www.combinatorics.ir

Transactions on Combinatorics
ISSN (print): 2251-8657, ISSN (on-line): 2251-8665
Vol. 5 No. 4 (2016), pp. 1-8.

www.ui.ac.ir

CACTI WITH EXTREMAL PI INDEX

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Communicated by Ivan Gutman

ABSTRACT. The vertex PI index $PI(G) = \sum_{xy \in E(G)}[n_{xy}(x) + n_{xy}(y)]$ is a distance-based molecular structure descriptor, where $n_{xy}(x)$ denotes the number of vertices which are closer to the vertex x than to the vertex y and which has been the considerable research in computational chemistry dating back to Harold Wiener in 1947. A connected graph is a cactus if any two of its cycles have at most one common vertex. In this paper, we completely determine the extremal graphs with the greatest and smallest vertex PI indices mong all cacti with a fixed number of vertices. As a consequence, we obtain the sharp bounds with corresponding extremal cacti and extend a known result.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For $x, y \in V(G)$, the distance $d(x, y)$ is the number of edges in a shortest path connecting x and y. A vertex is a pendant vertex if its neighborhood contains exactly one vertex. An edge of a graph is said to be pendant if one of its vertices is a pendant vertex. An edge $e \in E(G)$ is a cut edge if the graph deleting e contains two components.

A numerical representation that can preserve a structural property of a graph is mathematically defined as a graphic descriptor or a topological index. The Wiener index is the oldest and most thoroughly examined topological index used in chemistry. In 1947, Harold Wiener [24] applied Wiener index to determine physical properties of alkanes and defined as

$$W(G) = \sum_{\{x,y\} \subset V(G)} d(x, y).$$

MSC(2010): Primary: 05C90; Secondary: 05C05, 05C70.

Keywords: Distance, Extremal bounds, PI index, Cacti.

Received: 25 February 2016, Accepted: 28 February 2016.

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Compared to Wiener index, Szeged index was given by Klavžar and Gutman [15] in 1996 as follows:

$$Sz(G) = \sum_{xy \in E(G)} n_{xy}(x) n_{xy}(y),$$

where $n_{xy}(x)$ is the number of vertices $w \in V(G)$ such that $d(x,w) < d(y,w)$, $n_{xy}(y)$ is the number of vertices $w \in V(G)$ such that $d(x,w) > d(y,w)$ and $w \neq x, y$. Currently, various work relating Wiener index, Sz index and their chemical meaning have been already studied, referred to the surveys [1, 8, 9, 12]. Based on the considerable success of Wiener index and Sz index, Khadikar [16] proposed edge Padmakar-Ivan (PI$_e$) index in 2000 as follows:

$$PI_e(G) = \sum_{e=xy \in E(G)} [n_{ex}(e|G) + n_{ey}(e|G)],$$

where $n_{ex}(e|G)$ denotes the number of edges which are closer to the vertex x than to the vertex y, and $n_{ey}(e|G)$ denotes the number of edges which are closer to the vertex y than to the vertex x, respectively. The detailed applications of PI_e indices between chemistry and graph theory are investigated in [2]-[6],[16]-[18],[24]-[26]. As this definition does not count edges equidistant from both ends of the edge $e = xy$, Khalifeh et al. [19] continued to introduce a new PI index of vertex version below:

$$PI(G) = PI_v(G) = \sum_{xy \in E(G)} [n_{xy}(x) + n_{xy}(y)],$$

where $n_{xy}(x)$ is the number of vertices $w \in V(G)$ such that $d(x,w) < d(y,w)$, $n_{xy}(y)$ is the number of vertices $w \in V(G)$ such that $d(x,w) > d(y,w)$ and $w \neq x, y$. In addition, there are nice results regarding vertex PI index in the study of a computational complexity and the intersection between graph theory and chemistry. In [10], Das and Gutman obtained a lower bound on the vertex PI index of a connected graph in terms of numbers of vertices, edges, pendent vertices, and clique number. Hoji et al. [13] provided exact formulas for the vertex PI indices of Kronecker product of a connected graph G and a complete graph. Ilić and Milosavljević [14] established basic properties of weighted vertex PI index and proved some lower and upper bounds. Pattabiraman and Paulraja [21] presented the expressions for vertex PI indices of the strong product of a graph and the complete multipartite graph.

We explore another type of graphs: A graph is a cactus if it is connected and all of its blocks are either edges or cycles, i.e., any two of its cycles have at most one common vertex. Denote the cacti of n vertices and k pendent vertices as $\mathcal{C}_{n,k}$ with $n \geq k \geq 0$. Let $\lfloor x \rfloor$ be the largest integer which is less than or equal to x. Up to now, many results were obtained concerning the cacti between chemistry and graph theory. In [20], Li and Yang determined sharp upper and lower bounds of the cacti in $\mathcal{C}_{n,k}$ for special chemical indices of Zagreb indices. Feng and Yu [11] established the cacti in $\mathcal{C}_{n,k}$ with the smallest hyper-Wiener indices, which is a renovated version of Wiener index. Wang and Tan [22] characterized the extremal cacti having the largest Wiener and hyper-Wiener indices in $\mathcal{C}_{n,k}$. Wang and Kang [23] found the extremal bounds of another chemical index, Harary index, for the cacti $\mathcal{C}_{n,k}$. Chen [7] gave the first three smallest Gutman indices among the cacti.

Motivated by the results of chemical indices and their applications, it is worth noting that it may be much interesting to characterize the cacti in $\mathcal{C}_{n,k}$ with greatest and smallest vertex PI indices. The concept of vertex PI index yields the following fact.

Fact 1 *Let $G \in \mathcal{C}_{n,k}$ with $n \geq k \geq 0$, then*
(i) If G is C_3, C_4 or C_5, then $PI(G) = 0, 8, 10$.
(ii) If G is C_3 attaching a pendent edge e (say $C_3 \cup e$), then $PI(G) = 4$.

In this paper, we determine graphs with greatest and smallest vertex PI indices in $\mathcal{C}_{n,k}$, and provide the extremal cacti in Figs 1 and 2, which extends Das and Gutman's result[10] by excluding the number of edges and cliques for the cacti. Our main results are as follows.(In Figs 1 and 2, $\circ$ means that the vertex maybe exist.)

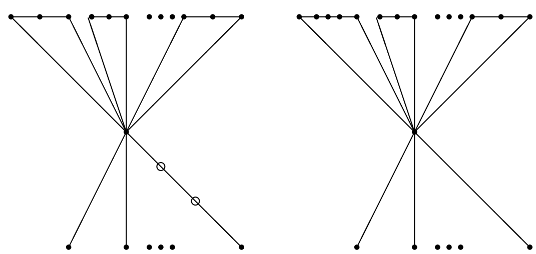

Fig. 1

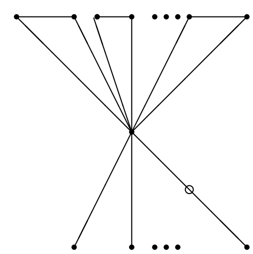

Fig. 2

Theorem 1.1. *Let $G \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_4, C_5\}$ with $n \geq k \geq 0$, then $PI(G) \leq (n-1+\lfloor\frac{n-k-1}{3}\rfloor)(n-2)$, where the equality holds if and only if G is a tree for $n \leq k+3$ and otherwise, one of the following statements holds(See Fig. 1):*
(i) All cycles have length 4 and there are at most $k+2$ cut edges.
(ii) All cycles have length 4 except one of length 6 and there are exact k pendent edges.

Theorem 1.2. *Let $G \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_4\}$ with $n \geq k \geq 0$, then $PI(G) \geq (n-1)(n-2) - 2\lfloor\frac{n-k-1}{2}\rfloor$, where the equality holds if and only if G is a tree for $n \leq k+2$ and otherwise, all cycles have length 3 and there are at most $k+1$ cut edges (See Fig. 2).*

2. **Main proofs**

Firstly, we provide some lemmas which are important in the proof of our main results.

Lemma 2.1. *Let $G \in \mathcal{C}_{n,k}$ and $e \in E(G)$. Then*
(i) $PI(e) \leq n-2$, the equality holds if e is a cut edge or an edge of an even cycle.
(ii) If e is an edge of an odd cycle C_o, then $PI(e) \leq n-3$. Furthermore, if $G = C_o$, then $PI(e) = n-3$.
(iii) For each odd cycle C of G, $PI(C) = (n-2)(|C|-1) - 2$.

Proof. Assume that $e = uv \in E(G)$. Since $PI(e)$ counts at most $n-2$ vertices, then $PI(e) \leq n-2$. If e is a cut edge, then $G - e$ contains two components G_1 and G_2. Thus, all vertices of G_1 are closer to one of $\{u, v\}$, say u, and all vertices of G_2 are closer to v. Thus, $PI(e) = n_e(u) + n_e(v) = n-2$ if e is a cut edge. Let $C = v_1 v_2 \dots v_a v_1$ be a cycle of G and $v_l v_l' \in E(C)$. Since G is a cactus, then $G - E(C)$

contains a components $B_1, B_2, \ldots, B_a$ such that $v_i \in V(B_i)$. If a is even, then $d(v_l, v_i) \neq d(v_l', v_i)$ for $1 \leq i \leq a$, and $d(v_l, u_i) \neq d(v_l', u_i)$ with $u_i \in V(B_i)$. We obtain that $PI(e) = n-2$ if C is even. Thus, (i) is true.

For $C = C_o$, a is odd. Then there exists a unique vertex $v_t \in V(C)$ such that $d(v_l, v_t) = d(v_l', v_t)$, that is, $PI(e) \leq n-3$. When $G = C_o$, we see $PI(e) = n-3$. Thus, (ii) is true.

For (iii), a is odd and $\sum_{i=1}^{a} |B_i| = n$. Note that if $d(v_l, v_t) = d(v_l', v_t)$ with $v_t \in V(C)$, then $d(v_l, u_t) = d(v_l', u_t)$ with $u_t \in V(B_t)$. Similarly, if $d(v_l, v_t) \neq d(v_l', v_t')$ with $v_t' \in V(C)$, then $d(v_l, u_t') \neq d(v_l', u_t')$ with $u_t' \in V(B_t)$. Thus, $PI(v_l, v_l') = n - 2 - |B_t|$ with $t \neq l, l'$. It induces that

$$\begin{aligned}
PI(C) &= \textstyle\sum_{e\in E(C)} PI(e) = \sum_{i=1}^{a}(n-2-|B_i|) \\
&= a(n-2) - \textstyle\sum_{i=1}^{a} |B_i| \\
&= |C|(n-2) - n \\
&= (|C|-1)(n-2) - 2
\end{aligned}$$

and Lemma 2.1 is true. □

Lemma 2.2. *Let C be a cycle of G. Define Transformation 1: $G_1 = G - xy$ with $xy \in E(G) - E(C)$ and Transformation 2: $G_2 = G + x'y'$, where at least one of $\{x', y'\}$ are in $V(G) - V(C)$. If $G_1, G_2 \in \mathcal{C}_{n,k}$ and $e \in E(C)$, then $PI(e) = PI_{G_1}(e) = PI_{G_2}(e)$.*

Proof. Let $C = v_1v_2\ldots v_av_1$, $v_l, v_l' \in E(C)$. Then $G - E(C)$ contains a components $B_1, B_2, \ldots, B_a$ such that $v_i \in V(B_i)$. Since G is a cactus, then for $v_i \in V(C)$, if $d(v_l, v_i) = d(v_l', v_i)$, we obtain $d(v_l, u_i) = d(v_l', u_i)$ with $u_i \in V(B_i)$. Similarly, if $d(v_l, v_i) \neq d(v_l', v_i)$, we obtain $d(v_l, u_i) \neq d(v_l', u_i)$ with $u_i \in V(B_i)$. Note that G_1 and G_2 contain the same cycle C as G, and the components B_j^i of $G_i - C$ with $v_j \in V(B_j^i)$ has the property that $V(B_j^i) = V(B_j^{i'})$. Then for $v_i \in V(C)$, if $d(v_l, v_i) = d(v_l', v_i)$, then $d_{G_1}(v_l, v_i) = d_{G_1}(v_l', v_i)$ and $d_{G_2}(v_l, v_i) = d_{G_2}(v_l', v_i)$, $d_{G_1}(v_l, u_i) = d_{G_1}(v_l', u_i)$ with $u_i \in V_{G_1}(B_i)$ and $d_{G_2}(v_l, u_i) = d_{G_2}(v_l', u_i)$ with $u_i \in V_{G_1}(B_i)$. Similarly, if $d(v_l, v_i) \neq d(v_l', v_i)$, then $d_{G_1}(v_l, v_i) \neq d_{G_1}(v_l', v_i)$ and $d_{G_2}(v_l, v_i) \neq d_{G_2}(v_l', v_i)$, $d_{G_1}(v_l, u_i) \neq d_{G_1}(v_l', u_i)$ with $u_i \in V_{G_1}(B_i)$ and $d_{G_2}(v_l, u_i) \neq d_{G_2}(v_l', u_i)$ with $u_i \in V_{G_2}(B_i)$. Thus, $PI(e) = PI_{G_1}(e) = PI_{G_2}(e)$ and Lemma 2.2 is true. □

Lemma 2.3. *If $G \in \mathcal{C}_{n,k}$ contains t_1 cycles of lengths $\{l_1, l_2, \ldots, l_{t_1}\}$ and $t_2 \geq k$ cut edges, then $PI(G)$ is unique and these cycles can be shared a common vertex $u_0, k-1$ pendent edges can be adjacent to u_0 and a path of length $t_2 - k + 1$ can be adjacent to u_0. (See Fig. 2)*

Proof. By Lemma 2.1 (i) and (iii), PI values with cycles of fixed lengths and fixd number of cut edges are determined. Then $PI(G) = \sum_{C \text{ is a cycle of G}} \sum_{e\in E(C)} PI(e) + \sum_{e \text{ is an cut edge of G}} PI(e)$ is unique. By recombining these cycles and cut edges, t_1 cycles can have a common vertex $u_0, k-1$ pendent edges can be adjacent to u_0 and a path of length $t_2 - k + 1$ can be adjacent to u_0. Thus, Lemma 2.3 is true. □

Lemma 2.4. *Let $G \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_5\}$, if $PI(G)$ attains the maximal value, then the length of each cycle, if any, is even.*

Proof. If G has a cycle, then $n \geq 3$. Assume that there is an odd cycle $C_{2t+1} = u_1u_2 \dots u_{2t}u_{2t+1}u_1$ with $t \geq 1$. If all vertices of C_{2t+1} have degree 2, then $G = C_{2t+1}$. Since $G \neq C_3, C_5$, then $n \geq 7$. By Lemma 2.1 (ii), $PI(e) = n - 3$ for $e \in E(C_{2t+1})$ and $PI(C_{2t+1}) = n(n-3)$. By Lemma 2.1 (iii), $PI(G) = (n-2)(2t) - 2$. We build a new graph $G' = (G - \{u_1u_{2t+1}\}) \cup \{u_1u_{2t-2}, u_{2t+1}\}$. Then G' contains a cycle $C'_1 = u_{2t-2}u_{2t-1}u_{2t}u_{2t+1}u_{2t-2}$ of length 4 and a cycle $C'_2 = u_1u_2 \dots u_{2t-2}u_1$ of length $2t-2$. By Lemma 2.1 (i), $PI(G') = PI(C'_1) + PI(C'_2) = (n-2)(2t+2)$. Thus, $PI(G') > PI(G)$, contradicted that $PI(G)$ is maximal.

Thus, there is a vertex of degree at least 3 in C_{2t+1}. If the vertex of degree 3 is unique, say u_1, then there exists a pendent path $u_1, v_1, v_2, \dots$. Set $G_0 = (G - \{u_1u_2\}) \cup \{u_2v_1\}$, then $G_0 \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_5\}$. By Lemma 2.1, we obtain $PI(G_1) > PI(G)$, a contradiction. If at least two vertices of $\{u_1, u_2, u_3\}$ has degree at least two, say u_1, u_2. Set $G_1 = G - \{u_1u_2\}$, then $G_1 \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_5\}$. By Lemma 2.1, we obtain $PI(G) = PI(C) + k(k+1) = k(k+3)$ and $PI(G_1) = (k+1)(k+3) > PI(G)$, a contradiction. If $t \geq 2$, we construct a new graph G_2 such that $G_2 = G - \{u_1, u_{2t+1}\} \cup \{u_1, u_{2t}\}$ with $d_G(u_{2t+1}) \geq 3$. Then $G_2 \in \mathcal{C}_{n,k}, C_{2t}$ is an even cycle and u_{2t}, u_{2t+1} is a cut edge. By Lemmas 2.1 and 2.2,

$$\begin{aligned} PI(G_2) - PI(G) &= (PI(u_{2t}u_{2t+1}) + PI(C_{2t})) - PI(C_{2t+1}) \\ &= (n-2)(2t+1) - [(n-2)(2t) - 2] \\ &> 0, \end{aligned}$$

contradicted that $PI(G)$ is maximal. Therefore, each cycle, if any, is even and Lemma 2.4 is true. □

Lemma 2.5. *Let $G \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e, C_5\}$ with $n \geq k+4$, if $PI(G)$ attains the maximal value, then all cycles are length 4 except at most one of them is 6.*

Proof. By Lemma 2.4, all cycles are even. If there exists an cycle $C = u_1u_2 \dots u_{2t}u_1$ with $t \geq 4$. Set $G_1 = (G - \{u_1u_{2t}\}) \cup \{u_1u_4, u_4u_{2t}\}$. Then $G_1 \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e\}$ and $|E(G_1)| = |E(G)| + 1$. Since each edge of G_1 is either a cut edge or an edge of an even cycle, then $PI(G_1) > PI(G)$ by Lemma 2.1 (i), that is, the length of cycles are at most 6. Now suppose that there are two cycles of length 6. By Lemma 2.3, we can assume these two cycles share a common vertex u_1, say $C_1 = u_1u_2 \dots u_6u_1$ and $C_2 = u_1v_2 \dots v_6u_1$. Set $G_2 = G - \{u_1u_2, u_3u_4, u_1v_2\} \cup \{u_1u_4, u_2v_2, u_3v_3, u_1v_3\}$. Then $G_2 \in \mathcal{C}_{n,k} - \{C_3, C_3 \cup e\}$ and $|E(G_2)| = |E(G)| + 1$. Since each edge of G_2 is either a cut edge or an edge of an even cycle, then $PI(G_1) > PI(G)$, that is, there are at most one cycle of length 6 and Lemma 2.5 is true. □

Lemma 2.6. *Let $G \in \mathcal{C}_{n,k} - \{C_4\}$, if $PI(G)$ attains the minimal value, then the length of each cycle, if any, is odd.*

Proof. Suppose G has an even cycle $C_{2t} = u_1u_2 \dots u_{2t}u_1$, then $n \geq k+4$ and $t \geq 2$. If all vertices of G have degree 2, then $G = C_{2t}$ and $n = 2t$. By Lemma 2.1 (i), $PI(G) = n(n-2) = 2t(2t-2)$. Since $G \neq C_4$ and $t \geq 3$, set $G_1 = (G - \{u_1u_2\}) \cup \{u_1u_4, u_2u_4\}$. Then $G_1 \in \mathcal{C}_{n,k} - \{C_4\}$, $C_{1,3} = u_2u_3u_4u_2$ is an odd cycle and $C_{1,2t-2} = u_1u_4u_5 \dots u_{2t}u_1$ is an even cycle. By Lemma 2.1 (i) and (iii), $PI(G_1) = PI(C_{1,3}) + PI(C_{1,2t-2}) = (n-2)2 - 2 + (n-2)(2t-2) = 2t(2t-2) - 2 < PI(G)$, contradicted that $PI(G)$ is minimal. If there exists a vertex u_2 with $d(u_2) \geq 3$, then we construct a new graph $G_2 = (G - \{u_1u_2\}) \cup \{u_1u_3\}$. Then $G_2 \in \mathcal{C}_{n,k}$, u_2u_3 is a cut edge and $C' = u_1u_3u_4 \dots u_{2t}u_1$ is an odd cycle. By Lemmas 2.1 and 2.3,

$$\begin{aligned} PI(G_2) - PI(G) &= (PI_{G_2}(u_2u_3) + PI_{G_2}(C')) - PI(C_{2t}) \\ &= [(n-2) + (n-2)(2t-2) - 2] - 2t(n-2) \\ &= -n < 0. \end{aligned}$$

Thus, $PI(G_2) < PI(G)$, contradicted that $PI(G)$ is minimal. Therefore, each cycle, if any, is odd and Lemma 2.6 is true. □

Lemma 2.7. *Let $G \in \mathcal{C}_{n,k} - \{C_4\}$ with $n \geq k+3$, if $PI(G)$ attains the minimal value, then all cycles have length* 3*.*

Proof. By Lemma 2.6, we only consider all cycles of G are odd. Suppose that there is an odd cycle of length greater than 3, say $C_{2t+1} = u_1u_2 \dots u_{2t+1}u_1$ with $t \geq 2$. Set a new graph $G_1 = (G - \{u_{2t-1}u_{2t}\}) \cup \{u_1u_{2t-1}, u_1u_{2t}\}$. Then $G_1 \in \mathcal{C}_{n,k}$ and we will show that $PI(G_1) < PI(G)$. Let $C_1 = u_1u_2 \dots u_{2t-1}u_1$ and $C_2 = u_1u_{2t}u_{2t+1}u_1$. By Lemma 2.1 (iii), $PI(C) = (n-2)(|C|-2)-2 = 2t(n-2)-2$ and $PI(C_1) + PI(C_2) = [(n-2)(|C_1|-2)-2] + [(n-2)(|C_2|-2)-2] = 2t(n-2)-4$. Thus, $PI(C_1) + PI(C_2) < PI(C)$. By Lemma 2.2, $PI(G_1) - PI(G) = PI(C_1) + PI(C_2) - PI(C) < 0$ and Lemma 2.7 is true. □

Now, we turn to prove the main results of this paper.

Proof. of Theorem 1.1, All length of cycles, if any, are even by Lemma 2.4. Since $e \in E(G)$ is either a cut edge or an edge of an even cycle, then $PI(e) = n-2$ by Lemma 2.1 (i). Thus, $PI(G) = |E(G)|(n-2)$ and it needs to maximize $|E(G)|$. For $n \leq k+3$, $\lfloor \frac{n-k-1}{3} \rfloor = 0$ and $PI(G) = (n-1)(n-2)$. Thus, Theorem 1.1 is true. For $n \geq k+4$, all length of cycles are 4 except at most one of them is 6 by Lemma 2.5. By Lemma 2.3, all cycles of G have a common vertex u_0, $k-1$ pendent edges are adjacent to u_0 and a path of length $t_2 - k + 1$ is adjacent to u_0.

Assume that there exist a cycle $C_6 = u_0u_1u_2u_3u_4u_5u_0$ and G contains more than $k+1$ cut edges, then G has a path $u_0, v_1, v_2, \dots$ of length more than 2. Set $G_1 = (G - \{u_2u_3\}) \cup \{u_2v_1, u_0u_3\}$, then $G_2 \in \mathcal{C}_{n,k}$ and $|E(G_2)| = |E(G)| + 1$. Since $e \in E(G_1)$ is either an cut edge or an edge of an even cycle, then $PI(e) = n-2$ and $PI(G_1) = (n-2)|E(G_1)| > PI(G) = (n-2)|E(G)|$, contradicted that $PI(G)$ is maximal. Thus, G contains exact k pendent edges. Next we will show that if all length of cycles are 4, then G contains at most $k+2$ cut edges. Otherwise, there exist a path $u_0v_1v_2 \dots$ of length at least 4 by Lemma 2.3. Set $G_2 = G \cup \{u_0v_3\}$, then $G_2 \in \mathcal{C}_{n,k}$ and $|E(G_2)| = |E(G)| + 1$. Since $e \in E(G_1)$ is either an cut edge or an edge of an even cycle, then $PI(e) = n-2$ and $PI(G_2) = (n-2)|E(G_2)| > PI(G) = (n-2)|E(G)|$, contradicted that $PI(G)$ is maximal. Note that for $n \geq k+4$, the number of cycles of G is $\lfloor \frac{n-k-1}{3} \rfloor$ and the number of edges of G is $n - 1 + \lfloor \frac{n-k-1}{3} \rfloor$. Thus, $PI(G) = (n - 1 + \lfloor \frac{n-k-1}{3} \rfloor)(n-2)$ and Theorem 1.1 is true. □

Proof. of Theorem 1.2, For $n \leq k+2$, $\lfloor \frac{n-k-1}{2} \rfloor = 0$ and $PI(G) = (n-1)(n-2)$ by Lemma 2.1. Thus, Theorem 1.2 is true. For $n \geq k+3$, the length of each edge of G is 3 by Lemma 2.7. Next we will show that G contains at most $k+1$ cut edges. Assume that G contains at least $k+2$ cut edges. By Lemma 2.3, all cycles of G have a common vertex $u_0, k-1$ pendent edges are adjacent to u_0 and a path of length at least $(k+2)-k+1 = 3$ is adjacent to u_0. Denote the path as $u_0v_1v_2v_3\ldots$, set $G_1 = G \cup \{u_0v_2\}$. By Lemma 2.1 (iii) and 2, $PI(G_1) - PI(G) = PI_{G_1}(v_0u_1u_2v_0) - PI(u_0v_1) - PI(v_1v_2) = [(n-2)(3-1)-2] - (n-2) - (n-2) = -2 < 0$. Thus, $PI(G_1) < PI(G)$, contradicted that $PI(G)$ is minimal. Note that for $n \geq k+3$, the number of cycles of length 3 is $\lfloor \frac{n-k-1}{2} \rfloor$ and the number of cut edges is $n-1-2\lfloor \frac{n-k-1}{2} \rfloor$. Thus,

$$\begin{aligned} PI(G) &= 2(n-3)(\lfloor \tfrac{n-k-1}{2} \rfloor) + (n-1-2\lfloor \tfrac{n-k-1}{2} \rfloor)(n-2) \\ &= (n-1)(n-2) - 2\lfloor \tfrac{n-k-1}{2} \rfloor, \end{aligned}$$

and Theorem 1.2 is true. □

Remark 2.8. *The maximal and minimal values of vertex PI vertices of cacti are uniqe, but the cacti achieved the maximal and minimal vertex PI index are not unique. All cacti satisfying the statements in Theorem 1.1 and Theorem 1.2 are arrived at the corresoponding sharp values. Fig 1 and Fig 2 are special examples achieved the sharp bounds.*

Acknowledgments

The first and second author was supported by Projects 11571134, 11371162 of NSFC, and by the Self-determined Research Funds of CCNU from the colleges basic research and operation of MOE., the second author was partially supported by the Summer Graduate Research Assistantship Program of Graduate School of University of Mississippi, the third author was partially supported by College of Liberal Arts Summer Research Grant of University of Mississippi.

References

[1] T. Al-Fozan, P. Manuel, I. Rajasingh and R. S. Rajan, Computing Szeged index of certain nanosheets using partition technique, *MATCH Commun. Math. Comput. Chem.*, **72** (2014) 339–353.

[2] A. R. Ashrafi and A. Loghman, PI index of zig-zag polyhex nanotubes, *MATCH Commun. Math. Comput. Chem.*, **55** (2006) 447–452.

[3] A. R. Ashrafi and A. Loghman, Padmakar-Ivan index of TUC4C8(S) nanotubes, *J. Comput. Theor. Nanosci.*, **3** (2006) 378–381.

[4] A. R. Ashrafi and A. Loghman, PI index of armchair polyhex nanotubes, *Ars Combin.*, **80** (2006) 193–199.

[5] A. R. Ashrafi, B. Manoochehrian and H. Yousefi-Azari, On the PI polynomial of a graph, *Util. Math.*, **71** (2006) 97–108.

[6] A. R. Ashrafi and F. Rezaei, PI index of polyhex nanotori, *MATCH Commun. Math. Comput. Chem.*, **57** (2007) 243–250.

[7] S. Chen, Cacti with the smallest, second smallest and third smallest Gutman index. *J. Comb. Optim.*, **31** (2016) 327–332.

[8] A. A. Dobrynin, R. Entringer and I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.*, **66** (2001) 211–249.

[9] A. A. Dobrynin, I. Gutman, S. Klavžzar and P. žZigert, Wiener index of hexagonal systems, *Acta Appl. Math.*, **72** (2002) 247–294.

[10] K. C. Das and I. Gutman, Bound for vertex PI index in terms of simple graph parameters, *Filomat*, **27** (2013) 1583–1587.

[11] L. Feng and G. Yu, On the hyper-Wiener index of cacti, *Util. Math.*, **93** (2014) 57–64.

[12] I. Gutman, S. Klavzar and B. Mohar, Fiftieth Anniversary of the Wiener Index, *Discrete Appl. Math.*, **80** (1997) 1–113.

[13] M. Hoji, Z. Luo and E. Vumar, Wiener and vertex PI indices of Kronecker products of graphs, *Discrete Appl. Math.*, **158** (2010) 1848–1855.

[14] A. Ilić and N. Milosavljević, The weighted vertex PI index, *Mathematical and Computer Modelling.*, **57** (2013) 623–631.

[15] S. Klavžar and I. Gutman, The Szeged and the Wiener Index of Graphs, *Appl. Math. Lett.*, **9** (1996) 45–49.

[16] P. V. Khadikar, On a Novel Structural Descriptor PI, *Nat. Acad. Sci. Lett.*, **23** (2000) 113–118.

[17] P. V. Khadikar, P. P. Kale, N. V. Deshpande, S. Karmarkar and V. K. Agrawal, Novel PI indices of hexagonal chains, *J. Math. Chem.*, **29** (2001) 143–150.

[18] P. V. Khadikar, S. Karmarkar and R. G. Varma, The estimation of PI index of polyacenes, *Acta Chim. Slov.*, **49** (2002) 755–771.

[19] M. H. Khalifeh, H. Yousefi-Azari and A. R. Ashrafi, Vertex and edge PI indices of Cartesian product graphs, *Discrete Appl. Math.*, **156** (2008) 1780–1789.

[20] S. Li, H. Yang and Q. Zhao, Sharp bounds on Zagreb indices of cacti with k pendant vertices. *Filomat*, **26** (2012) 1189–1200.

[21] K. Pattabiraman and P. Paulraja, Wiener and vertex PI indices of the strong product of graphs, *Discuss. Math. Graph Theory*, **32** (2012) 749–769.

[22] D. Wang and S. Tan, The maximum hyper-Wiener index of cacti, *J. Appl. Math. Comput.*, **47** (2015) 91–102.

[23] H. Wang and L. Kang, On the Harary index of cacti, *Util. Math.*, **96** (2015) 149–163.

[24] H. Wiener, Structural Determination of Paraffin Boiling Points, *J. Am. Chem. Soc.*, **69** (1947) 17–20.

[25] S. Wang and B. Wei, Multiplicative Zagreb indices of cacti, *Discrete Math. Algorithm. Appl.*, DOI:10.1142/S1793830916500403.

[26] S. Wang and B. Wei, Multiplicative Zagreb indices of k-trees, *Discrete Appl. Math.*, **180** (2015) 168–175.

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