

## The Hyper-Zagreb Index of Trees and Unicyclic Graphs

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**ABSTRACT.** Topological indices are widely used as mathematical tools to analyze different types of graphs emerged in a broad range of applications. The Hyper-Zagreb index ( $HM$ ) is an important tool because it integrates the first two Zagreb indices. In this paper, we characterize the trees and unicyclic graphs with the first four and first eight greatest  $HM$ -value, respectively.

**Keywords:** Hyper-Zagreb index, Vertex degree, Unicyclic graphs, Trees.

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### 1. INTRODUCTION

A nonnegative number is assigned to a graph  $G$  to define an associated topological index if it is the same for every isomorphic graph of  $G$ , i.e., it is graph invariant. Topological indices are appropriate tools to mathematically investigate and properly comprehend molecular structures and their properties

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such as complexity [9, 10]. The first topological index is proposed by Wiener [24] in order to examine chemical features of paraffin. Since trees demonstrate a remarkable importance in various applications, authors in [4] specifically investigate this index for this setting. Moreover, In [20], the extremal unicyclic graphs with respect to Wiener index is studied. The Hyper-Wiener index for acyclic structures is due to Randic, where later [15] extends this notion so that it applies applied for any connected graphs. An interested reader can explore some chemical applications of the Hyper-Wiener index in [12]. Zagreb indices were first suggested by Gutman et al. [13] in the 1970s, which absorbed attention of many scientists in different fields. The reader is encouraged to consult with [1, 3, 11, 14, 21, 25, 27] for more useful information. A comprehensive study on relations between the mentioned indices is found in [26].

All graphs in this paper are simple, finite and undirected. The vertex and edge sets of a graph  $G$  are shown by  $V(G)$  and  $E(G)$ , respectively. Also,  $n(G)$  denotes the number of vertices of  $G$ , which is called its order.

For a graph  $G$ , the *Hyper-Zagreb index* of  $G$  is defined as the following

$$HM(G) = \sum_{xy \in E(G)} (d_G(x) + d_G(y))^2, \quad (1.1)$$

where  $d_G(x)$  is the degree of vertex  $x$ . For the edge  $xy \in E(G)$ , if consider  $h_G(xy) := (d_G(x) + d_G(y))^2$ . Then, the above formulation can be equivalently written as

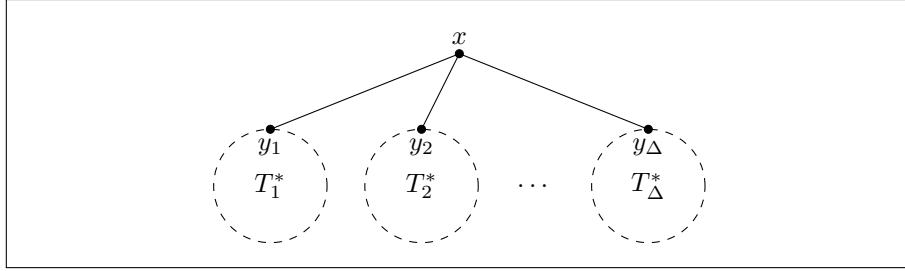
$$HM(G) = \sum_{xy \in E(G)} h_G(xy).$$

This was initially presented by Shirdel et al. [23] in 2013. They consider two simply connected graphs and compute this distance-based index for the resulted Cartesian product, composition, join and disjunction graphs. Gao et al. [7] discuss acyclic, unicyclic, and bicyclic graphs and find sharp bounds for their Hyper-Zagreb index. The degree of vertices is the main part of some other graph invariants such as irregularity and total irregularity, see [6, 17, 18, 19]. There is an extensive literature on this topic including [2, 5, 8, 22, 16].

## 2. PRELIMINARIES AND LEMMAS

In this section, we first bring several notations and definitions. Then, we propose different propositions which are essential for the subsequent section.

*Unicyclic graph*  $G$  of order  $n$  with circuit  $C_m = x_1x_2 \dots x_mx_1$  of length  $m$  is denoted by  $C_m^{u_1, u_2, \dots, u_k}(T_1, T_2, \dots, T_k)$  in which trees  $T_i$ 's for  $i = 1, 2, \dots, k$  are all nontrivial components of  $G - E(C_m)$  and  $u_i$  ( $i = 1, 2, \dots, k$ ) is the common vertex of  $T_i$  and  $C_m$ . Specially,  $G = C_n$  for  $k = 0$ . For convenience, we denote  $C_m^{u_1, u_2, \dots, u_k}(T_1, T_2, \dots, T_k)$  by  $C_m(T_1, T_2, \dots, T_k)$ , for any integer number  $k \geq 1$ . Let  $n(T_i) = l_i + 1$ ,  $i = 1, 2, \dots, k$ , then  $l = \sum_{i=1}^k l_i = n - m$ . Also, if

FIGURE 1. Tree  $T^x (T_1, T_2, \dots, T_\Delta)$ .

a tree  $T_i$  is the star  $S_{l_i+1}$  then we replace it by  $l_i$ , for example we denote  $C_4 (T_1, S_5, T_3, S_9)$  by  $C_4 (T_1, 4, T_3, 8)$ .

Let  $T$  be a tree with  $n$  vertices ( $n \geq 2$ ) such that  $x \in V(T)$  and  $x$  has a maximum degree of vertices in graph  $T$ , i.e.  $\Delta = d_T(x) = \max \{d_T(u), u \in V(T)\}$ .  $T$  is shown by  $T^x (T_1, T_2, \dots, T_\Delta)$ , where  $T_i = T_i^* + \{y_i x\}$ ,  $i = 1, 2, \dots, \Delta$ , and  $T_1^*, T_2^*, \dots, T_\Delta^*$  are trees with disjoint vertex sets and  $n_1, n_2, \dots, n_\Delta$  are numbers of their vertices, respectively. Therefore, we have  $|V(T_i)| = |V(T_i^*)| + 1 = n_i + 1$ ,  $i = 1, 2, \dots, \Delta$ , and  $n = |V(T)| = \sum_{i=1}^{\Delta} n_i + 1$  and  $y_i \in V(T_i^*)$ . Moreover,  $E(T_i) = E(T_i^*) \cup \{y_i x\}$  and  $V(T_i) = V(T_i^*) \cup \{x\}$  (see Figure 1).

The *coalescence* of  $G$  and  $H$  is denoted by  $G(u)oH(v)$  and obtained by identifying the vertex  $u$  of  $G$  with the vertex  $v$  of  $H$ .

**Lemma 2.1.** *Assume that  $z \in V(H)$  and  $\{u, w\} \subseteq V(G)$  such that the following conditions hold:*

- (a)  $d_G(u) \leq d_G(w)$ ,
- (b)  $\sum_{x \in N_G(u) \setminus \{w\}} d_G(x) \leq \sum_{x \in N_G(w) \setminus \{u\}} d_G(x)$ .

Moreover, let  $G_1 = G(u)oH(z)$  and  $G_2 = G(w)oH(z)$ , where  $G_1$  and  $G_2$  are as shown in Figure 2. Then,  $HM(G_2) \geq HM(G_1)$ , with the equality if and only if equality holds in both given conditions.

*Proof.* Recall that

$$\begin{aligned} \sum_{x \in N_G(w) \setminus \{u\}} h_{G_1}(xw) &= \sum_{x \in N_G(w) \setminus \{u\}} (d_G(x) + d_G(w))^2, \\ \sum_{x \in N_H(z)} h_{G_1}(xz) &= \sum_{x \in N_H(z)} (d_H(z) + d_G(u) + d_H(x))^2 \end{aligned}$$

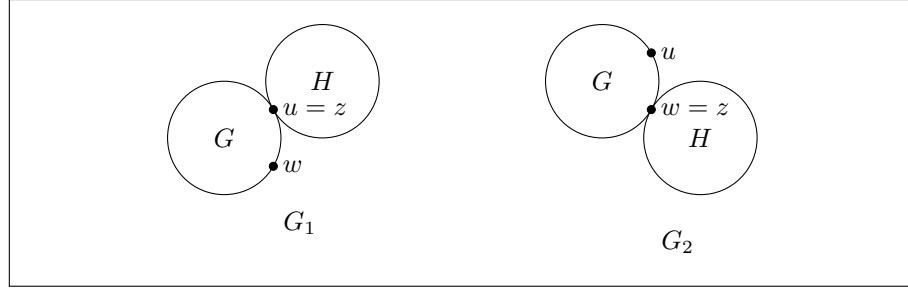


FIGURE 2. The transformation of two graphs.

and  $h_{G_1}(uw) = h_{G_2}(uw) = (d_G(z) + d_G(w) + d_H(x))^2$ . In addition, one has

$$\begin{aligned} \sum_{x \in N_H(z)} h_{G_2}(zx) &= \sum_{x \in N_H(z)} (d_H(z) + d_G(w) + d_H(x))^2, \\ \sum_{x \in N_G(u) \setminus \{w\}} h_{G_2}(xu) &= \sum_{x \in N_G(u) \setminus \{w\}} (d_G(u) + d_G(x))^2 \end{aligned}$$

and

$$\sum_{x \in N_G(w) \setminus \{u\}} h_{G_2}(xw) = \sum_{x \in N_G(w) \setminus \{x\}} (d_G(w) + d_G(x) + d_H(z))^2.$$

We consider two cases where either  $uw \in E(G)$  or  $uw \notin E(G)$ . First, suppose that  $uw \in E(G)$ . For  $i = 1$  and  $2$ , we have

$$\begin{aligned} HM(G_i) &= \sum_{\substack{xy \in E(G) \\ x, y \notin \{u, w\}}} h_G(xy) + \sum_{x \in N_G(u) \setminus \{w\}} h_{G_i}(xu) + \sum_{x \in N_G(w) \setminus \{u\}} h_{G_i}(xw) \\ &\quad + h_{G_i}(uw) + \sum_{x, y \neq z} h_H(xy) + \sum_{x \in N_H(z)} h_{G_i}(xz). \end{aligned}$$

On the other hand,

$$\sum_{x \in N_G(u) \setminus \{w\}} h_{G_1}(xu) = \sum_{x \in N_G(u) \setminus \{w\}} (d_G(u) + d_G(x) + d_H(x))^2.$$

Therefore,

$$\begin{aligned} &HM(G_2) - HM(G_1) \\ &= \sum_{x \in N_G(u) \setminus \{w\}} \left( (d_G(u) + d_G(x))^2 - (d_G(u) + d_G(x) + d_H(z))^2 \right) \\ &\quad + \sum_{x \in N_G(w) \setminus \{u\}} \left( (d_G(w) + d_G(x) + d_H(z))^2 - (d_G(w) + d_G(u))^2 \right) \\ &\quad + \sum_{x \in N_H(z)} \left( (d_H(z) + d_G(w) + d_H(x))^2 - (d_H(z) + d_G(u) + d_H(w))^2 \right) \end{aligned}$$

this implies that

$$\begin{aligned}
 HM(G_2) - HM(G_1) &\geq 2d_H(z)(d_G(u)(d_G(w) - 1) - d_G(u)(d_G(u) - 1)) \\
 &\quad + 2d_H(z) \left( \sum_{x \in N_G(w) \setminus \{u\}} d_G(u) - \sum_{x \in N_G(w) \setminus \{w\}} d_G(x) \right) \\
 &\geq 0.
 \end{aligned}$$

Now, suppose that  $uw \notin E(G)$ . Then, for  $i = 1$  and  $2$ , we have

$$\begin{aligned}
 HM(G_i) &= \sum_{\substack{xy \in E(G) \\ x, y \notin \{u, w\}}} h_G(xy) + \sum_{x \in N_G(u)} h_{G_i}(xu) + \sum_{x \in N_G(w)} h_{G_i}(xw) \\
 &\quad + \sum_{x, y \neq z} h_H(xy) + \sum_{x \in N_{G_i}} h_{G_i}(xz).
 \end{aligned}$$

Also, in this case one has

$$\sum_{x \in N_G(w) \setminus \{u\}} d_G(x) = \sum_{x \in N_G(w)} d_G(x), \quad \sum_{x \in N_G(u) \setminus \{w\}} d_G(x) = \sum_{x \in N_G(u)} d_G(x).$$

Hence, a similar approach as the previous case can be used to prove the result.  $\square$

**Lemma 2.2.** *Suppose  $u$  and  $v$  are vertices of graphs  $G_1$  and  $G_2$ , respectively. Let  $G$  be the graph obtained by joining  $u \in V(G_1)$  to  $v \in V(G_2)$  by an edge, and  $G'$  be the graph obtained by identifying  $u \in V(G_1)$  with  $v \in V(G_2)$  and attaching a pendent vertex to the common vertex as shown in Figure 3. Then if  $d_G(u), d_{G'}(v) \geq 2$ , we have  $HM(G) < HM(G')$ .*

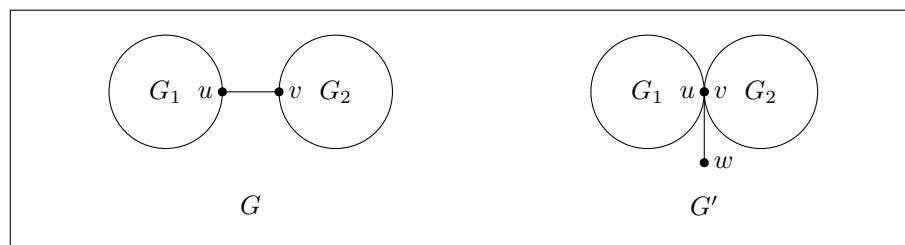


FIGURE 3. An illustration of graphs in Lemma 2.2.

*Proof.* Assume that the graph  $G'$  is obtained by identifying  $u \in V(G_1)$  with  $v \in V(G_2)$  and attaching a pendent vertex  $w$  to the common vertex. Then,

$$\begin{aligned} HM(G) = & h_G(uv) + \sum_{x \in N_{G_1}(u)} h_G(ux) + \sum_{x \in N_{G_2}(v)} h_G(vx) + \sum_{\substack{xy \in E(G_1) \\ u \notin \{x,y\}}} h_{G_1}(xy) \\ & + \sum_{\substack{xy \in E(G_2), v \notin \{x,y\}}} h_{G_2}(xy) \end{aligned}$$

and

$$\begin{aligned} HM(G') = & h_{G'}(uw) + \sum_{x \in N_{G_1}(u)} h_{G'}(ux) + \sum_{x \in N_{G_2}(v)} h_{G'}(vx) + \sum_{\substack{xy \in E(G_1) \\ u \notin \{x,y\}}} h_{G_1}(xy) \\ & + \sum_{\substack{xy \in E(G_2) \\ v \notin \{x,y\}}} h_{G_2}(xy). \end{aligned}$$

Since  $d_G(u) = d_{G_1}(u) + 1$ ,  $d_G(v) = d_{G_1}(v) + 1$ ,  $d_{G'}(w) = 1$  and  $d_{G'}(u) = d_{G'}(v) = d_{G_1}(u) + d_{G_2}(v) + 1$  we have

$$\sum_{x \in N_{G_1}(u)} h_G(ux) < \sum_{x \in N_{G_1}(u)} h_{G'}(ux), \quad \sum_{x \in N_{G_2}(v)} h_G(vx) < \sum_{x \in N_{G_2}(v)} h_{G'}(vx)$$

and  $h_G(uv) = h_{G'}(uw) = (d_{G_1}(u) + d_{G_2}(v) + 2)^2$ . Hence,

$$\begin{aligned} HM(G') - HM(G) = & \sum_{x \in N_{G_1}(u)} h_{G'}(ux) - \sum_{x \in N_{G_1}(u)} h_G(ux) \\ & + \sum_{x \in N_{G_2}(v)} h_{G'}(vx) - \sum_{x \in N_{G_2}(v)} h_G(vx) \\ & > 0. \end{aligned}$$

□

**Corollary 2.3.** Let  $T$  be a tree with  $n$  vertices. Then,  $HM(T) \leq HM(S_n)$ , with the equality if and only if  $T \cong S_n$ .

**Corollary 2.4.** Let  $G = C_m(T_1, T_2, \dots, T_k)$  be a unicyclic graph and  $n(T_i) = l_i + 1$ . Then,  $HM(G) \leq HM(C_m(l_1, l_2, \dots, l_k))$ , with the equality if and only if  $T_i \cong S_{l_i+1}$ ,  $i = 1, 2, \dots, k$ .

**Lemma 2.5.** Let  $G_1 = C_m(l_1, l_2, \dots, l_k)$  be a unicyclic graph and  $y_1u_i, u_iu_{i+1} \in E(C_m)$  such that  $d_{G_1}(y_1), d_{G_1}(u_i) \leq d_{G_1}(u_{i+1})$ , then for  $G_2 = C_m(l_1, \dots, l_{i-1}, l_{i+1} + l_i, l_{i+2}, \dots, l_k)$  one has that  $HM(G_1) < HM(G_2)$ .

*Proof.* Let  $G = C_m(l_1, \dots, l_{i-1}, l_{i+1}, l_{i+2}, \dots, l_k)$ , then  $2 = d_G(u_i) < 3 \leq d_G(u_{i+1})$ ; meaning that the condition (a) in Lemma 2.1 holds. Hence, we now

show that the second condition in this Lemma is also satisfied. Suppose that  $y_2u_{i+1} \in E(C_m)$ . By a simple calculation one can check that

$$\begin{aligned} \sum_{x \in N_G(u_i) \setminus \{u_{i+1}\}} d_G(x) &= d_G(y_1), \\ \sum_{x \in N_G(u_{i+1}) \setminus \{u_i\}} d_G(x) &= \sum_{\substack{x \in N_G(u_{i+1}) \setminus \{u_i\} \\ x \in V(C_m)}} d_G(x) + \sum_{\substack{x \in N_G(u_{i+1}) \setminus \{u_i\} \\ x \notin V(C_m)}} d_G(x) \\ &= d_G(y_2) + \sum_{\substack{x \in N_G(u_{i+1}) \setminus \{u_i\} \\ x \notin V(C_m)}} 1 \\ &= d_G(y_2) + d_G(u_{i+1}) - 2. \end{aligned}$$

Moreover,  $d_{G_1}(u_{i+1}) = d_G(u_{i+1})$  and  $d_G(y_1) = d_{G_1}(y_1)$ . On the other hand, since  $y_2 \in V(C_m)$  then  $d_G(y_2) \geq 2$ ; implying that  $d_G(y_2) - 2 \geq 0$ . So, we have

$$\sum_{x \in N_G(u_i) \setminus \{u_{i+1}\}} d_G(x) = d_G(y_1) = d_{G_1}(y_1) \leq d_{G_1}(u_{i+1}) = d_G(u_{i+1}) \leq \sum_{x \in N_G(u_{i+1}) \setminus \{u_i\}} d_G(x).$$

Therefore, the condition (b) of Lemma 2.1 holds, which completes the proof.  $\square$

**Lemma 2.6.** *Let  $G = C_m^{u_1, u_2, \dots, u_k} (l_1, l_2, \dots, l_k)$  be a unicyclic graph and  $k > 1$ . Then if  $u_i u_{i+1} \in E(C_m)$ ,  $i = 1, 2, \dots, k-1$ , then  $HM(G) < HM(C_m(n-m))$ . Otherwise, there exist positive integers  $l'_1, l'_2, \dots, l'_r$  ( $r \leq k$ ), such that  $HM(G) < HM(G') < HM(G'')$ , where  $G' = C_m^{v_1, v_2, \dots, v_r} (l'_1, l'_2, \dots, l'_r)$ ,  $G'' = C_m^{v_2, v_3, \dots, v_r} (l'_1 + l'_2, l'_3, \dots, l'_r)$ ,  $d_{G'}(v_i, v_j) \geq 2$  for  $1 \leq i < j \leq r$  and  $\{v_1, v_2, \dots, v_r\} \subseteq \{u_1, u_2, \dots, u_k\}$ .*

*Proof.*  $HM(G) < HM(G')$  is straightforward in light of Lemma 2.5. Now, by considering  $u = v_1, w = v_2$ ,  $H = S_{l'_1+1}$  and  $G = C_m^{v_2, v_3, \dots, v_r} (l'_2, l'_3, \dots, l'_r)$  and using Lemma 2.1 we can conclude that  $HM(G') < HM(G'')$ , as desired.  $\square$

**Lemma 2.7.** *Let  $G = C_m (l_1, l_2, \dots, l_k)$  be a unicyclic graph of order  $n$ . Then  $HM(G) \leq HM(C_m(n-m))$ , with equality if and only if  $k = 1$ .*

*Proof.* The proof is obtained by applying Lemmas 2.5 and 2.6.  $\square$

**Corollary 2.8.** *Let  $G = C_m (T_1, T_2, \dots, T_k)$  be a unicyclic graph and  $n(T_i) = l_i + 1$ ,  $i = 1, 2, \dots, k$ . Then,*

$$HM(G) \leq HM(C_m(l_1, l_2, \dots, l_k)) \leq HM(C_m(n-m)),$$

*with left equality if and only if  $T_i \cong S_{l_i+1}$ ,  $i = 1, 2, \dots, k$ , and right equality if and only if  $k = 1$ .*

**Lemma 2.9.** *Let  $G_1 = C_m(n-m)$  and  $G_2 = C_{m-1}(n-m+1)$ ,  $m \geq 4$ , be unicyclic graphs of order  $n$ . Then,  $HM(G_1) < HM(G_2)$ .*

*Proof.* By a simple calculation we have

$$\begin{aligned} HM(G_1) &= 4(m-2) + 2(n-m+4)^2 + (n-m)(n-m+3)^2 \\ &< 4(m-3) + 2(n-m+5)^2 + (n-m+1)(n-m+4)^2 \\ &= HM(G_2). \end{aligned}$$

As desired.  $\square$

**Lemma 2.10.** *Let  $G = C_m(T_1, T_2, \dots, T_k)$  be a unicyclic graph. Then,*

$$HM(G) = \sum_{i=1}^k \sum_{xy \in E(T_i)} h_G(xy) + \sum_{xy \in E(C_m)} h_G(xy).$$

*Proof.* The proof is trivial by the Hyper-Zagreb index definition (1.1).  $\square$

### 3. MAIN RESULTS

In this section, we characterize the trees and unicyclic graphs with the first four and first eight greatest HM-value, respectively.

**Theorem 3.1.** *Let  $T$  be a tree with  $n$  vertices. If  $T \not\cong S_n, T_n^1$  or  $T_n^2$ , then*

$$HM(T) \leq HM(T_n^3) < HM(T_n^2) < HM(T_n^1) < HM(S_n),$$

*with the equality if and if  $T \cong T_n^3$ , where  $T_n^1, T_n^2$  and  $T_n^3$  are given as in Figure 4.*

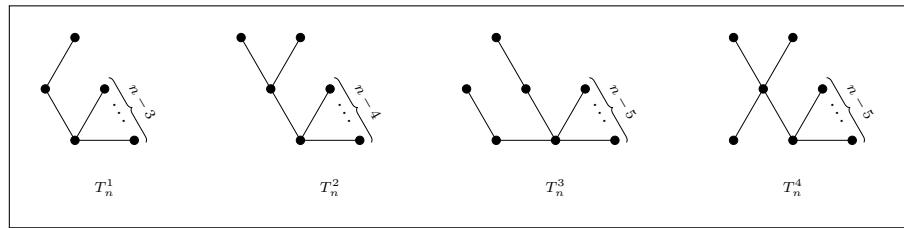


FIGURE 4. Some trees with large Hyper-Zagreb values.

Graph	HM-value
$S_n$	$n^3 - n^2$
$T_n^1$	$n^3 - 4n^2 + 7n + 6$
$T_n^2$	$n^3 - 7n^2 + 20n + 16$
$T_n^3$	$n^3 - 7n^2 + 20n$

TABLE 1. Trees with large Hyper-Zagreb values.

*Proof.* Using Table 1, we have  $HM(S_n) > HM(T_n^1) > HM(T_n^2) > HM(T_n^3)$ . Hence, we need to prove that  $HM(T) < HM(T_n^3)$  when  $T \not\cong T_n^3$ . Let  $T = T^x(T_1, T_2, \dots, T_\Delta)$ , where  $\Delta = d_T(x)$ . By Corollary 2.3, we have  $HM(T_i) \leq HM(S_{n_i})$ ,  $i = 1, 2, \dots, \Delta$ . Moreover, let  $T' = T^x(T'_1, T'_2, \dots, T'_\Delta)$ , where  $T'^*_i = S_{n_i}$ ,  $i = 1, 2, \dots, \Delta$ , then we have  $HM(T) \leq HM(T')$ . To complete the proof, we consider three different cases as follows:

*Case 1:* assume that  $d_T(y_i) = 1$ ,  $i = 1, 2, \dots, \Delta$ , then  $T = S_n$ . This is a contradiction to the assumption.

*Case 2:* assume that there exists  $y_t$  for  $t = 1, 2, \dots, \Delta$  such that  $d_T(y_t) \geq 2$  and  $d_T(y_i) = 1$  for  $i = 1, 2, \dots, \Delta$  and  $i \neq t$ . In this case, there are three subcases that can happen:

- (i) If  $|V(T_t^*)| = 2$ , then  $T \cong T_1^n$ . This is clearly a contradiction.
- (ii) If  $|V(T_t^*)| = 3$ , then we must consider that  $d_T(y_t) = 2$  or 3. The case  $d_T(y_t) = 3$  implies that  $T \cong T_n^2$ , which is a contradiction. If  $d_T(y_t) = 2$ , then

$$\begin{aligned} HM(T) &= (n-4)(n-2)^2 + (n-1)^2 + 16 + 9 \\ &= n^3 - 7n^2 + 18n + 10 \\ &< n^3 - 7n^2 + 20n \\ &= HM(T_n^3). \end{aligned}$$

- (iii) If  $|V(T_t^*)| \geq 4$ , then  $T = T^x \left( \overbrace{S_2, \dots, S_2}^{t-1 \text{ times}}, T_t, \overbrace{S_2, \dots, S_2}^{\Delta-t \text{ times}} \right)$ . By Corollary 2.3, the Hyper-Zagreb index for  $T$  is maximum when  $T_t^* = S_{n_t}$ . On the other hand, it follows from Lemma 2.1 that if  $n_t = 4$  than  $T$  has maximum  $HM$ -value, i.e. in this case  $T$  has maximum  $HM$ -value when  $T \cong T_n^4$  (see Figure 4). Hence, applying Lemma 2.1, it is clear that  $HM(T) \leq HM(T_n^4) < HM(T_n^3)$ .

*Case 3:* Suppose that there exist  $1 \leq s, t \leq \Delta$  such that  $d_T(y_s), d_T(y_t) \geq 2$ . Similar to previous, applying Corollary 2.3 and Lemma 2.1, it can concluded that  $HM(T) < HM(T_n^3)$ .  $\square$

**Theorem 3.2.** *Let  $G$  be a unicyclic graph of order  $n \geq 15$ . If  $G \not\cong C_3(n-3)$ ,  $C_3(1, n-4)$ ,  $C_3(T_{n-2}^1)$ ,  $C_4(n-2)$ ,  $C_3(2, n-5)$ ,  $C_3(1, 1, n-5)$  and  $C_3(T_{n-2}^2)$ . Then,*

$$\begin{aligned} HM(G) &\leq HM(C_3(T_{n-2}^3)) < HM(C_3(T_{n-2}^2)) < HM(C_3(1, 1, n-5)) \\ &< HM(C_3(2, n-5)) < HM(C_4(n-4)) < HM(C_3(T_{n-2}^1)) \\ &< HM(C_3(1, n-4)) < HM(C_3(n-3)), \end{aligned}$$

with the equality if and only if  $G \cong C_3(T_{n-2}^3)$  or  $G \cong C_3(P_3, 10)$  for  $n = 15$  (see Figure 5).

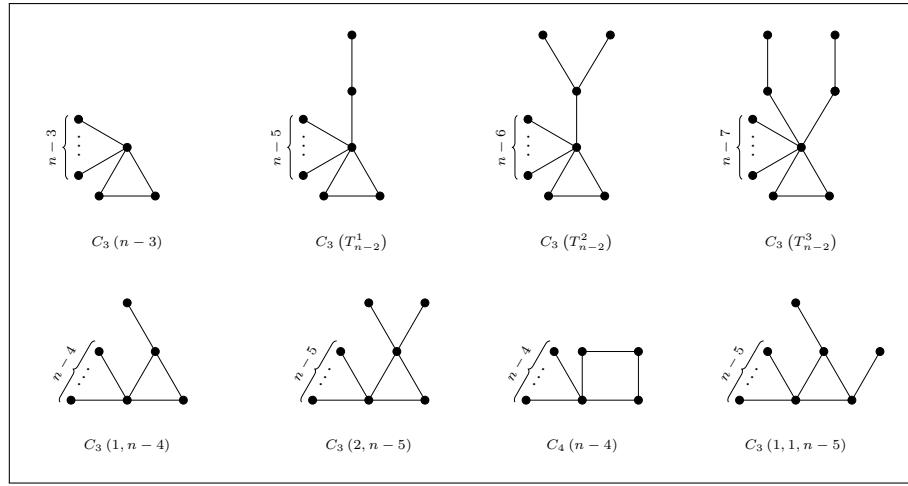


FIGURE 5. The unicyclic graphs with the first eight greatest Hyper-Zagreb.

Graph	HM-value
$C_3(n-3)$	$n^3 - n^2 + 4n + 18$
$C_3(1, n-4)$	$n^3 - 4n^2 + 11n + 38$
$C_3(T^1_{n-2})$	$n^3 - 4n^2 + 11n + 20$
$C_4(n-4)$	$n^3 - 4n^2 + 9n + 28$
$C_3(2, n-5)$	$n^3 - 7n^2 + 24n + 68$
$C_3(1, 1, n-5)$	$n^3 - 7n^2 + 24n + 48$
$C_3(T^2_{n-2})$	$n^3 - 7n^2 + 24n + 26$
$C_3(T^3_{n-2})$	$n^3 - 7n^2 + 24n + 10$

TABLE 2. Unicyclic graphs with large Hyper-Zagreb values.

*Proof.* Assume that  $G = C_m(T_1, T_2, \dots, T_k)$  be a unicyclic graph and  $n(T_i) = l_i + 1$ ,  $i = 1, 2, \dots, k$ . The given Table 2 provides the Hyper-Zagreb index of some graphs by which the result is trivial. It is enough to discuss about the equality case. If  $G \cong C_3(T^3_{n-2})$ , then  $HM(G) = HM(C_3(T^3_{n-2}))$ . Also, if  $G \cong C_3(P_3, 10)$  for  $n = 15$ , then  $HM(G) = 2170 = HM(C_3(T^3_{13}))$ . We now prove that  $HM(G) < HM(C_3(T^3_{n-2}))$ , where  $G \not\cong C_3(n-3)$ ,  $C_3(1, n-4)$ ,  $C_3(T^1_{n-2})$ ,  $C_4(n-2)$ ,  $C_3(2, n-5)$ ,  $C_3(1, 1, n-5)$  and  $C_3(T^2_{n-2})$ . We examine three cases of  $m = 3, 4$  and  $5$  for  $G = C_m(T_1, T_2, \dots, T_k)$  as follows:

*Case 1:*  $m = 3$ . We need to discuss three subcases that  $k = 1, 2$  and  $3$ .

(i)  $k = 1$ , then  $G = C_3(T_1)$ . By assumption, we know that  $T_1 \not\cong S_{n-2}, T_{n-2}^1, T_{n-2}^2$  and  $T_{n-2}^3$ . So, Theorem 3.1 implies that  $HM(T_1) < HM(T_{n-2}^3)$ . By Lemma 2.10, we get  $HM(G) < HM(C_3(T_{n-2}^3))$ .

(ii)  $k = 2$ , then  $G = C_3(T_1, T_2)$ . By assumption,  $G \not\cong C_3(1, n-4)$  and  $C_3(2, n-5)$ . By Corollaries 2.3, 2.4 and Lemmas 2.1, 2.10, the maximum value of  $HM(G)$  happens when  $G \cong C_3(3, n-6)$  or  $C_3(P_3, n-5)$ . The first case yields that

$$HM(G) \leq HM(C_3(3, n-6)) = n^3 - 10n^2 + 43n + 108.$$

Hence, we have (for  $n \geq 15$ ) that

$$\begin{aligned} HM(C_3(T_{n-3}^3)) - HM(G) &\geq HM(C_3(T_{n-3}^3)) - HM(C_3(3, n-6)) \\ &= (n^3 - 7n^2 + 24n + 10) \\ &\quad - (n^3 - 10n^2 + 43n + 108) \\ &= 3n^2 - 19n - 98 \\ &> 0. \end{aligned}$$

Similarly, for the second case we have

$$\begin{aligned} HM(C_3(T_{n-3}^3)) - HM(G) &\geq HM(C_3(T_{n-3}^3)) - HM(C_3(P_3, n-5)) \\ &= (n^3 - 7n^2 + 24n + 10) - (n^3 - 7n^2 + 22n + 40) \\ &= 2n - 30 \\ &> 0. \end{aligned}$$

This means that in both cases  $HM(G) < HM(C_3(T_{n-2}^3))$ .

(iii)  $k = 3$ , then  $G = C_3(T_1, T_2, T_3)$ . By Corollary 2.4, it is simple to see that  $HM(G) \leq HM(C_3(l_1, l_2, l_3))$ . On the other hand, since by assumption  $G \not\cong C_3(1, 1, n-5)$ , the Hyper-Zagreb index attains its maximum when  $G \cong C_3(1, 2, n-6)$ . Hence,

$$\begin{aligned} HM(C_3(T_{n-3}^3)) - HM(G) &\geq HM(C_3(T_{n-3}^3)) - HM(C_3(1, 2, n-6)) \\ &= (n^3 - 7n^2 + 24n + 10) - (n^3 - 10n^2 + 43n + 62) \\ &> 0. \end{aligned}$$

*Case 2:  $m = 4$ .* This needs to be analyzed for  $k = 1, 2, 3$  and 4.

(i)  $k = 1$ , then  $G = C_4(T_1)$ . Since  $G \not\cong C_4(n-4)$ , we have  $T_1 \not\cong S_{n-3}$ . Note that  $G$  has a maximum value of the Hyper-Zagreb index if  $T_1 \cong T_{n-3}^1$  by Theorem 3.1 and Lemma 2.10. Moreover, we have (for  $n \geq 15$ )

$$\begin{aligned} HM(C_3(T_{n-3}^3)) - HM(G) &\geq HM(C_3(T_{n-3}^3)) - HM(C_4(T_{n-3}^1)) \\ &= (n^3 - 7n^2 + 24n + 10) - (n^3 - 7n^2 + 22n + 20) \\ &> 0. \end{aligned}$$

(ii)  $k = 2$ , then  $G = C_4^{u_1, u_2}(T_1, T_2)_\alpha = C_4(T_1, T_2)_\alpha$ , where  $\alpha = d_G(u_1, u_2)$ .

By Lemma 2.1,  $G$  attains maximum  $HM$ -value if  $G \cong C_4(l_1, l_2)_{\alpha=1}$ .

This lemma also implies that

$$HM(C_4(l_1, l_2))_{\alpha=1} \leq HM(C_4(1, n-5))_{\alpha=1} = n^3 - 7n^2 + 22n + 38.$$

Therefore, for  $n \geq 15$ , we have

$$HM(G) \leq n^3 - 7n^2 + 22n + 38 < n^3 - 7n^2 + 24n + 10 = HM(C_3(T_{n-2}^3)).$$

(iii)  $k = 3$ , then  $G$  is considered as  $C_4(T_1, T_2, T_3)$ . By Corollary 2.4 and Lemmas 2.1, 2.10, for  $n \geq 15$  we have

$$\begin{aligned} HM(C_3(T_{n-2}^3)) - HM(G) &\geq HM(C_3(T_{n-2}^3)) - HM(C_4(l_1, l_2, l_3)) \\ &> HM(C_3(T_{n-2}^3)) - HM(C_4(1, n-5))_{\alpha=1} \\ &= (n^3 - 7n^2 + 24n + 10) - (n^3 - 7n^2 + 22n + 38) \\ &> 0. \end{aligned}$$

(iv)  $k = 4$ , then  $G = C_4(T_1, T_2, T_3, T_4)$ . In a similar way, one can see easily that  $HM(G) < HM(C_3(T_{n-2}^3))$ ; completing the proof of the second case.

*Case 3:*  $m \geq 5$ . Using Lemmas 2.9, 2.10 and Corollaries 2.3, 2.8, we conclude that (for  $n \geq 15$ )

$$\begin{aligned} HM(C_3(T_{n-2}^3)) - HM(G) &\geq HM(C_3(T_{n-2}^3)) - HM(C_m(l_1, l_2, \dots, l_k)) \\ &\geq HM(C_3(T_{n-2}^3)) - HM(C_m(n-m)) \\ &\geq HM(C_3(T_{n-2}^3)) - HM(C_5(n-5)) \\ &= (n^3 - 7n^2 + 24n + 10) - (n^3 - 7n^2 + 20n + 30) \\ &> 0. \end{aligned}$$

□

#### 4. CONCLUSION

In this paper, we studied the Hyper-Zagreb index and characterized the trees and unicyclic graphs with the first four and first eight greatest  $HM$ -value. It would be of interest to investigate its behavior on other classes of graphs with simple connectivity patterns and cyclic structures.

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