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On the Hyper Zagreb Index of Trees with a Specified Degree of Vertices

Muhammad Rizwan [1], Sana Shahab [2], Akhlaq Ahmad Bhatti [1], Muhammad Javaid [3,*] and Mohd Anjum [4]

1 Department of Sciences and Humanities, National University of Computer & Emerging Sciences, Lahore Campus, Lahore 54770, Pakistan; L165514@lhr.nu.edu.pk (M.R.); akhlaq.ahmad@nu.edu.pk (A.A.B.)
2 Department of Business Administration, College of Business Administration, Princess Nourah Bint Abdulrahman University, P.O. Box 84428, Riyadh 11671, Saudi Arabia; sshahab@pnu.edu.sa
3 Department of Mathematics, School of Science, University of Management and Technology, Lahore 54770, Pakistan
4 Department of Computer Engineering, Aligarh Muslim University, Aligarh 202002, India; mohdanjum@zhcet.ac.in
* Correspondence: muhammad.javaid@umt.edu.pk or javaidmath@gmail.com

Abstract: Topological indices are the numerical descriptors that correspond to some certain physico-chemical properties of a chemical compound such as the boiling point, acentric factor, enthalpy of vaporisation, heat of fusion, etc. Among these topological indices, the Hyper Zagreb index, is the most effectively used topological index to predict the acentric factor of some octane isomers. In the current work, we investigate the extremal values of the Hyper Zagreb index for some classes of trees.

Keywords: variable-sum connectivity index; hyper-Zagreb index; symmetric; chemical compound

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1. Introduction

Here, we only work with simple, connected, and finite tree graphs. We assume that in a graph $G(V(G), E(G))$, $V(G)$ and $E(G)$ represent the set of vertices and the set of edges, respectively. The degree of a vertex v is denoted by the symbol d_v or $d_v(G)$. The symbols Δ or $\Delta(G)$ represent a vertex's highest degree in a graph G. Every acyclic graph is called a tree, which is denoted by T. A leaf or a pendant vertex is a vertex of degree one. A branching vertex contains a degree more than or equal to three. We use the notation $N_G(v)$ to express the set of all neighbouring vertices to v. Further, we assume that $N_G[v] = N_G(v) \bigcup \{v\}$. The graph G' comes into existence when some transformations or operations are applied on G. In such a case, we assume d_t or $d_t(G)$ is the vertex degree of t in G, whereas $|V(G)| = |V(G')|$. For the undefined terminologies and notations related to this work, the reader can consult [1].

Graphs can be used to represent chemical substances (such as hydrocarbons) [2]. A topological descriptor is a number (or combination of numbers) that captures a certain characteristic of the graph. If a certain molecular property resembles the descriptor, it is considered a topological index. This particular type of descriptor, known as a topological index, can be used to analyse the physicochemical characteristics of chemical substances. During the past few years, there has been extensive research into the structural and analytical properties of topological indices in the field of mathematical chemistry [3–5]. For instance, topological indices have been used in (QSPR) and (QSAR) studies to model the properties of chemical compounds [6–8]. Topological indices have theoretical and practical appeal because they are now essential resources for the investigation of numerous real-world issues in fields such as computer science [9], physics [10], and ecology [11], among others.

Many topological index applications have been documented, the majority of which focus on investigating medical and pharmaceutical problems. A substantial and quickly growing field of study on this subject started midway through the 1990s, yielding a large amount of research, and this marked an important development in the study of topological indices mathematically. The work conducted by Erdös [12,13] should be particularly addressed within this scenario.

As an innovative method of describing heteroatoms in molecules, the idea of generalised molecular descriptors was put forth [14,15], in addition to evaluating structural variations [16]. The Zagreb types of topological indices and Zagreb polynomials for a few nanotubes covered by cycles were discussed in [17]. The regression relation between some topological indices and the sum-based geometric arithmetic index was determined in [18]. In [19], the authors showed the ability to use many topological indices for correlation, given the situation of typical temperatures of production; in addition, the authors assessed the common boiling temperatures of octane isomers. Siddiqui computed the exact formula for Zagreb indices and Zagreb polynomials for certain graphs, S_n, $S(n, C_3)$, and $S(n, C_4)$, with $n = 1, 2, 3$, and they also determined the corresponding graphs, see [20].

To achieve a forecast of a certain property of molecules, topological indices are primarily used; for more information, see [21–23]. Finding the extremal graphs on a collection of graphs that satisfy the limitations imposed by the parameters that minimise (or maximise) the value of a topological index, is hence a straightforward challenge [24–26].

Here, we present some topological indices related to our current work. In [27], the variable sum connectivity index was explored as,

$$\chi_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v)^\alpha,$$

with $\alpha \in R$.

Note that $\sum_{uv \in E(G)}(d_u + d_v) = \sum_{u \in V(G)}(d_u^2)$; consequently, χ_1 and $2\chi_{-1}$ denote the M_1 and (H harmonic index), respectively. See [28–31], etc., for more detail.

In 2004, Zhou et al. [32] developed the Hyper Zagreb index as

$$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2,$$

which has been widely studied in different areas.

The Hyper Zagreb index and a number of the physicochemical characteristics of alkanes have been well correlated: vapor pressure, boiling points, surface areas, etc. The enthalpy of vaporisation (HVAP), acentric factor, heat of fusion (DHVAP) of octane isomers, and entropy are among the physicochemical parameters that have been assessed using the Hyper Zagreb index HM(G) . In particular, the HM(G) highly correlates with the acentric factor [33]. By Δ/δ, we mean the maximum/minimum degree of a graph G; in terms of Δ and δ, the extreme values on the Hyper Zagreb index of graph G have been examined [34]. In [35], the extreme values for the first and second Hyper Zagreb indices were established. Additionally, using benzenoid hydrocarbons' boiling points as inputs, linear regression analysis was performed on degree-based indices. By comparison, the models corresponding to the other distance-based indices performed worse than the Hyper Zagreb index-based linear model.

In the current work, we characterize some nonsymmetric special classes of trees, which maximise or minimise the Hyper Zagreb index with n-vertex trees for (i) all odd degree vertices, (ii) fixed even degree vertices, and a (iii) fixed number of vertices of maximum degree.

2. Methodology

The following method was adopted to perform the research:

Step 1: We categorized the family of tree graphs into three different classes say, OT, $ET_{n,r}$, and $MT_{n,k}$.
Step 2: We constructed the lemmas to support our main results.
Step 3: Some graph operations were defined in lemmas to search our extremal graphs.

Step 4: By using the contradiction method and the lemmas, we obtained our main theorems in which we defined the exact formulas for the Hyper Zagreb index.

3. On the Minimum Hyper Zagreb Index of Trees with All Odd Degrees

Let OT be the collection of all n-vertex trees having an even number of vertices, and each vertex has an odd degree. In this section, we characterize the class of trees from OT, which contains the minimum value of the Hyper Zagreb index.

Lemma 1. *Let $T_{min} \in OT$ be a tree having a minimum Hyper Zagreb index. Let $P = x_0x_1 \ldots,$ $x_{i-1}x_i(= u)x_{i+1} \ldots, x_l$ be a path in T_{min}, which contains the vertex u, where the vertex u has the maximum degree among all x_i; $0 \leq i \leq l$, such that $d_u \geq 5$. We also assume that $x_{i-1}, x_{i+1}, u^1, u^2 \ldots, u^{d_u-2}$ are the vertices adjacent to u in T_{min}, and w^1 is a pendent vertex connected to u via u^1 (u^1 may be equal to w^1). We define $T^{(1)} = T_{min} - uu^2 - uu^3 + u^2w^1 + u^3w^1$, as shown in Figure 1. Clearly, $T^{(1)} \in OT$, and we have $HM(T_{min}) > HM(T^{(1)})$.*

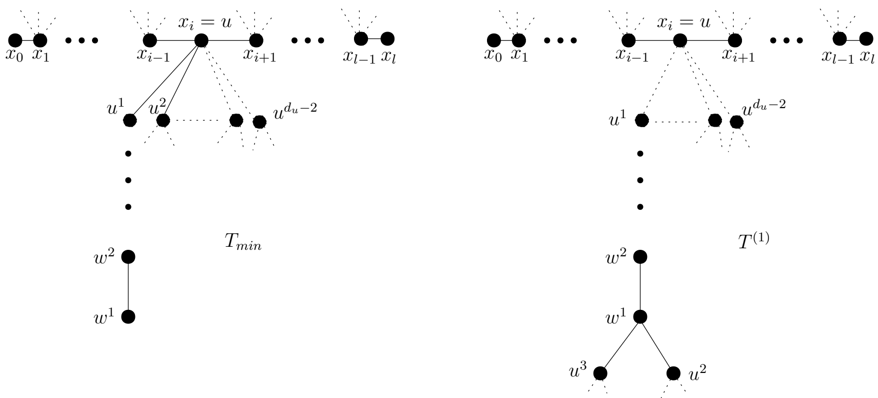

Figure 1. T_{min} and $T^{(1)}$ in Lemma 1.

Proof of Lemma 1. We first find the difference T_{min} - $T^{(1)}$ for the Hyper Zagreb index. Note that u and w^1 are the only vertices whose degrees differ in T_{min} and $T^{(1)}$. Therefore,

$$\begin{aligned}
HM(T_{min}) - HM(T^{(1)}) &= (d_u + d_{u^2})^2 + (d_u + d_{u^3})^2 + (d_{w^1} + d_{w^2})^2 + \sum_{\substack{t \in N(u) \\ t \neq u^2, u^3}} (d_u + d_t)^2 \\
&\quad - \sum_{\substack{t \in N(u) \\ t \neq u^2, u^3}} (d_u - 2 + d_t)^2 - (d_{w^1} + 2 + d_{w^2})^2 \\
&\quad - (d_{w^1} + 2 + d_{u^3})^2 - (d_{w^1} + 2 + d_{u^2})^2 \\
&= 2d_ud_{u^2} + 2(d_u)^2 + 2d_ud_{u^3} - 30 + 4d_u \\
&\quad + 4\sum_{\substack{t \in N(u) \\ t \neq u^2, u^3}} d_t - 4d_{w^2} - 6d_{u^3} - 6d_{u^2} \\
&= 2d_ud_{u^2} - 6d_{u^2} + 2d_ud_{u^3} - 6d_{u^3} + 2(d_u)^2 - 30 \\
&\quad + 4\sum_{\substack{t \in N(u) \\ t \neq u^2, u^3}} (d_u + d_t) - 4d_{w^2} > 0.
\end{aligned}$$

Since $d_u \geq d_{w^2}, d_{u^2} \geq 3, d_{u^3} \geq 3, \sum_{\substack{t \in N(u) \\ t \neq u^2, u^3}} d_t \geq 3$, a contradiction arises with our assumption. $\square$

Theorem 1. *If $T \in OT$, then $HM(T) \geq 26n - 56$, and the sign of equality holds, if and only if T possesses the degree sequence*

$$(\underbrace{3,3,\ldots,3,3}_{\frac{n-2}{2}},\underbrace{1,1,1,\ldots,1,1}_{\frac{n+2}{2}}).$$

Proof of Theorem 1. Let $T \in OT$ minimize the Hyper Zagreb index. We claim that there exist only the vertices of degree 1 and degree 3 in T. Suppose that on the contrary, there exists at least one vertex v of a degree greater or equal to $2t+1$, i.e., $d_v \geq 2t+1$, $t = 2,3,4\ldots$. According to Lemma 1, we obtain a tree $T^{(1)}$, such that $HM(T^{(1)}) < HM(T)$, which contradicts the choice of T, when we apply the transformation defined in Lemma 1 to every vertex v of degree $d_v \geq 2t+1$ successively. In every step from a tree $T^{(j)}$, we obtain a tree $T^{(j+1)}$ that contains a lower Hyper Zagreb index than its predecessor. We apply this transformation successively to obtain $T^{(k)}$. Clearly, $T^{(k)} \in OT$, and $HM(T^{(k)}) < HM(T)$, where T^k has the degree sequence

$$(\underbrace{3,3,\ldots,3,3}_{\frac{n-2}{2}},\underbrace{1,1,1,\ldots,1,1}_{\frac{n+2}{2}}),$$

and the proof is complete. □

4. On the Minimum and Maximum Hyper Zagreb Index of Trees with Fixed Even Degree Vertices

Let $ET_{n,r}$ denote the set of all n-vertex trees in which every tree has a fixed number of even degree vertices. Let the cardinality of the even degree vertices be denoted by r, such that $r \geq 1$ and $n \geq 5$.

Lemma 2. *Let $T_{min} \in ET_{n,r}$ be a tree having a minimum Hyper Zagreb index. Let $P = x_0x_1\ldots,x_{i-1}\,x_i(=u)x_{i+1}\ldots,x_l$ be a path in T_{min}, which contains the vertex u, where u has the maximum degree in $T_{min} \in ET_{n,r}$, such that $d_u \geq 4$, and $d_u \geq d_{x_i}; 0 \leq i \leq l$. We also assume that $x_{i-1}, x_{i+1}, u^1, u^2, u^3 \ldots, u^{d_u-2}$ are the vertices adjacent to u, and x_0, x_l are pendent vertices in T_{min}. We define $T^{(1)} = T_{min} - uu^1 - uu^2 + u^1x_l + u^2x_l$ (x_l may be equal to x_{i+1}), as shown in Figure 2. Clearly, $T^{(1)} \in ET_{n,r}$; then, $HM(T_{min}) > HM(T^{(1)})$.*

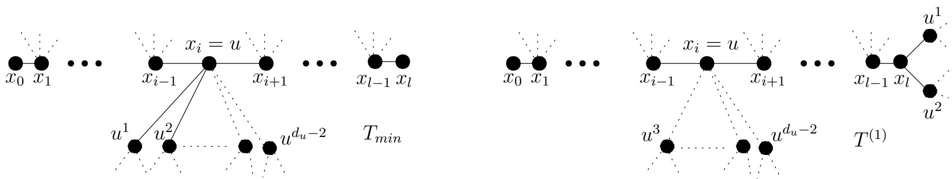

Figure 2. T_{min} and $T^{(1)}$ in Lemma 2.

Proof of Lemma 2. We first find the difference $T_{min} - T^{(1)}$ for the Hyper Zagreb index. Note that u and x_l are the only vertices whose degrees differ in T_{min} and $T^{(1)}$. Therefore,

$$\begin{aligned} HM(T_{min}) - HM(T^{(1)}) &= (d_u + d_{u^1})^2 + (d_u + d_{u^2})^2 + \sum_{\substack{t \in N(u) \\ t \neq u^1,u^2}} (d_u + d_t)^2 + (d_{x_l} + d_{x_{l-1}})^2 \\ &- \sum_{\substack{t \in N(u) \\ t \neq u^2,u^3}} (d_u - 2 + d_t)^2 + (d_{x_l} + 2 + d_{u^1})^2 \\ &+ (d_{x_l} + 2 + d_{u^2})^2 + (d_{x_l} + 2 + d_{x_{l-1}})^2 \\ &= 2d_ud_{u^1} + 2(d_u)^2 + 2d_ud_{u^2} - 30 + 4d_u \end{aligned}$$

$$+4 \sum_{\substack{t \in N(u) \\ t \neq u^2, u^3}} d_t - 6d_{u^1} - 6d_{u^2} - 4d_{x_{l-1}} > 0,$$

and since $d_{u^2} \geq 1, d_{u^3} \geq 1, \sum_{\substack{t \in N(u) \\ t \neq u^2, u^3}} d_t \geq 3$, is a contradiction. □

Lemma 3. *(a) Let u, z, v, and w be the vertices of a tree $T \in ET_{n,r}$ such that uz, zv, and $vw \in E(T)$, and $d_u(T) = 1, d_z(T) = 2, d_w(T) = 3$, and $d_v(T) = 3$. We define T' from T as $T' = T - uz - vw + zw + uv$; then, $HM(T') < HM(T)$.*

(b) Let u, y, z, v, w, and t be the vertices of tree $T \in ET_{n,r}$ such that uy, yz, zv, and $wt \in E(T)$, and $d_v(T) = d_w(T) = d_t(T) = d_u(T) = 3$, and $d_y(T) = d_z(T) = 2$ (v may coincide with w). We define T' as $T' = T - yz - zv - wt + zw + zt + yv$; then, $HM(T') < HM(T)$.

Proof of Lemma 3. (a) From the structure of T and T' we have,

$$HM(T) - HM(T') = 2(1 - d_w)(d_z - d_v) > 0,$$

and since $d_w = 3, d_z = 2$, and $d_v = 3$, this implies $HM(T) > HM(T')$.

(b) From the structure of T and T', we have,

$$HM(T) - HM(T') = 2(d_y d_z + d_z d_v + d_w d_t - d_y d_v - d_z d_t - d_w d_z) > 0,$$

and since $d_y = 2, d_z = 2, d_v = 3, d_w = 3$, and $d_t = 3$, this implies $HM(T) > HM(T')$. □

Thus, by Lemma 3, we conclude that in order to minimise the Hyper Zagreb index, we need to place the vertices of degree 2 between the vertices of degree 3, so that there is at least one vertex of degree 2 between any two vertices of degree 3 and the remaining vertices of degree 2 or one vertex of degree 2 and one vertex of degree 3. So, we conclude that the collection of all those trees, which contain n vertices with the degree sequence

$$(\underbrace{3, 3, \ldots, 3, 3}_{\frac{n-r-2}{2}}, \underbrace{2, 2, \ldots, 2, 2}_{r}, \underbrace{1, 1, 1, \ldots, 1, 1}_{\frac{n-r+2}{2}}),$$

must contain a particular arrangement of vertices of degree 2 as described above. Note that if $n > 3r + 2$, there are not enough vertices of degree 2 to be placed between any two vertices of degree 3. If $n \leq 3r + 2$, in order to minimise the Hyper Zagreb index, we have to first put at least one vertex of degree 2 between any two vertices of degree 3 (if it is possible), and the remaining vertices of degree 2 are placed arbitrarily between two vertices of degree 2 or between a vertex of degree 3 and a vertex of degree 2.

Theorem 2. *If $T \in ET_{n,r}$, where $1 \leq r < n - 2$, and $n \equiv r (mod\ 2)$, then $HM(T) \geq 25n - 9r - 50$ when $n \leq 3r + 2$, and $HM(T) \geq 26n - 12r - 56$ when $n > 3r + 2$. The sign of equality holds if and only if T possesses the degree sequence*

$$(\underbrace{3, 3, \ldots, 3, 3}_{\frac{n-r-2}{2}}, \underbrace{2, 2, \ldots, 2, 2}_{r}, \underbrace{1, 1, 1 \ldots, 1, 1}_{\frac{n-r+2}{2}}).$$

Proof of Theorem 2. Let $T \in ET_{n,r}$ minimise the Hyper Zagreb index. We claim that there does not exist any vertex of degree greater than 3 in T. To prove this claim, we suppose that on the contrary, there exists at least one vertex, say u, of a degree greater than 3 in T. According to Lemma 2, we can find another tree $T^{(1)}$, such that $HM(T) > HM(T^{(1)})$, which contradicts the choice of T. When we apply this transformation successively on every vertex u in T, we will find a sequence of trees $T^{(1)}, T^{(2)}, T^{(3)}, \ldots, T^{(r)}$ with the relation $HM(T) > HM(T^{(1)}) > HM(T^{(2)}) > \ldots > HM(T^{(r)})$. Having in mind Lemmas 2 and

Lemma 3 and the previous discussion, we conclude that the tree which minimises the Hyper Zagreb index contains the degree sequence with the particular arrangement of vertices defined above. Hence, $T^{(r)}$ has the degree sequence,

$$(\underbrace{3,3,\ldots,3,3}_{\frac{n-r-2}{2}},\underbrace{2,2,\ldots,2,2}_{r},\underbrace{1,1,1\ldots,1,1}_{\frac{n-r+2}{2}}).$$

□

Now, we provide some lemmas, which help us to prove Theorem 3.

Lemma 4. *Let $T_{max} \in ET_{n,r}$, with a maximum Hyper Zagreb index. Let $P = x_0x_1\ldots,x_i\ldots,x_l$ be a path in T_{max} containing the vertices $u = x_i$ and $v = x_j$, where $i,j \in \{1,2,3,\ldots,l-1\}, i \neq j$, such that for $t = 2,3,\ldots$, we have $d_v \geq d_u \geq 2t$. Let $x_{i-1}, x_{i+1}, u^1, u^2, \ldots, u^{d_u-2}$ be the vertices adjacent to the vertex u. We define $T^{(1)} = T_{max} - \sum_{t=1}^{2} u^t u + \sum_{t=1}^{2} u^t v$, as shown in Figure 3. Clearly, $T^{(1)} \in ET_{n,r}$; then, $HM(T_{max}) < HM(T^{(1)})$.*

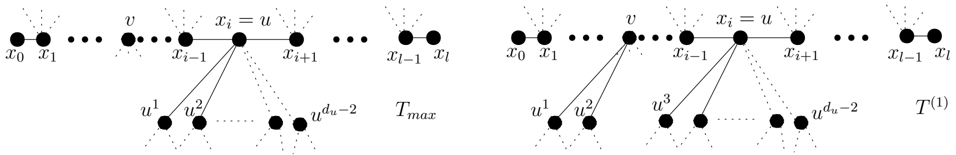

Figure 3. T_{max} and $T^{(1)}$ in Lemma 4.

Proof of Lemma 4. We first find the difference $T_{max} - T^{(1)}$ for the Hyper Zagreb index. Note that u and v are the only vertices whose degrees differ in T_{max} and $T^{(1)}$. Therefore,

$$\begin{aligned}
HM(T_{max}) - HM(T^{(1)}) = &\sum_{t=\sum_{j=1}^{2} u\hat{}j} (d_u + d_t)^2 + \sum_{\substack{s\in N(u)\\ s\neq \sum_{j=1}^{2} u^j}} (d_u + d_s)^2 + \sum_{\substack{r\in N(v)\\ r\neq t=\sum_{j=1}^{2}}} (d_v + d_r)^2 \\
&- \sum_{t=\sum_{j=1}^{2} u\hat{}j} (d_v + 2 + d_t)^2 + \sum_{\substack{s\in N(u)\\ s\neq \sum_{j=1}^{2} u^j}} (d_u - 2 + d_s)^2 + \sum_{\substack{r\in N(v)\\ r\neq t=\sum_{j=1}^{2}}} (d_v + 2 + d_r)^2 \\
&= 2\sum_{t=\sum_{j=1}^{2} u\hat{}j} d_u(d_t) + (d_u)^2 + 2\sum_{\substack{s\in N(u)\\ s\neq \sum_{j=1}^{2} u^j}} d_u(d_s) + 2\sum_{\substack{r\in N(v)\\ r\neq t=\sum_{j=1}^{2}}} d_v(d_r) \\
&-4 + 4d_u - 2\sum_{\substack{s\in N(u)\\ s\neq \sum_{j=1}^{2} u^j}} (d_u - 2)d_s - 4 - 4d_v - 2\sum_{t=\sum_{j=1}^{2} u\hat{}j} d_t(d_v + 2) \\
&-(d_v)^2 - 4 - 4d_v - 2\sum_{\substack{r\in N(v)\\ r\neq t=\sum_{j=1}^{2} u^j}} (d_v + 2)d_r,
\end{aligned}$$

and since $d_u \geq 4$ and $d_v \geq d_u$, we conclude $HM(T_{max}) < HM(T^{(1)})$. □

Lemma 5. *Let $T_{max} \in ET_{n,r}$ be a tree having a maximum Hyper Zagreb index. Let $P = x_0x_1\ldots,x_{i-1}$ $x_i(=u)x_{i+1}\ldots,x_l$ be a path in T_{max} containing the vertex $u = x_i \in V(T_{max})$, where $d_u \geq 2t$ and $d_{x_l} \geq 2t+1$; $t = 1,2,3,\ldots$, with $1 \leq i \leq l-1$. We also assume that $x_{l-1}, u^1, u^2, u^3 \ldots, u^{d_{x_l}-1}$ are the vertices adjacent to x_l in T_{max}. We define $T^{(1)} = T_{max} - \sum_{j=1}^{d_{x_l}-1} u^j x_l + \sum_{j=1}^{d_{x_l}-1} u^j u$ (x_l may be equal to x_{i+1}), as shown in Figure 4. Clearly, $T^{(1)} \in ET_{n,r}$; then, $HM(T_{max}) < HM(T^{(1)})$.*

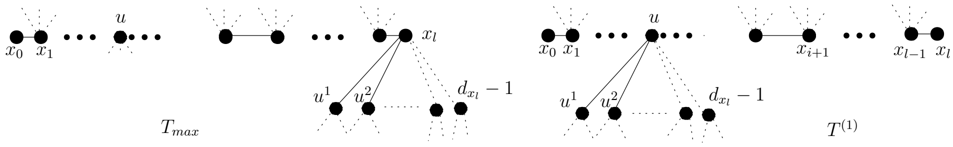

Figure 4. T_{max} and $T^{(1)}$ in Lemma 5.

Proof of Lemma 5. We first find the difference $T_{max} - T^{(1)}$ for the Hyper Zagreb index. Note that u and x_l are the only vertices whose degrees differ in T_{max} and $T^{(1)}$. Therefore,

$$\begin{aligned} HM(T_{max}) - HM(T^{(1)}) \quad &= \sum_{\substack{s\in N(u)\\ s\neq \sum_{j=1}^{d_{x_l}-1} u^j}} (d_u + d_s)^2 + \sum_{j=1}^{d_{x_l}-1} (d_{u^j} + d_{x_l})^2 + (d_{x_l} + d_{x_{l-1}})^2 \\ &- \sum_{j=1}^{d_{x_l}-1} (d_u + d_{x_l} - 1 + d_{u^j})^2 - \sum_{\substack{s\in N(u)\\ s\neq u^j, 1\leq j\leq d_{x_l}-1}} (d_u + d_{x_l} - 1 + d_s)^2 \\ &-(1 + d_{x_{l-1}})^2 \\ &= 2d_{x_l}(d_{x_{l-1}} - 1) - (d_u - 1)(d_u - 1 + 2d_{x_l}) \\ &-2\sum_{j=1}^{d_u-2} (d_u - 1)d_{u^j} - 1 + 2d_{x_l} - 2(d_u + d_s)(d_{x_l} - 1) - 1 - 2d_{x_{l-1}}, \end{aligned}$$

and since $2d_{x_l} < 2d_{x_l} + d_u - 1$ and $d_{x_{l-1}} - 1 \leq d_u - 1$, we conclude $HM(T_{max}) < HM(T^{(1)})$. □

Lemma 6. *Let u, z, v, and w be the vertices of a tree $T \in ET_{n,r}$, such that uz, zv, and $vw \in E(T)$, and $d_u(T) = 1, d_z(T) = 2t$, with $t = 2, 3, 4 \ldots, d_w(T) = 2$, and $d_v(T) = 2$. We define T' from T as $T' = T - uz - vw + zw + uv$; then, $HM(T') > HM(T)$.*

Proof of Lemma 6. From the structure of T and T', we have,

$$HM(T) - HM(T') = 2(d_u - d_w)(d_z - d_v) < 0,$$

and since $d_w > d_u$ and $d_z > d_v$, this implies $HM(T) < HM(T')$. □

Lemma 7. *If there exists a pendent vertex adjacent to a branching vertex in the tree $ET_{n,r}$ then the tree T_{max} does not contain a vertex of degree two with both non-pendent neighbours.*

Proof of Lemma 7. Suppose on the contrary that a pendent vertex u is adjacent to a vertex v of a degree greater than two, and there exists a vertex w of degree two, such that $N(w) = \{w_1, w_2\}$, and both w_1 and w_2 are non-pendent vertices. We define $T^{(1)} = T_{max} - ww_1 - ww_2 + uw + w_1w_2$, and clearly, $T^{(1)} \in ET_{n,r}$.

$$HM(T) - HM(T^{(1)}) = 2d_w(d_{w_1} + d_{w_2}) - 2d_{w_1}d_{w_2} - 2(d_u + d_v)^2 + (d_w)^2 - 2d_w d_u - (d_u)^2 - 1 < 0.$$

Hence, $HM(T) < HM(T^{(1)})$. □

Theorem 3. *If $T \in ET_{n,r}$, where $1 \leq r < n - 2$ and $n \equiv r (mod\ 2)$, then*

$$HM(T) \leq \begin{cases} k^3 + 4k^2 + 3k + 4r - 4 & \textit{for } \ n \geq 2k + 1, \\ k^3 + 3k^2 - k^2 r + 3k - 2kr + 17r - 17 & \textit{for } \ n < 2k + 1, \end{cases}$$

where k denotes the maximum degree of the vertex in T, the sign of equality can be easily obtained, if and only if T possesses the degree sequence

$$(n-r,\underbrace{2,2,\ldots,2,2}_{r-1},\underbrace{1,1,1\ldots,1,1}_{n-r}),$$

where $1 \le r < n-2$*.*

Proof of Theorem 3. Let $T \in ET_{n,r}$ maximise the Hyper Zagreb index. We consider the following two cases for completion of the proof of the above theorem.

Case 1

We claim that there does not exist any vertex of odd degree greater or equal to 3 in T. We suppose, on the contrary, that there exists at least one vertex of odd degree, say v, such that $d_v \ge 3$. According to the transformation defined in Lemma 4, we can find another tree $T_1^{(1)} \in ET_{n,r}$, such that $HM(T) < HM(T_1^{(1)})$, which contradicts the choice of T. If we apply this transformation successively on every vertex v, we find a sequence of trees $T_1^{(1)}, T_1^{(2)}, T_1^{(3)}, \ldots, T_1^{(s)}$ with the relation $HM(T) < HM(T_1^{(1)}) < HM(T_1^{(2)}) < \ldots < HM(T_1^{(s)})$. It is easy to understand that in $T_1^{(s)}$, there does not exist any branching vertex of odd degree.

Case 2

We claim that there exists only one branching vertex of an even degree in $T_1^{(s)}$. To prove this claim, we suppose, on the contrary, that there exists more than one branching vertex, say u, of even degree in $T_1^{(s)}$. Then, by Lemma 5, we can find another tree $T^{(s+1)} \in ET_{n,r}$, such that $HM(T_1^{(s)}) < HM(T_1^{(s+1)})$, and we obtain a contradiction. If we apply this transformation successively on every vertex having an even degree greater or equal to 4 in $T_1^{(s)}$, we find a sequence of trees $T_1^{(s+1)}, T_1^{(s+2)}, T_1^{(s+3)}, \ldots, T_1^{(r)}$ with the relation $HM(T_1^{(s)}) < HM(T_1^{(s+1)}) < HM(T_1^{(s+2)}) < \ldots < HM(T_1^{(r)})$. It is easy to understand that in $T_1^{(r)}$ there exists only one branching vertex of an even degree, and the remaining even degree vertices are of degree 2.

From the above discussion and Lemmas 4–7, it follows that a tree $T \in ET_{n,r}$, which maximises the Hyper Zagreb index, is a tree with only one branching vertex with degree k, such that an arbitrary vertex of degree one in $ET_{n,r}$ is adjacent to a vertex of degree 2 (for $n \ge 2k+1$), or there are exactly $n-k-1$ pendent vertices with neighbours of degree 2 (for $n < 2k+1$).

Therefore, if $T \in ET_{n,r}$, then $HM(T) = k^3 + 4k^2 + 3k + 4r - 4$ for $n \ge 2k+1$, and $HM(T) = k^3 + 3k^2 - k^2r + 3k - 2kr + 17r - 17$ for $n < 2k+1$. □

5. On the Minimum Hyper Zagreb Index of Trees with Fixed Vertices of Maximum Degree

Suppose that $MT_{n,k}$ is the collection of all n-vertex trees, where k represents the number of vertices of maximum degree. Here, we discover the graphs of trees that possess the lower bound for the Hyper Zagreb index from $MT_{n,k}$. Since P_n is only a member in $MT_{n,n-2}$, we consider $MT_{n,k}$ for $1 \le k \le n-3$.

Lemma 8. *If* $T_{min}^{(1)} \in MT_{n,k}$ *is a tree having a minimum Hyper Zagreb index, where* $1 \le k \le n-3$*, then the maximum degree of a vertex in* $T_{min}^{(1)}$ *equals 3.*

Proof of Lemma 8. We suppose that $\Delta \ge 4$, and the vertex u has the maximum degree Δ in $T_{min}^{(1)}$. We assume that $P = x_0x_1\ldots,x_{i-1}x_i(=u)x_{i+1}\ldots,x_l$ is the longest path in $T_{min}^{(1)}$ containing the vertex u. We also assume that the vertices $x_{i-1}, x_{i+1}, u^1, u^2\ldots, u^{\Delta-2}$ are the vertices adjacent to u in $T^{(1)}_{min}$, and w^1 is a pendent vertex connected to u via u^1 (u^1 may be equal to w^1). We define $T^{(1)} = T^{(1)}_{min} - uu^2 + u^2w^1$, as shown in Figure 5.

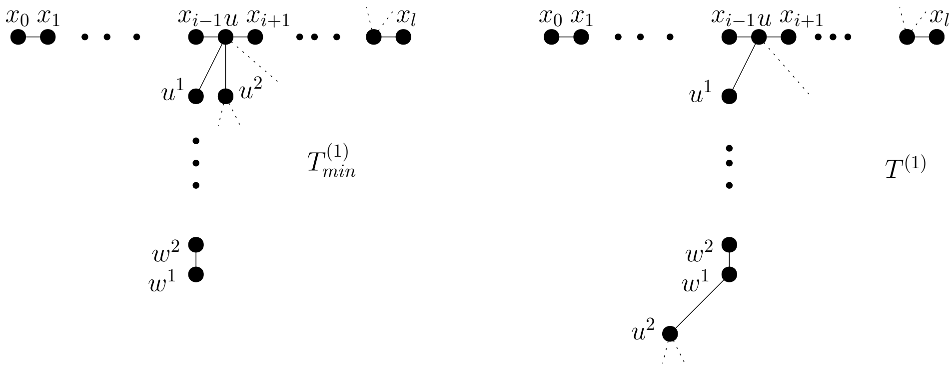

Figure 5. T_{max} and $T^{(1)}$ in Lemma 8.

$$\begin{aligned} HM(T^{(1)}_{min}) - HM(T^{(1)}) &= (d_u + d_{u^2})^2 + \sum_{\substack{s\in N(u)\\ s\neq u^2}} (d_u + d_s)^2 + (d_{w^1} + d_{w^2})^2 \\ &-(d_{w^1} + 1 + d_{w^2})^2 - (d_{w^1} + 1 + d_{u^2})^2 - \sum_{\substack{s\in N(u)\\ s\neq u^2}} (d_u - 1 + d_s)^2 \\ &= (d_u)^2 - 2(2 + d_{w^2}) + d_{u^2}(d_{u^2} + 2d_u) - (2 + d_{u^2})^2 + 2(d_u + d_s) > 0, \end{aligned}$$

and since $d_u \geq d_{w^2}$ and $d_{w^1} = 1$, this implies that $HM(T^{(1)}_{min}) > HM(T^{(1)})$.

It is easy to observe that $T^{(1)}$ contains $k-1$ vertices of degree Δ. In the same way, we apply the transformation defined in Lemma 8 on every vertex of degree Δ. In every step from a tree $T^{(j)}$, we obtain a tree $T^{(j+1)}$ that contains a lesser $HM(T)$ than its predecessor. We apply this transformation k times, and we reach a tree $T^{(k)}$ that contains k vertices of the maximum degree $\Delta - 1$. Clearly, $T^{(k)} \in MT_{n,k}$, and $HM(T^{(k)}) < HM(T^{(1)}_{min})$, which is a contradiction of the choice of $T^{(1)}_{min}$. □

Theorem 4. *If $T \in MT_{n,k}$, then $HM(T) \geq 16n + 18k - 32$ when $n \geq 3k + 2$, and $HM(T) \geq 14n - 24k - 32$ when $n < 3k + 2$. The sign of equality holds if and only if T possesses the degree sequence*

$$(\underbrace{3, 3, \ldots, 3, 3}_{k}, \underbrace{2, 2, \ldots, 2, 2}_{n-2k-2}, \underbrace{1, 1, 1 \ldots, 1, 1}_{k+2}.$$

Proof of Theorem 4. Let ${T_{min}}^{(1)} \in MT_{n,k}$ minimize the Hyper Zagreb index. According to Lemma 8, the degree sequence of the tree ${T_{min}}^{(1)}$ is

$$(\underbrace{3, 3, \ldots, 3, 3}_{k}, \underbrace{2, 2, \ldots, 2, 2}_{n-2k-2}, \underbrace{1, 1, 1 \ldots, 1, 1}_{k+2}),$$

where $k \leq n - 3$. The relation $\sum_{v\in V(T^{(1)}_{min})} d_v(T^{(1)}_{min}) = 2(n-1)$ gives $n_1 + 2n_2 + 3k = 2(n_1 + n_2 + k) - 2$,

$$n_1 = k + 2,$$

$$n_2 = n - 2k - 2.$$

Therefore,
for $n \geq 3k+2$, we have,

$$HM(T^{(1)}_{min}) = 16n + 18k - 32,$$

and for $n < 3k+2$, we have,

$$HM(T^{(1)}_{min}) = 14n - 24k - 32.$$

□

Corollary 1. *Let T^k be a tree with a minimum Hyper Zagreb index in the class of $MT_{n,k}$ and T^l be a tree with a minimum Hyper Zagreb index in the class of $MT_{n,l}$ $(k, l \leq n-3)$. If $k > l$, then $HM(T^k) > HM(T^l)$.*

6. Conclusions

Finding the extremal values (lower/upper bounds) of topological indices of a molecular structure has numerous applications in the field of chemical graph theory. These numerical values give important information regarding the physicochemical properties of the chemical compounds. In particular, investigating a topological index of a chemical tree sometimes gives a very good correlation to a physicochemical property of the chemical compound. The degree-based topological indices, such as the Hyper Zagreb index, have a very good correlation with the boiling point of benzenoid hydrocarbons and the acentric factor of some octane isomers. Therefore, in the current work, we computed the bounds of the Hyper Zagreb index of some specific tree structures, and the corresponding graphs were characterized. These extremal values not only help researchers to predict the properties of the chemical compounds but also significantly reduce the experimental costs.

However, it remains an open problem to study different topological indices for different classes of trees to predict the physicochemical properties of some chemical compounds.

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