
Preprint No. M 06/04

**A Method of Computing the PI
Index of Benzenoid Hydrocarbons
Using Orthogonal Cuts**

John, Peter E.; Khadikar, Padmakar V.;
Singh, Jyoti

Januar 2006

Impressum:

Hrsg.: Leiter des Instituts für Mathematik
Weimarer Straße 25
98693 Ilmenau

Tel.: +49 3677 69 3621

Fax: +49 3677 69 3270

<http://www.tu-ilmenau.de/ifm/>

ISSN xxxx-xxxx

ilmedia

Graphical Abstract

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

Peter E. John^a, Padmakar V. Khadikar^{b*} and Jyoti Singh^c

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 $n_{eu}(e/G)$ 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-Sizeged-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[#]

Peter E. John^{a*}, Padmakar V. Khadikar^b and Jyoti Singh^c

^a Department of Mathematics, Technical University of Ilmenau, PF 100565, 98684 Ilmenau, Germany

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

^{b*} Research Division, Laxmi Fumigation and Pest Control, Pvt. Ltd., 3, Khatipura, Indore 452 007, India, e-mail: pvkhadikar@rediffmail.com

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

e-mail: jyoti_singh07@rediffmail.com

Abstract

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.

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 indices¹. One of the oldest and most thoroughly examined molecular graph-based structural descriptor of organic molecule is the Wiener index or Wiener number²⁻⁹. 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.

*Author for correspondence (PEJ): Tel: + 49-3677-693630, e-mail: peter.john@tu-ilmenau.de

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 Gutman¹⁰⁻¹². 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:

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

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 literature¹⁵⁻⁴⁰. Furthermore, the derived PI index is very simple to calculate and has a discriminating power similar to that of W index, for details see ref⁹⁻¹¹. Earlier, one of the authors (PVK) described the methods for the calculation of PI index of hexagonal chains¹⁶. 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 Figs. 1, 2 and 3 one can see the difference of “co” and “sco”.

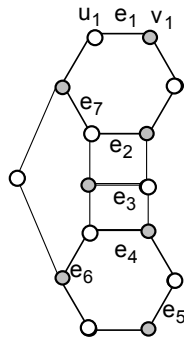


Figure 1

e_1 SCO e_2, e_3, e_4, e_5

e_5 SCO e_6, e_7, e_1

(sco : strongly codistant !)

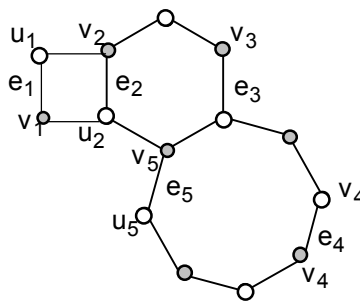


Figure 2

	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

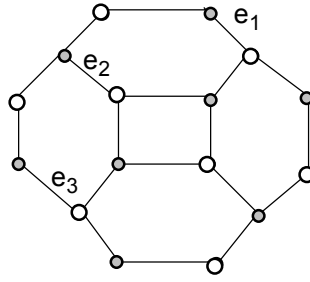


Figure 3

$e_1 \text{ sco } e_2, e_3$

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

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

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

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

Because of equation (1) is

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

With equation (2) become (3) the form

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

or

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

The sco relation satisfied the following statements:

- (i) reflexive property: For every edge $e \in E(G)$ is $e \text{ sco } e$,
- (ii) symmetric property: For edges $e, e' \in E(G)$ from $e' \text{ sco } e$ follow $e \text{ sco } e'$.

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

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

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

The sum in (5) is now

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

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

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

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

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

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

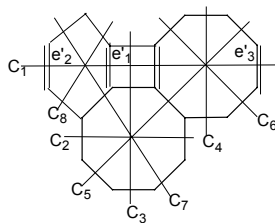
$$(9) \quad \text{PI}(G) = m^2 - \sum_{j=1}^k m_j^2$$

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

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

Examples:

Example 1 : G_1 is a sco-graph

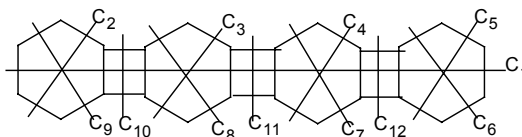


G_1

Thus, we have,

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

Example 2 : Phynalenes(P_h)



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

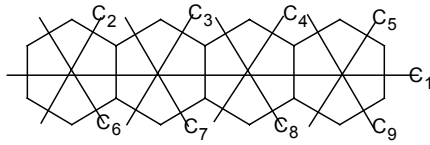
3. PI indices of benzenoid hydrocarbons using orthogonal cuts

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

where $m = 21$

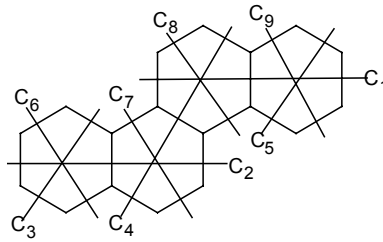
$m(C_1) = 5$ and $m(C_i) = 2$ for $i = 2, 3, \dots, 9$

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:

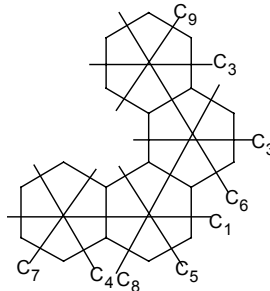
Example 4: Fibonacenes (F_h)



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

$= 441 - 51 = 390$

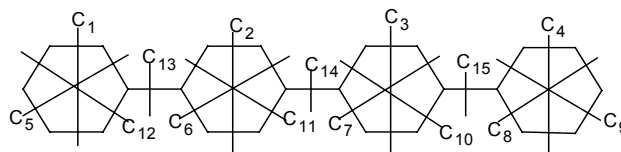
Example 5: Helicenes (H_h)



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

$= 390$

Example 6: Polyphenylenes(Poly)



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

4. Concluding Remarks

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

5. References

1. R. Todeschini and V. Consodni, *Handbook of Molecular Descriptors*, (Wiley-VCH, Weinheim (GER) 2000).
2. H. Wiener, Structural determination of Paraffin Boiling Points, *J. Am. Chem. Soc.* **69** (1947) 17-20.
3. H. Wiener, Correlation A Heat Of Isomerization and Differences in Heats of Vaporization of Isomers, among the Paraffin Hydrocarbons, *J. Am. Chem. Soc.* **69** (1947) 2636-2638.
4. H. Wiener, Influence of Interatomic Forces on Paraffin Properties, *J. Chem. phys.* **15** (1947) 766-767.
5. H. Wiener, Relationship of Physical Property of Isomeric Alkanes to Molecular Structure Surface Tension, Specific Dispersion and Critical Solution of Temperature in Aniline, *J. Phys. Colloid chem.* **52** (1948) 1082-1089.

6. H. Wiener, Vapour-Pressure Temperature Relations Among the Branched Paraffin Hydrocarbons, *J. Phys. Chem.* **52** (1948) 425-430.
7. Z. Mihalic, D. Veljan, D. Amic, S. Nikolic, D. Liavsic and N. Trinajstic, The Distance Matrix in Chemistry, *J. Math. Chem.* **11** (1992) 223-258.
8. I. Gutman, Y.N. Yeh, S. Lee and Y.L. Luo, Some Recent results in the Theory of the Wiener Number, *Indian J. Chem.* **32A** (1993) 651-661.
9. I. Gutman and O.E. Polansky, *Mathematical Concepts in Organic Chemistry* (Springer-Verlag, Berlin, 1986).
10. I. Gutman, A Formula for the Wiener Number of Tree and Its Extension to Graphs Containing Cycles, *Graph Theory Notes New York* **27** (1994) 9-15.
11. P.V. Khadikar, N.V. Deshpande, P.P. Kale, A. Dabrynin, I. Gutman and G. Domotor, The Szeged Index and an Analogy with the Wiener Index, *J. Chem. Inf. Comput. Sci.* **35** (1995) 545-550.
12. P.V. Khadikar, P.P. Kale, N.V. Deshpande, S. Karmarkar and V.K. Agrawal, Szeged Indices of Hexagonal Chains, *Commun. Math. Comput. Chem. (MATCH)* **43** (2001) 7-15.
13. P.V. Khadikar, On a Novel Structural Descriptor PI, *Nat. Acad. Sci. letters* **23** (2000) 113-118.
14. P.V. Khadikar, S. Karmarkar and V.K. Agrawal, A Novel PI Index and its Applications to QSPR/QSAR Studies, *J. Chem. Inf. Comput. Sci.* **41** (2001) 934-949.
15. V.K. Agrawal and P.V. Khadikar, QSAR Prediction of Toxicity of Nitrobenzene, *Biorg. Med. Chem.* **9** (2001) 3035-3040.
16. 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.
17. S. Singh, S. Joshi, A. Shrivastava and P.V. Khadikar, A Novel Method for Estimating Motor Octane Number (MON) – A Structure-Property Relationship Approach, *J. Sci. Ind. Res.* **61** (2002) 961-965.
18. P.V. Khadikar, A.V. Bajaj and D. Mandloi, Prediction of ¹³C Nuclear Magnetic Resonance Chemical Shifts ($\sum^{13}C_n$) in Alkanes and Cycloalkanes, *Indian J. Chem.* **41A** (2002) 2065-2067.
19. P.V. Khadikar, S. Karmarkar and R.G. Varma, On the Estimation of PI Index of Polyacenes, *Acta Chim. Slov.* **49** (2002) 755-771.
20. P.V. Khadikar, V.K. Agrawal and S. Karmarkar, Prediction of Lipophilicity of Polyacenes Using Quantitative Structure-activity Relationships, *Bioorg. Med. Chem.* **10** (2002) 3499-3507.

21. P.V. Khadikar, S. Karmarkar, S. Singh and A. Shrivastava, Use of the PI Index in Predicting Toxicity of Nitrobenzene Derivatives, *Bioorg. Med. Chem.* **10** (2002) 3163-3170.
22. P.V. Khadikar, S. Singh and A. Shrivastava, Novel Estimation of Lipophilic Behavior of Polychlorinated Biphenyls, *Bioorg. Med. Chem. Lett.* **12** (2002) 1125-1128.
23. P.V. Khadikar, A. Phadnis and A. Shrivastava, QSAR Study on Toxicity to Aqueous Organism Using PI Index, *Bioorg. Med. Chem.* **10** (2002) 1181-1188.
24. P.V. Khadikar, D. Mandloi, A.V. Bajaj and S. Joshi, QSAR Study on Solubility of Alkanes in Water and their Partition Coefficients in Different Solvent System using PI Index, *Bioorg. Med. Chem. Lett.* **13** (2003) 419-422.
25. P.V. Khadikar, S. Singh, D. Mandloi, S. Joshi and A.V. Bajaj, QSAR Study on Bioconcentration Factor (BCF) of Polyhalogenated Biphenyls Using the PI Index, *Bioorg. Med. Chem.* **11** (2003) 5045-5050.
26. P.V. Khadikar, S. Joshi, A.V. Bajaj and D. Mandloi, Correlations between the BenzeneCharacAcenes or Helicenes and Simple Molecular Descriptors, *Bioorg. Med. Chem. Lett.* **14** (2004) 1187-1191.
27. M. Jaiswal and P.V. Khadikar, QSAR Study on ¹³C NMR Chemical Shifts on Carbinol Carbon Atoms, *Bioorg. Med. Chem.* **12** (2004) 1793-1798.
28. M. Jaiswal, P.V. Khadikar and C.T. Supuran, QSAR Study on CA Inhibitory Activity of Disulfonamides: Effect of Halogen Substitution, *Bioorg. Med. Chem.* **12** (2004) 2477-2482.
29. M. Jaiswal and P.V. Khadikar, QSAR Study on Tadpole Narcosis Using PI Index: A Case of Heterogeneous Set of Compounds, *Bioorg. Med. Chem.* **12** (2004) 1731-1736.
30. M. Jaiswal, P.V. Khadikar, A. Scozzafava and C.T. Supuran, Carbonic Anhydrase Inhibitors: The First QSAR Study on Inhibition of Tumor Associated Isoenzyme IX with Aromatic and Heterocyclic-Sulfonamides, *Bioorg. Med. Chem. Lett.* **14** (2004) 3280-3290.
31. P.V. Khadikar, S. Singh, M. Jaiswal and M. Mandoli, Topological Estimation of Electronic Absorption Bands of Arene Absorption Spectra as a Tool for Modeling their Toxicity and Environmental Pollution, *Bioorg. Med. Chem. Lett.* **14** (2004) 4795-4801.
32. M. Jaiswal, P.V. Khadikar and C.T. Supuran, Topological Modeling of Lipophilicity Diureti Activity and Carbonic Inhibition Activity of Benzenesulfonamides: A Molecular Connectivity Approach, *Bioorg. Med. Chem. Lett.* **14** (2004) 5661-5666.
33. P.V. Khadikar, V. Shama, S. Karmarkar and C.T. Supuran, QSAR Studies on Benzene Sulfonamide Carbonic Anhydrase Inhibitors: Need of Hydrophobic Parameter for

- Topological Modeling of Binding Constants of Sulfonamides to Human CA-II, *Bioorg. Med. Chem. Lett.* **15** (2005) 923-930.
34. P.V. Khadikar, V. Sharma, S. Karmarkar and C.T. Supuran, Novel Use of Chemical Shift in NMR as Molecular Descriptor: A First Report on Modeling Carbonic Anhydrase Inhibitory Activity and Related Parameters, *Bioorg. Med. Chem. Lett.* **15** (2005) 931-936.
 35. M. Jaiswal and P.V. Khadikar, Use of Distance-Based Topological Indices for the Estimation of ^{13}C NMR Shifts: A Case of Benzene Derivatives, *J. Indian Chem. Soc.* **82** (2005) 247-249.
 36. A.R. Ashrafi and A. Loghman, PI Index of Armchair Polyhex Nanotubes, Personal communication.
 37. M. Jaiswal, P.V. Khadikar, D. Mandoli, M. Gupta, S. Karmarkar and R.S. Sisodia, *Bioinformatics, India* **3** (2002) 47-58.
 38. A.R. Ashrafi and A. Loghman, PI Index of $\text{TUC}_4\text{C}_8(\text{S})$ Nanotubes, Personal communication.
 39. A.R. Ashrafi and A. Logman, PI Index of Zig-Zag Polyhex Nanotubes, Personal communication.
 40. P.V. Khadikar, D. Mandloi and A.V. Bajaj, Novel Applications of PI index in Estimating Organic Reactivity-: CH: Acidity, s-Character and steric Energies, *Oxid. Commun.* **27** (2004) 23-28.