International Journal of Research Publication and Reviews

Journal homepage: www.ijrpr.com ISSN 2582-7421

Weighted Vertex PI Index of Crown and Fan Graph

A.Dhanalakshmi

Assistant Professor, Department of Mathematics, Sri Chandrasekharendra Saraswathi Viswa Mahavidyalaya, Kanchipuram, Tamilnadu, India

A B S T R A C T

In this paper we have given the definition of weighted vertex PI index. PI index gives the study of quantitative structure–activity relationship for the classification models used in the chemical, biological sciences, engineering, and nanotechnology. The weighted vertex PI index of a graph G was defined by

$$PI_w(G) = \sum_{e=uv} (d(u)+d(v))[n_u(e)+n_v(e)]$$

Here we have calculated the PI index for Crown and fan graph when it has $n \geq 6$ vertices.

Keywords: Weighted Vertex PI Index, Quantitative Structure

1. Introduction

Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of types of alkanes known as paraffins . In this paper, we consider another topological indices, named the Padmakar-Ivan index . An important aspect of modern toxicology research is the prediction of toxicity of chemicals from their molecular structures. Using PI index we study the toxicity of nitrobenzene derivatives. Also we report Quantitative Structure Toxicity Relationship using the PI index . In a series of papers, authors computed the PI index of some chemical graphs [1].

2. Molecular descriptor

Chemical compounds and drugs are often modeled as graphs where each vertex represents an atom of molecule, Fan and covalent bounds between atoms are represented by edges between the corresponding vertices. This graph derived from a chemical compounds is often called its Molecular graph, and can be different structures.

A. Iranmanesh and B. Soleimani [1], calculated the PI index of TUC4C8(R) nanotubes. They denoted the number of rhombus on the level one by p and length of cube by q .They have 2q rows of edges and 3q rows of vertices in TUC4C8(R) nanotubes.

Toufik Mansour and Mathias Schork [2] here they introduced the vertex PI index and szeged index of bridge graph are determined using these formulas the vertex PI and szeged indices of several graphs are computed.

M.H.KhalifeaH.Yousefi-Azaria..et.al they applied a matrix method to obtain exact formula for computing the szeged index of join and composition of graph. The join and composition of the vertex PI index of graph are also computed.

M.J Nadjafi-Araniet.al[3] the extremal values of this new topological index are computed .In particular we prove that for each n –vertex graph G of the extremal graph with respect to the vertex PI index $n(n-1) \leq PI_v(\mathrm{G}) \leq n\left\lfloor \frac{n}{2} \right\rfloor \left\lceil \frac{n}{2} \right\rceil$ also determined.

* *Corresponding author.*
E-mail address: dhana_amaresan@yahoo.com

Kinkar ch.Das1 and Ivan Gutman [5] estimates lower and upper bounds of PI index as well as the relationship between szeged and vertex PI indices.

Here DraganStevanovic [6]gives the sharp lower and upper bounds on the PI index of connected bicyclic graph with constant number of vertices and characterized the case of equality for both bounds.

In this paper, our objective is to find a mathematical technique, without using distance matrix, and apply the same to compute the PI index of crown and fan graphs. when it has $n \geq 6$ vertices.

3. Fan graph

A function graph is defined as the graph join where is the empty graph on nodes and is the path graph on nodes.If n≥6.[1]

4. Weighted Vertex of PI Index

A function graph is defined as the graph join where is the empty graph on nodes and is the path graph on nodes.If n≥6.[1]

Weighted vertex of PI index :

Let e=uv be an edge of the molecular graph G. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by n_u(e) . Analogously, n_v(e) is the number of vertices of G whose distance to the vertex v is smaller than the distance to the vertex u. Note that vertices equidistant to u and v are not counted. [1]

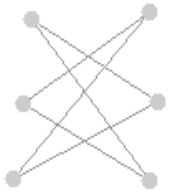
The weighted vertex PI index of a graph G was defined by

$PI_w(G)=\sum_{e=uv}(d(u)+d(v)[n_u(e)+n_v(e)]$

5. Crown Graph

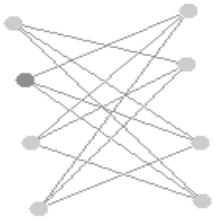
Calculating PI index for 6 vertices (.when n=3).

(i.e) K_3, K_3 graph



$PI_w(G)=[(2+2)(1+1)+(2+2)(1+1)+(2+2)(1+1)]$
$=8+8+8$
$=24.$

$K_{(4,4)}$

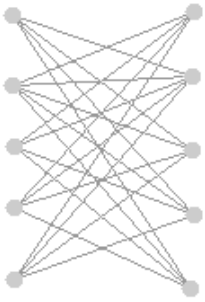


$PI_w(G)=[(3+3)(2+2)+(3+3)(2+2)+(3+3)(2+2) +(3+3)(2+2)]$

$=6(16)$

$=96$

$K_{(5,5)}$



$PI_w(G)=[8(3+3)+8(3+3)+8(3+3)+8(3+3)+8(3+3)]$

$=48+48+48+48+48$

$=240$

For "n" vertices ,

Let N denotes total number of degree of a vertices u and v .let n denote the total number of vertices of u or v.

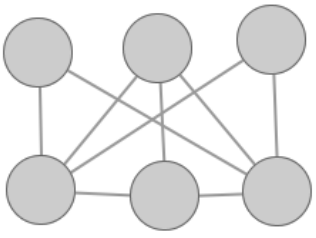
$PI_w(G)=n[N(N-2)]$

For eg; n=6 and N=10

$PI_w(G)=6[10(8)]=6[80]=480.$

6. Fan Graph

n =6 m=2

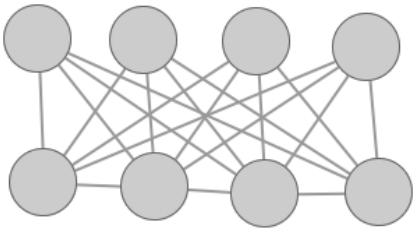


$PI_w(G) =[(4+3)(3+2)+(5+3)(4+2)+(4+3)(3+2)]$

$=2[7(5)]+8(6)$

$=118$

n =8 m=3



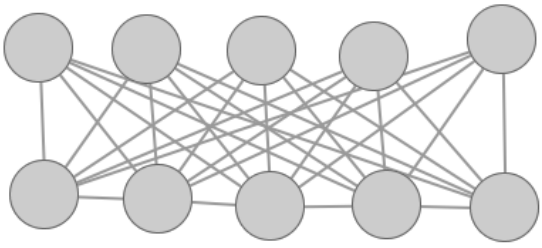
$PI_w(G)=[(5+4)(4+3)+(6+4)(5+3)+(6+4)(5+3)$

+(5+4)(4+3)]

=2[9(7)]+2[10(8)]

=126+160=286

n =10 m=4



$PI_w(G)$=[(6+5)(4+5)+(7+5)(6+4)+(7+5)(6+4) + 7+5)(6+4)+(6+5)(4+5)]

=2[11(9)]+3[12(10)]

=198+360

=558

For "n" vertices and "m" paths

$PI_w(G)=2(n+1)(n-1)+(m-1)(n-2)n$

7. Conclusion

We have given a definition of crown graph, and the extension of crown graph (nxn crown graph) and fan graph. And also we have given a general form for the molecule structure of some special graphs like crown, fan. It used in QSAR & QSPR studies.

REFERENCES

[1] PI Index of TUC4C8(R) Nanotubes A. Iranmanesh* and B. Soleimani Department of Mathematics, TarbiatModarresUniversity.MATCHCommun. Math. Comput. Chem. 57 (2007) 251-262 ISSN 0340 – 6253.

[2] The vertex PI index and Szeged index of bridge graphs Toufik Mansoura,Matthias Schorkb.Discrete Applied Mathematics157(2009)1600–1606.

[3] A matrix method for computing Szeged and vertex PI indices of join and composition of graphs, M.H. Khalifeh a, H. Yousefi-Azaria, A.R. AshrafibLinear Algebra and its Applications 429 (2008) 2702–2709.

[4] Extremal graphs with respect to the vertex PI index M.J.Nadjafi-Arani,G.H.Fath- Tabar , A.R.Ashrafi Applied Mathematics Letters 22 (2009) 1838–1840.

[5] Estimating the Vertex PI Index Kinkar Ch.DasaandIvan GutmanbZ. Naturforsch. 65a, 240–244 (2010); received March 7, 2009 / revised August 18, 2009.

[6] Bicyclic graphs with extremal values of PIindex , ŽanaKovijanićVukićevića, Dragan Stevanovićb,c, Discrete Applied Mathematics 161(2013)395-403