)$, let $d_G(v)$ denote the degree of v and let $N_G(v)$ denote the set of neighbours of v. A path $P = v_1v_2\dots v_t$ satisfying $d_G(v_1) \geq 3$, $d_G(v_i) = 2$ when $2 \leq i \leq t-1$, and $d_G(v_t) \geq 3$, is called an internal path of length $t-1$. A vertex of degree greater than 2 is called a branching vertex.

The augmented Zagreb (AZ) index of G, denoted by $\mathcal{AZ}(G)$, is defined [3] as

$$\mathcal{AZ}(G) = \sum_{uv\in E(G)} f(d_G(u), d_G(v)),$$

where $f(x,y) = \left(\frac{xy}{x+y-2}\right)^3$. This index was shown to have the best predicting ability for a variety of physicochemical properties among several tested vertex-degree-based topological indices (see [4, 5]). Hence, this topological index has attracted more and more attention in recent years. Consequently, various significant mathematical properties of the AZ index were obtained. Most of the known results on this index can be found in [1, 2, 6–8, 10].

In [3], Furtula et al. proved that the star is the unique tree having the minimum augmented Zagreb index among n-vertex trees. Lin et al. [8] and Xiao et al. [10] completely characterized the trees with the maximum augmented Zagreb index by proving that the n-vertex balanced double star uniquely maximizes AZ index for $n \geq 19$.

A tree T is a chemical tree if $d_T(v) \leq 4$ for every $v \in V(T)$. Let $\widetilde{T}_n$ be the set of all chemical trees of order n. A chemical tree $T \in \widetilde{T}_n$ is said to be an AZ-maximal/AZ-minimal chemical tree if T has the maximum/minimum AZ index among all chemical trees of n. In [9], the authors determined the maximum AZ index for chemical trees of order n, and the extremal chemical trees with the maximum AZ index were characterized. In the present paper, the minimum AZ index of chemical trees of order n is determined. The AZ-minimal chemical trees of order n are also characterized. Theorems 3.1 and 3.2 are the main results of this paper.

Note that S_n is a chemical tree for every $n \leq 5$. Thus, by a result reported in [3], the AZ-minimal chemical tree of order n is the star S_n for $n \leq 5$. Consequently, we assume $n \geq 6$ in the rest of this paper.

2. Lemmas

For a tree $T \in \widetilde{T}_n$, a vertex v with $d_T(v) = i$ is called an i-degree vertex, and an edge $e = uv$ with $d_T(u) = i$ and $d_T(v) = j$ is called an (i,j)-edge. The notations $n_i(T)$ and $m_{ij}(T)$ denote the number of i-degree vertices and the number of (i,j)-edges of T, respectively.

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Lemma 2.1 (see [6]). *Let* $f(x,y)=\left(\frac{xy}{x+y-2}\right)^3$ *with* $1\le x\le 4$ *and* $1\le y\le 4$. *Then*

(1) $f(1,y)$ *is strictly decreasing on* $y\ge 2$*;*

(2) $f(2,y)=8$*;*

(3) $f(3,y)$ *and* $f(4,y)$ *are strictly increasing on* y.

Lemma 2.2 (see [7]). *Let* $g(x)=\left(\frac{3x}{x+1}\right)^3-\left(\frac{4x}{x+2}\right)^3$ *with* $1\le x\le 4$. *Then* $g(x)$ *is strictly decreasing on* x.

Lemma 2.3. *Let* $T\in\widetilde{T}_n$ *be an AZ-minimal chemical tree. Then* $n_3(T)+n_4(T)\ge 1$.

Proof. Consider the tree $T_1\in\widetilde{T}_n$ depicted in Figure 2.1. Then

$$\mathcal{AZ}(T_1)=2f(1,3)+8(n-3)=\frac{27}{4}+8(n-3)<8(n-1)=\mathcal{AZ}(P_n),$$

which implies that the path P_n is not an AZ-minimal chemical tree. Thus, $n_3(T)+n_4(T)\ge 1$. □

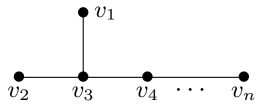


Figure 2.1: The chemical tree T_1 of order n, considered in the proof of Lemma 2.3.

From the definition of the AZ index, the next lemma follows.

Lemma 2.4. *Let* $T\in\widetilde{T}_n$ *be tree as depicted in Figure 2.2, where* $d_T(u)=d_T(v)\ge 2$. *Let* $T'=T-uu_1-vv_1+uv_1+vu_1$. *Then* $\mathcal{AZ}(T)=\mathcal{AZ}(T')$.

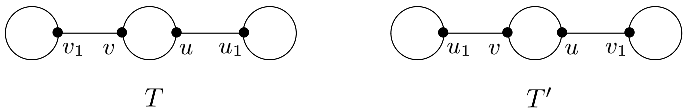


Figure 2.2: The chemical trees T and T' considered in Lemma 2.4.

Lemma 2.5. *If* $T\in\widetilde{T}_n$ *is an AZ-minimal chemical tree with* $n\ge 7$*, then* $m_{12}(T)=0$.

Proof. Suppose to the contrary that $m_{12}(T)\ne 0$. By Lemma 2.3, $n_3(T)+n_4(T)\ge 1$. Then, T is of the form as depicted in Figure 2.3, where $t\ge 2$ and $d_T(v)\ge 3$.

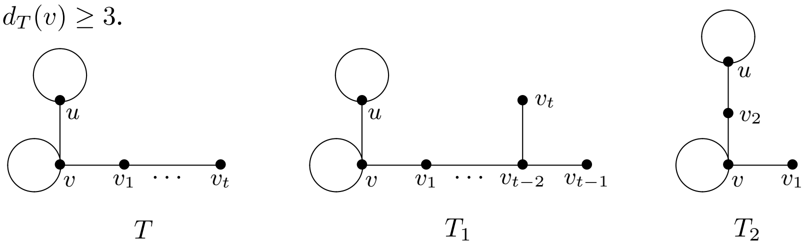


Figure 2.3: The chemical trees T, T_1, and T_2, considered in the proof of Lemma 2.5.

If $t\ge 3$, then let $T'=T_1=T-v_{t-1}v_t+v_{t-2}v_t$ (see Figure 2.3). So, $T'\in\widetilde{T}_n$. By Lemma 2.1, $f(3,d_T(v))\le f(3,4)=\frac{1728}{125}$. Thus,

$$\mathcal{AZ}(T')-\mathcal{AZ}(T)=\begin{cases}2f(1,3)+f(3,f(3,d_T(v))-24\le\frac{27}{4}+\frac{1728}{125}-24=-\frac{1713}{500} & \text{if } t=3,\\ 2f(1,3)-16=-\frac{37}{4} & \text{if } t\ge 4.\end{cases}$$

Hence, we have $\mathcal{AZ}(T')<\mathcal{AZ}(T)$, a contradiction. Therefore, $t=2$. Since $n\ge 7$, there is a vertex $x\in N_T(v)$ with $x\ne v_1$ such that $d_T(x)\ge 2$. Without loss of generality, we assume that $d_T(u)\ge 2$. Let $T'=T_2=T-vu-v_1v_2+vv_2+v_2u$ (see Figure 2.3). Then, $T'\in\widetilde{T}_n$ and by Lemma 2.1, $\mathcal{AZ}(T')-\mathcal{AZ}(T)=f(1,d_T(v))-f(d_T(u),d_T(v))<0$, which gives $\mathcal{AZ}(T')<\mathcal{AZ}(T)$, a contradiction. □

Lemma 2.6. *Let* $T\in\widetilde{T}_n$ *be an AZ-minimal chemical tree. Then* $m_{22}(T)\le 2$.

Proof. Suppose to the contrary that $m_{22}(T)\ge 3$. Then by Lemma 2.5, $m_{12}(T)=0$, which implies that every $(2,2)$-edge is on an internal path of T. By Lemma 2.4, we may assume that there is at most one internal path of T of length greater than 2. So, there is an internal path of T of length $t\ge 5$; that is, T is of the form as depicted in Figure 2.4, where $t\ge 5$, $d_T(v)\ge 3$, and $d_T(v_t)\ge 3$. Let $T'=T-v_3v_4+v_2v_4$ (see Figure 2.4). Then $T'\in\widetilde{T}_n$ and

$$\mathcal{AZ}(T')-\mathcal{AZ}(T)=f(1,3)-8=\frac{27}{8}-8=-\frac{37}{8}<0,$$

which yields $\mathcal{AZ}(T')<\mathcal{AZ}(T)$, a contradiction. □

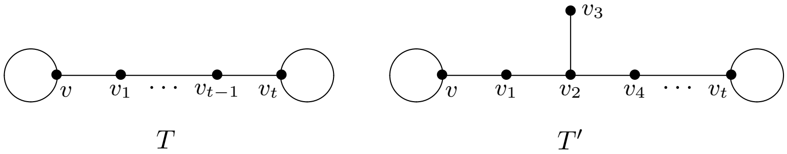


Figure 2.4: The chemical trees T and T' considered in the proof of Lemma 2.6.

Lemma 2.7. *Let $T \in \widetilde{T}_n$ be an AZ-minimal chemical tree. If $m_{22}(T) \neq 0$, then no two branching vertices are adjacent; that is, $m_{33}(T) = m_{34}(T) = m_{44}(T) = 0$.*

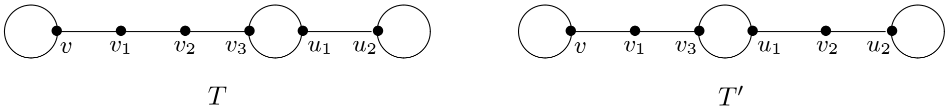


Figure 2.5: The chemical trees T and T' considered in the proof of Lemma 2.7.

Proof. Suppose to the contrary that $m_{22}(T) \neq 0$, and $u_1, u_2 \in V(T)$ are two adjacent branching vertices. Then T is of the form as depicted in Figure 2.5, where $d_T(u_1) \geq 3$, and $d_T(u_2) \geq 3$. Take $T' = T - v_1v_2 - v_2v_3 - u_1u_2 + v_1v_3 + u_1v_2 + v_2u_2$ as depicted in Figure 2.5. Then $T' \in \widetilde{T}_n$. By Lemma 2.1, $f(d_T(u_1), d_T(u_2)) \geq f(3,3) = \frac{729}{64}$. Hence,

$$\mathcal{AZ}(T') - \mathcal{AZ}(T) = 8 - f(d_T(u_1), d_T(u_2)) \leq 8 - \frac{729}{64} = -\frac{217}{64} < 0,$$

that is, $\mathcal{AZ}(T') < \mathcal{AZ}(T)$, a contradiction. □

Lemma 2.8. *Let $T \in \widetilde{T}_n$ be an AZ-minimal chemical tree. If $m_{22}(T) \neq 0$, then $n_3(T) = 0$.*

Proof. Suppose to the contrary that $m_{22}(T) \neq 0$ and $n_3(T) \neq 0$. Then T is of the form as depicted in Figure 2.6. By Lemma 2.7, no two branching vertices are adjacent. Then, $d_T(u_1) = 2$ and $d_T(u_i) \leq 2$ for $i = 2, 3$.

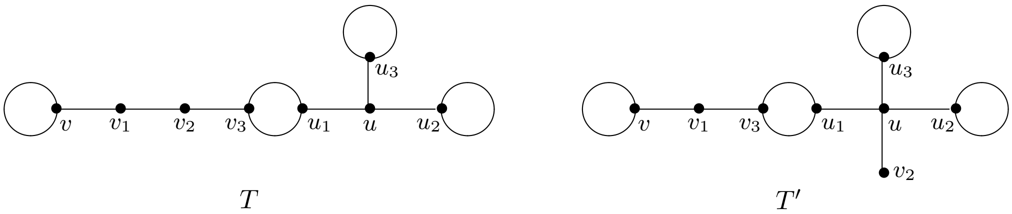


Figure 2.6: The chemical trees T and T' considered in the proof of Lemma 2.8.

Let $T' = T - v_1v_2 - v_2v_3 + v_1v_3 + uv_2$ (see Figure 2.6). By Lemma 2.2, $f(4, d_T(u_i)) - f(3, d_T(u_i)) \leq f(4,2) - f(3,2) = 0$ for $i = 2, 3$. Thus,

$$\mathcal{AZ}(T') - \mathcal{AZ}(T) = f(1,4) + \sum_{i=2}^{3} \big(f(4, d_T(u_i)) - f(3, d_T(u_i))\big) - 8 \leq \frac{64}{27} - 8 = -\frac{152}{27} < 0,$$

that is, $\mathcal{AZ}(T') < \mathcal{AZ}(T)$, a contradiction. □

Lemma 2.9. *Let $T \in \widetilde{T}_n$ be an AZ-minimal chemical tree, where $n \geq 7$. Then $m_{14}(T) \neq 0$.*

Proof. Suppose to the contrary that $m_{14}(T) = 0$. Then by Lemma 2.5, $m_{12}(T) = 0$, and so $m_{13}(T) \neq 0$ and $n_3(T) \neq 0$. By Lemma 2.8, $m_{22}(T) = 0$. Noting that $n \geq 7$, we have $n_3(T) \geq 2$. Then T is of the form as depicted in Figure 2.7, where $d_T(u) \geq 2$ and $d_T(v) \geq 2$. Without loss of generality, assume that $d_T(u) \geq d_T(v)$.

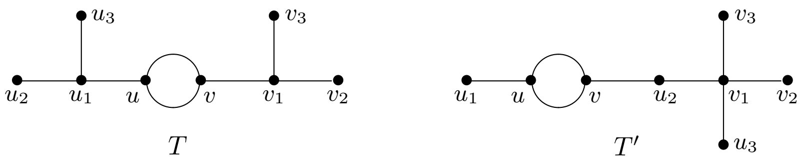


Figure 2.7: The chemical trees T and T' considered in the proof of Lemma 2.9.

If $d_T(u) \geq 3$, then let $T' = T - u_1u_2 - u_1u_3 - vv_1 + vu_2 + u_2v_1 + v_1u_3$, as depicted in Figure 2.7. So $T' \in \widetilde{T}_n$. By Lemma 2.1, $f(1, d_T(u)) \leq f(1,2) = 8$, $f(3, d_T(u)) \geq f(3,3) = \frac{729}{64}$, and $f(3, d_T(v)) \geq f(3,2) = 8$. Therefore,

$$\mathcal{AZ}(T') - \mathcal{AZ}(T) = 16 + 3f(1,4) + f(1, d_T(u)) - 4f(1,3) - f(3, d_T(u)) - f(3, d_T(v)) \leq 16 + \frac{64}{9} + 8 - \frac{27}{2} - \frac{729}{64} - 8 = -\frac{1025}{576} < 0,$$

Consequently, we have $\mathcal{AZ}(T') < \mathcal{AZ}(T)$, a contradiction.

If $d_T(u) = d_T(v) = 2$, then let $N_T(u) = \{u_1, u_0\}$ and take $T'' = T - uu_1 - u_1u_3 - vv_1 + vu_1 + u_2v_1 + v_1u_3$ (see Figure 2.8). So, $T'' \in \widetilde{T}_n$. Note that $m_{22}(T) = 0$. Then, $d_T(u_0) \geq 3$ and $f(1, d_T(u_0)) \leq f(1,3) = \frac{27}{8}$. Therefore,

$$\mathcal{AZ}(T'') - \mathcal{AZ}(T) = 3f(1,4) + f(1, d_T(u_0)) - 4f(1,3) \leq \frac{64}{9} + \frac{27}{8} - \frac{27}{2} = -\frac{217}{72} < 0,$$

which gives $\mathcal{AZ}(T'') < \mathcal{AZ}(T)$, a contradiction. □

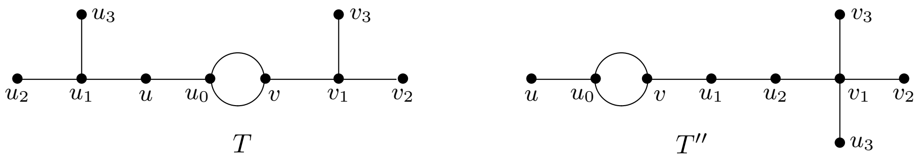


Figure 2.8: The chemical trees T and T'' considered in the proof of Lemma 2.9.

Lemma 2.10. *Let $T \in \widetilde{T}_n$ be an AZ-minimal chemical tree, where $n \geq 8$. Then $m_{44}(T) = 0$.*

Proof. Suppose to the contrary that $m_{44}(T) \neq 0$. By Lemma 2.9, $m_{14}(T) \neq 0$. Then by Lemma 2.4, we may assume that T is of the form as depicted in Figure 2.9. Let $T' = T - vu + v_1u$ (see Figure 2.9). Then $T' \in \widetilde{T}_n$. By Lemma 2.2, $f(3, d_T(v_i)) - f(4, d_T(v_i)) \leq f(3,1) - f(4,1) = \frac{217}{216}$ for $i = 2, 3$. Thus,

$$\mathcal{AZ}(T') - \mathcal{AZ}(T) = 16 + \sum_{i=2}^{3} \left(f(3, d_T(v_i)) - f(4, d_T(v_i))\right) - f(4,4) - f(1,4) \leq 16 + \frac{217}{108} - \frac{512}{27} - \frac{64}{27} = -\frac{359}{108} < 0,$$

that is, $\mathcal{AZ}(T') < \mathcal{AZ}(T)$, a contradiction. □

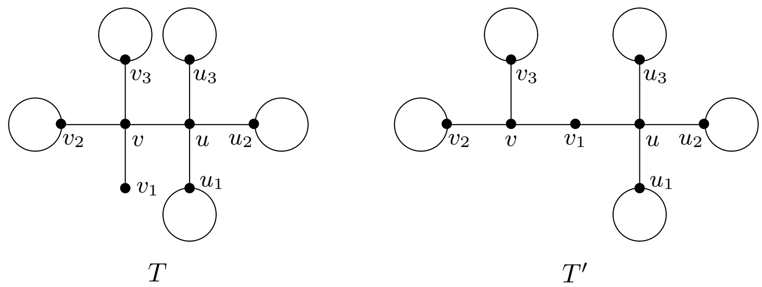


Figure 2.9: The chemical trees T and T' considered in the proof of Lemma 2.10.

Lemma 2.11. *Let $T \in \widetilde{T}_n$ be an AZ-minimal chemical tree with $n \geq 8$. Then $m_{34}(T) = 0$.*

Proof. Suppose to the contrary that $m_{34}(T) \neq 0$. By Lemma 2.9, $m_{14}(T) \neq 0$. Then by Lemma 2.4, we may assume that T is of the form as depicted in Figure 2.10. Without loss of generality, assume that $d_T(v_2) \geq d_T(v_3)$ and $d_T(v_5) \geq d_T(v_6)$.

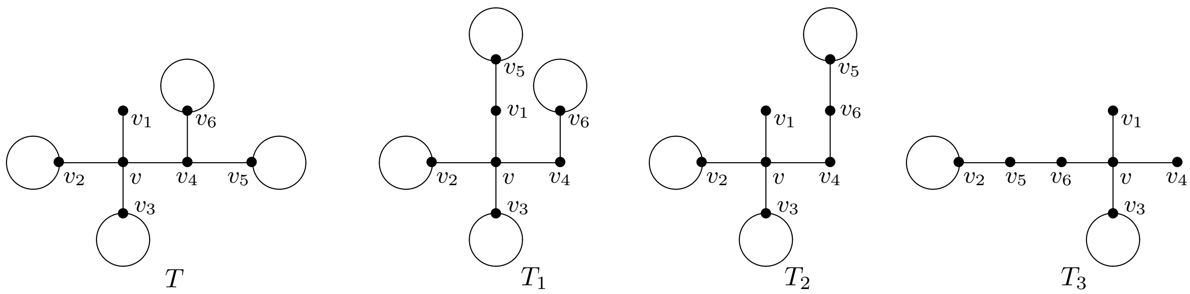


Figure 2.10: The chemical trees T, T_1, T_2, and T_3, considered in the proof of Lemma 2.11.

Case 1. $d_T(v_5) \geq 2$ and $d_T(v_6) \geq 2$.

Take $T' = T_1 = T - v_4v_5 + v_1v_5$ (see Figure 2.10). Then $T' \in \widetilde{T}_n$. By Lemma 2.1, $f(3, d_T(v_i)) \geq f(3,2) = 8$ for $i = 5, 6$. Thus,

$$\mathcal{AZ}(T') - \mathcal{AZ}(T) = 32 - f(3, d_T(v_5)) - f(3, d_T(v_6)) - f(3,4) - f(1,4) \leq 32 - 16 - \frac{1728}{125} - \frac{64}{27} = -\frac{656}{3375} < 0,$$

that is, $\mathcal{AZ}(T') < \mathcal{AZ}(T)$, a contradiction.

Case 2. $d_T(v_5) \geq 2$ and $d_T(v_6) = 1$.
Let $T' = T_2 = T - v_4v_5 + v_6v_5$ (see Figure 2.10). Then $T' \in \widetilde{T}_n$. By Lemma 2.1, $f(3, d_T(v_5)) \geq f(3, 2) = 8$. Hence,

$$\mathcal{AZ}(T') - \mathcal{AZ}(T) = 24 - f(1,3) - f(3,4) - f(3, d_T(v_5)) \leq 24 - \frac{27}{8} - \frac{1728}{125} - 8 = -\frac{1199}{1000} < 0,$$

which yields $\mathcal{AZ}(T') < \mathcal{AZ}(T)$, a contradiction.

Case 3. $d_T(v_5) = d_T(v_6) = 1$.
Since $n \geq 8$, we have $d_T(v_2) \geq 2$. Let $T' = T_3 = T - v_2v - v_4v_5 - v_4v_6 + v_2v_5 + v_5v_6 + v_6v$ (see Figure 2.10). Then $T' \in \widetilde{T}_n$. By Lemma 2.1, $f(4, d_T(v_2)) \geq f(4, 2) = 8$. Therefore,

$$\mathcal{AZ}(T') - \mathcal{AZ}(T) = 24 + f(1,4) - f(3,4) - 2f(1,3) - f(4, d_T(v_2)) \leq 24 + \frac{64}{27} - \frac{1728}{125} - \frac{27}{4} - 8 = -\frac{29749}{13500} < 0,$$

that is, $\mathcal{AZ}(T') < \mathcal{AZ}(T)$, a contradiction. $\square$

Lemma 2.12. *Let $T \in \widetilde{T}_n$ be an AZ-minimal chemical tree with $n \geq 8$. Then $m_{33}(T) = 0$.*

Proof. Suppose to the contrary that $m_{33}(T) \neq 0$. By Lemma 2.11, $m_{34}(T) = 0$. Then by Lemma 2.4, we may assume that T is of the form as depicted in Figure 2.11, where $d_T(u_i) \leq 2$ and $d_T(v_i) \leq 3$ for $i = 1, 2$. Without loss of generality, assume that $d_T(u_2) \geq d_T(u_1)$, $d_T(v_2) \geq d_T(v_1)$, and $d_T(v_2) \geq d_T(u_2)$. Let $T' = T - vv_1 + uv_1$ as (see Figure 2.11). Then $T' \in \widetilde{T}_n$ and

$$\mathcal{AZ}(T') - \mathcal{AZ}(T) = 16 + \sum_{i=1}^{2} \left(f(4, d_T(u_i)) - f(3, d_T(u_i))\right) + f(4, d_T(v_1)) - f(3,3) - f(3, d_T(v_1)) - f(3, d_T(v_2)).$$

If $d_T(u_2) = 1$, then $d_T(u_1) = 1$. Since $n \geq 8$, we have $d_T(v_2) \geq 2$. By Lemmas 2.1 and 2.2, $f(3, d_T(v_2)) \geq f(3, 2) = 8$ and $f(4, d_T(v_1)) - f(3, d_T(v_1)) \leq f(4, 3) - f(3, 3) = \frac{19467}{8000}$. Thus,

$$\mathcal{AZ}(T') - \mathcal{AZ}(T) \leq 16 + 2\left(\frac{64}{27} - \frac{27}{8}\right) + \frac{19467}{8000} - \frac{729}{64} - 8 = -\frac{320383}{108000} < 0,$$

that is, $\mathcal{AZ}(T') < \mathcal{AZ}(T)$, a contradiction. Hence, $d_T(u_2) = 2$, $d_T(u_1) \leq 2$, and $d_T(v_2) \geq 2$. By Lemmas 2.1 and 2.2, $f(3, d_T(v_2)) \geq f(3, 2) = 8$, $f(4, d_T(v_1)) - f(3, d_T(v_1)) \leq f(4, 3) - f(3, 3) = \frac{19467}{8000}$, and $f(4, d_T(u_i)) - f(3, d_T(u_i)) \leq f(4, 2) - f(3, 2) = 0$ for $i = 1, 2$. Consequently, we have

$$\mathcal{AZ}(T') - \mathcal{AZ}(T) \leq 16 + \frac{19467}{8000} - \frac{729}{64} - 8 = -\frac{3829}{4000} < 0,$$

a contradiction. $\square$

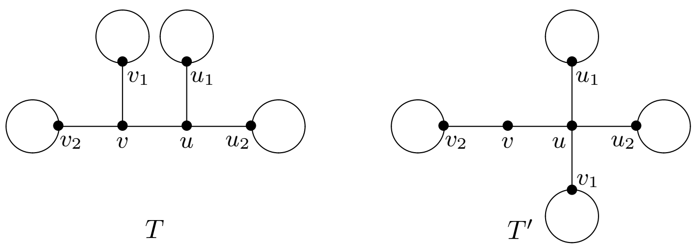


Figure 2.11: The chemical trees T and T' considered in the proof of Lemma 2.12.

Lemma 2.13. *Let $T \in \widetilde{T}_n$ be an AZ-minimal chemical tree with $n \geq 13$. Then $m_{13}(T) = 0$.*

Proof. Suppose to the contrary that $m_{13}(T) \neq 0$. From Lemmas 2.8, 2.9, 2.10, 2.11, and 2.12, it follows that $m_{14}(T) \neq 0$ and $m_{22}(T) = m_{44}(T) = m_{34}(T) = m_{33}(T) = 0$. Then, for every 3-degree or 4-degree vertex $v \in V(T)$, $d_T(x) \leq 2$ for $x \in N_T(v)$, and there is at least one 2-degree vertex in $N_T(v)$.

Case 1. $n_3(T) \geq 2$ and there is a 3-degree vertex $u \in V(T)$ such that $N_T(u)$ contains at last two 2-degree vertices.
In this case, T is of the form as depicted in Figure 2.12, where $d_T(v_0) = d_T(u_0) = 3$, $d_T(v_2) \leq 2$, and $d_T(u_2) \leq 2$. Take $T' = T_1 = T - uu_2 + vu_2$, as depicted in Figure 2.12. So, $T' \in \widetilde{T}_n$. By Lemma 2.2, $f(4, d_T(v_2)) - f(3, d_T(v_2)) \leq f(4, 2) - f(3, 2) = 0$ and $f(4, d_T(u_2)) - f(3, d_T(u_2)) \leq f(4, 2) - f(3, 2) = 0$. Thus,

$$\mathcal{AZ}(T') - \mathcal{AZ}(T) = f(1,4) + f(4, d_T(v_2)) + f(4, d_T(u_2)) - f(1,3) - f(3, d_T(v_2)) - f(3, d_T(u_2)) \leq \frac{64}{27} - \frac{27}{8} = -\frac{217}{216} < 0,$$

that is, $\mathcal{AZ}(T') < \mathcal{AZ}(T)$, a contradiction.

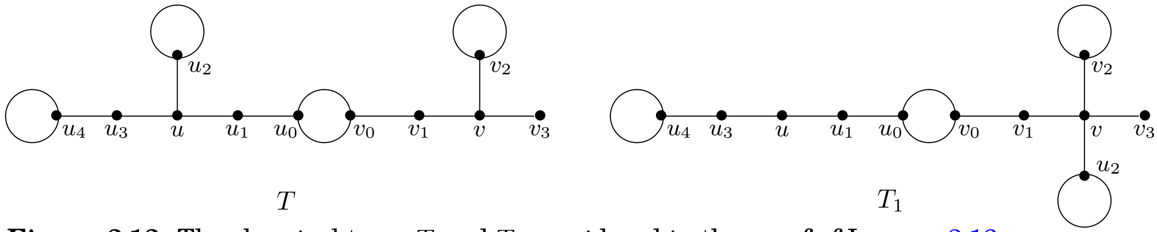


Figure 2.12: The chemical trees T and T_1 considered in the proof of Lemma 2.13.

Case 2. $n_3(T) \geq 2$ and for every 3-degree vertex $v \in V(T)$, $N_T(v)$ contains a unique 2-degree vertex.
In this case, T is of the form as depicted in Figure 2.13, where $d_T(u_0) \geq 3$, $d_T(v_0) \geq 3$, $d_T(u_2) \leq 2$, and $d_T(v_2) \leq 2$. Note that $n \geq 13$. So, $u_0 \neq v$. Take $T' = T_2 = T - uu_1 - uu_2 - v_1v + v_1u_3 + uv + vu_2$, as depicted in Figure 2.13. Then $T' \in \widetilde{T}_n$. By Lemma 2.1, $f(1, d_T(u_0)) \leq f(1,3) = \frac{27}{8}$. Thus,

$$\mathcal{AZ}(T') - \mathcal{AZ}(T) = 3f(1,4) + f(1, d_T(u_0)) - 4f(1,3) \leq \frac{64}{9} + \frac{27}{8} - \frac{27}{2} = -\frac{217}{72} < 0,$$

that is, $\mathcal{AZ}(T') < \mathcal{AZ}(T)$, a contradiction.

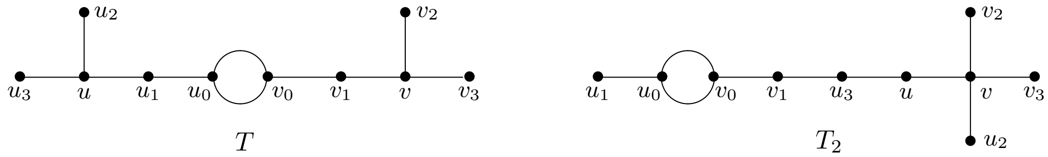


Figure 2.13: The chemical trees T and T_2 considered in the proof of Lemma 2.13.

Case 3. $n_3(T) = 1$.
Note that $n \geq 13$. Then $n_4(T) \neq 0$. If for every 4-degree vertex $w \in V(T)$, $N_T(w)$ contains three 1-degree vertices, then we have $n_4(T) \leq 2$ and $n = 4n_4(T) + 4 \leq 12$ (since $n_3(T) = 1$ and $m_{13}(T) \neq 0$), which is a contradiction. Thus, there is a 4-degree vertex $u \in V(T)$ such that $N_T(u)$ contains at lest two 2-degree vertices. That is, T is of the form as depicted in Figure 2.14. Let $T' = T_3 = T - u_3u_4 + v_3u_4$ (see Figure 2.14). Then, $T' \in \widetilde{T}_n$ and

$$\mathcal{AZ}(T') - \mathcal{AZ}(T) = f(1,4) - f(1,3) = \frac{64}{27} - \frac{27}{8} = -\frac{217}{216} < 0,$$

that is, $\mathcal{AZ}(T') < \mathcal{AZ}(T)$, a contradiction. □

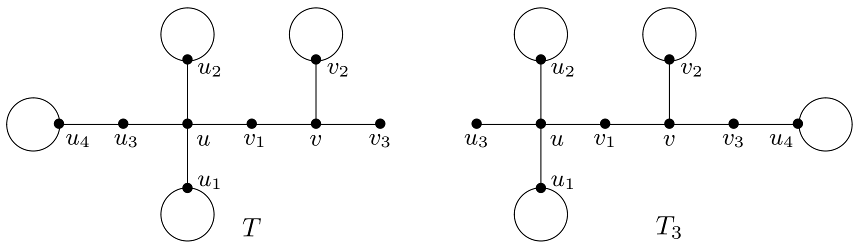


Figure 2.14: The chemical trees T and T_3 considered in the proof of Lemma 2.13.

Lemma 2.14. *Let $T \in \widetilde{T}_n$ be an AZ-minimal chemical tree with $n \geq 13$. Then $n_3(T) \leq 2$.*

Proof. Suppose to the contrary that $n_3(T) \geq 3$. Let $u, v \in V(T)$ be two 3-degree vertices. By Lemmas 2.11, 2.12, and 2.13, all vertices in $N_T(u)$ and $N_T(v)$ are 2-degree vertices. Then, T is of the form as depicted in Figure 2.15, where $d_T(u_i) = 2$ and $d_T(v_i) = 2$ for $i = 1, 2, 3$. Take $T' = T - vv_3 + uv_3$ (see Figure 2.15). Then, $T' \in \widetilde{T}_n$ and $\mathcal{AZ}(T') = \mathcal{AZ}(T)$. Note that $n_3(T') = n_3(T) - 2 \geq 1$, and both vv_1, vv_2, are $(2,2)$-edges of T'. By Lemma 2.8, it is a contradiction. □

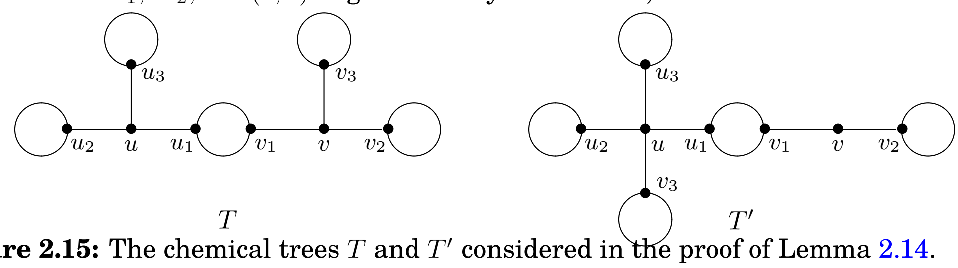


Figure 2.15: The chemical trees T and T' considered in the proof of Lemma 2.14.

3. AZ-minimal chemical trees of order $n \geq 6$

For any chemical tree $T \in \widetilde{T}_n$, the following equations hold:

$$n_1(T) + n_2(T) + n_3(T) + n_4(T) = n, \tag{1}$$
$$n_1(T) + 2n_2(T) + 3n_3(T) + 4n_4(T) = 2(n-1), \tag{2}$$
$$m_{12}(T) + m_{13}(T) + m_{14}(T) = n_1(T), \tag{3}$$
$$m_{12}(T) + 2m_{22}(T) + m_{23}(T) + m_{24}(T) = 2n_2(T), \tag{4}$$
$$m_{13}(T) + m_{23}(T) + 2m_{33}(T) + m_{34}(T) = 3n_3(T), \tag{5}$$
$$m_{14}(T) + m_{24}(T) + m_{34}(T) + 2m_{44}(T) = 4n_4(T). \tag{6}$$

Note that

$$n-1 = |E(T)| = m_{12}(T) + m_{13}(T) + m_{14}(T) + m_{22}(T) + m_{23}(T) + m_{24}(T) + m_{33}(T) + m_{34}(T) + m_{44}(T),$$

and for $y = 1, 2, 3, 4$,

$$f(2,y) = 8, f(1,3) = \frac{27}{8}, f(1,4) = \frac{64}{27}, f(3,3) = \frac{729}{64}, f(3,4) = \frac{1728}{125}, f(4,4) = \frac{512}{27}.$$

Thus,

$$\begin{aligned}\mathcal{AZ}(T) =& \sum_{1\leq i\leq j\leq 4} f(i,j)m_{ij}(T)\\ =&8\left(m_{12}(T)+m_{22}(T)+m_{23}(T)+m_{24}(T)\right) + \frac{27}{8}m_{13}(T) + \frac{64}{27}m_{14}(T) + \frac{729}{64}m_{33}(T) + \frac{1728}{125}m_{34}(T) + \frac{512}{27}m_{44}(T)\\ =&8(n-1) + \left(\frac{27}{8}-8\right)m_{13}(T) + \left(\frac{64}{27}-8\right)m_{14}(T) + \left(\frac{729}{64}-8\right)m_{33}(T) + \left(\frac{1728}{125}-8\right)m_{34}(T) + \left(\frac{512}{27}-8\right)m_{44}(T)\\ =&8(n-1) - \frac{37}{8}m_{13}(T) - \frac{152}{27}m_{14}(T) + \frac{217}{64}m_{33}(T) + \frac{728}{125}m_{34}(T) + \frac{296}{27}m_{44}(T).\end{aligned} \tag{7}$$

Theorem 3.1. *Let $6 \leq n \leq 12$. Then $T \in \widetilde{T}_n$ is an AZ-minimal chemical tree if and only if T is of the form as depicted in Figure 3.1 in terms of n.*

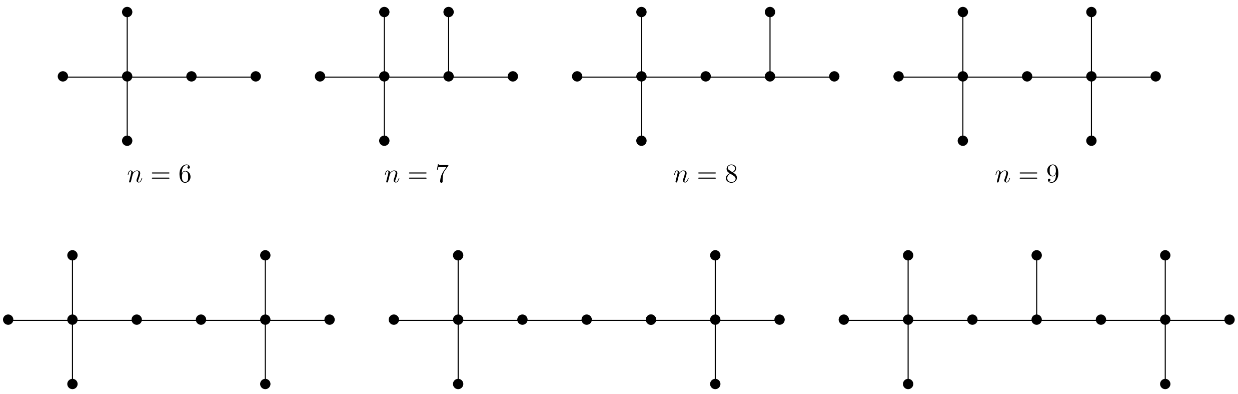


Figure 3.1: The AZ-minimal chemical trees of order $6 \leq n \leq 12$.

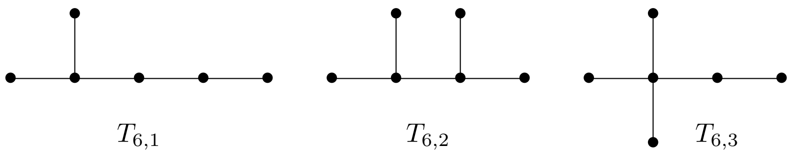


Figure 3.2: The chemical trees $T_{6,1}$, $T_{6,2}$ and $T_{6,3}$ of order 6.

Proof. Let $T \in \widetilde{T}_n$ be an AZ-minimal chemical tree, where $6 \leq n \leq 12$. By Lemma 2.3, $n_3(T) + n_4(T) \geq 1$.

If $n = 6$, then T is one of the three trees $T_{6,1}$, $T_{6,2}$, $T_{6,3}$, depicted in Figure 3.2. By elementary calculations, one has $\mathcal{AZ}(T_{6,1}) > \mathcal{AZ}(T_{6,2}) > \mathcal{AZ}(T_{6,3})$. Thus, $T = T_{6,3}$.

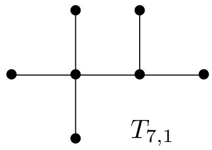


Figure 3.3: The chemical tree $T_{7,1}$ of order 7.

If $n = 7$, then by Lemmas 2.5 and 2.9, $m_{12}(T) = 0$ and $m_{14}(T) \neq 0$. Hence, $T = T_{7,1}$ (see Figure 3.3).

Finally, assume that $8 \leq n \leq 12$. By Lemmas 2.5, 2.6, 2.8, 2.9, 2.10, 2.11 and 2.12, $m_{12}(T) = m_{33}(T) = m_{34}(T) = m_{44}(T) = 0$, $m_{14}(T) \neq 0$, $m_{22}(T) \leq 2$, and if $n_3(T) \neq 0$ then $m_{22}(T) = 0$. Thus, $T = T_{8,1}$ if $n = 8$, $T = T_{9,1}$ if $n = 9$, $T = T_{10,1}$ if $n = 10$, $T \in \{T_{11,1}, T_{11,2}, T_{11,3}\}$ if $n = 11$, and $T \in \{T_{12,1}, T_{12,2}\}$ if $n = 12$, (see Figure 3.4). By simple calculations, one has $\mathcal{AZ}(T_{11,1}) < \mathcal{AZ}(T_{11,2}) < \mathcal{AZ}(T_{11,3})$ and $\mathcal{AZ}(T_{12,1}) < \mathcal{AZ}(T_{12,2})$. Therefore, $T = T_{11,1}$ if $n = 11$, and $T = T_{12,1}$ if $n = 12$. $\square$

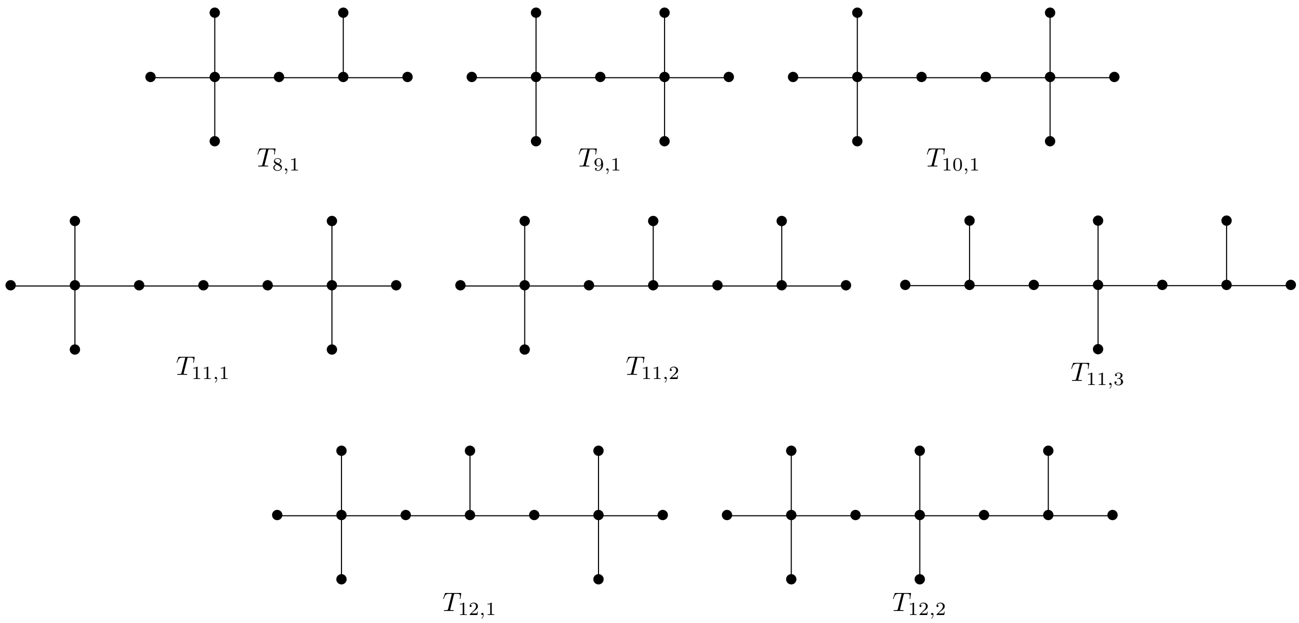


Figure 3.4: The chemical trees of orders 8–12 used in the proof of Theorem 3.1.

Theorem 3.2. *Let $n \geq 13$ and $T \in \widetilde{T}_n$.*

(1). *If $n \equiv 0 \pmod 4$, then*

$$\mathcal{AZ}(T) \geq \frac{4(35n - 92)}{27}.$$

The equation holds if and only if $n_3(T) = 1$, $n_4(T) = \frac{n-4}{4}$, $m_{12}(T) = m_{13}(T) = m_{22}(T) = m_{33}(T) = m_{34}(T) = m_{44}(T) = 0$, and $m_{14}(T) = \frac{n+2}{2}$.

(2). *If $n \equiv 1 \pmod 4$, then*

$$\mathcal{AZ}(T) \geq \frac{4(35n - 111)}{27}.$$

The equation holds if and only if $n_3(T) = 0$, $n_4(T) = \frac{n-1}{4}$, $m_{12}(T) = m_{13}(T) = m_{22}(T) = m_{33}(T) = m_{34}(T) = m_{44}(T) = 0$, and $m_{14}(T) = \frac{n+3}{2}$.

(3). *If $n \equiv 2 \pmod 4$, then*

$$\mathcal{AZ}(T) \geq \frac{4(35n - 92)}{27}.$$

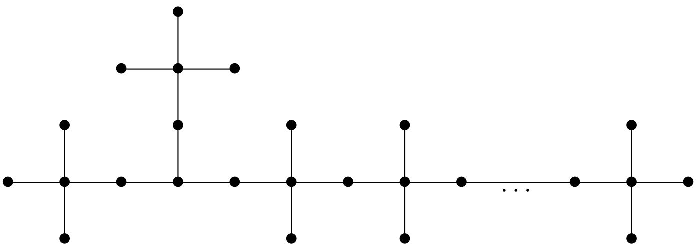
The equation holds if and only if $n_3(T) = 0$, $n_4(T) = \frac{n-2}{4}$, $m_{12}(T) = m_{13}(T) = m_{33}(T) = m_{34}(T) = m_{44}(T) = 0$, $m_{22}(T) = 1$, and $m_{14}(T) = \frac{n+2}{2}$.

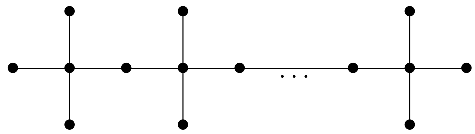
(4). *If $n \equiv 3 \pmod 4$, then*

$$\mathcal{AZ}(T) \geq \frac{4(35n - 73)}{27}.$$

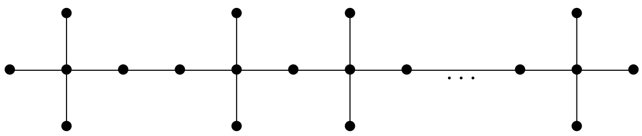
The equation holds if and only if $T = T_1$ when $n \in \{15, 19\}$, while $T \in \{T_1, T_2\}$ when $n \geq 23$, where $n_3(T_1) = 0$, $n_4(T_1) = \frac{n-3}{4}$, $m_{12}(T_1) = m_{13}(T_1) = m_{33}(T_1) = m_{34}(T_1) = m_{44}(T_1) = 0$, $m_{22}(T_1) = 2$, $m_{14}(T_1) = \frac{n+1}{2}$, $n_3(T_2) = 2$, $n_4(T_2) = \frac{n-7}{4}$, $m_{12}(T_2) = m_{13}(T_2) = m_{22}(T_2) = m_{33}(T_2) = m_{34}(T_2) = m_{44}(T_2) = 0$, and $m_{14}(T_2) = \frac{n+1}{2}$.

For every considered case, an AZ-minimal chemical tree $T \in \widetilde{T}_n$ is shown in Figure 3.5.

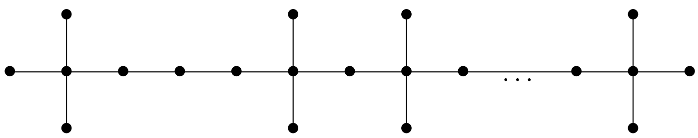




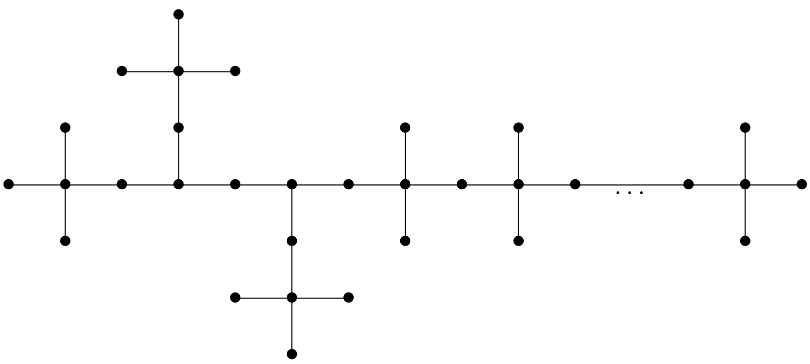
$T \in \widetilde{T}_n$ (where $n \geq 13$ and $n \equiv 0 \pmod 4$) $T \in \widetilde{T}_n$ (where $n \geq 13$ and $n \equiv 1 \pmod 4$)



$T \in \widetilde{T}_n$ (where $n \geq 13$ and $n \equiv 2 \pmod 4$)



$T_1 \in \widetilde{T}_n$ (where $n \geq 13$ and $n \equiv 3 \pmod 4$)



$T_2 \in \widetilde{T}_n$ (where $n \geq 23$ and $n \equiv 3 \pmod 4$)

Figure 3.5: The AZ-minimal chemical trees of orders $n \geq 13$.

Proof. Let $T \in \widetilde{T}_n$ be an AZ-minimal chemical tree, where $n \geq 13$. By Lemmas 2.5, 2.6, and 2.8–2.14, we have that $m_{12}(T) = m_{13}(T) = m_{33}(T) = m_{34}(T) = m_{44}(T) = 0$, $m_{14}(T) \neq 0$, $m_{22}(T) \leq 2$, $n_3(T) \leq 2$, and if $n_3(T) \neq 0$ then $m_{22}(T) = 0$.

Case 1. $n_3(T) = 0$.
By (1), (2) and (3), one has $n_1(T) = 2n_4(T) + 2 = m_{14}(T)$ and $n_2(T) = n - 2 - 3n_4(T)$. Then, from (4) and (5) it follows that

$$4n_4(T) = m_{14}(T) - 2m_{22}(T) + 2n_2(T) = 2n_4(T) + 2 - 2m_{22}(T) + 2n - 4 - 6n_4(T),$$

that is, $4n_4(T) = n - 1 - m_{22}(T)$.

If $m_{22}(T) = 0$, then $n_4(T) = \frac{n-1}{4}$. Thus, $n \equiv 1 \pmod 4$ and $m_{14}(T) = 2n_4(T) + 2 = \frac{n+3}{2}$. Now, by using (7), one has

$$\mathcal{AZ}(T) = 8(n-1) - \frac{152}{27} \cdot \frac{n+3}{2} = \frac{4(35n - 111)}{27}. \tag{8}$$

If $m_{22}(T) = 1$, then $n_4(T) = \frac{n-2}{4}$. So, $n \equiv 2 \pmod 4$ and $m_{14}(T) = \frac{n+2}{2}$. From (7), it follows that

$$\mathcal{AZ}(T) = 8(n-1) - \frac{152}{27} \cdot \frac{n+2}{2} = \frac{4(35n - 92)}{27}. \tag{9}$$

If $m_{22}(T) = 2$, then $n_4(T) = \frac{n-3}{4}$. Hence, $n \equiv 3 \pmod 4$ and $m_{14}(T) = \frac{n+1}{2}$. By utilizing (7), one has

$$\mathcal{AZ}(T) = 8(n-1) - \frac{152}{27} \cdot \frac{n+1}{2} = \frac{4(35n - 73)}{27}. \tag{10}$$

Case 2. $n_3(T) \neq 0$.
In this case, $m_{22}(T) = 0$ and $n_3(T) \leq 2$. By using (1), (2), and (3), one has $n_1(T) = m_{14}(T) = n_3(T) + 2n_4(T) + 2$ and $n_2(T) = n-2-2n_3(T)-3n_4(T)$. From (4), (5), and (6), it follows that $3n_3(T)+4n_4(T)-2n_2(T) = m_{14}(T) = n_3(T)+2n_4(T)+2$. Then $3n_3(T) + 4n_4(T) - 2(n - 2 - 2n_3(T) - 3n_4(T)) = m_{14}(T) = n_3(T) + 2n_4(T) + 2$; that is, $4n_4(T) = n - 1 - 3n_3(T)$.

If $n_3(T) = 1$, then $n_4(T) = \frac{n-4}{4}$. Thus, $n \equiv 0 \pmod 4$ and $m_{14}(T) = n_3(T) + 2n_4(T) + 2 = \frac{n+2}{2}$. By using (7), one has

$$\mathcal{AZ}(T) = 8(n-1) - \frac{152}{27} \cdot \frac{n+2}{2} = \frac{4(35n-92)}{27}.$$

If $n_3(T) = 2$, then $n_4(T) = \frac{n-7}{4}$. Hence, $n \equiv 3 \pmod 4$ and $m_{14}(T) = n_3(T) + 2n_4(T) + 2 = \frac{n+1}{2}$. From (7), it follows that

$$\mathcal{AZ}(T) = 8(n-1) - \frac{152}{27} \cdot \frac{n+1}{2} = \frac{4(35n-73)}{27}.$$

In this case, note that $m_{13}(T) = m_{33}(T) = m_{34}(T) = 0$. Thus, by using (5), one has $m_{23}(T) = 3n_3(T) = 6$. Hence, $n_2(T) \geq m_{23}(T) - 1 = 5$. Also, observe that

$$n_2(T) = n - 2 - 2n_3(T) - 3n_4(T) = n - 6 - \frac{3n-21}{4} = \frac{n-3}{4},$$

which implies that $n \geq 23$. □

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