The PI Index of Gated Amalgam

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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 index of gated amalgam.

Keywords: PI index, Organic molecule, Wiener index, Gated amalgam.

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1. Introduction

Wiener index (W) and Szeged index (Sz) are introduced to reflect certain structural features of organic molecules [1-6]. [7, 8] introduced another index called Padmaker-Ivan (PI) index. PI index is a very useful number in chemistry, as demonstrated in literature [8-16]. In [8] 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 [9] authors pointed out that PI index is superior to ${}^0X$, ${}^2X$ and logP indices for modeling Tadpole narcosis. In [10] the authors reported quantitative structure—toxicity relationship (QSTR) study using the PI index. They have used 41 monosubstituted nitrobenzene for this purpose. The results have shown that the PI index alone is not an appropriate index for modeling toxicity of nitrobenzene derivatives. Combining PI index with other distance-based topological indices resulted in statistically significant models and excellent results were obtained in pentaparametric models. For the previous results about PI index, please see [17, 18, 19].

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

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

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 [18]. In the following we write n_{eu} instead of $n_{eu}(e|G)$ for short.

The organization of the paper is as follows: in section 2 we present some preliminaries, in section 3 we present our main result—Theorem 3.1 which provides a general technique to use mathematical induction.

2. Preliminaries

For basic definitions cited in this paper, please see [20, 21] for further details.

Definition 2.1. The *interval* I(u, v) between vertices u and v of a connected graph G is the set of vertices of all shortest paths between u and v in G. A subgraph H of G is a *convex subgraph* if for any vertices $u, v \in V(H)$ we have $I(u,v) \subseteq V(H)$. A subgraph H of graph G is called *gated subgraph* in G if for every $x \in V(G)$ there exists a vertex u in H such that $u \in I(x,v)$ for all $v \in V(H)$. If for some x such a vertex u in V(H) exists, it must be unique. It is called the *gate* of x in H and we denote it $g_H(x)$. The intersection of gated subgraphs is a gated subgraph and a gated subgraph is always convex subgraph [22, 23].

Definition 2.2. Let G_1 and G_2 be gated subgraphs of graph G such that $G_1 \cup G_2 = G$ and $G_1 \cap G_2 \neq \phi$. If there are no edges between

$V(G_1)\setminus V(G_2)$ and $V(G_2)\setminus V(G_1)$, G is called a *gated amalgam* of G_1 and G_2 [23].

Definition 2.3. Let G be the gated amalgam of G_1 and G_2, $H = G_1 \mathrm{I}\ G_2$. Define *gate map* $g_i : V(G_i) \to V(H)$ as follows: for $\forall x \in V(G_i), g_i(x) = g_H(x)$, i = 1, 2.

Definition 2.4. Let G be the gated amalgam of G_1 and G_2, $H = G_1 \mathrm{I}\ G_2$, let $g_1 : V(G_1) \to V(H)$ and $g_2 : V(G_2) \to V(H)$ be the gate maps respectively.

For $xy \in E(G_1) - E(H)$, let $u = g_1(x)$, $v = g_1(y)$, define l_{xy} as follows: (1) If $d(x, g_1(x)) = d(y, g_1(y))$ and $g_1(x) \neq g_1(y)$, define l_{xy} = (n_{uv} in G_2) — (n_{uv} in H); (2) If $d(x, g_1(x)) = d(y, g_1(y))$ and $g_1(x) = g_1(y)$, define l_{xy} = 0; (3) If $d(x, g_1(x)) \neq d(y, g_1(y))$, define $l_{xy} = |E(G_2)| - |E(H)|$.

For $xy \in E(G_2) - E(H)$, let $u = g_2(x)$, $v = g_2(y)$, define m_{xy} as follows: (1) If $d(x, g_2(x)) = d(y, g_2(y))$ and $g_2(x) \neq g_2(y)$, define m_{xy} = (n_{uv} in G_1) — (n_{uv} in H); (2) If $d(x, g_2(x)) = d(y, g_2(y))$ and $g_2(x) = g_2(y)$, define m_{xy} = 0; (3) If $d(x, g_2(x)) \neq d(y, g_2(y))$, define $m_{xy} = |E(G_1)| - |E(H)|$.

Where (n_{uv} in G_i) means the number of edges of G_i which are not equidistant from u and v in G_i, i = 1, 2; So does (n_{uv} in H).

3. Main Results

Theorem 3.1. *Let G be the gated amalgam of* G_1 *and* G_2, $H = G_1 \cap G_2$, $g_1 : V(G_1) \to V(H)$ *and* $g_2 : V(G_2) \to V(H)$ *be the gate maps respectively. Then*

$$PI(G) = PI(G_1) + PI(G_2) - PI(H) + \sum_{xy \in E(G_1)-E(H)} l_{xy} + \sum_{xy \in E(G_2)-E(H)} m_{xy},$$

where l_{xy} *and* m_{xy} *are defined in Definition 2.4.*

Proof. Claim 1: H is a connected subgraph of G.

In fact, by Definition 2.1 and Definition 2.2 we know that H is a gated subgraph of G. By Definition 2.1 H is a convex subgraph of G. For $\forall u, v \in V(H)$, since we suppose G is a connected graph in this paper, there exists one of the shortest (u, v)—paths P in G. Because H is a convex subgraph of G, by Definition 2.1 we have $V(P) \subseteq V(H)$. Hence, P is contained in H. Claim 1 follows.

Case 1. $xy \in E(H)$.

Since (n_{xy} in H) is counted twice by (n_{xy} in G_1) and (n_{xy} in G_2), by the definition of PI index we have

$$(n_{xy} \text{ in G}) = (n_{xy} \text{ in } G_1)$$

$+(n_{xy}$ in $G_2)$ $-$ $(n_{xy}$ in H),

which are terms of $PI(G_1)+PI(G_2)-PI(H)$ respectively.

Case 2. $xy \in E(G_1)-E(H)$.

Subcase 2.1. Suppose $d(x,g_1(x))=d(y,g_1(y))$ and $g_1(x)\neq g_1(y)$.

Claim 2: $g_1(x)g_1(y)\in E(H)$.

Otherwise, by Claim 1 there exists one of the shortest $(g_1(x),g_1(y))-$ paths $P_1=u_1u_2...u_n$ in H, where $n\geq 3$, $u_1=u=g_1(x)$, $u_n=v=g_1(y)$. By Definition 2.1 and Definition 2.2 H is a gated subgraph of G. By Definition 2.1 H is a convex subgraph of G, we have $V(P_1)\subseteq V(H)$. Hence, P_1 is also one of the shortest $(g_1(x),g_1(y))-$ paths in G. Let $P_2=x_1x_2...x_m$ be the shortest $(x,g_1(x))-$path in G, $P_3=y_1y_2...y_m$ be the shortest $(y,g_1(y))-$path in G, where $x_1=x$, $x_m=g_1(x)$, $y_1=y$, $y_m=g_1(y)$.

Let $P_4=\{xy\}\cup P_3$, $P_5=P_1\cup P_2$. Because $|E(P_2)|=|E(P_3)|$ we have

$$|E(P_4)|<|E(P_5)|,$$

Thus, $g_1(x)$ is not a gate from x to $g_1(y)$, which is a contradiction. Claim 2 follows.

By Claim 2 and the definition of PI index we have

$$(n_{xy} \text{ in G}) = (n_{xy} \text{ in } G_1)$$

$$+ (n_{uv} \text{ in } G_2) - (n_{uv} \text{ in H})$$

$$= (n_{xy} \text{ in } G_1) + l_{xy},$$

which are terms of $PI(G_1) + \sum_{xy \in E(G_1) - E(H)} l_{xy}$ respectively.

Subcase 2.2. Suppose $d(x, g_1(x)) = d(y, g_1(y))$ and $g_1(x) = g_1(y)$.

Thus, all edges in $E(G_2)$ are equidistant from $g_1(x)$ (or $g_1(y)$), hence, all edges of $E(G_2)$ are equidistant from x and y. Thus, we have

$$(n_{xy} \text{ in G}) = (n_{xy} \text{ in } G_1)$$

$$= (n_{xy} \text{ in } G_1) + l_{xy},$$

which are terms of $PI(G_1) + \sum_{xy \in E(G_1) - E(H)} l_{xy}$ respectively.

Subcase 2.3 Suppose $d(x, g_1(x)) \neq d(y, g_1(y))$.

Claim 3: $g_1(x) = g_1(y)$.

Otherwise, suppose $g_1(x) \neq g_1(y)$. Without loss of generality, let $d(x, g_1(x)) < d(y, g_1(y))$. Let P_6 be one of the shortest $(x, g_1(x))$ – path in G and P_7 be one of the shortest $(y, g_1(y))$ – paths in G. Denote $P_8 = P_6 \cup \{xy\}$, $P_9 = P_1 \cup P_7$, where P_1 is the shortest $(g_1(x), g_1(y))$ – path in H, $n \geq 2$, defined in Claim 2. Because

$d(x, g_1(x)) < d(y, g_1(y))$ we have

$$|E(P_8)| < |E(P_9)|.$$

However, P_8 does not pass through $g_1(y)$. That is, $g_1(y)$ is not the gate of y, which is a contradiction. Claim 3 follows.

By Claim 3 all edges in $E(G_2) - E(H)$ are equidistant from $g_1(x)$ (or $g_1(y)$). Since $d(x, g_1(x)) \neq d(y, g_1(y))$, all edges in $E(G_2) - E(H)$ are not equidistant from x and y. By the definition of PI index we have

$$(n_{xy} \text{ in G}) = (n_{xy} \text{ in } G_1) + |E(G_2)| - |E(H)|$$

$$= (n_{xy} \text{ in } G_1) + l_{xy},$$

which are terms of $PI(G_1) + \sum_{xy \in E(G_1) - E(H)} l_{xy}$ respectively.

Similarly, we can discuss Case 3:

Case 3. $xy \in E(G_2) - E(H)$.

The theorem follows.

By Theorem 3.1 the following theorem is obvious.

Theorem 3.2. *Let G be the graph obtained by identifying of a vertex of graphs G_1 and G_2, let the identified vertex be w. Then*

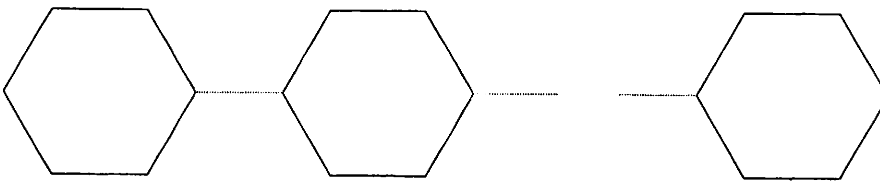
$$PI(G) = PI(G_1) + PI(G_2)$$
$$+ |T_1||E(G_2)| + |T_2||E(G_1)|,$$

where

$$T_i = \{xy \in E(G_i) \mid d(x, w) \neq d(y, w)\}, i = 1, 2.$$

Remark: Theorem 3.1 provides a technique to prove theorems about PI indices by mathematical induction. In the following we use two examples to show that Theorem 3.1 with mathematical induction is a general method to prove theorems about PI indices, for the original proofs, please see [17].

Define polyphenylene with h hexagons as follows, denote it PO_h:



PO_h

Figure 1. Polyphenylene

Theorem 3.3[17]. $PI(PO_h) = 49h^2 - 27h + 2$.

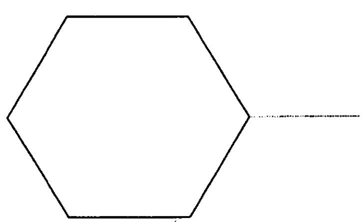
Proof. By mathematical induction.

(1). When h = 1, PO_1 is a 6-cycle, Theorem 3.3 follows clearly.

(2). Suppose

$$PI(PO_{h-1}) = 49(h-1)^2 - 27(h-1) + 2$$

holds, $h \geq 2$. Let $G = PO_h$, G_1 be as follows and $G_2 = PO_{h-1}$.



G

Figure 2. G_1 in the proof of Theorem 3.3.

By the definition of PI index, it is easy to see that

$$PI(G_1) = 36.$$

Obviously, we have

$$|T_1| = 7,$$
$$|T_2| = 7h - 8.$$

By Theorem 3.2 Theorem 3.3 follows.

Consider a polyacene having h hexagons as follows, denote it L_h.

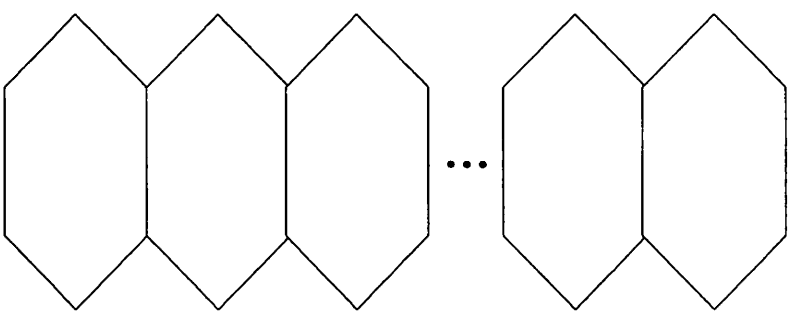


Figure 3. Polyacene

Theorem 3.4[17]. $PI(L_h) = 24h^2$.

Proof. By mathematical induction.

(1). When h = 1, L_1 is a hexagon, Theorem 3.4 follows clearly.

(2). Suppose $h \geq 2$ and $PI(L_{h-1}) = 24(h-1)^2$ holds.

Let G_1 be the left hexagon of L_h, G_2 be L_{h-1} and H be K_2. By Theorem 3.1 Theorem 3.4 follows.

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