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A Lower Bound for the First Hyper-Zagreb Index of Trees with given Roman Domination Number

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Abstract

In graph theory, the first Hyper-Zagreb index $HM_1(\mathcal{G})$ is calculated by summing the squares of the degrees of adjacent vertices u and v in molecular graphs. A Roman dominating function (RDF) on a graph $\mathcal{G}$ is a function $z : \mathcal{V}(\mathcal{G}) \to \{0, 1, 2\}$, where $\mathcal{V}(\mathcal{G})$ is the vertex set, with the requirement that for each vertex v with $z(v) = 0$, there exists an adjacent vertex u such that $z(u) = 2$. The Roman domination number (RDN) denoted as $\zeta_R(\mathcal{G})$ and represents as the minimum total weight of all vertices under an RDF, and it plays a significant role in network analysis. In this paper, we present a new lower bound for the $HZ_1(\mathcal{T})$ for trees $\mathcal{T}$ with order n and $\zeta_R(\mathcal{T})$. These findings enhance our understanding of tree structures, providing chemists with a valuable tool for analyzing molecular stability and reactivity. By establishing mathematical bounds on the $HZ_1(\mathcal{T})$, this research supports more precise predictions of molecular properties and aids in efficient experimental planning in chemical graph theory.

Keywords: Tree; Roman domination number; first hyper Zagreb index; Bound.

1. Introduction

The focus of this work is on graphs that are simple, undirected, and connected. Let us represent such a graph as $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ in which the variables $\mathcal{V}$ and $\mathcal{E}$, respectively, represent the sets of vertices and edges. The collection of vertices connected to a vertex u by an edge is called the open neighborhood of that vertex, and it is represented by the notation $N(v) = u \in \mathcal{V} \mid uv \in \mathcal{E}$ for every vertex $u \in \mathcal{V}$. The number of edges that interact with vertex u in the graph $\mathcal{G}$ is the degree of that vertex, represented by $\eta_{\mathcal{T}}(u)$. A pendant vertex is a vertex u in $\mathcal{G}$ with $\eta_{\mathcal{T}}(u) = 1$.

The longest path connecting any two leaves on a tree is its diameter. To describe the tree derived from $\mathcal{T}$, we remove the vertices $v_1, \ldots, v_k$. We do this by using the notation $\mathcal{T} - \{v_1, \ldots, v_k\}$. To indicate the

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path with n vertices, use the symbol $\mathcal{P}_n$. The reference book [13] should be consulted for any definitions of graph theory notations or terms not included here.

A chemical molecule can be seen as a graph, with the edges representing the bonds of chemicals between the atoms and the vertices representing the atoms. This model makes it possible to analyze molecular structures and characteristics using principles from graph theory. Chemist uses the $HM_1(\mathcal{G})$, as a topological metric to measure how connected atoms and bonds are within a molecule. Understanding the structure and characteristics of molecules is made easier with the use of this index, particularly when studying chemical reactions and molecular interactions. Topological indices (TIs) serve as mathematical parameters for analyzing different properties of these molecules. Among these indices, degree-based ones like the $HM_1(\mathcal{G})$ have garnered significant attention. The $HM_1(\mathcal{G})$ was introduced by Shirdel et al. [25] in 2013. $HM_1(\mathcal{G})$ is defined as follows:

$$HM_1(\mathcal{G}) = \sum_{uv \in \mathcal{E}(\mathcal{G})} (\eta_{\mathcal{G}}(u) + \eta_{\mathcal{G}}(v))^2.$$

For more in-depth exploration of the Hyper-Zagreb indices, refer to [23, 26, 11, 14, 8].

Suppose we have an undirected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where the collection of vertices is $\mathcal{V}$, and the set of edges is $\mathcal{E}$. If every vertex u in $\mathcal{V}$ is either a part of $\mathcal{D}$ or related to a vertex in $\mathcal{D}$, then that subset $\mathcal{D} \subseteq \mathcal{V}$ is called a dominance set. Stated differently, any vertex $u \in \mathcal{V}$ must either be an adjacent vertex v in $\mathcal{D}$ or belong to $\mathcal{D}$, which implies the existence of an edge $uv \in \mathcal{E}$. Within graph theory, the study of domination in graphs has been a busy field of study [13].

For any vertex $v \in \mathcal{V}$ for which $z(v) = 0$ has at least one nearby vertex $u \in N(v)$ with $z(u) = 2$, the function $z : \mathcal{V} \to \{0, 1, 2\}$ is referred to as a RDF. The *weight* of z is defined as the sum $z(\mathcal{V}) = \sum_{v \in \mathcal{V}} z(v)$. The RDN and denoted as $\zeta_R(\mathcal{G})$ of a graph $\mathcal{G}$ is the minimum weight of a RDN on $\mathcal{V}$. This concept ensures that all undefended vertex is protected by a strongly defended neighboring vertex.

Research on the relationships between TIs and domination numbers in graphs has been extensive and remains an active area of study [4, 5, 7, 20, 3]. For instance, Borovićanin and Furtula examined extremal Zagreb indices (ZI) of $\mathcal{T}$ for specific DNs [5]. Maximum value on ZI for $\mathcal{T}$, uni-cycle (UC), and bi-cycle (BC) graphs with particular TDN were derived by Mojdeh et al. [20]. Maitreyi et al. [19] established upper bounds for the atom-bond sum-connectivity (ABS) index in trees of fixed order with a given maximum degree, addressing an open problem by Hussain, Liu, and Hua. Li et al. [15] identified extremal graphs maximizing the ABS index under constraints such as clique and chromatic numbers, while Noureen et al. [22] extended this analysis to tricyclic graphs. Wang and Zhou [27] examined unicyclic graphs, deriving the ABS index maximum for a fixed diameter. Beyond ABS, Zou and Zhong [30] established a lower bound for the modified Randić index in line graphs of trees, generalizing results from Wang et al. [30] and Zhang and Wu, thereby refining inequalities in topological indices.

Further investigations by Du examined the maximal ZI_1 for trees with a specified RDN, focusing on connections between the RDN and the ZI_1 a research theme spanning five decades [9]. Studies on the Randić index by Hasni et al. provided an upper bound for trees based on their number of vertices with TDN and identified extremal trees within this context [12]. Shahid Zaman et al. [29] examined M-polynomials' coindices, linking topological indices to antiviral drugs' properties using quadratic regression. Similarly, Shahid Zaman [28] employed QSPR modeling to correlate anticancer drugs' molecular descriptors with their physicochemical attributes. Additionally, extremal graphs were characterized, with upper bounds identified for the ZI of UC and BC graphs with assigned RDNs, furthering insights into extremal behaviors within these indices. Recently, Ali et al. [1] derived lower bounds for HZ_2 in terms of graph order and the RDN. Liu et al. investigate extremal values of ZI in Eulerian graphs, analyze TIs in random pentagonal chain networks, and explore minimization of the Kirchhoff index in graphs with fixed vertex bipartiteness, identifying key structural properties across these studies [17, 18, 16, 21, 10, 24, 2].

A significant gap exists in the literature regarding minimum values for the HZ_1 of $\mathcal{T}$ expressed in terms of tree vertices and their RDN. Addressing this gap would enhance our comprehension of the structural properties linking the Hyper-Zagreb index with domination-related parameters.

This research contributes to advancing theoretical understanding in graph theory, particularly benefiting applications in chemical graph theory by providing insights into TIs based on Roman domination. The findings will offer valuable tools for studying molecular stability and electronic properties in chemistry, where understanding these graph indices is crucial.

2. A lower bound for the trees with a particular Roman dominance number in the first Hyper-Zagreb index

First, we present a lemma from the literature that supports our results.

Lemma 2.1. [6] For $n \geq 3$, RDN of $\mathcal{P}_n$ is $\zeta_R(\mathcal{P}_n) = \lceil \frac{2n}{3} \rceil$.

We establish new lower bounds for the $HM_1(\mathcal{T})$ index, derived in terms of the RDN and the order of the graph. Let $M(n, \zeta_R)$ represent a proposed lower bound for $HM_1(\mathcal{T})$. We demonstrate that $HM_1(\mathcal{T})$ is indeed bounded below using Lemma 2.2 and Theorem 2.3. Specifically, we define

$$M(n, \zeta_R) = \frac{50n}{3} - 30 - \zeta_R.$$

In order to prove the main Theorem 2.3, we now show the following lemma.

Lemma 2.2. Suppose $\mathcal{T}$ be a tree with order $n \geq 3$, Roman domination number ζ_R, and a vertex $u \in \mathcal{V}(\mathcal{T})$ such that $\eta_{\mathcal{T}}(u) = x \geq 3$, $N(u) = \{b_1, b_2, \ldots, b_x\}$, $\eta_{\mathcal{T}}(b_l) = w \geq 2$ and $\eta_{\mathcal{T}}(b_k) = 1$, $\forall\ k \in \{1, 2, \ldots, x-1\}$. If we take $\mathcal{T}' = \mathcal{T}' - b_1$, and $\zeta_R(\mathcal{T}') = \zeta_R(\mathcal{T})$, then $HM_1(\mathcal{T}) > M(n, \zeta_R)$.

Proof. Assume that $M(n, \zeta_R) = \frac{50n}{3} - 30 - \zeta_R$.

$$\begin{aligned}
HM_1(\mathcal{T}) =& HM_1(\mathcal{T}') + (x-1)(x+1)^2 + (x+w)^2 - (x-2)x^2 - (x+w-1))^2, \\
=& HM_1(\mathcal{T}') + 3x^2 + x + 2w - 2, \\
\geq& \frac{50(m-1)}{3} - 30 - \zeta_R(\mathcal{T}) + 3x^2 + x + 2w - 2, \\
=& M(n, \zeta_R) + 3x^2 + x + 2w - \frac{56}{3},
\end{aligned}$$

Suppose that $z(x, w) = 3x^2 + x + 2w - \frac{56}{3}$, $z(x, w) > 0$, $\forall\ x \geq 3$ and $w \geq 2$. Therefore, $HM_1(\mathcal{T}) \geq M(n, \zeta_R) + z(x, w) > M(n, \zeta_R)$. □

Given a tree with a specified RDN, we establish a lower bound for the first Hyper-Zagreb index as follows.

Theorem 2.3. Let $\mathcal{T}$ be a tree graph of order n with Roman domination number ζ_R. The lower bound of the $HM_1(\mathcal{T})$ is

$$HM_1(\mathcal{T}) \geq M(n, \zeta_R).$$

The equality hold if and only if $\mathcal{T} \cong \mathcal{P}_n$ where $n \equiv 0\ (mod\ 3)$.

Proof. We start by introducing the order n. For any tree with equality of order $n \geq 4$, the outcome is instantaneous if and only if $\mathcal{T} = \mathcal{P}_n$. If $n \geq 5$, then any tree $\mathcal{T}'$ with order $h' < h$ will have the same result. Let $\mathcal{T}$ represent an order n tree. To start, let $\Delta(\mathcal{T}) = 2$. Afterward, $\mathcal{T} = \mathcal{P}_n$. Lemma 2.1 says that if

$n \equiv k\ (mod\ 3)$, then $\zeta_R = \zeta_R(\mathcal{P}_n) = \frac{2n+k}{3}$, we obtain:

$$\begin{aligned} HM_1(\mathcal{P}_n) =& 16n - 30, \\ =& 16n - 30 - \zeta_R + \frac{2n+k}{3}, \\ =& 16n - 30 - \zeta_R + \frac{2n}{3} + \frac{k}{3}, \\ =& \frac{50n}{3} - 30 - \zeta_R + \frac{k}{3}, \\ \geq& \frac{50n}{3} - 30 - \zeta_R, \end{aligned}$$

and equality is maintained if and only if $n \equiv 0\ (mod\ 3)$.
Let $v_1 \dots v_{d+1}$ be a diametrical path of $\mathcal{T}$ and assume that $\Delta(\mathcal{T}) \geq 3$ and v_1 and v_{d+1} are obviously pendent vertices.
Assume that $\mathcal{T}' = \mathcal{T} - v_1$. The relationship between $HM_1(\mathcal{T}) = HM_1(\mathcal{T}') + 2\eta_{\mathcal{T}}(v_3) + (\eta_{\mathcal{T}}(v_2))^2 + 4\eta_{\mathcal{T}}(v_2)$ and $\zeta_R(\mathcal{T}) - 1 \leq \zeta_R(\mathcal{T}') \leq \zeta_R(\mathcal{T})$ is readily apparent. Using the induction hypothesis on $\mathcal{T}'$, if $max\{\eta_{\mathcal{T}}(v_2), \eta_{\mathcal{T}}(v_3)\} \geq 3$ or $\eta_{\mathcal{T}}(v_2) = \eta_{\mathcal{T}}(v_3) = 2$ and $\zeta_R(\mathcal{T}) - 1 = \zeta_R(\mathcal{T})$, then we obtain:

$$\begin{aligned} HM_1(\mathcal{T}) \geq& HM_1(\mathcal{T}') + 2\eta_{\mathcal{T}}(v_3) + (\eta_{\mathcal{T}}(v_2))^2 + 4\eta_{\mathcal{T}}(v_2), \\ \geq& \frac{50(n-1)}{3} - 30 - \zeta_R(\mathcal{T}') + 2\eta_{\mathcal{T}}(v_3) + (\eta_{\mathcal{T}}(v_2))^2 + 4\eta_{\mathcal{T}}(v_2), \\ \geq& \frac{50n}{3} - 30 - \zeta_R(\mathcal{T}) + 2\eta_{\mathcal{T}}(v_3) + (\eta_{\mathcal{T}}(v_2))^2 + 4\eta_{\mathcal{T}}(v_2) - \frac{50}{3}, \\ \geq& \frac{50n}{3} - 30 - \zeta_R(\mathcal{T}) + 18 - \frac{50}{3}, \\ >& \frac{50n}{3} - 30 - \zeta_R(\mathcal{T}) = M(n, \zeta_R). \end{aligned}$$

Therefore, we assume that $\zeta_R(\mathcal{T}) = \zeta_R(\mathcal{T}')$ and $\eta_{\mathcal{T}}(v_2) = \eta_{\mathcal{T}}(v_3) = 2$. Then, we need to have $z(v_1) = z(v_3) = 0$ and $z(v_2) = 2$ for every $\zeta_R(\mathcal{T})$-function z. It is evident that $\zeta_R(\mathcal{T}'') = \zeta_R(\mathcal{T} - \{v_1, v_2, v_3\}) + 2$ as a result. Assume that $\mathcal{T}'' = \mathcal{T} - \{v_1, v_2, v_3\}$. Consequently, $\zeta_R(\mathcal{T}'') = \zeta_R(\mathcal{T}) - 2$. We know that $|V(\mathcal{T}'')| \geq 3$ since $\Delta(\mathcal{T}) \geq 3$. $HM_1(\mathcal{T}) - HM_1(\mathcal{T}'') \geq 30 + 4\ (\eta_{\mathcal{T}}(v_4))^2 + \sum_{v \in N(v_4) - \{v_3\}} \eta_{\mathcal{T}}(v)$ is easily verifiable. Using the induction hypothesis on $\mathcal{T}''$ and the knowledge that $\zeta_R(\mathcal{T}'') = \zeta_R(\mathcal{T}) - 2$ and $max\{\eta_{\mathcal{T}}(v_4), \eta_{\mathcal{T}}(v_5)\} \geq 3$, we obtain:

$$\begin{aligned} HM_1(\mathcal{T}) \geq& HM_1(\mathcal{T}'') + 30 + 4(\eta_{\mathcal{T}}(v_4))^2 + \sum_{v \in N(v_4) - \{v_3\}} \eta_{\mathcal{T}}(v), \\ \geq& \frac{50(n-3)}{3} - 30 - (\zeta_R(\mathcal{T}) - 2) + 30 + 4\ (\eta_{\mathcal{T}}(v_4))^2 + (\eta_{\mathcal{T}}(v_5))^2, \\ \geq& \frac{50n}{3} - 30 - \zeta_R(\mathcal{T}) + 32 + 4\ (\eta_{\mathcal{T}}(v_4))^2 + (\eta_{\mathcal{T}}(v_5))^2 - \frac{150}{3}, \\ \geq& \frac{50n}{3} - 30 - \zeta_R(\mathcal{T}) + 52 - \frac{150}{3}, \\ >& \frac{50n}{3} - 30 - \zeta_R(\mathcal{T}) = M(n, \zeta_R). \end{aligned}$$

Let us assume that $\gamma_{\mathcal{T}}(v_2) = 3$. If $\gamma_{\mathcal{T}}(v_3) = 2$, we can make use of Lemma 2.2 to obtain the desired outcome. On the other hand, if $\gamma_{\mathcal{T}}(v_3) = x \geq 3$, let us define $N(v_2) = \{v_1, v_3, u_1\}$ and $N(v_3) = \{v_2, v_4, b_1, b_2, \dots, b_{x-2}\}$. Here, $\gamma_{\mathcal{T}}(b_l) = k_l$ for $l \leq x - 2$, and we set $\gamma_{\mathcal{T}}(v_4) = w$. Now consider

$\mathcal{T}'' = \mathcal{T} - \{v_1, v_2, u_1\}$. Under these conditions, we have $\zeta_R(\mathcal{T}) = \zeta_R(\mathcal{T}'') + 2$, leading to:

$$\begin{aligned} HM_1(\mathcal{T}) =& HM_1(\mathcal{T}'') + x^2 + 8x + 2w + 40 + \sum_{i=1}^{x-1}(x + k_i) - \sum_{i=1}^{x-1}(x + k_i - 1), \\ \geq& \frac{50(n-3)}{3} - 30 - (\zeta_R - 2) + x^2 + 8x + 2w + 40 + x - 2, \\ =& M(m, \zeta_R) + x^2 + 9x + 2w - 10. \end{aligned}$$

Suppose $\beta(x, w) = x^2 + 9x + 2w - 10$ if $x \geq 3$, and $w \geq 2$, then $\beta(x, w) > 0$. So, $HM_1(\mathcal{T}) \geq M(n, \zeta_R) + \beta(x, w) > M(n, \zeta_R)$.
Since $\eta_{\mathcal{T}}(v_4) = \eta_{\mathcal{T}}(v_5) = 2$, we can assume this. Since $\Delta(\mathcal{T}) \geq 3$, we can infer that $\Delta(\mathcal{T}'') \geq 3$. Given the induction hypothesis for $\mathcal{T}''$ and the knowledge that $\zeta_R(\mathcal{T}'') = \zeta_R(\mathcal{T}) - 2$, we can now calculate:

$$\begin{aligned} HM_1(\mathcal{T}) \geq& HM_1(\mathcal{T}'') + 30 + 4\ (\eta_{\mathcal{T}}(v_4))^2 + \sum_{v \in N(v_4) - \{v_3\}} \eta_{\mathcal{T}}(v), \\ \geq& \frac{50(n-3)}{3} - 30 - (\zeta_R(\mathcal{T}) - 2) + 30 + 4\ (\eta_{\mathcal{T}}(v_4))^2 + (\eta_{\mathcal{T}}(v_5))^2, \\ \geq& \frac{50n}{3} - 30 - \zeta_R(\mathcal{T}) + 32 + 4\ (\eta_{\mathcal{T}}(v_4))^2 + (\eta_{\mathcal{T}}(v_5))^2 - \frac{150}{3}, \\ \geq& \frac{50n}{3} - 30 - \zeta_R(\mathcal{T}) + 52 - \frac{150}{3}, \\ >& \frac{50n}{3} - 30 - \zeta_R(\mathcal{T}) = M(n, \zeta_R). \end{aligned}$$

Hence, the theorem is proved. □

3. Conclusion

In this study, we established a new lower bound for the $HZ_1(\mathcal{T})$ in terms of the order and RDN, given by

$$M(n, \zeta_R) = \frac{50n}{3} - 30 - \zeta_R.$$

This result provides chemists with a valuable tool for predicting molecular properties associated with stability and reactivity. Since the Hyper-Zagreb index is closely linked to the electronic structure of molecules, especially in relation to π-electron systems, this lower bound can assist in estimating molecular behavior without extensive experimental data. By understanding these mathematical bounds, chemists can better infer molecular characteristics, streamline experimental planning, and support the development of new compounds in a more efficient and theoretically grounded manner.

Declarations

Author Contribution Statement All authors contributed equally to the paper.

Declaration of competing interest The authors have no conflict of interest to disclose.

Data availability statements All the data used to find the results is included in the manuscript.

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Ethical statement This article contains no studies with humans or animals.

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