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ON MINIMAL TREES WITH RESPECT TO HYPER-ZAGREB INDICES

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Abstract. Zagreb indices are among the foremost topological indices in mathematical chemistry. These indices are crucial for investigating the total π-electron energy of alternant hydrocarbons and are utilized to study various aspects of molecular properties, including complexity, chirality, ZE-isomerism, and hetero-systems. In this paper, we focus on two well-known modifications of these indices: the first and second hyper-Zagreb indices. For a finite simple graph Γ, these indices are expressed as

$$HM_1(\Gamma) = \sum_{\vartheta\omega \in E(\Gamma)} (d_\Gamma(\vartheta) + d_\Gamma(\omega))^2 \quad \text{and} \quad HM_2(\Gamma) = \sum_{\vartheta\omega \in E(\Gamma)} (d_\Gamma(\vartheta) d_\Gamma(\omega))^2,$$

where $E(\Gamma)$ denotes the edge set of Γ and $d_\Gamma(\vartheta)$ indicates the degree of the vertex ϑ in Γ. In this paper, we introduce graph transformations on trees and connected graphs that minimize the first and second hyper-Zagreb indices. Accordingly, we determine the minimum values of these indices within the class of all trees with a given number of vertices and a specified maximum vertex degree. Additionally, we characterize the corresponding minimal trees. Our results will be extended to all connected graphs with a given order and maximum vertex degree.

1. Introduction

Let Γ be a simple connected graph with vertex set $V(\Gamma)$ and edge set $E(\Gamma)$. For a vertex $\vartheta \in V(\Gamma)$, the open neighborhood $N_\Gamma(\vartheta)$ is defined as the set of all vertices in Γ that are adjacent to ϑ. The degree $d_\Gamma(\vartheta)$ of the vertex ϑ is defined as the number of vertices in its open neighborhood, i.e., the

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order of $N_\Gamma(\vartheta)$. For any two vertices $\vartheta, \omega \in V(\Gamma)$, the distance $d_\Gamma(\vartheta, \omega)$ is the length of any shortest path connecting them. As usual, P_n and S_n are the path and the star of order n, respectively.

A tree is defined as an acyclic-connected graph. In a tree, a vertex with degree one is referred to as a leaf, and the neighbor of a leaf is said to be a support vertex. A support vertex that is incident to more than one leaf is called a strong support vertex, and a support vertex that has at most one non-leaf neighbor is called an end-support vertex.

A rooted tree is a tree in which a particular vertex is selected as the root. If ϑ is a non-root vertex in a rooted tree, the neighbor of ϑ that lies on the path between ϑ and the root is referred to as the parent of ϑ. A tree that has at most one vertex ω of the degree larger than two is called a spider with center ω. The path connecting a leaf of the spider to its center is known as a leg of the spider.

An invariant is a property of a graph that depends solely on its abstract structure and is unaffected by its depiction or the labeling of its vertices and edges. Such invariants are also known as topological indices. Topological indices have attained a significant recognition due to their applications in chemistry and other scientific fields [10].

Zagreb indices are among the foremost topological indices in mathematical chemistry. These indices were proposed by Gutman and Trinajstić [22] in 1972 and were further elaborated by Gutman *et al.* [21] in 1975. They are formulated for a simple graph Γ as

$$M_1(\Gamma) = \sum_{\vartheta \in V(\Gamma)} d(\vartheta)^2 = \sum_{\vartheta\omega \in E(\Gamma)} (d_\Gamma(\vartheta) + d_\Gamma(\omega)) \text{ and } M_2(\Gamma) = \sum_{\vartheta\omega \in E(\Gamma)} d_\Gamma(\vartheta) d_\Gamma(\omega).$$

The Zagreb indices have been extensively investigated, mainly due to their role in investigating the total π-electron energy of alternant hydrocarbons. Additionally, they have been used to assess molecular complexity, chirality, ZE–isomerism, and hetero-systems. For comprehensive literature on these indices, see the review papers [1, 9] and the references cited therein.

After the introduction of Zagreb indices, various modifications have been proposed, among which Zagreb coindices [11, 3], hyper-Zagreb indices [36, 39], leap Zagreb indices [30, 40], reformulated Zagreb indices [28, 23], generalized Zagreb index [6, 5], multiplicative Zagreb indices [38, 18, 12], entire Zagreb indices [4, 26], augmented Zagreb index [15], Zagreb connection indices [20, 33, 37], exponential Zagreb indices [24, 31, 7], and ad-hoc Lanzhou index [2] can be mentioned. To learn more about various variants of Zagreb indices, see the review paper [19].

The first and second hyper-Zagreb indices are well-known variants of the Zagreb indices. The first index, denoted as HM_1, was proposed by Shirdel *et al.* [36] in 2013 and the second one, denoted as HM_2, was introduced by Wei *et al.* [39] in 2016. They are expressed for a simple graph Γ as

$$HM_1(\Gamma) = \sum_{\vartheta\omega \in E(\Gamma)} (d_\Gamma(\vartheta) + d_\Gamma(\omega))^2 \text{ and } HM_2(\Gamma) = \sum_{\vartheta\omega \in E(\Gamma)} (d_\Gamma(\vartheta) d_\Gamma(\omega))^2.$$

Some mathematical and chemical properties of the hyper-Zagreb indices have been established so far. Rajasekharaiah and Murthy [32] conducted a linear regression analysis that included the

HM_1 and HM_2 indices alongside other topological indices. Their study demonstrated that the linear model based on the HM_1 index provided a better fit for predicting the boiling points of benzenoid hydrocarbons compared to models based on other invariants. Keerthi *et al.* [25] showed that the HM_1 index is well correlated with several physico-chemical characteristics, such as enthalpy of vaporisation, acentric factor, heat of fusion, and entropy of octane isomers. Particularly, they found that the HM_1 index has a high correlation with the acentric factor of octane isomers. Shirdel *et al.* [36], Gao *et al.* [16], Basavanagoud *et al.* [8] and Modabish *et al.* [29] studied the HM_1 index and, or HM_2 index for various special graphs and operations on graphs. Gao *et al.* [17] investigated extremal graphs with respect to the HM_1 index among trees, unicyclic graphs, and bicyclic graphs. Rezapour *et al.* [34] determined the trees and unicyclic graphs with the first four and first eight greatest HM_1 values, respectively. Falahati-Nezhad and Azari [14], Milovanović *et al.* [27], and Elumali *et al.* [13] established some upper and, or lower bounds on the HM_1 index. Rizwan *et al.* [35] characterized certain non-symmetric special collections of trees that maximize or minimize the HM_1 index. Wei *et al.* [39] investigated the HM_1 and HM_2 indices for carbon nanocones $CNC_k[n]$ and Keerthi *et al.* [25] computed the values of these indices for fractal and Cayley tree dendrimers.

In this paper, we intend to further investigate the mathematical properties of the first and second hyper-Zagreb indices by computing their minimum values over the set of all trees and connected graphs with a fixed order and maximum vertex degree. More precisely, we first suggest graph transformations that decrease the HM_1 and HM_2 indices. Based on these transformations, we obtain lower bounds for the HM_1 and HM_2 indices within the class of all trees with a given order and maximum vertex degree. The minimal trees that attain these lower bounds are also characterized. Finally, we extend our results to determine the minimum values of the mentioned indices for all connected graphs with a given order and maximum degree, identifying the corresponding minimal graphs.

The following observation, which will be used in the proof of our main theorems, is a direct consequence of the definition of the hyper-Zagreb indices.

Observation 1. *For a connected graph Γ and any $\varrho \notin E(\Gamma)$, the following inequalities hold:*

$$HM_1(\Gamma + \varrho) > HM_1(\Gamma) \quad \text{and} \quad HM_2(\Gamma + \varrho) > HM_2(\Gamma).$$

2. Main result

Throughout the section, $T(n, \Delta)$ denotes the class of all trees with n vertices and maximum vertex degree Δ.

Proposition 2.1. *Let $T \in T(n, \Delta)$ be a tree, and let $\rho \in V(T)$ be a vertex with degree Δ. If there is an end-support vertex in T, different from ρ, whose degree is at least three, then there exists another tree $T' \in T(n, \Delta)$ such that $HM_1(T) > HM_1(T')$ and $HM_2(T) > HM_2(T')$.*

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Proof. Let T be a rooted tree with root ρ. Let $\eta \neq \rho$ be an end-support vertex of degree $d_T(\eta) = k \geq 3$, which has the maximum distance from ρ. Denote the open neighborhood of η as $N_T(\eta) = \{\eta_1, \eta_2, \dots, \eta_k\}$. We may assume that η_k is the parent of η. Let T' denote a tree constructed from $T - \eta_1$ by attaching a pendant edge $\eta_2\eta_1$. Define

$$S = \{\eta\eta_i \mid 1 \leq i \leq k\} \text{ and } S' = (S \cup \{\eta_1\eta_2\}) - \{\eta\eta_1\}.$$

Clearly, $T' \in T(n, \Delta)$ and we have

$$\sum_{\vartheta\omega \notin S} (d_T(\vartheta) + d_T(\omega))^2 = \sum_{\vartheta\omega \notin S'} (d_{T'}(\vartheta) + d_{T'}(\omega))^2.$$

By definition, we have

$$\begin{aligned} HM_1(T) &= \sum_{\vartheta\omega \notin S} (d_T(\vartheta) + d_T(\omega))^2 + \sum_{\vartheta\omega \in S} (d_T(\vartheta) + d_T(\omega))^2 \\ &= \sum_{\vartheta\omega \notin S} (d_T(\vartheta) + d_T(\omega))^2 + \sum_{i=3}^{k} (d_T(\eta) + d_T(\eta_i))^2 + 2(k+1)^2, \end{aligned} \tag{2.1}$$

and

$$\begin{aligned} HM_1(T') &= \sum_{\vartheta\omega \notin S'} (d_{T'}(\vartheta) + d_{T'}(\omega))^2 + \sum_{\vartheta\omega \in S'} (d_{T'}(\vartheta) + d_{T'}(\omega))^2 \\ &= \sum_{\vartheta\omega \notin S'} (d_{T'}(\vartheta) + d_{T'}(\omega))^2 + \sum_{i=3}^{k} (d_T(\eta) + d_T(\eta_i) - 1)^2 + (k+1)^2 + 9. \end{aligned} \tag{2.2}$$

By (2.1) and (2.2), we have

$$\begin{aligned} HM_1(T) - HM_1(T') =& \sum_{i=3}^{k} (d_T(\eta) + d_T(\eta_i))^2 + 2(k+1)^2 \\ & - \sum_{i=3}^{k} (d_T(\eta) + d_T(\eta_i) - 1)^2 - (k+1)^2 - 9 \\ >& k^2 + 2k - 8. \end{aligned}$$

Since $k \geq 3$, we have $HM_1(T) - HM_1(T') > 0$. Additionally,

$$\begin{aligned} HM_2(T) &= \sum_{\vartheta\omega \notin S} (d_T(\vartheta)\, d_T(\omega))^2 + \sum_{\vartheta\omega \in S} (d_T(\vartheta)\, d_T(\omega))^2 \\ &= \sum_{\vartheta\omega \notin S} (d_T(\vartheta)\, d_T(\omega))^2 + \sum_{i=3}^{k} (d_T(\eta)\, d_T(\eta_i))^2 + 2(k+1)^2, \end{aligned} \tag{2.3}$$

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and

$$\begin{aligned} HM_2(T') &= \sum_{\vartheta\omega\notin S'} (d_{T'}(\vartheta)\, d_{T'}(\omega))^2 + \sum_{\vartheta\omega\in S'} (d_{T'}(\vartheta)\, d_{T'}(\omega))^2 \\ &= \sum_{\vartheta\omega\notin S'} (d_{T'}(\vartheta)\, d_{T'}(\omega))^2 + \sum_{i=3}^{k}(d_T(\eta)\, d_T(\eta_i)-1)^2 + (k+1)^2 + 9. \end{aligned} \tag{2.4}$$

By (2.3) and (2.4), we have

$$\begin{aligned} HM_2(T) - HM_2(T') &= \sum_{i=3}^{k}(d_T(\eta)\, d_T(\eta_i))^2 + 2k^2 - \sum_{i=3}^{k}((d_T(\eta)-1)\, d_T(\eta_i))^2 - 4(k-1)^2 - 4 \\ &= (2k-1)\sum_{i=3}^{k} d_T(\eta_i)^2 - 2(k-2)^2 \\ &\geq (2k-1)(k+1) - 2(k-2)^2 \\ &= 9k-9. \end{aligned}$$

Since $k \geq 3$, we have $HM_2(T) - HM_2(T') > 0$. □

Proposition 2.2. *Let $T \in T(n,\Delta)$ be a tree, and let $\rho \in V(T)$ be a vertex with degree Δ. If there is a support vertex in T, different from ρ, whose degree is at least three, then there exists another tree $T' \in T(n,\Delta)$ such that $HM_1(T) > HM_1(T')$ and $HM_2(T) > HM_2(T')$.*

Proof. Consider T as a rooted tree with root ρ. Let $\eta \neq \rho$ be a support vertex with degree $d_T(\eta) = k \geq 3$, which is at the maximum distance from ρ. Denote the open neighborhood of η as $N_T(\eta) = \{\eta_1, \eta_2, \ldots, \eta_k\}$. We may assume that η_k is the parent of η. Proposition 2.1 implies that η is not an end-support vertex. Suppose $d_T(\eta_1) = 1$ and $d_T(\eta_i) = 2$ for $2 \leq i \leq k-1$. Let T_1 be the component of $T - \eta\eta_2$ that contains η_2. We may assume that $T_1 = \eta_2\gamma_1\gamma_2\cdots\gamma_t$, $t \geq 1$. Then, we have $d_T(\gamma_i) = 2$, for $1 \leq i \leq t-1$, and $d_T(\gamma_t) = 1$. Denote by T' the tree constructed from $T - \eta_1$ by attaching a pendant edge $\gamma_t\eta_1$. First let us consider the case when $t = 1$ and define

$$S = \{\eta\eta_i \mid 1 \leq i \leq k\} \cup \{\eta_2\gamma_1\} \text{ and } S' = (S \cup \{\eta_1\gamma_1\}) - \{\eta\eta_1\}.$$

Clearly, $T' \in T(n,\Delta)$ and we have

$$\sum_{\vartheta\omega\notin S} (d_T(\vartheta) + d_T(\omega))^2 = \sum_{\vartheta\omega\notin S'} (d_{T'}(\vartheta) + d_{T'}(\omega))^2.$$

Then

$$\begin{aligned}
HM_1(T)-HM_1(T') =&\sum_{i=3}^{k}(d_T(\eta)+d_T(\eta_i))^2+(d_T(\eta)+d_T(\eta_1))^2\\
&+(d_T(\eta)+d_T(\eta_2))^2+(d_T(\eta_2)+d_T(\gamma_1))^2\\
&-\sum_{i=3}^{k}(d_{T'}(\eta)+d_{T'}(\eta_i))^2-(d_{T'}(\eta)+d_{T'}(\eta_2))^2\\
&-(d_{T'}(\eta_1)+d_{T'}(\gamma_1))^2-(d_{T'}(\eta_2)+d_{T'}(\gamma_1))^2\\
=&\sum_{i=3}^{k}(d_T(\eta)+d_T(\eta_i))^2+(k+1)^2+(k+2)^2+9\\
&-\sum_{i=3}^{k}(d_T(\eta)+d_T(\eta_i)-1)^2-(k+1)^2-25\\
>&k^2+4k-12,
\end{aligned}$$

and

$$\begin{aligned}
HM_2(T)-HM_2(T') =&\sum_{i=2}^{k}(d_T(\eta)\,d_T(\eta_i))^2+(d_T(\eta)\,d_T(\eta_1))^2+(d_T(\eta_2)\,d_T(\gamma_1))^2\\
&-\sum_{i=2}^{k}(d_{T'}(\eta)\,d_{T'}(\eta_i))^2-(d_{T'}(\eta_1)\,d_{T'}(\gamma_1))^2-(d_{T'}(\eta_2)\,d_{T'}(\gamma_1))^2\\
=&\sum_{i=2}^{k}(d_T(\eta)\,d_T(\eta_i))^2+k^2+4-\sum_{i=2}^{k}((d_T(\eta)-1)\,d_T(\eta_i))^2-16-4\\
=&(2k-1)\sum_{i=2}^{k}d_T(\eta_i)^2+k^2-16\\
\geq&4(2k-1)(k-1)-k^2-16\\
=&9k^2-12k-12.
\end{aligned}$$

Using the fact that $k\geq 3$, we have $HM_1(T)-HM_1(T')>0$ and $HM_2(T)-HM_2(T')>0$.

Now, let $t\geq 2$ and define

$$S=\{\eta\eta_i \mid 1\leq i\leq k\}\cup\{\gamma_{t-1}\gamma_t\} \text{ and } S'=(S\cup\{\eta_1\gamma_t\})-\{\eta\eta_1\}.$$

Clearly, $T'\in T(n,\Delta)$ and we have

$$\sum_{\vartheta\omega\notin S}(d_T(\vartheta)+d_T(\omega))^2=\sum_{\vartheta\omega\notin S'}(d_{T'}(\vartheta)+d_{T'}(\omega))^2.$$

Hence,

$$\begin{aligned}
HM_1(T)-HM_1(T') =& \sum_{i=3}^{k}(d_T(\eta)+d_T(\eta_i))^2+(d_T(\eta)+d_T(\eta_1))^2\\
&+(d_T(\eta)+d_T(\eta_2))^2+(d_T(\gamma_{t-1})+d_T(\gamma_t))^2\\
&-\sum_{i=3}^{k}(d_{T'}(\eta)+d_{T'}(\eta_i))^2-(d_{T'}(\eta)+d_{T'}(\eta_2))^2\\
&-(d_{T'}(\eta_1)+d_{T'}(\gamma_t))^2-(d_{T'}(\gamma_{t-1})+d_{T'}(\gamma_t))^2\\
=&\sum_{i=3}^{k}(d_T(\eta)+d_T(\eta_i))^2+(k+1)^2+(k+2)^2+9\\
&-\sum_{i=3}^{k}(d_T(\eta)+d_T(\eta_i)-1)^2-(k+1)^2-25\\
>&k^2+4k-12,
\end{aligned}$$

and

$$\begin{aligned}
HM_2(T)-HM_2(T') =& \sum_{i=2}^{k}(d_T(\eta)\,d_T(\eta_i))^2+(d_T(\eta)\,d_T(\eta_1))^2+(d_T(\gamma_{t-1})\,d_T(\gamma_t))^2\\
&-\sum_{i=2}^{k}(d_{T'}(\eta)\,d_{T'}(\eta_i))^2-(d_{T'}(\eta_1)\,d_{T'}(\gamma_1))^2-(d_{T'}(\gamma_{t-1})\,d_{T'}(\gamma_t))^2\\
=&\sum_{i=2}^{k}(d_T(\eta)\,d_T(\eta_i))^2+k^2+4-\sum_{i=2}^{k}((d_T(\eta)-1)\,d_T(\eta_i))^2-16-4\\
=&(2k-1)\sum_{i=2}^{k}d_T(\eta_i)^2+k^2-16\\
\geq&4(2k-1)(k-1)-k^2-16\\
=&9k^2-12k-12.
\end{aligned}$$

Given that $k\geq 3$, we have $HM_1(T)-HM_1(T')>0$ and $HM_2(T)-HM_2(T')>0$. □

Proposition 2.3. *Let $T\in T(n,\Delta)$ be a tree, and let $\rho\in V(T)$ have degree Δ. If there exists a vertex in T, different from ρ, whose degree is at least three, then there exists another tree $T'\in T(n,\Delta)$ such that $HM_1(T)>HM_1(T')$ and $HM_2(T)>HM_2(T')$.*

Proof. Consider T as a rooted tree with root ρ. Let $\eta\neq\rho$ be a vertex with degree $d_T(\eta)=k\geq 3$, which is at the maximum distance from ρ. Denote the open neighborhood of η as $N_T(\eta)=\{\eta_1,\eta_2,\ldots,\eta_k\}$. We may assume that η_k is the parent of η. By Propositions 2.1 and 2.2, η is not a support vertex. Let T_1 and T_2 be the components of $T-\{\eta\eta_1,\eta\eta_2\}$ that contain η_1 and η_2, respectively. We can assume that $T_1=\eta_1\gamma_1\gamma_2\cdots\gamma_t$, $t\geq 1$ and $T_2=\eta_2\lambda_1\lambda_2\cdots\lambda_l$, $l\geq 1$. Then we have $d_T(\gamma_i)=d_T(\lambda_j)=2$,

$1 \leq i \leq t-1$, $1 \leq j \leq l-1$, and $d_T(\gamma_t) = d_T(\lambda_l) = 1$. Denote by T' the tree constructed from $T - T_1$ by attaching a path $\lambda_l \eta_1 \gamma_1 \gamma_2 \cdots \gamma_t$. Let $l = 1$. Then define

$$S = \{\eta\eta_i \mid 1 \leq i \leq k\} \cup \{\eta_2\omega_1\} \text{ and } S' = (S \cup \{\eta_1\lambda_1\}) - \{\eta\eta_1\}.$$

Clearly, $T' \in T(n, \Delta)$ and we have

$$\sum_{\vartheta\omega \notin S} (d_T(\vartheta) + d_T(\omega))^2 = \sum_{\vartheta\omega \notin S'} (d_{T'}(\vartheta) + d_{T'}(\omega))^2.$$

Hence,

$$\begin{aligned}
HM_1(T) - HM_1(T') =& \sum_{i=3}^{k} (d_T(\eta) + d_T(\eta_i))^2 + (d_T(\eta) + d_T(\eta_1))^2 \\
& + (d_T(\eta) + d_T(\eta_2))^2 + (d_T(\eta_2) + d_T(\lambda_1))^2 \\
& - \sum_{i=3}^{k} (d_{T'}(\eta) + d_{T'}(\eta_i))^2 - (d_{T'}(\eta) + d_{T'}(\eta_2))^2 \\
& - (d_{T'}(\eta_1) + d_{T'}(\lambda_1))^2 - (d_{T'}(\eta_2) + d_{T'}(\lambda_1))^2 \\
=& \sum_{i=3}^{k} (d_T(\eta) + d_T(\eta_i))^2 + 2(k+2)^2 + 9 \\
& - \sum_{i=3}^{k} (d_T(\eta) + d_T(\eta_i) - 1)^2 - (k+1)^2 - 32 \\
>& k^2 + 6k - 16,
\end{aligned}$$

and

$$\begin{aligned}
HM_2(T) - HM_2(T') =& \sum_{i=2}^{k} (d_T(\eta)\, d_T(\eta_i))^2 + (d_T(\eta)\, d_T(\eta_1))^2 + (d_T(\eta_2)\, d_T(\lambda_1))^2 \\
& - \sum_{i=2}^{k} (d_{T'}(\eta)\, d_{T'}(\eta_i))^2 - (d_{T'}(\eta_1)\, d_{T'}(\lambda_1))^2 - (d_{T'}(\eta_2)\, d_{T'}(\lambda_1))^2 \\
=& \sum_{i=2}^{k} (d_T(\eta)\, d_T(\eta_i))^2 + 4k^2 + 4 - \sum_{i=2}^{k} ((d_T(\eta) - 1)\, d_T(\eta_i))^2 - 16 - 16 \\
=& (2k-1) \sum_{i=2}^{k} d_T(\eta_i)^2 + 4k^2 - 28 \\
>& 4k^2 - 28.
\end{aligned}$$

By using the fact that $k \geq 3$, we have $HM_1(T) - HM_1(T') > 0$ and $HM_2(T) - HM_2(T') > 0$. Now let $l \geq 2$. Assume that

$$S = \{\eta\eta_i \mid 1 \leq i \leq k\} \cup \{\lambda_{l-1}\lambda_l\} \text{ and } S' = (S \cup \{\eta_1\lambda_l\}) - \{\eta\eta_1\}.$$

Clearly, $T' \in T(n,\Delta)$ and we have

$$\sum_{\vartheta\omega\notin S}(d_T(\vartheta)+d_T(\omega))^2=\sum_{\vartheta\omega\notin S'}(d_{T'}(\vartheta)+d_{T'}(\omega))^2.$$

Hence,

$$\begin{aligned}
HM_1(T)-HM_1(T')=&\sum_{i=3}^{k}(d_T(\eta)+d_T(\eta_i))^2+(d_T(\eta)+d_T(\eta_1))^2\\
&+(d_T(\eta)+d_T(\eta_2))^2+(d_T(\lambda_{l-1})+d_T(\lambda_l))^2\\
&-\sum_{i=3}^{k}(d_{T'}(\eta)+d_{T'}(\eta_i))^2-(d_{T'}(\eta)+d_{T'}(\eta_2))^2\\
&-(d_{T'}(\eta_1)+d_{T'}(\lambda_l))^2-(d_{T'}(\lambda_{l-1})+d_{T'}(\lambda_l))^2\\
=&\sum_{i=3}^{k}(d_T(\eta)+d_T(\eta_i))^2+2(k+2)^2+9\\
&-\sum_{i=3}^{k}(d_T(\eta)+d_T(\eta_i)-1)^2-(k+1)^2-32\\
>&k^2+6k-16,
\end{aligned}$$

and

$$\begin{aligned}
HM_2(T)-HM_2(T')=&\sum_{i=2}^{k}(d_T(\eta)\,d_T(\eta_i))^2+(d_T(\eta)\,d_T(\eta_1))^2+(d_T(\lambda_{l-1})\,d_T(\lambda_l))^2\\
&-\sum_{i=2}^{k}(d_{T'}(\eta)\,d_{T'}(\eta_i))^2-(d_{T'}(\eta_1)\,d_{T'}(\lambda_l))^2-(d_{T'}(\lambda_{l-1})\,d_{T'}(\lambda_l))^2\\
=&\sum_{i=2}^{k}(d_T(\eta)\,d_T(\eta_i))^2+4k^2+4-\sum_{i=2}^{k}((d_T(\eta)-1)\,d_T(\eta_i))^2-16-16\\
=&(2k-1)\sum_{i=2}^{k}d_T(\eta_i)^2+4k^2-28\\
>&4k^2-28.
\end{aligned}$$

Since $k\geq 3$, we have $HM_1(T)-HM_1(T')>0$ and $HM_2(T)-HM_2(T')>0$. This completes the proof. □

By Propositions 2.1, 2.2, and 2.3, we can conclude that among all trees $T\in T(n,\Delta)$, the minimum values of the $HM_1(T)$ and $HM_2(T)$ are achieved by spiders. Now, we determine the specific spiders that attain the minimum values of the $HM_1(T)$ and $HM_2(T)$.

Proposition 2.4. *Let $T \in T(n, \Delta)$ be a spider with $\Delta \geq 3$ legs, where the length of two of the legs is 2 or greater. Then there exists another spider $T' \in T(n, \Delta)$ such that $HM_1(T) > HM_1(T')$ and $HM_2(T) > HM_2(T')$.*

Proof. Let ρ denote the center of T, and consider the two legs $\rho\gamma_1\gamma_2 \cdots \gamma_t$ and $\rho\lambda_1\lambda_2 \cdots \lambda_l$, where $l, t \geq 2$, both having lengths of 2 or greater. Let T' be the tree constructed from $T - \{\gamma_1\gamma_2\}$ by attaching the edge $\lambda_l\gamma_2$. By definition, we have

$$HM_1(T) - HM_1(T') = (\Delta + 2)^2 + 9 - 32 = (\Delta + 2)^2 - 23,$$

and

$$HM_2(T) - HM_2(T') = 4\Delta^2 + 4 - \Delta^2 - 16 = 3\Delta^2 - 12.$$

Therefore we conclude that, $HM_1(T) - HM_1(T') > 0$ and $HM_2(T) - HM_2(T') > 0$, which were the desired results. □

Theorem 2.5. *Let $T \in T(n, \Delta)$ have $n \geq 4$ vertices. Then*

$$HM_1(T) \geq 16n + \Delta^3 + 2\Delta^2 - 13\Delta - 20,$$

when $\Delta < n - 1$, and the equality is achieved if and only if T is a spider with exactly one leg of length greater than or equal to 2. Additionally,

$$HM_1(T) = \Delta(\Delta + 1)^2,$$

when $\Delta = n - 1$.

Proof. If $\Delta = n - 1$, then $T \cong S_n$ and $HM_1(T) = \Delta(\Delta + 1)^2$. Now, if $\Delta = 2$ then $T \cong P_n$, for which

$$HM_1(P_n) = 16n - 30 = 16n + \Delta^3 + 2\Delta^2 - 13\Delta - 20.$$

Therefore, we assume that $3 \leq \Delta \leq n - 2$. Let $T' \in T(n, \Delta)$ be a tree with $n \geq 4$ such that $HM_1(T') \leq HM_1(T)$ for every tree $T \in T(n, \Delta)$. Let ρ be a vertex of T' with degree $d_{T'}(\rho) = \Delta$, and let T' be rooted at ρ. By choosing T', Propositions 2.1, 2.2, and 2.3, we conclude that T' must be a spider whose center is ρ. Then, by Proposition 2.4, it follows that T' must be a spider with exactly one leg of length at least two and we have

$$\begin{aligned} HM_1(T') =& (\Delta + 2)^2 + (\Delta - 1)(\Delta + 1)^2 + 16(n - \Delta - 2) + 9 \\ =& 16n + \Delta^3 + 2\Delta^2 - 13\Delta - 20, \end{aligned}$$

from which the desired result is achieved. □

With an argument similar to that of the previous case, we obtain:

Theorem 2.6. *Let $T \in T(n, \Delta)$ have $n \geq 4$ vertices. Then*

$$HM_2(T) \geq 16n + \Delta^3 + 3\Delta^2 - 16\Delta - 28,$$

when $\Delta < n-1$, and the equality is achieved if and only if T is a spider with exactly one leg of length greater than or equal to 2*. Additionally,*

$$HM_2(T) = \Delta^3,$$

when $\Delta = n-1$.

The Observation 1 and Theorems 2.5 and 2.6 yield the following corollary.

Corollary 2.7. *Let Γ be a connected graph with n vertices and maximum degree Δ. Then*

$$HM_1(\Gamma) \geqslant \begin{cases} 16n + \Delta^3 + 2\Delta^2 - 13\Delta - 20 & \text{if } \Delta < n-1 \\ \\ \Delta(\Delta+1)^2 & \text{if } \Delta = n-1, \end{cases}$$

and

$$HM_2(\Gamma) \geqslant \begin{cases} 16n + \Delta^3 + 3\Delta^2 - 16\Delta - 28 & \text{if } \Delta < n-1 \\ \\ \Delta^3 & \text{if } \Delta = n-1, \end{cases}$$

with equality if and only if Γ is a spider with at most one leg of length greater than or equal to 2.

3. Conclusion

In this paper, we focused on two variants of the well-known Zagreb indices, namely the first and second hyper-Zagreb indices, which have shown better performance than some previously introduced indices. These indices exhibit a strong correlation with certain physico-chemical characteristics, such as the enthalpy of vaporization, acentric factor, heat of fusion, and entropy of octane isomers.

We presented several graph transformations that reduce the values of the first and second hyper-Zagreb indices. These transformations were applied to determine the minimum values of these indices within the class of trees with order n and maximum degree Δ. Additionally, we demonstrated that within this class, the mentioned indices achieve their minimum values at spiders with at most one leg of length at least two. Our results are also applicable to all connected graphs with a specified order and maximum degree. Given that many families of chemical graphs associated with molecular structures can be represented as trees, our findings may enhance the understanding of the physico-chemical features of these structures.

For future research, we propose investigating additional extremal problems related to the hyper-Zagreb indices across various collections of connected graphs, including trees, unicyclic graphs, bicyclic graphs, tricyclic graphs, and, more generally, c-cyclic graphs, while fixing certain graph parameters such as size, girth, radius, diameter, number of pendant vertices, and domination number.

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