Extremal (Chemical) Graphs with Respect to the General Multiplicative Zagreb Indices

Xiaoling Sun and Jianwei Du*

Abstract—**The first and second general multiplicative Zagreb indices are modified versions of the well-known Zagreb indices. In this paper, we determine the extremal values of the first and second general multiplicative Zagreb indices among all n-vertex (chemical) trees, (chemical) unicyclic graphs, (chemical) bicyclic graphs, (chemical) tricyclic graphs, (chemical) tetracyclic graphs and (chemical) pentacyclic graphs.**

Index Terms—**General multiplicative Zagreb indices, Extremal graph, Chemical graph.**

I. Introduction

In this paper, just simple connected graphs are considered. For such a graph G, we represent the sets of vertices and edges by $V(G)$ and $E(G)$, respectively. Let us use $d_G(x)$ (or simply $d(x)$) to denote the degree of vertex x in G. The notation $n_k(G)$ (n_k for short) denotes the number of vertices with degree k in G. Let $G - xy$ and $G + xy$ be the graphs obtained from G by deleting the edge $xy \in E(G)$ and by adding the edge $xy \notin E(G)$ $(x, y \in V(G))$, respectively. A graph G of order n is called a tree, unicyclic graph, bicyclic graph, tricyclic graph, tetracyclic graph, pentacyclic graph, if it has $n-1+r$ edges such that $r = 0, 1, 2, 3, 4, 5$, respectively. For other terminologies and notations not defined here, readers can refer to [8].

In mathematical chemistry and chemical graph theory, the topological indices are one of the useful tools to characterize the physical or chemical properties of molecules, and they play a significant role in pharmacology, chemistry, etc. (see [14], [15], [24]). The famous Zagreb indices, first introduced by Gutman and Trinajstić [17], are used to examine the structure dependence of total π-electron energy on molecular orbital. The first and second Zagreb indices (denoted by M_1 and M_2) of a graph G are defined as

$$M_1(G) = \sum_{x\in V(G)} d(x)^2,\ M_2(G) = \sum_{xy\in E(G)} d(x)d(y).$$

Todeschini et al. [25] proposed two versions of Zagreb indices which are now called the first and second multiplicative Zagreb indices (denoted by Π_1 and Π_2), and they are expressed as below:

$$\Pi_1(G) = \prod_{x\in V(G)} d(x)^2,$$
$$\Pi_2(G) = \prod_{xy\in E(G)} d(x)d(y) = \prod_{x\in V(G)} d(x)^{d(x)}.$$

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Xiaoling Sun is an associate professor of the School of Mathematics, North University of China, Taiyuan 030051, China (e-mail: sunxiaoling@nuc.edu.cn).

Jianwei Du is an associate professor of the School of Mathematics, North University of China, Taiyuan 030051, China (Corresponding author, e-mail: jianweidu@nuc.edu.cn).

Recently, Vetrík et al [22] introduced a generalized form of the multiplicative Zagreb indices, which are named the first and second general multiplicative Zagreb indices (denoted by P_1^α and P_2^α). And they are defined by

$$P_1^\alpha(G) = \prod_{x\in V(G)} d(x)^\alpha,$$
$$P_2^\alpha(G) = \prod_{xy\in E(G)} (d(x)d(y))^\alpha = \prod_{x\in V(G)} d(x)^{\alpha d(x)}, \quad (1)$$

where $\alpha \neq 0$ is a real number. In [22], the maximum and minimum general multiplicative Zagreb indices of trees with fixed number of vertices or branching vertices or segments or pendant vertices were determined by Vetrík et al, and the corresponding extremal trees were identified. In [9] and [10], the extremal trees, quasi-tree graphs and quasi-unicyclic graphs with a perfect matching, as well as the extremal quasi-tree graphs and quasi-unicyclic graphs with given order and number of pendant vertices with respect to general multiplicative Zagreb indices were obtained by the authors of this paper. For other recent mathematical investigations on general multiplicative Zagreb indices, we refer the readers to [1]–[3], [7], [21], [23].

A chemical (or molecular) graph is a graph G with $d(x) \leq 4$ for all $x \in V(G)$. In recent years, studying the extremal values of topological indices on chemical (or molecular) graphs has become an important research subject [4]–[6], [11]–[13], [18]–[20], [26]. Therefore, in this work, we provide the first seven maximum (resp. minimum) P_1^α and the first seven minimum (resp. maximum) P_2^α of trees or chemical trees for $\alpha > 0$ (resp. for $\alpha < 0$); the first three maximum (resp. minimum) P_1^α and the first three minimum (resp. maximum) P_2^α of unicyclic graphs or chemical unicyclic graphs for $\alpha > 0$ (resp. for $\alpha < 0$); the first three maximum (resp. minimum) P_1^α and the first three minimum (resp. maximum) P_2^α of bicyclic graphs or chemical bicyclic graphs for $\alpha > 0$ (resp. for $\alpha < 0$); the first eight maximum (resp. minimum) P_1^α and the first seven minimum (resp. maximum) P_2^α of tricyclic graphs for $\alpha > 0$ (resp. for $\alpha < 0$); the first seven maximum (resp. minimum) P_1^α and the first six minimum (resp. maximum) P_2^α of chemical tricyclic graphs for $\alpha > 0$ (resp. for $\alpha < 0$); the first four maximum (resp. minimum) P_1^α and the first three minimum (resp. maximum) P_2^α of tetracyclic graphs or chemical tetracyclic graphs for $\alpha > 0$ (resp. for $\alpha < 0$); the first four maximum (resp. minimum) P_1^α and the first three minimum (resp. maximum) P_2^α of pentacyclic graphs or chemical pentacyclic graphs for $\alpha > 0$ (resp. for $\alpha < 0$).

II. Preliminaries

Lemma 2.1: [10] Let $l_1(x) = \frac{x+c}{x}$. Then $l_1(x)$ is strictly decreasing in $x \geq 1$, where $c \geq 1$ is an integer.

TABLE I
DEGREE DISTRIBUTIONS (DD) OF TREES WITH $2 \leq n_1 \leq 6$ AND THEIR P_1^α, P_2^α

$No.$	n_6	n_5	n_4	n_3	n_2	n_1	$n_i(i \geq 7)$	P_1^α	P_2^α
A_1	0	0	0	0	$n-2$	2	0	$(2^n \cdot 0.2500)^\alpha$	$(4^n \cdot 0.0625)^\alpha$
A_2	0	0	0	1	$n-4$	3	0	$(2^n \cdot 0.1875)^\alpha$	$(4^n \cdot 0.1055)^\alpha$
A_3	0	0	1	0	$n-5$	4	0	$(2^n \cdot 0.1250)^\alpha$	$(4^n \cdot 0.2500)^\alpha$
A_4	0	0	0	2	$n-6$	4	0	$(2^n \cdot 0.1406)^\alpha$	$(4^n \cdot 0.1780)^\alpha$
A_5	0	1	0	0	$n-6$	5	0	$(2^n \cdot 0.0781)^\alpha$	$(4^n \cdot 0.7629)^\alpha$
A_6	0	0	1	1	$n-7$	5	0	$(2^n \cdot 0.0938)^\alpha$	$(4^n \cdot 0.4219)^\alpha$
A_7	0	0	0	3	$n-8$	5	0	$(2^n \cdot 0.1055)^\alpha$	$(4^n \cdot 0.3003)^\alpha$
A_8	1	0	0	0	$n-7$	6	0	$(2^n \cdot 0.0469)^\alpha$	$(4^n \cdot 2.8477)^\alpha$
A_9	0	1	0	1	$n-8$	6	0	$(2^n \cdot 0.0586)^\alpha$	$(4^n \cdot 1.2875)^\alpha$
A_{10}	0	0	2	0	$n-8$	6	0	$(2^n \cdot 0.0625)^\alpha$	$(4^n \cdot 1.0000)^\alpha$
A_{11}	0	0	1	2	$n-9$	6	0	$(2^n \cdot 0.0703)^\alpha$	$(4^n \cdot 0.7119)^\alpha$
A_{12}	0	0	0	4	$n-10$	6	0	$(2^n \cdot 0.0791)^\alpha$	$(4^n \cdot 0.5068)^\alpha$

TABLE II
DD OF UNICYCLIC GRAPHS WITH $n_1 \leq 2$ AND THEIR P_1^α, P_2^α

$No.$	n_4	n_3	n_2	n_1	$n_i(i \geq 5)$	P_1^α	P_2^α
U_1	0	0	n	0	0	$(2^n \cdot 1.0000)^\alpha$	$(4^n \cdot 1.0000)^\alpha$
U_2	0	1	$n-2$	1	0	$(2^n \cdot 0.7500)^\alpha$	$(4^n \cdot 1.6875)^\alpha$
U_3	1	0	$n-3$	2	0	$(2^n \cdot 0.5000)^\alpha$	$(4^n \cdot 4.0000)^\alpha$
U_4	0	2	$n-4$	2	0	$(2^n \cdot 0.5625)^\alpha$	$(4^n \cdot 2.8477)^\alpha$

TABLE III
DD OF BICYCLIC GRAPHS WITH $n_1 \leq 1$ AND THEIR P_1^α, P_2^α

$No.$	n_5	n_4	n_3	n_2	n_1	$n_i(i \geq 6)$	P_1^α	P_2^α
B_1	0	1	0	$n-1$	0	0	$(2^n \cdot 2.0000)^\alpha$	$(4^n \cdot 64.0000)^\alpha$
B_2	0	0	2	$n-2$	0	0	$(2^n \cdot 2.2500)^\alpha$	$(4^n \cdot 45.5625)^\alpha$
B_3	1	0	0	$n-2$	1	0	$(2^n \cdot 1.2500)^\alpha$	$(4^n \cdot 195.3125)^\alpha$
B_4	0	1	1	$n-3$	1	0	$(2^n \cdot 1.5000)^\alpha$	$(4^n \cdot 108.0000)^\alpha$
B_5	0	0	3	$n-4$	1	0	$(2^n \cdot 1.6875)^\alpha$	$(4^n \cdot 76.8867)^\alpha$

TABLE IV
DD OF TRICYCLIC GRAPHS WITH $n_1 = 0$ AND THEIR P_1^α, P_2^α

$No.$	n_6	n_5	n_4	n_3	n_2	n_1	$n_i(i \geq 7)$	P_1^α	P_2^α
D_1	1	0	0	0	$n-1$	0	0	$(2^n \cdot 3.0000)^\alpha$	$(4^n \cdot 1.1664\times10^4)^\alpha$
D_2	0	1	0	1	$n-2$	0	0	$(2^n \cdot 3.7500)^\alpha$	$(4^n \cdot 0.5273\times10^4)^\alpha$
D_3	0	0	2	0	$n-2$	0	0	$(2^n \cdot 4.0000)^\alpha$	$(4^n \cdot 0.4096\times10^4)^\alpha$
D_4	0	0	1	2	$n-3$	0	0	$(2^n \cdot 4.5000)^\alpha$	$(4^n \cdot 0.2916\times10^4)^\alpha$
D_5	0	0	0	4	$n-4$	0	0	$(2^n \cdot 5.0625)^\alpha$	$(4^n \cdot 0.2076\times10^4)^\alpha$

TABLE V
DD OF TRICYCLIC GRAPHS WITH $n_1 = 1$ AND THEIR P_1^α, P_2^α

$No.$	n_7	n_6	n_5	n_4	n_3	n_2	n_1	$n_i(i \geq 8)$	P_1^α	P_2^α
D_6	1	0	0	0	0	$n-2$	1	0	$(2^n \cdot 1.7500)^\alpha$	$(4^n \cdot 5.1471\times10^4)^\alpha$
D_7	0	1	0	0	1	$n-3$	1	0	$(2^n \cdot 2.2500)^\alpha$	$(4^n \cdot 1.9683\times10^4)^\alpha$
D_8	0	0	1	1	0	$n-3$	1	0	$(2^n \cdot 2.5000)^\alpha$	$(4^n \cdot 1.2500\times10^4)^\alpha$
D_9	0	0	1	0	2	$n-4$	1	0	$(2^n \cdot 2.8125)^\alpha$	$(4^n \cdot 0.8899\times10^4)^\alpha$
D_{10}	0	0	0	2	1	$n-4$	1	0	$(2^n \cdot 3.0000)^\alpha$	$(4^n \cdot 0.6912\times10^4)^\alpha$
D_{11}	0	0	0	1	3	$n-5$	1	0	$(2^n \cdot 3.3750)^\alpha$	$(4^n \cdot 0.4921\times10^4)^\alpha$
D_{12}	0	0	0	0	5	$n-6$	1	0	$(2^n \cdot 3.7969)^\alpha$	$(4^n \cdot 0.3503\times10^4)^\alpha$

TABLE VI
DD OF TRICYCLIC GRAPHS WITH $n_1 = 2$ AND THEIR P_1^α, P_2^α

$No.$	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	$n_i(i \geq 9)$	P_1^α	P_2^α
D_{13}	1	0	0	0	0	0	$n-3$	2	0	$(2^n \cdot 1.0000)^\alpha$	$(4^n \cdot 26.2144\times10^4)^\alpha$
D_{14}	0	1	0	0	0	1	$n-4$	2	0	$(2^n \cdot 1.3125)^\alpha$	$(4^n \cdot 8.6858\times10^4)^\alpha$
D_{15}	0	0	1	0	1	0	$n-4$	2	0	$(2^n \cdot 1.5000)^\alpha$	$(4^n \cdot 4.6656\times10^4)^\alpha$
D_{16}	0	0	1	0	0	2	$n-5$	2	0	$(2^n \cdot 1.6875)^\alpha$	$(4^n \cdot 3.3215\times10^4)^\alpha$
D_{17}	0	0	0	2	0	0	$n-4$	2	0	$(2^n \cdot 1.5625)^\alpha$	$(4^n \cdot 3.8147\times10^4)^\alpha$
D_{18}	0	0	0	1	1	1	$n-5$	2	0	$(2^n \cdot 1.8750)^\alpha$	$(4^n \cdot 2.1094\times10^4)^\alpha$
D_{19}	0	0	0	1	0	3	$n-6$	2	0	$(2^n \cdot 2.1094)^\alpha$	$(4^n \cdot 1.5017\times10^4)^\alpha$
D_{20}	0	0	0	0	3	0	$n-5$	2	0	$(2^n \cdot 2.0000)^\alpha$	$(4^n \cdot 1.6384\times10^4)^\alpha$
D_{21}	0	0	0	0	2	2	$n-6$	2	0	$(2^n \cdot 2.2500)^\alpha$	$(4^n \cdot 1.1664\times10^4)^\alpha$
D_{22}	0	0	0	0	1	4	$n-7$	2	0	$(2^n \cdot 2.5313)^\alpha$	$(4^n \cdot 0.8304\times10^4)^\alpha$
D_{23}	0	0	0	0	0	6	$n-8$	2	0	$(2^n \cdot 2.8477)^\alpha$	$(4^n \cdot 0.5912\times10^4)^\alpha$

TABLE VII
DD OF TETRACYCLIC GRAPHS WITH $n_1 = 0$ AND THEIR P_1^α, P_2^α

$No.$	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	$n_i(i \geq 9)$	P_1^α	P_2^α
E_1	1	0	0	0	0	0	$n-1$	0	0	$(2^n \cdot 4.0000)^\alpha$	$(4^n \cdot 4.1943 \times 10^6)^\alpha$
E_2	0	1	0	0	0	1	$n-2$	0	0	$(2^n \cdot 5.2500)^\alpha$	$(4^n \cdot 1.3897 \times 10^6)^\alpha$
E_3	0	0	1	0	1	0	$n-2$	0	0	$(2^n \cdot 6.0000)^\alpha$	$(4^n \cdot 0.7465 \times 10^6)^\alpha$
E_4	0	0	1	0	0	2	$n-3$	0	0	$(2^n \cdot 6.7500)^\alpha$	$(4^n \cdot 0.5314 \times 10^6)^\alpha$
E_5	0	0	0	2	0	0	$n-2$	0	0	$(2^n \cdot 6.2500)^\alpha$	$(4^n \cdot 0.6104 \times 10^6)^\alpha$
E_6	0	0	0	1	1	1	$n-3$	0	0	$(2^n \cdot 7.5000)^\alpha$	$(4^n \cdot 0.3375 \times 10^6)^\alpha$
E_7	0	0	0	1	0	3	$n-4$	0	0	$(2^n \cdot 8.4375)^\alpha$	$(4^n \cdot 0.2403 \times 10^6)^\alpha$
E_8	0	0	0	0	3	0	$n-3$	0	0	$(2^n \cdot 8.0000)^\alpha$	$(4^n \cdot 0.2621 \times 10^6)^\alpha$
E_9	0	0	0	0	2	2	$n-4$	0	0	$(2^n \cdot 9.0000)^\alpha$	$(4^n \cdot 0.1866 \times 10^6)^\alpha$
E_{10}	0	0	0	0	1	4	$n-5$	0	0	$(2^n \cdot 10.1250)^\alpha$	$(4^n \cdot 0.1329 \times 10^6)^\alpha$
E_{11}	0	0	0	0	0	6	$n-6$	0	0	$(2^n \cdot 11.3906)^\alpha$	$(4^n \cdot 0.0946 \times 10^6)^\alpha$

TABLE VIII
DD OF TETRACYCLIC GRAPHS WITH $n_1 = 1$ AND THEIR P_1^α, P_2^α

$No.$	n_9	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	$n_i(i \geq 10)$	P_1^α	P_2^α
E_{12}	1	0	0	0	0	0	0	$n-2$	1	0	$(2^n \cdot 2.2500)^\alpha$	$(4^n \cdot 24.2138 \times 10^6)^\alpha$
E_{13}	0	1	0	0	0	0	1	$n-3$	1	0	$(2^n \cdot 3.0000)^\alpha$	$(4^n \cdot 7.0779 \times 10^6)^\alpha$
E_{14}	0	0	1	0	0	1	0	$n-3$	1	0	$(2^n \cdot 3.5000)^\alpha$	$(4^n \cdot 3.2942 \times 10^6)^\alpha$
E_{15}	0	0	1	0	0	0	2	$n-4$	1	0	$(2^n \cdot 3.9375)^\alpha$	$(4^n \cdot 2.3452 \times 10^6)^\alpha$
E_{16}	0	0	0	1	1	0	0	$n-3$	1	0	$(2^n \cdot 3.7500)^\alpha$	$(4^n \cdot 2.2781 \times 10^6)^\alpha$
E_{17}	0	0	0	1	0	1	1	$n-4$	1	0	$(2^n \cdot 4.5000)^\alpha$	$(4^n \cdot 1.2597 \times 10^6)^\alpha$
E_{18}	0	0	0	1	0	0	3	$n-5$	1	0	$(2^n \cdot 5.0625)^\alpha$	$(4^n \cdot 0.8968 \times 10^6)^\alpha$
E_{19}	0	0	0	0	2	0	1	$n-4$	1	0	$(2^n \cdot 4.6875)^\alpha$	$(4^n \cdot 1.0300 \times 10^6)^\alpha$
E_{20}	0	0	0	0	1	2	0	$n-4$	1	0	$(2^n \cdot 5.0000)^\alpha$	$(4^n \cdot 0.8000 \times 10^6)^\alpha$
E_{21}	0	0	0	0	1	1	2	$n-5$	1	0	$(2^n \cdot 5.6250)^\alpha$	$(4^n \cdot 0.5695 \times 10^6)^\alpha$
E_{22}	0	0	0	0	1	0	4	$n-6$	1	0	$(2^n \cdot 6.3281)^\alpha$	$(4^n \cdot 0.4055 \times 10^6)^\alpha$
E_{23}	0	0	0	0	0	3	1	$n-5$	1	0	$(2^n \cdot 6.0000)^\alpha$	$(4^n \cdot 0.4424 \times 10^6)^\alpha$
E_{24}	0	0	0	0	0	2	3	$n-6$	1	0	$(2^n \cdot 6.7500)^\alpha$	$(4^n \cdot 0.3149 \times 10^6)^\alpha$
E_{25}	0	0	0	0	0	1	5	$n-7$	1	0	$(2^n \cdot 7.5938)^\alpha$	$(4^n \cdot 0.2242 \times 10^6)^\alpha$
E_{26}	0	0	0	0	0	0	7	$n-8$	1	0	$(2^n \cdot 8.5430)^\alpha$	$(4^n \cdot 0.1596 \times 10^6)^\alpha$

TABLE IX
DD OF PENTACYCLIC GRAPHS WITH $n_1 = 0$ AND THEIR P_1^α, P_2^α

$No.$	n_{10}	n_9	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	$n_i(i \geq 11)$	P_1^α	P_2^α
F_1	1	0	0	0	0	0	0	0	$n-1$	0	0	$(2^n \cdot 5.0000)^\alpha$	$(4^n \cdot 25.0000 \times 10^8)^\alpha$
F_2	0	1	0	0	0	0	0	1	$n-2$	0	0	$(2^n \cdot 6.7500)^\alpha$	$(4^n \cdot 6.5377 \times 10^8)^\alpha$
F_3	0	0	1	0	0	0	1	0	$n-2$	0	0	$(2^n \cdot 8.0000)^\alpha$	$(4^n \cdot 2.6844 \times 10^8)^\alpha$
F_4	0	0	1	0	0	0	0	2	$n-3$	0	0	$(2^n \cdot 9.0000)^\alpha$	$(4^n \cdot 1.9110 \times 10^8)^\alpha$
F_5	0	0	0	1	0	1	0	0	$n-2$	0	0	$(2^n \cdot 8.7500)^\alpha$	$(4^n \cdot 1.6085 \times 10^8)^\alpha$
F_6	0	0	0	1	0	0	1	1	$n-3$	0	0	$(2^n \cdot 10.5000)^\alpha$	$(4^n \cdot 0.8894 \times 10^8)^\alpha$
F_7	0	0	0	1	0	0	0	3	$n-4$	0	0	$(2^n \cdot 11.8125)^\alpha$	$(4^n \cdot 0.6332 \times 10^8)^\alpha$
F_8	0	0	0	0	2	0	0	0	$n-2$	0	0	$(2^n \cdot 9.0000)^\alpha$	$(4^n \cdot 1.3605 \times 10^8)^\alpha$
F_9	0	0	0	0	1	1	0	1	$n-3$	0	0	$(2^n \cdot 11.2500)^\alpha$	$(4^n \cdot 0.6151 \times 10^8)^\alpha$
F_{10}	0	0	0	0	1	0	2	0	$n-3$	0	0	$(2^n \cdot 12.0000)^\alpha$	$(4^n \cdot 0.4778 \times 10^8)^\alpha$
F_{11}	0	0	0	0	1	0	1	2	$n-4$	0	0	$(2^n \cdot 13.5000)^\alpha$	$(4^n \cdot 0.3401 \times 10^8)^\alpha$
F_{12}	0	0	0	0	1	0	0	4	$n-5$	0	0	$(2^n \cdot 15.1875)^\alpha$	$(4^n \cdot 0.2421 \times 10^8)^\alpha$
F_{13}	0	0	0	0	0	2	1	0	$n-3$	0	0	$(2^n \cdot 12.5000)^\alpha$	$(4^n \cdot 0.3906 \times 10^8)^\alpha$
F_{14}	0	0	0	0	0	2	0	2	$n-4$	0	0	$(2^n \cdot 14.0625)^\alpha$	$(4^n \cdot 0.2781 \times 10^8)^\alpha$
F_{15}	0	0	0	0	0	1	2	1	$n-4$	0	0	$(2^n \cdot 15.0000)^\alpha$	$(4^n \cdot 0.2160 \times 10^8)^\alpha$
F_{16}	0	0	0	0	0	1	1	3	$n-5$	0	0	$(2^n \cdot 16.8750)^\alpha$	$(4^n \cdot 0.1538 \times 10^8)^\alpha$
F_{17}	0	0	0	0	0	1	0	5	$n-6$	0	0	$(2^n \cdot 18.9844)^\alpha$	$(4^n \cdot 0.1095 \times 10^8)^\alpha$
F_{18}	0	0	0	0	0	0	4	0	$n-4$	0	0	$(2^n \cdot 16.0000)^\alpha$	$(4^n \cdot 0.1678 \times 10^8)^\alpha$
F_{19}	0	0	0	0	0	0	3	2	$n-5$	0	0	$(2^n \cdot 18.0000)^\alpha$	$(4^n \cdot 0.1194 \times 10^8)^\alpha$
F_{20}	0	0	0	0	0	0	2	4	$n-6$	0	0	$(2^n \cdot 20.2500)^\alpha$	$(4^n \cdot 0.0850 \times 10^8)^\alpha$
F_{21}	0	0	0	0	0	0	1	6	$n-7$	0	0	$(2^n \cdot 22.7813)^\alpha$	$(4^n \cdot 0.0605 \times 10^8)^\alpha$
F_{22}	0	0	0	0	0	0	0	8	$n-8$	0	0	$(2^n \cdot 25.6289)^\alpha$	$(4^n \cdot 0.0431 \times 10^8)^\alpha$

TABLE X
DD OF PENTACYCLIC GRAPHS WITH $n_1 = 1$ AND THEIR P_1^α, P_2^α

$No.$	n_{11}	n_{10}	n_9	n_8	n_7	n_6	n_5	n_4	n_3	n_2	n_1	$n_i(i \geq 12)$	P_1^α	P_2^α
F_{23}	1	0	0	0	0	0	0	0	0	$n-2$	1	0	$(2^n \cdot 2.7500)^\alpha$	$(4^n \cdot 17.8320 \times 10^9)^\alpha$
F_{24}	0	1	0	0	0	0	0	0	1	$n-3$	1	0	$(2^n \cdot 3.7500)^\alpha$	$(4^n \cdot 42.1875 \times 10^8)^\alpha$
F_{25}	0	0	1	0	0	0	0	1	0	$n-3$	1	0	$(2^n \cdot 4.5000)^\alpha$	$(4^n \cdot 15.4968 \times 10^8)^\alpha$
F_{26}	0	0	1	0	0	0	0	0	2	$n-4$	1	0	$(2^n \cdot 5.0625)^\alpha$	$(4^n \cdot 11.0324 \times 10^8)^\alpha$
F_{27}	0	0	0	1	0	0	1	0	0	$n-3$	1	0	$(2^n \cdot 5.0000)^\alpha$	$(4^n \cdot 8.1920 \times 10^8)^\alpha$
F_{28}	0	0	0	1	0	0	0	1	1	$n-4$	1	0	$(2^n \cdot 6.0000)^\alpha$	$(4^n \cdot 4.5298 \times 10^8)^\alpha$
F_{29}	0	0	0	1	0	0	0	0	3	$n-5$	1	0	$(2^n \cdot 6.7500)^\alpha$	$(4^n \cdot 3.2249 \times 10^8)^\alpha$
F_{30}	0	0	0	0	1	1	0	0	0	$n-3$	1	0	$(2^n \cdot 5.2500)^\alpha$	$(4^n \cdot 6.0036 \times 10^8)^\alpha$
F_{31}	0	0	0	0	1	0	1	0	1	$n-4$	1	0	$(2^n \cdot 6.5625)^\alpha$	$(4^n \cdot 2.7143 \times 10^8)^\alpha$
F_{32}	0	0	0	0	1	0	0	2	0	$n-4$	1	0	$(2^n \cdot 7.0000)^\alpha$	$(4^n \cdot 2.1083 \times 10^8)^\alpha$
F_{33}	0	0	0	0	1	0	0	1	2	$n-5$	1	0	$(2^n \cdot 7.8750)^\alpha$	$(4^n \cdot 1.5009 \times 10^8)^\alpha$
F_{34}	0	0	0	0	1	0	0	0	4	$n-6$	1	0	$(2^n \cdot 8.8594)^\alpha$	$(4^n \cdot 1.0685 \times 10^8)^\alpha$
F_{35}	0	0	0	0	0	2	0	0	1	$n-4$	1	0	$(2^n \cdot 6.7500)^\alpha$	$(4^n \cdot 2.2958 \times 10^8)^\alpha$
F_{36}	0	0	0	0	0	1	1	1	0	$n-4$	1	0	$(2^n \cdot 7.5000)^\alpha$	$(4^n \cdot 1.4580 \times 10^8)^\alpha$
F_{37}	0	0	0	0	0	1	0	2	1	$n-5$	1	0	$(2^n \cdot 9.0000)^\alpha$	$(4^n \cdot 0.8062 \times 10^8)^\alpha$
F_{38}	0	0	0	0	0	1	0	1	3	$n-6$	1	0	$(2^n \cdot 10.1250)^\alpha$	$(4^n \cdot 0.5740 \times 10^8)^\alpha$
F_{39}	0	0	0	0	0	1	0	0	5	$n-7$	1	0	$(2^n \cdot 11.3906)^\alpha$	$(4^n \cdot 0.4086 \times 10^8)^\alpha$
F_{40}	0	0	0	0	0	0	3	0	0	$n-4$	1	0	$(2^n \cdot 7.8125)^\alpha$	$(4^n \cdot 1.1921 \times 10^8)^\alpha$
F_{41}	0	0	0	0	0	0	2	1	1	$n-5$	1	0	$(2^n \cdot 9.3750)^\alpha$	$(4^n \cdot 0.6592 \times 10^8)^\alpha$
F_{42}	0	0	0	0	0	0	2	0	3	$n-6$	1	0	$(2^n \cdot 10.5469)^\alpha$	$(4^n \cdot 0.4693 \times 10^8)^\alpha$
F_{43}	0	0	0	0	0	0	1	3	0	$n-5$	1	0	$(2^n \cdot 10.0000)^\alpha$	$(4^n \cdot 0.5120 \times 10^8)^\alpha$
F_{44}	0	0	0	0	0	0	1	2	2	$n-6$	1	0	$(2^n \cdot 11.2500)^\alpha$	$(4^n \cdot 0.3645 \times 10^8)^\alpha$
F_{45}	0	0	0	0	0	0	1	1	4	$n-7$	1	0	$(2^n \cdot 12.6563)^\alpha$	$(4^n \cdot 0.2595 \times 10^8)^\alpha$
F_{46}	0	0	0	0	0	0	1	0	6	$n-8$	1	0	$(2^n \cdot 14.2383)^\alpha$	$(4^n \cdot 0.1847 \times 10^8)^\alpha$
F_{47}	0	0	0	0	0	0	0	4	1	$n-6$	1	0	$(2^n \cdot 12.0000)^\alpha$	$(4^n \cdot 0.2831 \times 10^8)^\alpha$
F_{48}	0	0	0	0	0	0	0	3	3	$n-7$	1	0	$(2^n \cdot 13.5000)^\alpha$	$(4^n \cdot 0.2016 \times 10^8)^\alpha$
F_{49}	0	0	0	0	0	0	0	2	5	$n-8$	1	0	$(2^n \cdot 15.1875)^\alpha$	$(4^n \cdot 0.1435 \times 10^8)^\alpha$
F_{50}	0	0	0	0	0	0	0	1	7	$n-9$	1	0	$(2^n \cdot 17.0860)^\alpha$	$(4^n \cdot 0.1022 \times 10^8)^\alpha$
F_{51}	0	0	0	0	0	0	0	0	9	$n-10$	1	0	$(2^n \cdot 19.2217)^\alpha$	$(4^n \cdot 0.0727 \times 10^8)^\alpha$

Lemma 2.2: [10] Let $l_2(x) = \frac{(x+c)^{x+c}}{x^x}$. Then $l_2(x)$ is strictly increasing in $x \geq 1$, where $c \geq 1$ is an integer.

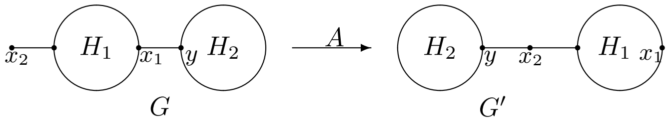

Fig. 1. Transformation A

Transformation A: Let H_1 and H_2 be two graphs with vertices $x_1, x_2 \in V(H_1)$, $y \in V(H_2)$ such that $d_{H_1}(x_1) \geq 2$, $d_{H_1}(x_2) = 1$, as shown in Fig. 1. Let G be the graph obtained from H_1 and H_2 by attaching vertices x_1 and y. Set $G' = G - x_1y + x_2y$, as shown in Fig. 1.

Lemma 2.3: Suppose G and G' are graphs in Fig. 1, then $P_1^\alpha(G) < P_1^\alpha(G')$, $P_2^\alpha(G) > P_2^\alpha(G')$ for $\alpha > 0$, and $P_1^\alpha(G) > P_1^\alpha(G')$, $P_2^\alpha(G) < P_2^\alpha(G')$ for $\alpha < 0$.

Proof: By (1) and Lemma 2.1, Lemma 2.2, for $\alpha > 0$, we deduce that

$$\frac{P_1^\alpha(G)}{P_1^\alpha(G')} = \frac{(d_{H_1}(x_1)+1)^\alpha}{2^\alpha d_{H_1}(x_1)^\alpha} = \left(\frac{\frac{d_{H_1}(x_1)+1}{d_{H_1}(x_1)}}{\frac{2}{1}}\right)^\alpha < 1$$

and

$$\frac{P_2^\alpha(G)}{P_2^\alpha(G')} = \frac{(d_{H_1}(x_1)+1)^{\alpha(d_{H_1}(x_1)+1)}}{2^{2\alpha} d_{H_1}(x_1)^{\alpha d_{H_1}(x_1)}} = \left(\frac{\frac{(d_{H_1}(x_1)+1)^{(d_{H_1}(x_1)+1)}}{d_{H_1}(x_1)^{d_{H_1}(x_1)}}}{\frac{2^2}{1^1}}\right)^\alpha > 1.$$

Similarly, we can draw conclusions for $\alpha < 0$. ■

III. Main result

Lemma 3.1: [16] An n-vertex tree T belongs to one of equivalence classes given in Table I if and only if T satisfies the condition $2 \leq n_1(T) \leq 6$.

Theorem 3.1: Let T^* be a tree of order n. For $n \geq 10$, $T_1 \in A_1, T_2 \in A_2, T_3 \in A_4, T_4 \in A_3, T_5 \in A_7, T_6 \in A_6$, $T_7 \in A_{12}$ (see Table I), and $T \in T^* \setminus \{T_1, T_2, \cdots, T_7\}$, then $P_1^\alpha(T_1) > P_1^\alpha(T_2) > P_1^\alpha(T_3) > P_1^\alpha(T_4) > P_1^\alpha(T_5) > P_1^\alpha(T_6) > P_1^\alpha(T_7) > P_1^\alpha(T)$ and $P_2^\alpha(T_1) < P_2^\alpha(T_2) < P_2^\alpha(T_3) < P_2^\alpha(T_4) < P_2^\alpha(T_5) < P_2^\alpha(T_6) < P_2^\alpha(T_7) < P_2^\alpha(T)$ for $\alpha > 0$. Furthermore, we have $P_1^\alpha(T_1) < P_1^\alpha(T_2) < P_1^\alpha(T_3) < P_1^\alpha(T_4) < P_1^\alpha(T_5) < P_1^\alpha(T_6) < P_1^\alpha(T_7) < P_1^\alpha(T)$ and $P_2^\alpha(T_1) > P_2^\alpha(T_2) > P_2^\alpha(T_3) > P_2^\alpha(T_4) > P_2^\alpha(T_5) > P_2^\alpha(T_6) > P_2^\alpha(T_7) > P_2^\alpha(T)$ for $\alpha < 0$.

Proof: By using Table I, for $\alpha > 0$, we have $P_1^\alpha(T_1) > P_1^\alpha(T_2) > P_1^\alpha(T_3) > P_1^\alpha(T_4) > P_1^\alpha(T_5) > P_1^\alpha(T_6) > P_1^\alpha(T_7)$ and $P_2^\alpha(T_1) < P_2^\alpha(T_2) < P_2^\alpha(T_3) < P_2^\alpha(T_4) < P_2^\alpha(T_5) < P_2^\alpha(T_6) < P_2^\alpha(T_7)$. If $n_1(T) = 5$ or 6, then from the data in Table I, the result holds. If $n_1(T) \geq 7$, then by using Transformation A repeatedly, one can obtain a tree T' such that $n_1(T') = 6$. By Lemma 2.3, $P_1^\alpha(T') > P_1^\alpha(T)$ and $P_2^\alpha(T') < P_2^\alpha(T)$ for $\alpha > 0$. Moreover, by Table I, $P_1^\alpha(T_7) \geq P_1^\alpha(T')$ and $P_2^\alpha(T_7) \leq P_2^\alpha(T')$ for $\alpha > 0$, which yields the result.

Similarly, the conclusions for $\alpha < 0$ can be proved. ■

Lemma 3.2: [16] An n-vertex unicyclic graph U belongs to one of equivalence classes given in Table II if and only if U satisfies the condition $n_1(U) \leq 2$.

Theorem 3.2: Let U^* be a unicyclic graph of order n. For $n \geq 5$, $G_1 \in U_1, G_2 \in U_2, G_3 \in U_4$ (see Table II), and $U \in U^* \setminus \{G_1, G_2, G_3\}$, then $P_1^\alpha(G_1) > P_1^\alpha(G_2) > P_1^\alpha(G_3) > P_1^\alpha(U)$ and $P_2^\alpha(G_1) < P_2^\alpha(G_2) < P_2^\alpha(G_3) < P_2^\alpha(U)$ for $\alpha > 0$. Furthermore, we have $P_1^\alpha(G_1) < P_1^\alpha(G_2) < P_1^\alpha(G_3) < P_1^\alpha(U)$ and $P_2^\alpha(G_1) > P_2^\alpha(G_2) > P_2^\alpha(G_3) > P_2^\alpha(U)$ for $\alpha < 0$

Proof: By using Table II, for $\alpha > 0$, we have $P_1^\alpha(G_1) > P_1^\alpha(G_2) > P_1^\alpha(G_3)$ and $P_2^\alpha(G_1) < P_2^\alpha(G_2) < P_2^\alpha(G_3)$. If $n_1(U) = 2$, then the theorem holds from the data in Table II. If $n_1(U) \geq 3$, then by using Transformation A repeatedly, one can obtain a unicyclic graph U' such that $n_1(U') = 2$. By Lemma 2.3, $P_1^\alpha(U') > P_1^\alpha(U)$ and $P_2^\alpha(U') < P_2^\alpha(U)$ for $\alpha > 0$. Moreover, by the data displayed in Table II, $P_1^\alpha(G_3) \geq P_1^\alpha(U')$ and $P_2^\alpha(G_3) \leq P_2^\alpha(U')$ for $\alpha > 0$, which yields the result.

Similarly, the case of $\alpha < 0$ can be proved. ■

Lemma 3.3: [16] An n-vertex bicyclic graph B belongs to one of equivalence classes given in Table III if and only if B satisfies the condition $n_1(B) \leq 1$.

Theorem 3.3: Let B^* be a bicyclic graph of order n. For $n \geq 7$, $G_1 \in B_2, G_2 \in B_1, G_3 \in B_5$ (see Table III), and $B \in B^* \setminus \{G_1, G_2, G_3\}$, then $P_1^\alpha(G_1) > P_1^\alpha(G_2) > P_1^\alpha(G_3) > P_1^\alpha(B)$ and $P_2^\alpha(G_1) < P_2^\alpha(G_2) < P_2^\alpha(G_3) < P_2^\alpha(B)$ for $\alpha > 0$. Furthermore, we have $P_1^\alpha(G_1) < P_1^\alpha(G_2) < P_1^\alpha(G_3) < P_1^\alpha(B)$ and $P_2^\alpha(G_1) > P_2^\alpha(G_2) > P_2^\alpha(G_3) > P_2^\alpha(B)$ for $\alpha < 0$.

Proof: By using Table III, for $\alpha > 0$, we have $P_1^\alpha(G_1) > P_1^\alpha(G_2) > P_1^\alpha(G_3)$ and $P_2^\alpha(G_1) < P_2^\alpha(G_2) < P_2^\alpha(G_3)$. If $n_1(B) = 1$, then the theorem holds from the data in Table III. If $n_1(B) \geq 2$, then by using Transformation A repeatedly, one can obtain a bicyclic graph B' such that $n_1(B') = 1$. By Lemma 2.3, $P_1^\alpha(B') > P_1^\alpha(B)$ and $P_2^\alpha(B') < P_2^\alpha(B)$ for $\alpha > 0$. Moreover, by the data displayed in Table III, $P_1^\alpha(G_3) \geq P_1^\alpha(B')$ and $P_2^\alpha(G_3) \leq P_2^\alpha(B')$ for $\alpha > 0$, which yields the result.

Similarly, the results for $\alpha < 0$ can be proved. ■

Lemma 3.4: [16] An n-vertex tricyclic graph D belongs to one of equivalence classes given in Tables IV-VI if and only if D satisfies the condition $n_1(D) \leq 2$.

Theorem 3.4: Let D^* be a tricyclic graph of order n. For $n \geq 11$, $G_1 \in D_5, G_2 \in D_4, G_3 \in D_3, G_4 \in D_{12}, G_5 \in D_2, G_6 \in D_{11}, G_7 \in D_1$ or $D_{10}, G_8 \in D_{23}$, (see Tables IV-VI), and $D \in D^* \setminus \{G_1, G_2, \cdots, G_8\}$, then $P_1^\alpha(G_1) > P_1^\alpha(G_2) > P_1^\alpha(G_3) > P_1^\alpha(G_4) > P_1^\alpha(G_5) > P_1^\alpha(G_6) > P_1^\alpha(G_7) > P_1^\alpha(G_8) > P_1^\alpha(D)$ for $\alpha > 0$ and $P_1^\alpha(G_1) < P_1^\alpha(G_2) < P_1^\alpha(G_3) < P_1^\alpha(G_4) < P_1^\alpha(G_5) < P_1^\alpha(G_6) < P_1^\alpha(G_7) < P_1^\alpha(G_8) < P_1^\alpha(D)$ for $\alpha < 0$; For $n \geq 11$, $H_1 \in D_5, H_2 \in D_4, H_3 \in D_{12}, H_4 \in D_3, H_5 \in D_{11}, H_6 \in D_2, H_7 \in D_{23}$ (see Tables IV-VI), and $D' \in D^* \setminus \{H_1, H_2, \cdots, H_7\}$, then $P_2^\alpha(H_1) < P_2^\alpha(H_2) < P_2^\alpha(H_3) < P_2^\alpha(H_4) < P_2^\alpha(H_5) < P_2^\alpha(H_6) < P_2^\alpha(H_7) < P_2^\alpha(D')$ for $\alpha > 0$ and $P_2^\alpha(H_1) > P_2^\alpha(H_2) > P_2^\alpha(H_3) > P_2^\alpha(H_4) > P_2^\alpha(H_5) > P_2^\alpha(H_6) > P_2^\alpha(H_7) > P_2^\alpha(D')$ for $\alpha < 0$.

Proof: By using Tables IV-VI, for $\alpha > 0$, we have $P_1^\alpha(G_1) > P_1^\alpha(G_2) > P_1^\alpha(G_3) > P_1^\alpha(G_4) > P_1^\alpha(G_5) > P_1^\alpha(G_6) > P_1^\alpha(G_7) > P_1^\alpha(G_8)$ and $P_2^\alpha(H_1) < P_2^\alpha(H_2) < P_2^\alpha(H_3) < P_2^\alpha(H_4) < P_2^\alpha(H_5) < P_2^\alpha(H_6) < P_2^\alpha(H_7)$. If $n_1(D) \leq 2$ or $n_1(D') \leq 2$, we can get the results from the data given in Tables IV-VI. If $n_1(D) \geq 3$ or

$n_1(D') \geq 3$, then by using Transformation A repeatedly, one can obtain a tricyclic graph D'' such that $n_1(D'') = 2$. By Lemma 2.3, $P_1^\alpha(D'') > P_1^\alpha(D)$ and $P_2^\alpha(D'') < P_2^\alpha(D')$ for $\alpha > 0$. Moreover, by the data displayed in Table VI, we have $P_1^\alpha(G_8) \geq P_1^\alpha(D'')$ and $P_2^\alpha(H_7) \leq P_2^\alpha(D'')$ for $\alpha > 0$, which yields the result.

Similarly, the case of $\alpha < 0$ can be proved. ■

Lemma 3.5: [16] An n-vertex tetracyclic graph G belongs to one of equivalence classes given in Tables VII and VIII if and only if G satisfies the condition $n_1(G) \leq 1$.

Theorem 3.5: Let G^* be a tetracyclic graph of order n. For $n \geq 12$, $G_1 \in E_{11}, G_2 \in E_{10}, G_3 \in E_9, G_4 \in E_{26}$, (see Tables VII and VIII), and $G \in G^* \setminus \{G_1, G_2, G_3, G_4\}$, then $P_1^\alpha(G_1) > P_1^\alpha(G_2) > P_1^\alpha(G_3) > P_1^\alpha(G_4) > P_1^\alpha(G)$ for $\alpha > 0$ and $P_1^\alpha(G_1) < P_1^\alpha(G_2) < P_1^\alpha(G_3) < P_1^\alpha(G_4) < P_1^\alpha(G)$ for $\alpha < 0$; For $n \geq 12$, $H_1 \in E_{11}, H_2 \in E_{10}, H_3 \in E_{26}$ (see Tables VII and VIII), and $G' \in G^* \setminus \{H_1, H_2, H_3\}$, then $P_2^\alpha(H_1) < P_2^\alpha(H_2) < P_2^\alpha(H_3) < P_2^\alpha(G')$ for $\alpha > 0$ and $P_2^\alpha(H_1) > P_2^\alpha(H_2) > P_2^\alpha(H_3) > P_2^\alpha(G')$ for $\alpha < 0$.

Proof: By using Tables VII and VIII, for $\alpha > 0$, we have $P_1^\alpha(G_1) > P_1^\alpha(G_2) > P_1^\alpha(G_3) > P_1^\alpha(G_4)$ and $P_2^\alpha(H_1) < P_2^\alpha(H_2) < P_2^\alpha(H_3)$. If $n_1(G) \leq 1$ or $n_1(G') \leq 1$, we can get the results from the data given in Tables VII and VIII. If $n_1(G) \geq 2$ or $n_1(G') \geq 2$, then by using Transformation A repeatedly, one can obtain a tetracyclic graph G'' such that $n_1(G'') = 1$. By Lemma 2.3, $P_1^\alpha(G'') > P_1^\alpha(G)$ and $P_2^\alpha(G'') < P_2^\alpha(G')$ for $\alpha > 0$. Moreover, by the data displayed in Table VIII, $P_1^\alpha(G_4) \geq P_1^\alpha(G'')$ and $P_2^\alpha(H_3) \leq P_2^\alpha(G'')$ for $\alpha > 0$, which yields the result.

Similarly, the results for $\alpha < 0$ can be proved. ■

Lemma 3.6: [16] An n-vertex pentacyclic graph H belongs to one of equivalence classes given in Tables IX and X if and only if H satisfies the condition $n_1(H) \leq 1$.

Theorem 3.6: Let H^* be a pentacyclic graph of order n. For $n \geq 16$, $G_1 \in F_{22}, G_2 \in F_{21}, G_3 \in F_{20}, G_4 \in F_{51}$, (see Tables IX and X), and $H \in H^* \setminus \{G_1, G_2, G_3, G_4\}$, then $P_1^\alpha(G_1) > P_1^\alpha(G_2) > P_1^\alpha(G_3) > P_1^\alpha(G_4) > P_1^\alpha(H)$ for $\alpha > 0$ and $P_1^\alpha(G_1) < P_1^\alpha(G_2) < P_1^\alpha(G_3) < P_1^\alpha(G_4) < P_1^\alpha(H)$ for $\alpha < 0$; For $n \geq 12$, $H_1 \in F_{22}, H_2 \in F_{21}, H_3 \in F_{51}$ (see Tables IX and X), and $H' \in H^* \setminus \{H_1, H_2, H_3\}$, then $P_2^\alpha(H_1) < P_2^\alpha(H_2) < P_2^\alpha(H_3) < P_2^\alpha(H')$ for $\alpha > 0$ and $P_2^\alpha(H_1) > P_2^\alpha(H_2) > P_2^\alpha(H_3) > P_2^\alpha(H')$ for $\alpha < 0$.

Proof: By using Tables IX and X, for $\alpha > 0$, we have $P_1^\alpha(G_1) > P_1^\alpha(G_2) > P_1^\alpha(G_3) > P_1^\alpha(G_4)$ and $P_2^\alpha(H_1) < P_2^\alpha(H_2) < P_2^\alpha(H_3)$. If $n_1(H) \leq 1$ or $n_1(H') \leq 1$, we can get the results from the data given in Tables IX and X. If $n_1(H) \geq 2$ or $n_1(H') \geq 2$, then by using Transformation A repeatedly, one can obtain a pentacyclic graph H'' such that $n_1(H'') = 1$. By Lemma 2.3, $P_1^\alpha(H'') > P_1^\alpha(H)$ and $P_2^\alpha(H'') < P_2^\alpha(H')$ for $\alpha > 0$. Moreover, by the data displayed in Table X, $P_1^\alpha(G_4) \geq P_1^\alpha(H'')$ and $P_2^\alpha(H_3) \leq P_2^\alpha(H'')$ for $\alpha > 0$, which yields the result.

Similarly, the case of $\alpha < 0$ can be proved. ■

IV. Corollaries

Remark 4.1: For any extremal graphs in Theorems 3.1-3.3, 3.5 and 3.6, the maximum degree of these extremal graphs is less than or equal to 4, so Theorems 3.1-3.3, 3.5 and 3.6 hold for chemical tree, chemical unicyclic graph, chemical bicyclic graph, chemical tetracyclic graph and chemical pentacyclic graph, respectively.

Note that for $D \in D_1$ or D_2 in Table IV, D is not a chemical tricyclic graph, by Theorem 3.4, we have the following theorem.

Theorem 4.2: Let D^* be a chemical tricyclic graph of order n. For $n \geq 11$, $G_1 \in D_5, G_2 \in D_4, G_3 \in D_3, G_4 \in D_{12}, G_5 \in D_{11}, G_6 \in D_{10}, G_7 \in D_{23}$, (see Tables IV-VI), and $D \in D^* \setminus \{G_1, G_2, \cdots, G_7\}$, then $P_1^\alpha(G_1) > P_1^\alpha(G_2) > P_1^\alpha(G_3) > P_1^\alpha(G_4) > P_1^\alpha(G_5) > P_1^\alpha(G_6) > P_1^\alpha(G_7) > P_1^\alpha(D)$ for $\alpha > 0$ and $P_1^\alpha(G_1) < P_1^\alpha(G_2) < P_1^\alpha(G_3) < P_1^\alpha(G_4) < P_1^\alpha(G_5) < P_1^\alpha(G_6) < P_1^\alpha(G_7) < P_1^\alpha(D)$ for $\alpha < 0$; For $n \geq 11$, $H_1 \in D_5, H_2 \in D_4, H_3 \in D_{12}, H_4 \in D_3, H_5 \in D_{11}, H_6 \in D_{23}$ (see Tables IV-VI), and $D' \in D^* \setminus \{H_1, H_2, \cdots, H_6\}$, then $P_2^\alpha(H_1) < P_2^\alpha(H_2) < P_2^\alpha(H_3) < P_2^\alpha(H_4) < P_2^\alpha(H_5) < P_2^\alpha(H_6) < P_2^\alpha(D')$ for $\alpha > 0$ and $P_2^\alpha(H_1) > P_2^\alpha(H_2) > P_2^\alpha(H_3) > P_2^\alpha(H_4) > P_2^\alpha(H_5) > P_2^\alpha(H_6) > P_2^\alpha(D')$ for $\alpha < 0$.

Note that $\Pi_1(G) = P_1^2(G)$ and $\Pi_2(G) = P_2^1(G)$ for a (chemical) graph G, by Theorems 3.1-3.6, Theorem 4.2 and Remark 4.1, one can derive the following corollaries.

Corollary 4.1: Let T^* be a tree or a chemical tree of order n. For $n \geq 10$, $T_1 \in A_1, T_2 \in A_2, T_3 \in A_4, T_4 \in A_3, T_5 \in A_7, T_6 \in A_6$, $T_7 \in A_{12}$ (see Table I), and $T \in T^* \setminus \{T_1, T_2, \cdots, T_7\}$, then $\Pi_1(T_1) > \Pi_1(T_2) > \Pi_1(T_3) > \Pi_1(T_4) > \Pi_1(T_5) > \Pi_1(T_6) > \Pi_1(T_7) > \Pi_1(T)$ and $\Pi_2(T_1) < \Pi_2(T_2) < \Pi_2(T_3) < \Pi_2(T_4) < \Pi_2(T_5) < \Pi_2(T_6) < \Pi_2(T_7) < \Pi_2(T)$.

Corollary 4.2: Let U^* be a unicyclic graph or a chemical unicyclic graph of order n. For $n \geq 5$, $G_1 \in U_1, G_2 \in U_2, G_3 \in U_4$ (see Table II), and $U \in U^* \setminus \{G_1, G_2, G_3\}$, then $\Pi_1(G_1) > \Pi_1(G_2) > \Pi_1(G_3) > \Pi_1(U)$ and $\Pi_2(G_1) < \Pi_2(G_2) < \Pi_2(G_3) < \Pi_2(U)$.

Corollary 4.3: Let B^* be a bicyclic graph or a chemical bicyclic graph of order n. For $n \geq 7$, $G_1 \in B_2, G_2 \in B_1, G_3 \in B_5$ (see Table III), and $B \in B^* \setminus \{G_1, G_2, G_3\}$, then $\Pi_1(G_1) > \Pi_1(G_2) > \Pi_1(G_3) > \Pi_1(B)$ and $\Pi_2(G_1) < \Pi_2(G_2) < \Pi_2(G_3) < \Pi_2(B)$.

Corollary 4.4: (i) Let D^* be a tricyclic graph of order n. For $n \geq 11$, $G_1 \in D_5, G_2 \in D_4, G_3 \in D_3, G_4 \in D_{12}, G_5 \in D_2, G_6 \in D_{11}, G_7 \in D_1$ or $D_{10}, G_8 \in D_{23}$, (see Tables IV-VI), and $D \in D^* \setminus \{G_1, G_2, \cdots, G_8\}$, then $\Pi_1(G_1) > \Pi_1(G_2) > \Pi_1(G_3) > \Pi_1(G_4) > \Pi_1(G_5) > \Pi_1(G_6) > \Pi_1(G_7) > \Pi_1(G_8) > \Pi_1(D)$; For $n \geq 11$, $H_1 \in D_5, H_2 \in D_4, H_3 \in D_{12}, H_4 \in D_3, H_5 \in D_{11}, H_6 \in D_2, H_7 \in D_{23}$ (see Tables IV-VI), and $D' \in D^* \setminus \{H_1, H_2, \cdots, H_7\}$, then $\Pi_2(H_1) < \Pi_2(H_2) < \Pi_2(H_3) < \Pi_2(H_4) < \Pi_2(H_5) < \Pi_2(H_6) < \Pi_2(H_7) < \Pi_2(D')$.

(ii) Let D^* be a chemical tricyclic graph of order n. For $n \geq 11$, $G_1 \in D_5, G_2 \in D_4, G_3 \in D_3, G_4 \in D_{12}, G_5 \in D_{11}, G_6 \in D_{10}, G_7 \in D_{23}$, (see Tables IV-VI), and $D \in D^* \setminus \{G_1, G_2, \cdots, G_7\}$, then $\Pi_1(G_1) > \Pi_1(G_2) > \Pi_1(G_3) > \Pi_1(G_4) > \Pi_1(G_5) > \Pi_1(G_6) > \Pi_1(G_7) > \Pi_1(D)$; For $n \geq 11$, $H_1 \in D_5, H_2 \in D_4, H_3 \in D_{12}, H_4 \in D_3, H_5 \in D_{11}, H_6 \in D_{23}$ (see Tables IV-VI), and $D' \in D^* \setminus \{H_1, H_2, \cdots, H_6\}$, then $\Pi_2(H_1) < \Pi_2(H_2) < \Pi_2(H_3) < \Pi_2(H_4) < \Pi_2(H_5) < \Pi_2(H_6) < \Pi_2(D')$.

Corollary 4.5: Let G^* be a tetracyclic graph or a chemical tetracyclic graph of order n. For $n \geq 12$, $G_1 \in E_{11}, G_2 \in E_{10}, G_3 \in E_9, G_4 \in E_{26}$, (see Tables VII and VIII), and $G \in G^* \setminus \{G_1, G_2, G_3, G_4\}$, then $\Pi_1(G_1) >$

$\Pi_1(G_2) > \Pi_1(G_3) > \Pi_1(G_4) > \Pi_1(G)$; For $n \geq 12$, $H_1 \in E_{11}, H_2 \in E_{10}, H_3 \in E_{26}$ (see Tables VII and VIII), and $G' \in G^* \setminus \{H_1, H_2, H_3\}$, then $\Pi_2(H_1) < \Pi_2(H_2) < \Pi_2(H_3) < \Pi_2(G')$.

Corollary 4.6: Let H^* be a pentacyclic graph or a chemical pentacyclic graph of order n. For $n \geq 16$, $G_1 \in F_{22}, G_2 \in F_{21}, G_3 \in F_{20}, G_4 \in F_{51}$, (see Tables IX and X), and $H \in H^* \setminus \{G_1, G_2, G_3, G_4\}$, then $\Pi_1(G_1) > \Pi_1(G_2) > \Pi_1(G_3) > \Pi_1(G_4) > \Pi_1(H)$; For $n \geq 12$, $H_1 \in F_{22}, H_2 \in F_{21}, H_3 \in F_{51}$ (see Tables IX and X), and $H' \in H^* \setminus \{H_1, H_2, H_3\}$, then $\Pi_2(H_1) < \Pi_2(H_2) < \Pi_2(H_3) < \Pi_2(H')$.

V. Conclusion

The vertices and edges of graphs represent the atoms and the chemical bonds of a compound, respectively. So we can use graph theory to characterize these chemical structures. The mathematical properties of general multiplicative Zagreb indices deserve further study since they can be used to detect the chemical compounds which may have desirable properties. Namely, if one can find some properties well-correlated with these two descriptors for some value of α, then the extremal graphs should correspond to compounds with minimum or maximum value of that property. Furthermore, one such property has already been found for multiplicative Zagreb indices.

Through out this paper, we determine the extremal general multiplicative Zagreb indices of n-vertex (chemical) trees, (chemical) unicyclic graphs, (chemical) bicyclic graphs, (chemical) tricyclic graphs, (chemical) tetracyclic graphs and (chemical) pentacyclic graphs. Furthermore, we apply these results directly to multiplicative Zagreb indices. We will consider the extremal values with respect to general multiplicative Zagreb indices of other chemical graphs as a near future work.

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