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EXTREMAL CHEMICAL TREES WITH RESPECT TO HYPER-ZAGREB INDEX

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Abstract. Suppose G is a molecular graph with edge set $E(G)$. The hyper-Zagreb index of G is defined as $HM(G) = \sum_{uv\in E(G)}[deg_G(u) + deg_G(v)]^2$, where $deg_G(u)$ is the degree of a vertex u in G. In this paper, all chemical trees of order $n \geq 12$ with the first twenty smallest hyper-Zagreb index are characterized.

1. Introduction

Throughout this paper, all graphs will be assumed to be finite, undirected and simple. The vertex and edge set of such a graph is denoted by $V(G)$ and $E(G)$, respectively. The notation $deg_G(v)$ denotes the degree of a vertex v in G and $N[v, G]$ stands for the set of all vertices adjacent to v. A vertex of degree one is called a pendant vertex and we use $\Delta = \Delta(G)$ to denote the maximum degree of vertices in G. Suppose $n_i = n_i(G)$ denotes the number of vertices of degree i in G, then it is obvious that $\sum_{i=1}^{\Delta(G)} n_i = |V(G)|$. We also use the notation $m_{i,j}(G)$ for the number of edges in G connecting a vertex of degree i to a vertex of degree j.

Choose the subset W of $V(G)$ and define the subgraph $G - W$ to construct from G by deleting the vertices of W and all edges incident to a vertex in W. In a similar way, if $E' \subseteq E(G)$, then $G - E'$ denotes the subgraph of G obtained by deleting the edges of E'. In the case that $W = \{v\}$ and $E' = \{xy\}$, the subgraphs $G - W$ and $G - E'$ will be written as $G - v$ and $G - xy$, respectively. Furthermore, if x and y are not adjacent in G, then $G + xy$ is the graph obtained from G by adding the edge xy.

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A connected acyclic graph is called a tree and the path and star graphs on n vertices will be denoted by P_n and S_n, respectively. The chemical graph theory is one of the most important topic in mathematical chemistry that investigate the chemical problems by graph theory language. Topological indices are main tools of chemical graph theory and simply we can say that they are graph invariants applicable in chemistry [7, 11].

The Zagreb indices that was introduced by Ivan Gutman and Nanad Trinajstić [14], are most important degree-based topological indices in mathematical chemistry. These numbers are used by various researchers in QSPR/QSAR studies [1, 16, 20] and also some mathematicians studied their mathematical properties, see [1, 4, 5, 6, 12, 13] for details.

In an exact phrase, the first and the second Zagreb indices of a graph G are defined as $M_1(G) = \sum_{uv\in E(G)}[deg_G(u)+deg_G(v)]$ and $M_2(G) = \sum_{uv\in E(G)}[deg_G(u)deg_G(v)]$, respectively. There are some modification and generalization of Zagreb indices. The hyper-Zagreb index is one of such modified version which introduced by Shirdel, et al. in 2013 [19] as $HM(G) = \sum_{uv\in E(G)}[deg_G(u) + deg_G(v)]^2$. It is worth mentioning that in 2010, Zhou and Trinajstić introduced the general sum-connectivity index [22] as $\chi^\alpha(G) = \sum_{uv\in E(G)}[deg_G(u) + deg_G(v)]^\alpha$, where $\chi^1(G) = M_1(G)$ and $\chi^2(G) = HM(G)$.

In [19], the authors computed Hyper Zagreb index for the cartesian product, composition, join and disjunction of graphs. Basavanagoud et al. [3] corrects some errors in [19] and gave the correct expressions for hyper-Zagreb index of some other graph operations. Pattabiraman et al. [17] obtained the hyper Zagreb index and its coindex of the edge corona product graph, double graph and Mycielskian graphs. Veylaki et al. [21] defined the hyper-Zagreb coindex of graph G as $\overline{HM}(G) = \sum_{uv\in E(\overline{G})}[deg_G(u) + deg_G(v)]^2$. They also presented some identities for $HM(\overline{G})$ and $\overline{HM}^2(G)$. In [15], Gutman determined some basic relations between $HM(\overline{G})$ and $\overline{HM}^2(G)$.

Basavanagoud et al. [2] characterized the expressions for forgotten topological index, hyper-Zagreb index and coindex for generalized transformation graphs and their complements. In [9], Elumalai et al. established, analyzed and compared some new upper bounds on the hyper-Zagreb index in terms of the number of vertices and edges, maximum and minimum vertex degrees, first and second Zagreb indices, harmonic index, and inverse edge degree. Falahati-Nejad et al. [10] presented some

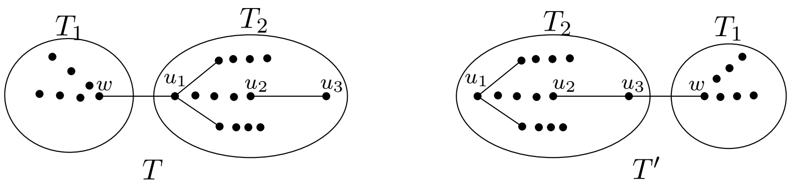

Figure 1. The chemical trees T_1, T_2, T and T' in Transformation A.

upper and lower bounds for the hyper-Zagreb index in terms of some chemical parameters and relate this index to various well-known molecular descriptors. In [18] Rezapour et al. characterized the trees and unicyclic graphs with the first four and first eight greatest hyper Zagreb index, respectively.

In this paper, we aim to determine extremal chemical trees with respect to hyper-Zagreb index via applying some graph operations decreasing hyper Zagreb index and the chemical trees of order $n \geq 12$ with the first twenty smallest hyper Zagreb index will be presented.

2. Some Graph Transformations

In this section, some graph transformations are presented that decrease the Hyper-Zagreb index of chemical trees.

Transformation A**.** Suppose that T_1 is a chemical tree with given vertex w. In addition, suppose that T_2 is another chemical tree with given vertices u_1, u_2 and u_3, such that $d_{T_2}(u_1) = 2$ *or* 3, $d_{T_2}(u_3) = 1$ and $u_2u_3 \in E(T_2)$. let T be the chemical tree obtained from T_1 and T_2 by attaching vertices w, u_1, and $T' = T - wu_1 + wu_3$. The above referred chemical trees have been illustrated in Fig. 1.

Lemma 2.1. *Let* T *and* T' *be two chemical trees as shown in Fig. 1. Then we have* $HM(T') < HM(T)$.

Proof. We distinguish the following cases:
Case 1. $u_1 \neq u_2$. In this case suppose that $N[u_1, T_2] = \{f_1, f_2, ..., f_{d_{T_2}(u_1)}\}$ and $d_{T_2}(f_i) = d_i$, for $i = 1, 2, .., d_{T_2}(u_1)$. We have

$$HM(T) - HM(T') = (d_{T_1}(w) + d_{T_2}(u_1) + 2)^2 + (d_{T_2}(u_2) + 1)^2$$

$$
\begin{aligned}
&+\sum_{i=1}^{d_{T_2}(u_1)}(d_i+d_{T_2}(u_1)+1)^2-\Big((d_{T_1}(w)+3)^2\\
&+(d_{T_2}(u_2)+2)^2+\sum_{i=1}^{d_{T_2}(u_1)}(d_i+d_{T_2}(u_1))^2\Big)\\
&> d_{T_2}(u_1)^2+d_{T_1}(w)(2d_{T_2}(u_1)-2)+5d_{T_2}(u_1)\\
&-(2d_{T_2}(u_2)+8)\geq 0 \quad \text{as } d_{T_2}(u_1)\geq 2.
\end{aligned}
$$

Case 2. $u_1 = u_2$. Suppose $N[u_1, T_2] = \{f_1(:= u_3), f_2, ..., f_{d_{T_2}(u_1)}\}$, $d_{T_2}(f_i) = d_i$, for $i = 2, .., d_{T_2}(u_1)$. Then,

$$
\begin{aligned}
HM(T)-HM(T') &= (d_{T_1}(w)+d_{T_2}(u_1)+2)^2+(d_{T_2}(u_1)+2)^2\\
&+\sum_{i=2}^{d_{T_2}(u_1)}(d_i+d_{T_2}(u_1)+1)^2-\Big((d_{T_1}(w)+3)^2+(d_{T_2}(u_1)+2)^2\\
&+\sum_{i=2}^{d_{T_2}(u_1)}(d_i+d_{T_2}(u_1))^2\Big)\\
&> (d_{T_1}(w)+d_{T_2}(u_1)+2)^2-(d_{T_1}(w)+3)^2>0 \quad \text{as } d_{T_2}(u_1)\geq 2.
\end{aligned}
$$

which completes the proof. □

Transformation B**.** Suppose that T_1 and T_2 are two chemical trees with given vertices $w \in V(T_1)$ and $\{u_1, u_2\} \subseteq V(T_2)$ such that $1 \leq d_{T_1}(w) \leq 3$, $d_{T_2}(u_1) = 2$ *or* 3, $d_{T_2}(u_2) = 1$ and $u_1u_2 \in E(T_2)$. In addition, suppose that $P_k := v_0v_1 \dots v_k$ is a path, of length $k \geq 0$. let T be the chemical tree obtained from T_1, T_2 and P_k by adding the edges wu_1, u_2v_0, and $T' = T - \{wu_1, u_2v_0\} + \{wv_0, v_ku_1\}$. The above referred chemical trees have been illustrated in Fig. 2.

Lemma 2.2. *Let T and T' be two chemical trees as shown in Fig. 2. Then we have $HM(T') < HM(T)$.*

Proof. By definition,

$$
\begin{aligned}
HM(T)-HM(T') &= (d_{T_1}(w)+d_{T_2}(u_1)+2)^2+(d_{T_2}(u_1)+3)^2+3^2\\
&- \Big((d_{T_1}(w)+3)^2+(d_{T_2}(u_1)+3)^2+(d_{T_2}(u_1)+2)^2\Big)\\
&= 2d_{T_1}(w)d_{T_2}(u_1)-2d_{T_1}(w)>0 \quad \text{as } d_{T_2}(u_1)\geq 2,
\end{aligned}
$$

proving the lemma. □

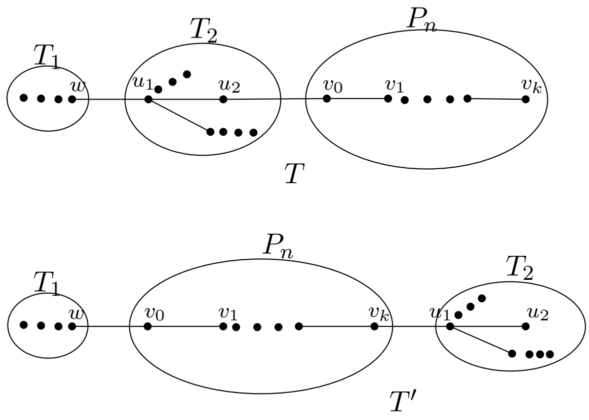

Figure 2. The chemical trees T_1, T_2, P_k, T and T' in Transformation B.

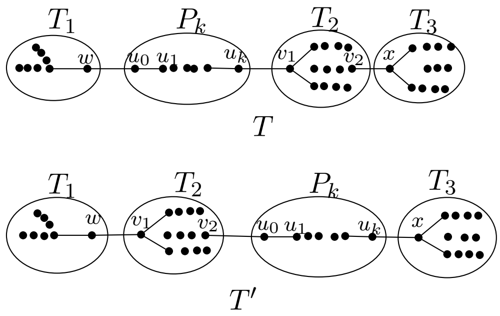

Figure 3. The chemical trees T_1, T_2, T_3, P_k, T and T' in Transformation C.

Transformation C**.** Suppose that T_1, T_2 and T_3 are three chemical trees with given vertices $w \in V(T_1)$, $\{v_1, v_2\} \subseteq V(T_2)$ and $x \in V(T_3)$ such that $d_{T_1}(w) = 1$, $d_{T_2}(v_2) = 2$ *or* 3 and $d_{T_3}(x) = 2$ *or* 3. In addition, suppose that $P_k := u_0u_1 \dots u_k$ is a path, of length $k \geq 0$. let T be the chemical tree obtained from T_1, T_2, T_3 and P_k by adding the edges wu_0, u_kv_1, v_2x and $T' = T - \{wu_0, u_kv_1, v_2x\} + \{wv_1, v_2u_0, u_kx\}$. The above referred chemical trees have been illustrated in Fig. 3.

Lemma 2.3. *Let* T *and* T' *be two chemical trees as shown in Fig. 3. Then* $HM(T') < HM(T)$.

Proof. By definition,

$$\begin{aligned} HM(T)-HM(T') &= 4^2+(d_{T_2}(v_2)+d_{T_3}(x)+2)^2 \\ &- \Big((d_{T_2}(v_2)+3)^2+(d_{T_2}(x)+3)^2\Big) \\ &= 2\Big(d_{T_2}(v_2)d_{T_3}(x)+1-(d_{T_2}(v_2)+d_{T_3}(x))\Big) \\ &> 0 \ \text{ as } d_{T_2}(v_2),\ d_{T_3}(x)\geq 2, \end{aligned}$$

proving the lemma. □

3. Main Results

For positive integers $x_1,\ldots,x_m$, and $y_1,\ldots,y_m$, let $T(x_1^{(y_1)},\ldots,x_m^{(y_m)})$ be the class of trees with x_i vertices of the degree y_i, $i=1,\ldots,m$. Note that this class may be empty.

Lemma 3.1. (*See* [8]) *If G is a chemical tree with n vertices, then $n_1(G)=n_3(G)+2n_4(G)+2$ and $n_2(G)=n-(2n_3(G)+3n_4(G)+2)$.*

Lemma 3.2. (*See* [8]) *There is a tree of order n (>2) in $T(x_1^{(y_1)},\ldots,x_m^{(y_m)})$ if and only if $\sum_{i=1}^{m}x_iy_i=2n-2$.*

Remark 3.3. Note that if $n\geq 13$, then by Lemma 3.2, our classes of chemical trees are nonempty sets.

Notations: For a positive number $n\geq 13$, let:

$$\begin{aligned} H(n) &= \{T\in T(4^{(3)},(n-10)^{(2)},6^{(1)})\mid\ m_{1,2}(T)=0\ ,\ m_{1,3}(T)=6\ ,m_{2,2}(T)=n-13, \\ &\qquad m_{2,3}(T)=6,\ m_{3,3}(T)=0\} \\ F(n) &= \{T\in T(1^{(4)},1^{(3)},(n-7)^{(2)},5^{(1)})\mid\ m_{1,2}(T)=0\ ,\ m_{1,3}(T)=2\ ,\ m_{1,4}(T)=3\ , \\ &\qquad m_{2,2}(T)=n-8\ ,\ m_{2,3}(T)=1,\ m_{2,4}(T)=1\ ,\ \textit{and}\ m_{3,4}(T)=0\}. \end{aligned}$$

It is easy to see that for each $T_1\in H(n)$, $T_2\in F(n)$ *and* $T_3:=P_n$,

$$HM(T_1) = 16n+38, \tag{3.1}$$

$$HM(T_2) = 16n+40, \tag{3.2}$$

$$HM(T_3) = 16n-30. \tag{3.3}$$

Theorem 3.4. *Let $\acute{T}$ be a chemical tree with $n \geq 13$ vertices and $\Delta(\acute{T}) = 3$, such that $n_3(\acute{T}) \geq 4$. if $\acute{T} \notin H(n)$. Then, for each $T \in H(n)$, $HM(T) < HM(T')$.*

Proof. We have two separate classes as follows
CASE 1. $\acute{T} \in T(4^{(3)}, (n-10)^{(2)}, 6^{(1)})$. Since $\acute{T} \notin H(n)$, $\acute{T}$ has at least one of the following conditions: $m_{1,2}(T) \neq 0$, $m_{1,3}(T) \neq 6$,$m_{2,2}(T) \neq n-13$, $m_{2,3}(T) \neq 6$ *or* $m_{3,3}(T) \neq 0$.
We now apply repeated applications of Transformations B and C to obtain a chemical tree $Q \in H(n)$. By Lemmas 2.2 and 2.3, $HM(T) = HM(Q) < HM(T')$, as desird.
CASE 2. $n_3(\acute{T}) \geq 5$. Since $n_3(\acute{T}) \geq 5$, by repeated applications of Transformation A we obtain a chemical tree $G \in T(4^{(3)}, (n-10)^{(2)}, 6^{(1)})$. If $G \in H(n)$, then by Lemma 2.1, $HM(T) = HM(G) < HM(T')$. Otherwise, we obtain the result by replacing $\acute{T}$ with G in Case 1. □

Theorem 3.5. *Let $\acute{T}$ be a chemical tree with $n \geq 8$ vertices and $\Delta(\acute{T}) = 4$. Then, if $\acute{T} \notin F(n) \cup T(1^{(4)}, (n-5)^{(2)}, 4^{(1)})$, $T \in F(n)$, then $HM(T) < HM(T')$.*

Proof. We have three cases as follows:
CASE 1. $\acute{T} \in T(1^{(4)}, 1^{(3)}, (n-7)^{(2)}, 5^{(1)})$. Since $\acute{T} \notin H(n)$, $\acute{T}$ has at least one of the following conditions: $m_{1,2}(T) \neq 0$, $m_{1,3}(T) \neq 2$, $m_{1,4}(T) \neq 3$, $m_{2,2}(T) \neq n-8$, $m_{2,3}(T) \neq 1$, $m_{2,4}(T) \neq 1$, *or* $m_{3,4}(T) \neq 0$. By repeated applications of Transformations B and C we obtain a chemical tree $Q \in H(n)$. We now apply Lemmas 2.2 and 2.3, to prove $HM(T) = HM(Q) < HM(T')$.
CASE 2. $n_4(\acute{T}) \geq 2$. Since $n_4(\acute{T}) \geq 2$, by repeated applications of Transformation A we obtain a chemical tree $G \in T(1^{(4)}, 1^{(3)}, (n-7)^{(2)}, 5^{(1)})$. If $G \in F(n)$, then by Lemma 2.1, $HM(T) = HM(G) < HM(T')$. Otherwise, we obtain the result by replacing $\acute{T}$ with G in Case 1.
CASE 3. $n_4(\acute{T}) = 1$ and $n_3(\acute{T}) \geq 2$. Since $n_3(\acute{T}) \geq 2$, by repeated applications of Transformation A we obtain a chemical tree $Q \in T(1^{(4)}, 1^{(3)}, (n-7)^{(2)}, 5^{(1)})$. If $Q \in F(n)$, then by Lemma 2.1, $HM(T) = HM(Q) < HM(T')$. Otherwise, we obtain the result by replacing $\acute{T}$ with Q in Case 1. □

Remark 3.6. Let $T_1 := P_n$, $T_2 \in G_1$, $T_3 \in G_2$, $T_4 \in G_3$, $T_5 \in I_1$, $T_6 \in I_2$, $T_7 \in I_3$, $T_8 \in I_6$, $T_9 \in I_4$, $T_{10} \in I_7$, $T_{11} \in I_5$, $T_{12} \in I_8$, $T_{13} \in I_9$, $T_{14} \in L_1$, $T_{15} \in L_2$, $T_{16} \in L_7$, $T_{17} \in L_3$, $T_{18} \in L_8$, $T_{19} \in A_1$, $T_{20} \in L_4$, $T_{21} \in L_9$, $T_{22} \in L_{13}$, $T_{23} \in$

Table 1. The Chemical Trees in Class $T(1^{(4)}, (n-5)^{(2)}, 4^{(1)})$.

Notation	$m_{2,4}$	$m_{1,4}$	$m_{1,2}$	$m_{2,2}$	HM
A_1	1	3	1	n-6	16n+24
A_2	2	2	2	n-7	16n+28
A_3	3	1	3	n-8	16n+32
A_4	4	0	4	n-9	16n+36

Table 2. The Chemical Trees in Class $T(3^{(3)}, (n-8)^{(2)}, 5^{(1)})$.

Notation	$m_{3,3}$	$m_{2,3}$	$m_{1,2}$	$m_{1,3}$	$m_{2,2}$	HM
L_1	0	4	0	5	n-10	16n+20
L_2	0	5	1	4	n-11	16n+22
L_3	0	6	2	3	n-12	16n+24
L_4	0	7	3	2	n-13	16n+26
L_5	0	8	4	1	n-14	16n+28
L_6	0	9	5	0	n-15	16n+30
L_7	1	2	0	5	n-9	16n+22
L_8	1	3	1	4	n-10	16n+24
L_9	1	4	2	3	n-11	16n+26
L_{10}	1	5	3	2	n-12	16n+28
L_{11}	1	6	4	1	n-13	16n+30
L_{12}	1	7	5	0	n-14	16n+32
L_{13}	2	1	1	4	n-9	16n+26
L_{14}	2	2	2	3	n-10	16n+28
L_{15}	2	3	3	2	n-11	16n+30
L_{16}	2	4	4	1	n-12	16n+32
L_{17}	2	5	5	0	n-13	16n+34

Table 3. The Chemical Trees in Class $T(2^{(3)}, (n-6)^{(2)}, 4^{(1)})$.

Notation	$m_{3,3}$	$m_{2,3}$	$m_{1,2}$	$m_{1,3}$	$m_{2,2}$	HM
I_1	0	2	0	4	n-7	16n+2
I_2	0	3	1	3	n-8	16n+4
I_3	0	4	2	2	n-9	16n+6
I_4	0	5	3	1	n-10	16n+8
I_5	0	6	4	0	n-11	16n+10
I_6	1	1	1	3	n-7	16n+6
I_7	1	2	2	2	n-8	16n+8
I_8	1	3	3	1	n-9	16n+10
I_9	1	4	4	0	n-10	16n+12

Table 4. The Chemical Trees in Class $T(1^{(3)}, (n-4)^{(2)}, 3^{(1)})$.

Notation	$m_{2,3}$	$m_{1,2}$	$m_{1,3}$	$m_{2,2}$	HM
G_1	1	1	2	n-5	16n-14
G_2	2	2	1	n-6	16n-12
G_3	3	3	0	n-7	16n-10

$L_5,\ T_{24} \in L_{10},\ T_{25} \in L_{14},\ T_{26} \in A_2,\ T_{27} \in L_6,\ T_{28} \in L_{11},\ T_{29} \in L_{15},\ T_{30} \in L_{12},\ T_{31} \in L_{16},\ T_{32} \in A_3,\ T_{33} \in L_{17},\ T_{34} \in A_4,\ T_{35} \in H(n)$ *and* $T_{36} \in F(n)$.

Theorem 3.7. *If* $n \geq 13$ *and* $T \in \tau(n) \diagdown \{T_1, T_2, ..., T_{35}\}$, *then*
$HM(T_1) < HM(T_2) < HM(T_3) < HM(T_4) < HM(T_5) < HM(T_6) < HM(T_7) = HM(T_8) < HM(T_9) = HM(T_{10}) < HM(T_{11}) = HM(T_{12}) < HM(T_{13}) < HM(T_{14}) < HM(T_{15}) = HM(T_{16}) < HM(T_{17}) = HM(T_{18}) = HM(T_{19}) < HM(T_{20}) = HM(T_{21}) = HM(T_{22}) < HM(T_{23}) = HM(T_{24}) = HM(T_{25}) = HM(T_{26}) < HM(T_{27}) = HM(T_{28}) = HM(T_{29}) < HM(T_{30}) = HM(T_{31}) = HM(T_{32}) < HM(T_{33}) < HM(T_{34}) < HM(T_{35}) = 16n + 38 < HM(T)$.

Proof. The proof follows from Tables 1, 2, 3, 4 and Equations 3.1, 3.3. To explain, we note that
$HM(T_1) < HM(T_2) < HM(T_3) < HM(T_4) < HM(T_5) < HM(T_6) < HM(T_7) = HM(T_8) < HM(T_9) = HM(T_{10}) < HM(T_{11}) = HM(T_{12}) < HM(T_{13}) < HM(T_{14}) < HM(T_{15}) = HM(T_{16}) < HM(T_{17}) = HM(T_{18}) = HM(T_{19}) < HM(T_{20}) = HM(T_{21}) = HM(T_{22}) < HM(T_{23}) = HM(T_{24}) = HM(T_{25}) = HM(T_{26}) < HM(T_{27}) = HM(T_{28}) = HM(T_{29}) < HM(T_{30}) = HM(T_{31}) = HM(T_{32}) < HM(T_{33}) < HM(T_{34}) < HM(T_{35}) = 16n + 38$. If $\Delta(G) = 3$ and $n_3(G) \geq 4$ then the proof follows from Theorem 3.4 and Equations 3.1. Suppose $\Delta(T) = 4$. If $n_4(T) \geq 2$ or ($n_4(T) = 1$ and $n_3(T) \geq 1$), then Theorem 3.5 and Equations 3.2 gives us the result. Otherwise, $T \in \{T_1, T_2, ..., T_{35}\}$. ☐

Remark 3.8. *If* $n = 12$, *then*
$HM(T_1) < HM(T_2) < HM(T_3) < HM(T_4) < HM(T_5) < HM(T_6) < HM(T_7) = HM(T_8) < HM(T_9) = HM(T_{10}) < HM(T_{11}) = HM(T_{12}) < HM(T_{13}) < HM(T_{14}) < HM(T_{15}) = HM(T_{16}) < HM(T_{17}) = HM(T_{18}) = HM(T_{19}) < HM(T_{21}) = HM(T_{22}) < HM(T_{24}) = HM(T_{25}) = HM(T_{26}) < HM(T_{29}) < HM(T_{31}) = HM(T_{32}) < HM(T_{34}) < HM(T') = HM(T_{36}) = 16n + 40 < HM(T)$.

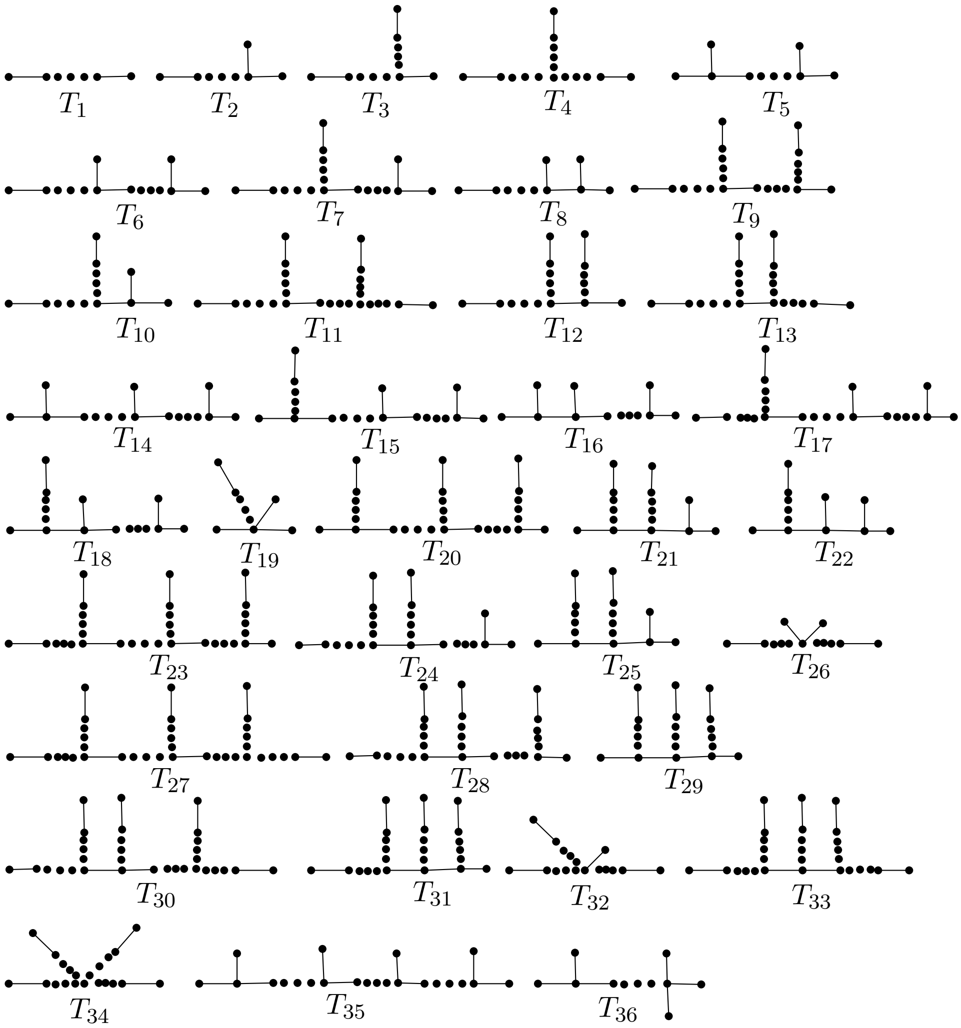

Figure 4. The chemical trees in Remark 3.6

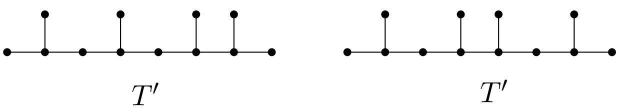

Figure 5. The chemical tree T' in Remark 3.8.

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