PI INDICES FOR SOME CLASSES OF BICYCLIC GRAPHS

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Abstract

The Padmakar-Ivan (PI) index is a Wiener-Szeged-like topological index which reflects certain structural features of organic molecules. In this paper we study the PI indices of bicyclic graphs whose cycles do not share two or more common vertices.

INTRODUCTION

Wiener index (W) and Szeged index (Sz) were introduced to reflect certain structural features of organic molecules [1-3]. [4, 5] introduced another index called Padmaker-Ivan (PI) index. PI index is a very useful number in chemistry, as demonstrated in literature [5-13]. In [5] authors studied the applications of PI index to QSRP/QSAR. It turned out that the PI index has a similar discriminating function as Wiener index and Szeged index, sometimes it gave better results. Hence, PI index as a topological index is worth studying. In [6] authors pointed out that PI index is superior to ^0X, ^2X and logP indices for modeling Tadpole narcosis. For the previous results about PI index, see [14-19].

Let G be a simple connected graph. The PI index of graph G is defined as follows:

$$PI(G) = \sum[n_{eu}(e|G) + n_{ev}(e|G)],$$

where for edge e = uv $n_{eu}(e|G)$ is the number of edges of G lying closer to u than v, $n_{ev}(e|G)$ is the number of edges of G lying closer to v than u and summation goes over all edges of G. The edges which are equidistant from u and v are not considered for the calculation of PI index [15]. In the following we write n_{eu} instead of $n_{eu}(e|G)$.

PRELIMINARIES

Definition 2.1[20]. A graph G is called a bicyclic graph if there exist two edges $e_1, e_2 \in E(G)$ such that $G - \{e_1, e_2\}$ is a spanning tree of G. That is, G is a bicyclic graph if and only if G is a simple connected graph with n vertices and n + 1 edges.

Definition 2.2. Let $e = uv \in E(G)$ and $e \in E(C_{2k+1})$, where $C_{2k+1} = x_1x_2 \dots x_{2k+1}x_1$, $x_1 = u$, $x_{2k+1} = v$. Let

$$E_{k+1} = \{e_1 \in E(G) - E(C_{2k+1}) | \text{ the shortest paths from } u \text{ to } e_1 \text{ and from } v \text{ to } e_1 \text{ must pass through } x_{k+1} \text{ respectively}\}.$$

We call E_{k+1} the attached edges at vertex x_{k+1}. Let $h_{k+1} = |E_{k+1}|$.

Lemma 2.3[5]. (1). Let C_{2n+1} be an odd cycle, $n \geq 1$, we have

$$PI(C_{2n+1}) = 2n(2n + 1).$$

(2). Let C_{2n} be an even cycle, $n \geq 2$, we have

$$PI(C_{2n}) = 4n(n - 1).$$

MAIN RESULT

Theorem 3.1. Let G be a bicycle graph whose cycles do not share two or more common vertices, $n = |V(G)|$.

(1). When G contains two odd cycles C_{2k+1} and C_{2t+1}, we have

$$PI(G) = n(n-1) + 2(k + t);$$

(2). When G contains two even cycles C_{2k} and C_{2t}, we have

$$PI(G) = n(n+1) - 2(k + t);$$

(3). When G contains an odd cycle C_{2k+1} and an even cycle C_{2t}, we have

$$PI(G) = n^2 + 2(k - t).$$

Proof. Claim 1: Let $e = uv \in E(G)$. When e is not contained in any cycle, we have

$$n_{eu} + n_{ev} = n.$$

In fact, suppose e_1 is equidistant from u and v, there exist two shortest paths P_1 and P_2 from u to e_1 and from v to e_1 respectively, where $e_1 \neq e$. Hence,

$$W = \{e\} \cup P_1 \cup P_2 \cup \{e_1\}$$

is a closed walk which contains a cycle containing e, a contradiction. Claim 1 follows.

Claim 2: Let C be an even cycle, $e = uv \in E(C)$, we have

$$n_{eu} + n_{ev} = n - 1.$$

In fact, let $C = x_1x_2 \dots x_{2k}x_1$, where $x_1 = u$, $x_{2k} = v$. By the definition of G there are two edges x_1x_{2k} and x_kx_{k+1} which are equidistant from u and v. Similarly, x_ix_{i+1} is not equidistant from u and v, where $x_ix_{i+1} \in E(C)$, $i \neq k$, $i \neq 2k$, $x_{2k+1} = x_1$.

Let $e_2 \in E(G) - E(C)$, let P_3 and P_4 be the two shortest paths from u to e_2 and from v to e_2 respectively.

Case 2.1. $e_2 \in E(C_1)$, where C_1 is a cycle and $C_1 \neq C$.

By the definition of G, P_3 and P_4 must pass through the same vertex x_j to e_2, where $x_j \in V(C)$. Let $z \in V(P_3) \cap V(P_4)$ and z be the first vertex from u to e_2 along P_3. Since

$$|E(P_3)| = |E(P_4)|,$$

we have

$$|E(P_3(u,z)| = |E(P_4(v, z))|.$$

Define

$$C_2 = P_3(u,z) \cup P_4(v, z) \cup \{uv\}.$$

Obviously, C_2 is an odd cycle contained by C, which is a contradiction. Hence, e_2 is not equidistant from u and v.

Case 2.2. e_2 is contained in no cycle.

Similarly, we can prove that e_2 is not equidistant from u and v.

By Definition 2.1 we have $|E(G)| = n + 1$. Claim 2 follows.

Claim 3: For an odd cycle C_{2k+1}, $e = uv \in E(C_{2k+1})$, $n = |V(G)|$, we have

$$\sum_{e \in E(C_{2k+1})} [n_{eu}(e \mid G) + n_{ev}(e \mid G)] = 2k(n+1).$$

In fact, by the definition of G and Lemma 2.3 we have

$$n_{eu}(e|C_{2k+1}) + n_{ev}(e|C_{2k+1}) = 2k.$$

Let $r = |E(G)| - |E(C_{2k+1})|$, by Definition 2.1 we have $r = n - 2k$. By Definition 2.2 we have $r = h_1 + h_2 + \ldots + h_{2k+1}$.

Without loss of generality, let $e = uv$, $C_{2k+1} = x_1x_2\ldots x_{2k+1}x_1$, where $x_1 = u$, $x_{2k+1} = v$. By the definition of G we have $d(u, x_{k+1}) = d(v, x_{k+1})$. Hence, by the definition of G and Definition 2.2 we know that the edges in E_{k+1} are equidistant from u and v, hence, they have no contributions to $n_{eu}(e|G) + n_{ev}(e|G)$. Similarly, the edges in E_j are not equidistant from u and v, hence, they have contributions to $n_{eu}(e|G) + n_{ev}(e|G)$, $j \neq k + 1$. Thus, we have

$$n_{eu}(e|G) + n_{ev}(e|G) = 2k + r - h_{k+1}.$$

By symmetry we have

$$\sum_{e \in E(C_{2k+1})} [n_{eu}(e \mid G) + n_{ev}(e \mid G)]$$

$$= 2k(2k + 1) + r - h_1 + \ldots + r - h_{2k+1}$$

$$= 2k(2k + 1) + 2kr$$

$$= 2k(n + 1).$$

Claim 3 follows.

By Claim 1, Claim 2 and Claim 3 we have

(1). When G contains two odd cycles C_{2k+1} and C_{2t+1}, we have

$$PI(G) = 2k(n+1) + 2t(n+1) + n(n+1-2k-1-2t-1)$$
$$= n(n-1) + 2(k+t);$$

(2). When G contains two even cycles C_{2k} and C_{2t}, we have

$$PI(G) = 2k(n-1) + 2t(n-1) + n(n+1-2k-2t)$$
$$= n(n+1) - 2(k+t);$$

(3). When G contains an odd cycle C_{2k+1} and an even cycle C_{2t}, we have

$$PI(G) = 2k(n+1) + 2t(n-1) + n(n+1-2k-1-2t)$$
$$= n^2 + 2(k-t).$$

The theorem follows.

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