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Graphical Abstract

A Method of Computing the PI Index of Benzenoid Hydrocarbons Using Orthogonal Cuts[#]

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The Padmakar-Ivan (PI) index of a graph G is defined as PI (G) = Σ [n_{eu}(e|G)+n_{ev}(e|G)], where for edge e=(u,v) are 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 PI index is a Wiener-Szeged-Like topological index developed very recently. In this paper we describe a method of computing PI index of benzenoid hydrocarbons (H) using orthogonal cuts. The method requires the finding of number of edges in the orthogonal cuts in a benzenoid system (H) and the edge number of H – a task significantly simpler than the calculation of PI index directly from its definition.

Running head: The PI Index

Key words: benzenoid hydrocarbons, cuts in benzenoid graphs

A Method of Computing the PI Index of Benzenoid Hydrocarbons Using Orthogonal Cuts[#]

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Abstract

The Padmakar-Ivan (PI) index of a graph G is defined as PI (G) = Σ [n_{eu}(e|G)+n_{ev}(e|G)], where for edge e=(u,v) are n_{eu} (e|G) the number of edges of G lying closer to u than v, and 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 PI index is a Wiener-Szeged-like topological index developed very recently. In this paper we describe a method of computing PI index of benzenoid hydrocarbons (H) using orthogonal cuts. The method requires the finding of number of edges in the orthogonal cuts in a benzenoid system (H) and the edge number of H – a task significantly simpler than the calculation of PI index directly from its definition.

1. Introduction

Numbers reflecting certain structural features of organic molecules that are obtained from the molecular graph are usually called graph invariants or more commonly topological indices[1]. One of the oldest and most thoroughly examined molecular graph-based structural descriptor of organic molecule is the Wiener index or Wiener number[2-9]. This quantity is equal to the sum of distances between all pairs of vertices of the respective molecular graph.

[#] On the eve of 70th anniversary of both Prof. Padmakar V. Khadikar and his wife Mrs. Kusum Khadikar.
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The Wiener index (W) is applicable to acyclic (tree) graphs only. For cyclic compounds a novel molecular-graph-based descriptor, refered to as the Szeged index, Sz is putforward by Gutman [10-12]. This is considered as the modification of Wiener index to cyclic graph. It is based on distance in the molecular graph but is not of the same type as the Wiener index, W. For acyclic systems(trees) Sz and W coincide. Consequently, one of the authors (PVK) introduced yet another index called Padmakar-Ivan (PI) index [13,14]. The PI index of a graph G is defined as:

$$PI = PI(G) = \Sigma [n_{eu}(e|G)+n_{ev}(e|G)] \quad (1)$$

where for edge e = (u,v) 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 "equidistant" from u and v are not consider for the calculation of PI index. Since PI index is different for acyclic graphs several applications of PI index are reported in the literature [15-40]. Furthermore, the derived PI index is very simple to calculate and has a discriminating power similar to that of W index, for details see ref [9-11]. Earlier, one of the authors (PVK) described the methods for the calculation of PI index of hexagonal chains[16]. In this paper we simplify these methods using orthogonal cuts.

2. Calculation of the PI index of a bipartite graph from orthogonal cuts.

It is worthy mentioning that in the following derivation we changed the property " equidistant" by "strongly codistant" ("sco").

Let G = (V, E) be the embedding of a connected, planar and bipartite graph in the Euclidean plane; V = V(G) and E = E(G) are the vertex and the edge set of G, respectively. The number of edges of G is denoted by m = m(G) = | E |.

Let d (x, y) denote the length of a shortest path connecting vertices $x, y \in V$.

Edge $e = (u, v) \in E$ has end vertices $u, v \in V$.

Edge e' = (u', v') $\in$ E is called *codistant* to edge e = (u, v) (briefly: e' *co* e) if and only if d (u, u') = d (v, v') or d (u, v') = d (v, u').

Edge e' = (u', v') $\in$ E is called *strongly codistant* to edge e = (u, v) (briefly: e' *sco* e) if and only if d (u, u') = d (v, v') = i and d (u, v') = d (v, u') = i+1, or vice versa, and i = 0,1,…

In Figs. 1, 2 and 3 one can see the difference of “co” and “sco”.

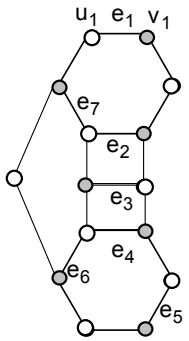


Figure 1

e_1 sco e_2, e_3, e_4, e_5
e_5 sco e_6, e_7, e_1
(sco : strongly codistant !)

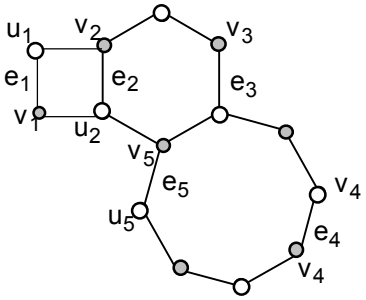


Figure 2

	u_2 v_2	u_3 v_3	u_4 v_4
u_1	2 1	4 3	6 7
v_1	1 2	3 4	5 6

e_1 sco e_2, e_3

and

e_1 co e_2, e_3, e_4

---

e_4 co e_1, e_5

and

e_4 sco e_5

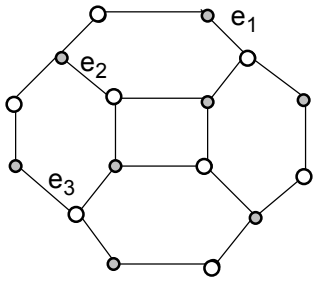


Figure 3

e_1 sco e_2, e_3

An *orthogonal cut* C (e) with respect to edge e is the set of all edges $e' \in E$ which are strongly codistant to e: C (e): = $\{e' \in E \mid e'$ *sco* $e\}$.

Let C*(e) denote the *complement of* C(e) *with respect to edge set* E:

C* (e): = $\{e^* \in E \mid e^*$ *nsco* $e\}$, " e^* *nsco* e" means that e^* not strongly codistant to e.

Let m(e) = |C(e)| denote the number of strongly codistant edges of G with respect to edge e, and m*(e) = |C*(e)| = | E – C(e)|.

Clearly, for every edge $e \in E$ is

(2) $$m = m(e) + m^*(e).$$

Because of equation (1) is

(3) $$PI(G) = \sum_{e \in E(G)} m^*(e).$$

With equation (2) become (3) the form

(4) $$PI(G) = \sum_{e \in E(G)} [m - m(e)],$$

or

(5) $$PI(G) = m^2 - \sum_{e \in E(G)} m(e).$$

The sco relation satisfied the following statements:

(i) reflexive property: For every edge $e \in E(G)$ is e *sco* e,

(ii) symmetric property: For edges $e,e' \in E(G)$ from e' *sco* e follow e *sco* e'.

Not for all bipartite graphs is valid (see Figure 1)

(iii) transitive property: For edges $e,e',e'' \in E(G)$ from e *sco* e' and e' *sco* e'' follow e *sco* e''.

Graph G is called a *strongly codistance graph* (briefly: *sco graph*) if and only if the edge relation "*sco"* is an equivalence relation for subset C = C(e) of E = E(G)(properties (i), (ii) and (iii) are satisfied). In such a graph G is for every edge $e\# \in C(e)$ also C(e#) = C(e); the set C(e) is denoted an *orthogonal cut* with respect to edge e of G. For an sco graph G the edge set E = E(G) is the union of pairwise disjoint equivalence classes of orthogonal cuts $C_j = C_j(G)$, j = 1,2,…,k of graph G. Let $m_j = |C_j|$ the number of edges of orthogonal cut C_j.

The sum in (5) is now

$$\sum_{e\in E(G)} m(e) = \sum_{j=1}^{k} \sum_{e\in C_j} m(e) . \qquad (6)$$

The number m(e) is for every edge $e \in C_j$ in an sco graph G the same, namely m(e) = $m(C_j) = m_j$ and the internal sum of the right hand side of (6) is

$$\sum_{e\in C_j} m(e) = m_j^{\,2} , \qquad (7)$$

and the sum of the left hand side of equation (6) is

$$\sum_{e\in E(G)} m(e) = \sum_{j=1}^{k} m_j^{\,2} . \qquad (8)$$

Now the new formula for the PI index of an sco graph (follow from (5) and (8)) is

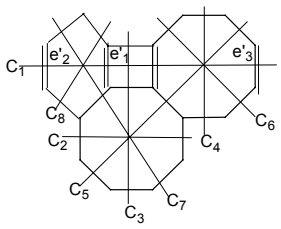
$$PI(G) = m^2 - \sum_{j=1}^{k} m_j^{\,2} \qquad (9)$$

If $\mathbf{C} = \mathbf{C}(G) = \{C_1, C_2, ..., C_k\}$ denote the set of all orthogonal cuts of G then is another form of equation (9):

$$PI(G) = m^2 - \sum_{C\in \mathbf{C}} m(C)^2 . \qquad (10)$$

Examples:

Example 1 : G_1 is a sco-graph

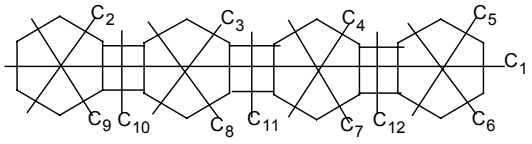


G_1

Thus, we have,

$PI(G_1) = 21^2 - 1.4^2 - 3.3^2 - 4.2^2 = 382$

Example 2 : Phynalenes(P_h)



$PI(P_h) = [30^2 - [1(8)^2 + 11(2)^2] = 792$

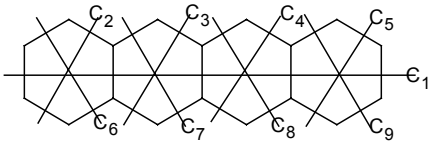
3. PI indices of benzenoid hydrocarbons using orthogonal cuts

Let us now discuss the applications of orthogonal cut methodology for the calculations of PI indices of benzenoid hydrocarbons.

Note that the graph of a benzenoid hydrocarbon is a sco graph. Therefore is equation (10) applicable. Here some further examples.

Consider the case of polyacene given below:

Example 3: L_h



Therefore, PI (L_h) = $m^2 - \Sigma\, m(C)$

where m = 21

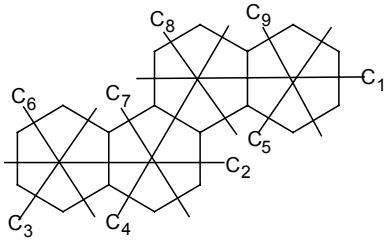
m (C_1) = 5 and m (C_i) = 2 for i = 2,3,…,9

i.e. PI (L_h) = $[21^2-[8(2)^2 + 1\,(5)^2]$

= 441-57 = 384

Similarly, we can compute PI indices of Fibonacenes, Helicenes and Polyphenylenes using the following examples:

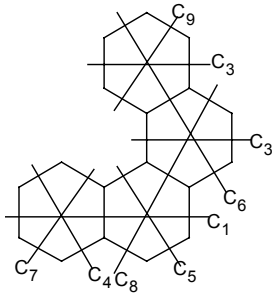
Example 4:Fibonacenes (F_h)



PI (F_h) = $21^2-[3(3)^2 + 6\,(2)^2]$

= 441 – 51 = 390

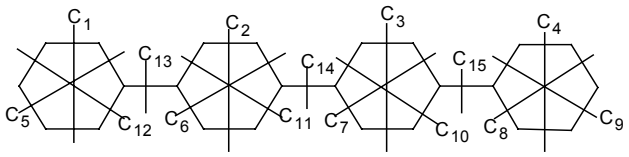
Example 5:Helicenes(H_h)



PI (H_h) = $21^2-[3(3)^2 + 6\,(2)^2]$

=390

Example 6: Polyphenylenes(Poly)



$$PI\ (Poly) = 27^2 - [\ 12\ (2)^2 + 3\ (1)^2]$$
$$= 682$$

4. Concluding Remarks

The methodology for the computation of PI indices of benzenoid hydrocarbons is better than the one base on eq. (1). The new orthogonal cut method proposed by us requires only the total number of edges and the number of edges involved in the orthogonal cut. The case of Polyphenyls indicates simply to consider the number of edges in all types of edge-cuts.

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