

A method of computing the PI index of benzenoid hydrocarbons using orthogonal cuts[#]

Peter E. John*

*Department of Mathematics, Technical University of Ilmenau, PF 100565,
98684 Ilmenau, Germany*

E-mail: peter.john@tu-ilmenau.de

Padmakar V. Khadikar

*Research Division, Laxmi Fumigation and Pest Control, Pvt. Ltd., 3, Khatipura,
Indore 452 007, India*

E-mail: pvkhadikar@rediffmail.com

Jyoti Singh

Department of Chemistry, A.P.S. University, Rewa 486 003, India

Received 6 February 2006; revised 15 February 2006

The Padmakar–Ivan (PI) index of a graph G is defined as $PI(G) = \sum[n_{eu}(e|G) + n_{ev}(e|G)]$, 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.

KEY WORDS: benzenoid hydrocarbons, cuts in benzenoid graphs

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

[#]On the eve of 70th anniversary of both Prof. Padmakar V. Khadikar and his wife Mrs. Kusum Khadikar.

*Corresponding author.

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.

The Wiener index (W) is applicable to acyclic (tree) graphs only. For cyclic compounds a novel molecular-graph-based descriptor, referred to as the Szeged index (Sz) is put forward by Gutman [10] and Khadikar et al. [11,12]. This is considered as the modification of W to cyclic graph. It is based on distance in the molecular graph but is not of the same type as the 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:

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

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 considered 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 [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 $i = 0, 1, \dots$

In figures 1–3 one can see the difference of “co” and “sco”.

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 : $C(e) := \{e' \in E | e' \text{ sco } e\}$.

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

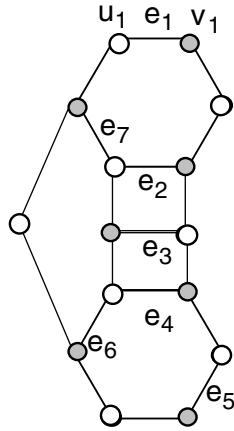
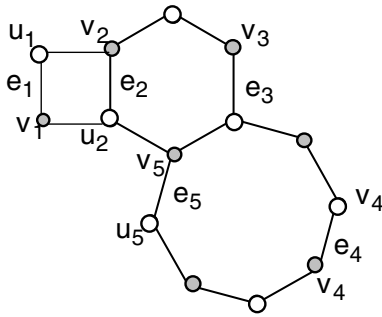


Figure 1. e_1 sco e_2, e_3, e_4, e_5 ; e_5 sco e_6, e_7, e_1 (sco: strongly codistant !).



	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

Figure 2. 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 .

$C^*(e) := \{e^* \in E | e^* nsco e\}$, “ $e^* nsco e$ ” 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

$$m = m(e) + m^*(e). \tag{2}$$

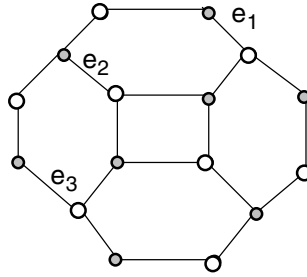


Figure 3. e_1 sco e_2, e_3 .

Because of equation (1) is

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

With equation (2) become (3) the form

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

or

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

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)–(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 $C_j = C_j(G)$, $j = 1, 2, \dots, k$, of graph G . Let $m_j = |C_j|$ the number of edges of orthogonal cut C_j .

The sum in (5) is now

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

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

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

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

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

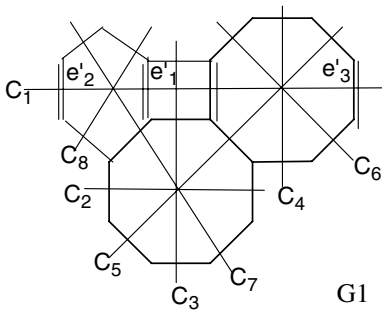
Now the new formula for the PI index of an sco graph (follow from (5) and (8)) is

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

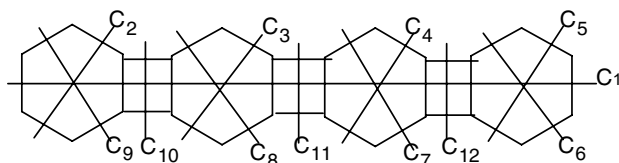
If $C = C(G) = \{C_1, C_2, \dots, C_k\}$ denote the set of all orthogonal cuts of G then is another form of equation (9):

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

Example 1. G_1 is a sco-graph.



Thus, we have,
 $PI(G_1) = 21^2 - 1.4^2 - 3.3^2 - 4.2^2 = 382.$

Example 2. Phynalenes (P_h)

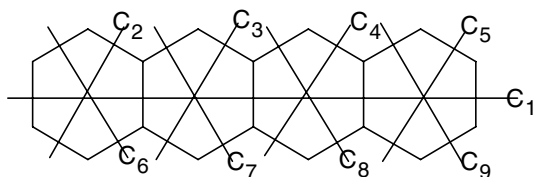
$$\text{PI}(P_h) = [30^2 - [1(8)^2 + 11(2)^2]] = 792.$$

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, equation (10) is applicable. Here some further examples.

Consider the case of polyacene given below:

Example 3. L_h 

$$\text{Therefore, } \text{PI}(L_h) = m^2 - \sum m(C),$$

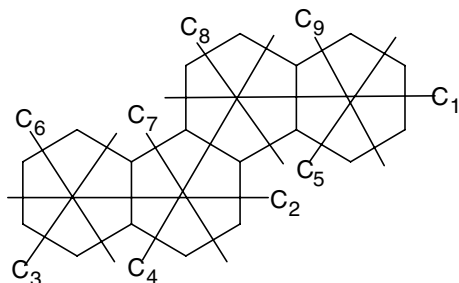
where $m = 21$.

$$m(C_1) = 5 \text{ and } m(C_i) = 2 \text{ for } i = 2, 3, \dots,$$

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

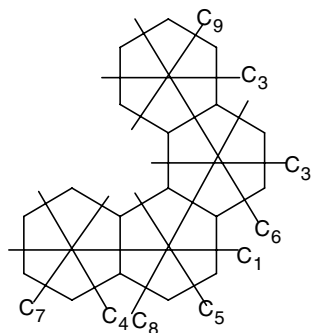
$$= 441 - 57 = 384.$$

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

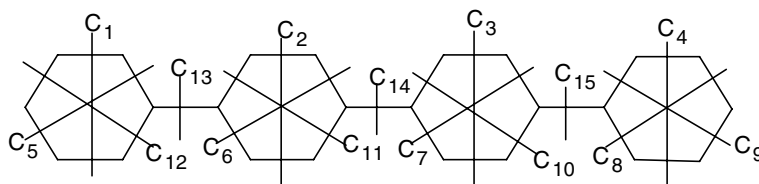
Example 4. Fibonacenes (F_h)

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

$$= 441 - 51 = 390.$$

Example 5. Helicenes (H_h)

$$\begin{aligned} \text{PI}(H_h) &= 21^2 - [3(3)^2 + 6(2)^2] \\ &= 390. \end{aligned}$$

Example 6. Polyphenylenes(Poly)

$$\begin{aligned} \text{PI}(\text{Poly}) &= 27^2 - [12(2)^2 + 3(1)^2] \\ &= 682. \end{aligned}$$

4. Concluding remarks

The methodology for the computation of PI indices of benzenoid hydrocarbons is better than the one based on equation (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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