



## Extremal $c$ -cyclic graphs with respect to the general multiplicative first Zagreb index

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**Abstract.** The general multiplicative first Zagreb index of a simple graph  $H$  is expressed as the product of the weights  $(\deg_H(\omega))^\alpha$  over all vertices  $\omega$  of  $H$ , where  $\deg_H(\omega)$  shows the degree of  $\omega$ , and  $\alpha \neq 0$  is a real number. The cyclomatic number of a connected graph  $H$  is given by  $c = \epsilon - \nu + 1$ , where  $\epsilon$  and  $\nu$  are the size and order of  $H$ , respectively. In this paper, we present sharp bounds for the general multiplicative first Zagreb index of simple connected graphs with cyclomatic number  $c$  focusing on the cases when  $c=0, 1$ , and  $2$ . We also extend our findings to molecular trees and to all simple connected graphs with the maximum degree  $\Delta$  and cyclomatic number  $c$ , where  $\Delta \geq 2c$ . In addition, we identify the graphs reaching these bounds.

### 1. Introduction

Denote by  $H$  a simple connected graph, by  $V(H)$  its vertex set, and by  $E(H)$  its edge set. For  $\omega \in V(H)$ , the set  $N_H(\omega) = \{v \in V(H) : \omega v \in E(H)\}$  is called the open neighborhood of  $\omega$  in  $H$ . The degree  $\deg_H(\omega)$  of  $\omega$  is the cardinality of  $N_H(\omega)$  and the distance  $d_H(\omega, v)$  between  $\omega, v \in V(H)$  is the number of edges in any shortest  $(\omega, v)$ -path in  $H$ . A pendant vertex is a vertex of degree 1. If  $|V(H)| = \nu$  and  $|E(H)| = \epsilon$ , then the number  $c = \epsilon - \nu + 1$  is called the cyclomatic number of  $H$ . Trees, unicyclic graphs, and bicyclic graphs are simple connected graphs whose cyclomatic numbers are  $c = 0$ ,  $c = 1$ , and  $c = 2$ , respectively. For any notations and terminology not introduced in this work, readers are directed to consult standard references in graph theory, such as Bondy and Murty [4] and West [36].

Vertex-degree-based topological indices are graph invariants whose formulas are dependent to the vertex degrees of the graph. These indices are useful in analyzing different properties of chemical structures including the viscosity, entropy, enthalpy of vaporization, gyration radius, boiling point, etc (see for example [16]).

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The first Zagreb index [12] is among the oldest and the best-known vertex-degree-based indices in mathematical chemistry. It was considered in 1972 by Gutman and Trinajstić within studying the total  $\pi$ -electron energy of alternant hydrocarbons. It is expressed for a graph  $H$  as

$$M_1(H) = \sum_{\omega \in V(H)} (\deg_H(\omega))^2.$$

Alternatively, it can be defined as

$$M_1(H) = \sum_{v\omega \in E(H)} (\deg_H(v) + \deg_H(\omega)).$$

The first Zagreb index reflects the extent of branching of the molecular carbon-atom skeleton [26]. For comprehensive, transparent information on the first Zagreb index, see [2, 5, 9, 20, 24, 38, 40] and the references given therein.

In the last decades, various variants of the first Zagreb index have been put forward [11], among which the first multiplicative Zagreb index attracted much attention. This index was proposed by Todeschini and Consonni [27] in 2010 and formulated for a graph  $H$  as

$$\Pi_1(H) = \prod_{\omega \in V(H)} (\deg_H(\omega))^2.$$

It should be noted that the  $\Pi_1$  index is the square of the Narumi-Katayama index [3, 19, 21] given by

$$NK(H) = \prod_{\omega \in V(H)} \deg_H(\omega).$$

The mathematical and chemical properties of the  $\Pi_1$  index have been well examined in the literature. We refer readers to [8, 10, 18, 19, 25, 28, 32–35, 37] for its extremal problems, [7, 13] for its behavior under composite graphs, [17] for the examination over Eulerian graphs and [23, 39] for studying through molecular graphs.

In 2018, Vetrík and Balachandran [29] proposed a generalization for the  $\Pi_1$  index. This invariant, named the general multiplicative first Zagreb index, is formulated by

$$P_1^\alpha(H) = \prod_{\omega \in V(H)} (\deg_H(\omega))^\alpha,$$

where  $\alpha \neq 0$  is a real quantity. Note that the cases  $\alpha = 1, 2$  pertain to the Narumi-Katayama index and first multiplicative Zagreb index, respectively.

Some extremal problems on the general multiplicative first Zagreb index have been examined so far. Vetrík and Balachandran [29] obtained the extreme values of the  $P_1^\alpha$  index for trees with a given order, a given number of branching vertices, a given number of pendant vertices, and a given number of segments, and determined the related extremal trees. In addition, they presented bounds (lower and upper) on the  $P_1^\alpha$  index for trees and unicyclic graphs of a given order and perfect matching and of a given order and matching number and determined the trees and unicyclic graphs that reach the bounds [31]. Vetrík and Balachandran [30] also examined the  $P_1^\alpha$  index for graphs with a given clique number. Alfuraidean *et al.* [1] examined the  $P_1^\alpha$  index for graphs with a low cyclomatic number. Javed *et al.* [15] considered the extremal  $(v, e)$ -graphs with respect to the  $P_1^\alpha$  index. Ismail *et al.* [14] presented a unified approach for the extreme values of the exponential of  $P_1^\alpha$  index over bicyclic, unicyclic, and tree graphs. Du and Sun [6] examined the extreme values of quasi-unicyclic graphs with respect to the  $P_1^\alpha$  index. Noureen *et al.* [22] investigated the importance of the  $P_1^\alpha$  index in anticipation of the enthalpy of formation of hydrocarbons. They also studied chemical trees with a given order and a given number of branching vertices or segments with respect to  $P_1^\alpha$  index.

In this paper, we aim to find the solutions for some other extremal problems on the  $P_1^\alpha$  index. More precisely, we present sharp bounds on the  $P_1^\alpha$  index within the class of all simple connected graphs with cyclomatic number  $c$ , in the special cases where  $c = 0, 1$ , and  $2$ . The results are extended to all molecular trees (trees with maximum degree 4 or less) and to all graphs with the maximum degree  $\Delta$  and cyclomatic number  $c$  for which  $\Delta \geq 2c$ . In addition to the extremal values, the respective extremal graphs are determined.

## 2. Trees

In this section,  $\mathcal{T}(v, \Delta)$  indicates the family of trees on  $v$  vertices whose maximum degree is  $\Delta$ . A tree with a special vertex selected as the root is called a rooted tree. A tree with at most one vertex of degree greater than two is called a spider and the vertex possessing the maximum degree is its center (see Figure 1). A path between the center and any pendant vertex of the spider is called a leg. By convention, a path on  $v$  vertices, denoted by  $P_v$ , may be regarded as a spider with one or two legs.

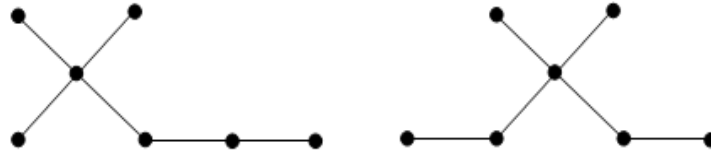


Figure 1: The spider graphs with  $v = 7$  and  $\Delta = 4$ .

**Lemma 2.1.** Denote by  $T$  a tree in  $\mathcal{T}(v, \Delta)$  rooted at  $\omega$ , where  $\deg_T(\omega) = \Delta$ . If  $T$  contains a vertex other than  $\omega$  with degree three or more, then  $\mathcal{T}(v, \Delta)$  includes a tree  $T_1$  with  $P_1^\alpha(T_1) < P_1^\alpha(T)$  if  $\alpha < 0$  and  $P_1^\alpha(T_1) > P_1^\alpha(T)$  if  $\alpha > 0$ .

*Proof.* Denote by  $v$  an element of the set  $\{u \in V(T) : u \neq \omega, \deg_T(u) \geq 3\}$ , having the greatest distance from  $\omega$ . Let  $N_T(v) = \{v_1, v_2, \dots, v_k\}$ , and  $v_k$  be on the path in  $T$  from  $\omega$  to  $v$ . Then  $\deg_T(v_i) \in \{1, 2\}$  for  $1 \leq i \leq k-1$ . Therefore there exists three cases.

**Case 1.** There are at least two pendant vertices in  $N_T(v)$ .

Suppose that  $v_1$  and  $v_2$  are two pendant vertices and let  $T_1 = (T - \{vv_1\}) \cup \{v_1v_2\}$ . Then

$$\begin{aligned} \frac{P_1^\alpha(T)}{P_1^\alpha(T_1)} &= \frac{(\deg_T(v_1))^\alpha (\deg_T(v_2))^\alpha (\deg_T(v))^\alpha}{(\deg_{T_1}(v_1))^\alpha (\deg_{T_1}(v_2))^\alpha (\deg_{T_1}(v))^\alpha} \\ &= \frac{1^\alpha 1^\alpha k^\alpha}{1^\alpha 2^\alpha (k-1)^\alpha} = \left( \frac{k}{2(k-1)} \right)^\alpha. \end{aligned}$$

Since  $k \geq 3$ , then  $\frac{k}{2(k-1)} < 1$ . Therefore, if  $\alpha > 0$ , then  $P_1^\alpha(T_1) > P_1^\alpha(T)$  and if  $\alpha < 0$ , then  $P_1^\alpha(T_1) < P_1^\alpha(T)$ .

**Case 2.** There is exactly one pendant vertex in  $N_T(v)$ .

Suppose that  $v_1$  is a pendant vertex and  $vu_1u_2 \dots u_l$  ( $l \geq 2$ ) is a path in  $T$  and  $u_1 = v_2$ . Let  $T_1 = (T - \{vv_1\}) \cup \{v_1u_l\}$ . Then

$$\begin{aligned} \frac{P_1^\alpha(T)}{P_1^\alpha(T_1)} &= \frac{(\deg_T(v_1))^\alpha (\deg_T(u_l))^\alpha (\deg_T(v))^\alpha}{(\deg_{T_1}(v_1))^\alpha (\deg_{T_1}(u_l))^\alpha (\deg_{T_1}(v))^\alpha} \\ &= \frac{1^\alpha 1^\alpha k^\alpha}{1^\alpha 2^\alpha (k-1)^\alpha} = \left( \frac{k}{2(k-1)} \right)^\alpha. \end{aligned}$$

Since  $k \geq 3$ , then  $\frac{k}{2(k-1)} < 1$ . Therefore, if  $\alpha > 0$ , then  $P_1^\alpha(T_1) > P_1^\alpha(T)$  and if  $\alpha < 0$ , then  $P_1^\alpha(T_1) < P_1^\alpha(T)$ .

**Case 3.** All vertices in  $N_T(v)$  except  $v_k$  have degree two.

Let  $vx_1x_2\dots x_t$  and  $vu_1u_2\dots u_l$  be two paths in  $T$  with  $x_1 = v_1$ ,  $u_1 = v_2$  and  $t, l \geq 2$ . Assume that  $T_1 = (T - \{vv_1\}) \cup \{v_1u_l\}$ . Then

$$\begin{aligned}\frac{P_1^\alpha(T)}{P_1^\alpha(T_1)} &= \frac{(\deg_T(u_l))^\alpha (\deg_T(v))^\alpha}{(\deg_{T_1}(u_l))^\alpha (\deg_{T_1}(v))^\alpha} \\ &= \frac{1^\alpha k^\alpha}{2^\alpha (k-1)^\alpha} = \left(\frac{k}{2(k-1)}\right)^\alpha.\end{aligned}$$

Since  $k \geq 3$ , then  $\frac{k}{2(k-1)} < 1$ . Therefore, if  $\alpha > 0$ , then  $P_1^\alpha(T_1) > P_1^\alpha(T)$  and if  $\alpha < 0$ , then  $P_1^\alpha(T_1) < P_1^\alpha(T)$ .  $\square$

The proof of Lemma 2.1 did not depend on the degree of the root vertex. By the same argument, one can obtain a similar lemma for rooted trees whose roots can be on vertices of arbitrary degree.

**Lemma 2.2.** Denote by  $T$  a tree in  $\mathcal{T}(v, \Delta)$  rooted at  $\omega$ , where  $\deg_T(\omega) = k$ . If  $T$  contains a vertex other than  $\omega$  of degree three or more, then  $\mathcal{T}(v, \Delta)$  includes a tree  $T_1$  with  $P_1^\alpha(T_1) < P_1^\alpha(T)$  if  $\alpha < 0$  and  $P_1^\alpha(T_1) > P_1^\alpha(T)$  if  $\alpha > 0$ .

Here is the first main theorem of this paper.

**Theorem 2.3.** If  $T \in \mathcal{T}(v, \Delta)$ , then

$$P_1^\alpha(T) \geq \Delta^\alpha 2^{(v-\Delta-1)\alpha},$$

when  $\alpha < 0$  and

$$P_1^\alpha(T) \leq \Delta^\alpha 2^{(v-\Delta-1)\alpha},$$

when  $\alpha > 0$ . The equality occurs if and only if  $T$  is a spider.

*Proof.* Let  $\alpha < 0$  (resp.  $\alpha > 0$ ) and  $T_1 \in \mathcal{T}(v, \Delta)$  such that  $P_1^\alpha(T) \geq P_1^\alpha(T_1)$  (resp.  $P_1^\alpha(T_1) \geq P_1^\alpha(T)$ ) for all  $T \in \mathcal{T}(v, \Delta)$ . Distinguish a vertex  $\omega \in V(T_1)$  with  $\deg_{T_1}(\omega) = \Delta$  as the root of  $T_1$ . By Lemma 2.1,  $T_1$  must be a spider whose center is  $\omega$ . Then  $P_1^\alpha(T) \geq P_1^\alpha(T_1) = \Delta^\alpha 2^{(v-\Delta-1)\alpha}$ , when  $\alpha < 0$  and  $P_1^\alpha(T) \leq P_1^\alpha(T_1) = \Delta^\alpha 2^{(v-\Delta-1)\alpha}$ , when  $\alpha > 0$ .  $\square$

From Theorem 2.3 the next corollaries are concluded.

**Corollary 2.4.** Denote by  $T$  a molecular tree of order  $v$  and  $\Delta = 4$ . Then  $P_1^\alpha(T) \geq 4^\alpha 2^{(v-5)\alpha}$ , when  $\alpha < 0$  and  $P_1^\alpha(T) \leq 4^\alpha 2^{(v-5)\alpha}$ , when  $\alpha > 0$ . The equality happens if and only if  $T$  is a molecular tree with exactly one vertex of degree more than two.

**Corollary 2.5.** Denote by  $T$  a molecular tree of order  $v$  and  $\Delta = 3$ . Then  $P_1^\alpha(T) \geq 3^\alpha 2^{(v-4)\alpha}$ , when  $\alpha < 0$  and  $P_1^\alpha(T) \leq 3^\alpha 2^{(v-4)\alpha}$ , when  $\alpha > 0$ . The equality happens if and only if  $T$  is a molecular tree with exactly one vertex of degree more than two.

**Lemma 2.6.** The function  $f(y) = y^\alpha 2^{(v-y-1)\alpha}$  for  $y \geq 2$  is decreasing when  $\alpha > 0$  and is increasing when  $\alpha < 0$ .

*Proof.* If  $f(y) = y^\alpha 2^{(v-y-1)\alpha}$ , then

$$\begin{aligned}f'(y) &= \alpha y^{\alpha-1} 2^{(v-y-1)\alpha} - \alpha \ln(2) y^\alpha 2^{(v-y-1)\alpha} \\ &= \alpha y^{\alpha-1} 2^{(v-y-1)\alpha} (1 - y \ln(2)).\end{aligned}$$

Since  $y \geq 2$ , then  $1 - y \ln(2) \leq 1 - 2 \ln(2) \approx -0.3862$ . Thus  $f(y)$  is decreasing when  $\alpha > 0$  and is increasing when  $\alpha < 0$ .  $\square$

The following result reported in [29] is a direct consequence of Theorem 2.3 and Lemma 2.6.

**Corollary 2.7.** [29] If  $T$  is a  $v$ -vertex tree, then  $P_1^\alpha(T) \geq 2^{(v-2)\alpha}$ , when  $\alpha < 0$  and  $P_1^\alpha(T) \leq 2^{(v-2)\alpha}$ , when  $\alpha > 0$ . The equality happens if and only if  $T = P_v$ .

### 3. Unicyclic graphs

Throughout this section,  $\mathcal{U}(v, \Delta)$  indicates the family of  $v$ -vertex unicyclic graphs whose maximum degree is  $\Delta$ . A unicyclic graph containing at most one vertex of degree 3 or more is called a cephalopod graph (see Figure 2). The vertex possessing the maximum degree is its center and the paths attached to the center are its arms.

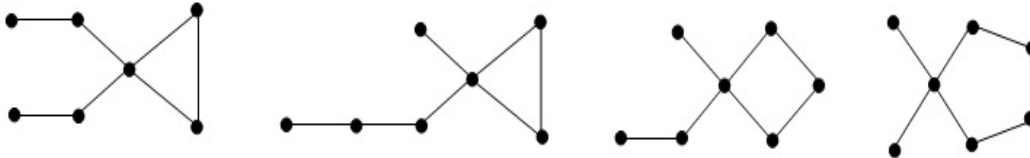


Figure 2: The cephalopod graphs with  $v = 7$  and  $\Delta = 4$ .

**Lemma 3.1.** Let  $U \in \mathcal{U}(v, \Delta)$  in which the degree of the vertices on its unique cycle is not equal to  $\Delta$ . Then  $\mathcal{U}(v, \Delta)$  possesses a unicyclic graph  $U_1$  having the vertex of maximum degree  $\Delta$  on its cycle with  $P_1^\alpha(U_1) < P_1^\alpha(U)$  if  $\alpha < 0$  and  $P_1^\alpha(U_1) > P_1^\alpha(U)$  if  $\alpha > 0$ .

*Proof.* Assume that  $\deg_U(v) = \Delta$  and let  $u \in V(U)$  with  $\deg_U(u) = k \geq 3$  lies on the cycle of  $U$ , for which  $d_U(v, u)$  is the minimum. Suppose that  $N_U(u) = \{u_1, u_2, \dots, u_k\}$  and  $N_U(v) = \{v_1, v_2, \dots, v_\Delta\}$ , where  $v_\Delta$  is on  $(u, v)$ -path.

Denote by  $T_v$  the rooted tree possessing the maximum possible number of vertices connected to  $v$  and  $v_\Delta \notin V(T_v)$ . By Lemma 2.2, we can convert  $T_v$  to a spider  $T'_v$  on the same order and  $\deg_{T'_v}(v) = \Delta - 1$  legs centered at  $v$ , for that  $P_1^\alpha(T'_v) \leq P_1^\alpha(T_v)$  if  $\alpha < 0$  and  $P_1^\alpha(T'_v) \geq P_1^\alpha(T_v)$  if  $\alpha > 0$ . Let  $U^* \in \mathcal{U}(v, \Delta)$  be derived from  $U$  by omitting  $T_v$  and adding  $T'_v$ . From Lemma 2.2,  $P_1^\alpha(U^*) \leq P_1^\alpha(U)$  if  $\alpha < 0$  and  $P_1^\alpha(U^*) \geq P_1^\alpha(U)$  if  $\alpha > 0$ .

Denote by  $x_1, \dots, x_{\Delta-1}$  the pendant vertices of  $T'_v$  and by  $y_1, \dots, y_l$  the vertices of degree 2 of  $T'_v$ . Suppose that  $U_1 \in \mathcal{U}(v, \Delta)$  is derived from  $U^*$  by removing  $V(T'_v)$  and adding  $ux_1, \dots, ux_{\Delta-k}$  and the path  $v_\Delta v y_1 \dots y_l x_{\Delta-k+1} \dots x_{\Delta-1}$ . Then

$$\begin{aligned} \frac{P_1^\alpha(U)}{P_1^\alpha(U_1)} &= \frac{(\deg_U(u))^\alpha (\deg_U(v))^\alpha \prod_{\Delta-k+1 \leq i \leq \Delta-2} (\deg_U(x_i))^\alpha}{(\deg_{U_1}(u))^\alpha (\deg_{U_1}(v))^\alpha \prod_{\Delta-k+1 \leq i \leq \Delta-2} (\deg_{U_1}(x_i))^\alpha} \\ &= \frac{k^\alpha \Delta^\alpha 1^{(k-2)\alpha}}{\Delta^\alpha 2^\alpha 2^{(k-2)\alpha}} = \left( \frac{k}{2^{k-1}} \right)^\alpha. \end{aligned}$$

Since  $k \geq 3$ , then  $\frac{k}{2^{k-1}} < 1$ . Therefore, if  $\alpha > 0$ , then  $P_1^\alpha(U_1) > P_1^\alpha(U)$  and if  $\alpha < 0$ , then  $P_1^\alpha(U_1) < P_1^\alpha(U)$ .  $\square$

The subsequent lemma is a consequence of Lemma 2.2, and its proof is hence not given.

**Lemma 3.2.** Let  $U \in \mathcal{U}(v, \Delta)$  in which the degree of at least one of the vertices on its unique cycle is  $\Delta$  and the degree of at least one of the vertices not being on its unique cycle is at least three. Then  $\mathcal{U}(v, \Delta)$  contains a unicyclic graph  $U_1$  with  $P_1^\alpha(U_1) < P_1^\alpha(U)$  if  $\alpha < 0$  and  $P_1^\alpha(U_1) > P_1^\alpha(U)$  if  $\alpha > 0$ .

**Lemma 3.3.** Let  $\mathcal{U}(v, \Delta)$  possess a unicyclic graph  $U$  such that all vertices of degree three or more lie on its cycle. If  $U$  contains at least two such vertices, then  $\mathcal{U}(v, \Delta)$  includes a unicyclic graph  $U_1$  with  $P_1^\alpha(U_1) < P_1^\alpha(U)$  if  $\alpha < 0$  and  $P_1^\alpha(U_1) > P_1^\alpha(U)$  if  $\alpha > 0$ .

*Proof.* Assume that  $\deg_U(u) = \Delta \geq 3$ . Let  $u \neq v$  with degree  $k \geq 3$  and  $N_U(v) = \{v_1, v_2, \dots, v_k\}$  where  $v_1$  and  $v_2$  are on the cycle. Denote by  $T_v$  the rooted tree possessing the maximum possible number of vertices

connected to  $v$  and  $v_1, v_2 \notin V(T_v)$ . By Lemma 2.2, we can convert  $T_v$  to a spider  $T'_v$  on the same order and  $\deg_{T'_v}(v) = \Delta - 2$  whose center is on  $v$ , with  $P_1^\alpha(T'_v) \leq P_1^\alpha(T_v)$  if  $\alpha < 0$  and  $P_1^\alpha(T'_v) \geq P_1^\alpha(T_v)$  if  $\alpha > 0$ . Let  $U^* \in \mathcal{U}(v, \Delta)$  be derived from  $U$  by omitting  $T_v$  and adding  $T'_v$ . By Lemma 2.2,  $P_1^\alpha(U^*) \leq P_1^\alpha(U)$  if  $\alpha < 0$  and  $P_1^\alpha(U^*) \geq P_1^\alpha(U)$  if  $\alpha > 0$ .

Denote by  $x_1, \dots, x_{k-2}$  the pendant vertices of  $T'_v$  and by  $y_1, \dots, y_l$  the vertices of degree 2 of  $T'_v$ . Assume  $U_1 \in \mathcal{U}(v, \Delta)$  is derived from  $U^*$  by removing  $V(T'_v)$ , the edge  $vv_1$  and adding the path  $v_1y_1 \dots y_lx_1 \dots x_{k-2}v$ . Then

$$\begin{aligned} \frac{P_1^\alpha(U)}{P_1^\alpha(U_1)} &= \frac{(\deg_U(v))^\alpha \prod_{1 \leq i \leq k-2} (\deg_U(x_i))^\alpha}{(\deg_{U_1}(v))^\alpha \prod_{1 \leq i \leq k-2} (\deg_{U_1}(x_i))^\alpha} \\ &= \frac{k^\alpha 1^{(k-2)\alpha}}{2^\alpha 2^{(k-2)\alpha}} = \left( \frac{k}{2^{k-1}} \right)^\alpha. \end{aligned}$$

Since  $k \geq 3$ , then  $\frac{k}{2^{k-1}} < 1$ . Therefore, if  $\alpha > 0$ , then  $P_1^\alpha(U_1) > P_1^\alpha(U)$  and if  $\alpha < 0$ , then  $P_1^\alpha(U_1) < P_1^\alpha(U)$ .  $\square$

The second main theorem of the paper is as follows.

**Theorem 3.4.** *If  $U \in \mathcal{U}(v, \Delta)$ , then*

$$P_1^\alpha(U) \geq \Delta^\alpha 2^{(v-\Delta+1)\alpha},$$

*when  $\alpha < 0$  and*

$$P_1^\alpha(U) \leq \Delta^\alpha 2^{(v-\Delta+1)\alpha},$$

*when  $\alpha > 0$ . The equality happens if and only if  $U$  is a cephalopod graph with  $v$  vertices and  $\Delta - 2$  arms.*

*Proof.* Assume that,  $\alpha < 0$  (resp.  $\alpha > 0$ ) and  $U_1 \in \mathcal{U}(v, \Delta)$  such that  $P_1^\alpha(U) \geq P_1^\alpha(U_1)$  (resp.  $P_1^\alpha(U_1) \geq P_1^\alpha(U)$ ) for all  $U \in \mathcal{U}(v, \Delta)$ . Consider a vertex  $\omega \in V(U_1)$  with  $\deg_{U_1}(\omega) = \Delta$ . According to Lemmas 3.1, 3.2, and 3.3,  $U_1$  must be a cephalopod centered at  $\omega$ . Then  $P_1^\alpha(U) \geq P_1^\alpha(U_1) = \Delta^\alpha 2^{(v-\Delta+1)\alpha}$ , when  $\alpha < 0$  and  $P_1^\alpha(U) \leq P_1^\alpha(U_1) = \Delta^\alpha 2^{(v-\Delta+1)\alpha}$ , when  $\alpha > 0$ .  $\square$

In the same way as Lemma 2.6, we deduce the following lemma.

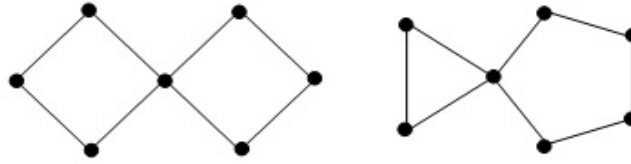
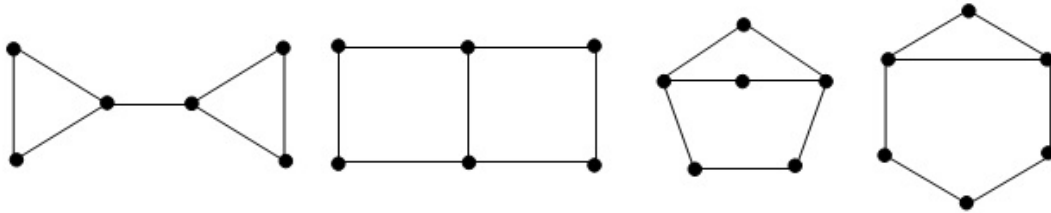
**Lemma 3.5.** *The function  $f(y) = y^\alpha 2^{(v-y+1)\alpha}$  for  $y \geq 2$  is decreasing when  $\alpha > 0$  and is increasing when  $\alpha < 0$ .*

Theorem 3.4 and Lemma 3.5 yield the following corollary.

**Corollary 3.6.** *If  $U$  is a  $v$ -vertex unicyclic graph, then  $P_1^\alpha(U) \geq 2^{v\alpha}$ , when  $\alpha < 0$  and  $P_1^\alpha(U) \leq 2^{v\alpha}$ , when  $\alpha > 0$ . The equality occurs if and only if  $U = C_v$ , where  $C_v$  is the  $v$ -vertex cycle.*

#### 4. Bicyclic graphs

In this section,  $\mathcal{B}(v, \Delta)$  indicates the family of  $v$ -vertex bicyclic graphs whose maximum degree equals  $\Delta$ . A bicyclic graph in  $\mathcal{B}(v, \Delta)$  with  $\Delta \geq 4$  is called a butterfly graph if it possesses exactly one vertex of degree  $\Delta$  such that its two cycles share this vertex,  $v - \Delta + 3$  vertices of degree 2 and  $\Delta - 4$  pendant vertices (see Figure 3). A bicyclic graph in  $\mathcal{B}(v, 3)$  is called a dumbbell graph if it possesses exactly 2 vertices of degree 3 and  $v - 2$  vertices of degree 2 (see Figure 4).

Figure 3: The butterfly graphs with  $v = 7$  and  $\Delta = 4$ .Figure 4: The dumbbell graphs with  $v = 6$ .

The next theorems are obtained by the transitions described for trees and unicycle graphs. Therefore, their proof is omitted.

**Theorem 4.1.** *If  $B \in \mathcal{B}(v, \Delta)$  and  $\Delta \geq 4$ , then*

$$P_1^\alpha(B) \geq \Delta^\alpha 2^{(v-\Delta+3)\alpha},$$

*when  $\alpha < 0$  and*

$$P_1^\alpha(B) \leq \Delta^\alpha 2^{(v-\Delta+3)\alpha},$$

*when  $\alpha > 0$ . The equality happens if and only if  $B$  is a butterfly graph.*

**Theorem 4.2.** *If  $B \in \mathcal{B}(v, 3)$ , then*

$$P_1^\alpha(B) \geq 3^{2\alpha} 2^{(v-2)\alpha},$$

*when  $\alpha < 0$  and*

$$P_1^\alpha(B) \leq 3^{2\alpha} 2^{(v-2)\alpha},$$

*when  $\alpha > 0$ . The equality happens if and only if  $B$  is a dumbbell graph.*

In the same way as Lemma 2.6, we get the next lemma.

**Lemma 4.3.** *The function  $f(y) = y^\alpha 2^{(v-y+3)\alpha}$  for  $y \geq 4$  is decreasing when  $\alpha > 0$  and is increasing when  $\alpha < 0$ .*

As a consequence of Theorem 4.1 and Lemma 4.3, we arrive at:

**Corollary 4.4.** *If  $B \in \mathcal{B}(v, \Delta)$  and  $\Delta \geq 4$ , then  $P_1^\alpha(B) \geq 4^\alpha 2^{(v-1)\alpha}$ , when  $\alpha < 0$  and  $P_1^\alpha(B) \leq 4^\alpha 2^{(v-1)\alpha}$ , when  $\alpha > 0$ . The equality happens if and only if  $B$  is a bicyclic graph with exactly one vertex of degree 4 and  $v - 1$  vertices of degree 2.*

## 5. $c$ -cyclic graphs

Let  $C(v, \Delta)$  indicate the family of  $v$ -vertex  $c$ -cyclic graphs whose maximum degree is  $\Delta$ . Similar to the arguments given for trees, unicycle graphs, and bicyclic graphs, we reach the subsequent theorem for the  $c$ -cyclic graphs with  $\Delta \geq 2c$ .

**Theorem 5.1.** If  $H \in C(v, \Delta)$  with  $\Delta \geq 2c$ , then

$$P_1^\alpha(H) \geq \Delta^\alpha 2^{(v-\Delta+2c-1)\alpha},$$

when  $\alpha < 0$  and

$$P_1^\alpha(H) \leq \Delta^\alpha 2^{(v-\Delta+2c-1)\alpha},$$

when  $\alpha > 0$ . The equality happens if and only if  $H$  is a  $c$ -cyclic graph with exactly one vertex of degree more than two.

By the same way of Lemma 2.6, we arrive at:

**Lemma 5.2.** The function  $f(y) = y^\alpha 2^{(v-y+2c-1)\alpha}$  for  $y \geq 2c$  and  $c > 0$  is decreasing when  $\alpha > 0$  and is increasing when  $\alpha < 0$ .

From Theorem 5.1 and Lemma 5.2, we get the next corollary.

**Corollary 5.3.** If  $H \in C(v, \Delta)$  with  $\Delta \geq 2c$  and  $c > 0$ , then  $P_1^\alpha(H) \geq c^\alpha 2^{v\alpha}$ , when  $\alpha < 0$  and  $P_1^\alpha(H) \leq c^\alpha 2^{v\alpha}$ , when  $\alpha > 0$ . The equality case happens if and only if  $H$  is a  $c$ -cyclic graph with exactly one vertex of degree  $2c$  and  $v - 1$  vertices of degree 2.

## 6. Conclusion

This paper has established sharp bounds for the general multiplicative first Zagreb index in simple connected graphs, focusing particularly on the cases of cyclomatic numbers  $c=0, 1$ , and 2. We have further extended these results to molecular trees and graphs with maximum degree satisfying  $\Delta \geq 2c$ . Our analysis characterizes the extremal graphs that achieve these bounds, providing precise structural insights. These findings contribute to a deeper understanding of the multiplicative first Zagreb index in relation to graph parameters such as cyclomatic number and maximum vertex degree.

The results presented here not only generalize and refine known bounds but also open new directions for future research. Extensions to graphs with higher cyclomatic numbers or other classes of molecular graphs could yield further valuable inequalities. Additionally, the interplay between multiplicative Zagreb indices and other graph invariants remains an important area for exploration. It is anticipated that these advances will enhance the application of topological indices in chemical graph theory and related disciplines.

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## Availability of data and materials

The paper includes or uses no datasets.

## Conflicts of Interest

The authors declare that they have no conflict of interest.

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