THE PUBLISHING HOUSE
OF THE ROMANIAN ACADEMY

CHEMISTRY
Research article

A STUDY OF THE NANOSTAR DENDRIMER BY PADMAKAR-IVAN INDEX

JAFAR ASADPOUR[1]

[1] Department of Mathematics, Miyaneh Branch, Islamic Azad University, Miyaneh, Iran
Corresponding author: Jafar ASADPOUR, E-mail: jafar_asadpour@yahoo.com

Received September 20, 2013

The Padmakar-Ivan index of a graph G is the sum over all edges *uv* of *G* of the number of edges which are not equidistant from the vertices *u* and *v*. In this paper we compute the *PI* index of extended bridge graphs. This is an efficient method of finding these indices especially when the extended bridge graph has a molecular graph of dendrimers form.

Key words: PI index, Extended bridge graph, Nanostar dendrimer.

INTRODUCTION

The Wiener index is one of the oldest descriptors concerned with the molecular graph. This index was first proposed by H. Wiener[18] and it is concerned with the determination of the boiling points of paraffins. Wieners original definition was different, but equivalent, from that which was written above. The definition of Wiener index in terms of distances between vertices of a graph is due to Hosoya[17]. In mathematical research, the Wiener index has been first studied in[9], and for a long time mathematicians were not aware of the importance of the Wiener index in mathematical chemistry. In theoretical chemistry molecular structure descriptor, also called topological indices, are used to understand the properties of chemical compounds. By now there are many different types of such indices for a general graph $G=(V,E)$. Here, apart from the Wiener index, we are interested in indices such as the Szeged index and the vertex PadmakarIvan index, the so called PI_v index of a graph. The Szeged index is a topological index closely related to the Wiener index and is a summation of vertexmultiplicative type and coincides with the Wiener index in the case that the graph G is a tree. Since the Szeged index takes into account how the vertices of the graph G are distributed, it is natural to define an index that takes into account the distribution of the edges of G. All the indices mentioned above, when applied to chemical graphs have many chemical applications and it was shown that the PI_v index is related to the Szeged index of a graph, and all of them have connections with the physicochemical properties of many complex compounds. For the topological indices associated to a graph two groups of problems can be distinguished in the theory of topological indices. One is to ask the dependence of the index to the graph and the other is the calculation of these indices efficiently, the greatest progress in solving the above problems was made for trees and hexagonal systems by Gutman *et al.* in[10]. In this paper we will develop a method to calculate Padmakar-Ivan index of the extended bridge graphs with several examples of molecular graphs. Throughout this paper all the graphs are simple and connected.

PRELIMINARIES

Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively.

We denote the distance between two arbitrary vertices x and y of G by $d_G(x,y)$ ($d(x,y)$ for short). It is defined as the number of edges in the minimal path connecting the vertices x and y. Given an edge $e=uv\in E(G)$ of G, we define the distance of e to a vertex $w\in V(G)$ as the minimum of the distances of its ends to w, i.e. $d(w,e)=min\{d(w,u), d(w,v)\}$. Let us denote the number of edges lying closer to the vertex u than to the vertex v by $m_u(e|G)$ and the number of edges lying closer to the vertex v than to the vertex u by $m_v(e|G)$, thus $m_u(e|G)=|\{f\in E(G)|d(u,f)<d(v,f)\}|$, and similarly for $m_v(e|G)$. The Padmakar-Ivan (*PI*) index of a graph *G* is defined as

$$PI(G)=\sum_{e\in E(G)} m_e(G)$$

where $m_e(G)=m_v(e|G)+m_u(e|G)$ is the number of edges of G that are not equidistant from the two ends of the edge e. Let $\{G_i\}$ be a set of finite pair wise disjoint graphs with $v_i\in V(G_i)$. The bridge graph

$B(G_1,G_2, \dots ,G_n) =B(G_1,G_2, \dots ,G_n;v_1,v_2, \dots , v_n)$

of $\{G_i\}$ with respect to the vertices $\{v_i\}$ is the graph obtained from the graphs $G_1,G_2, \dots ,G_n$ by connecting the vertices v_i and v_{i+1} by an edge for all $i=1, 2, \dots , n-1$. Define

$G_n(H, v)=B(H,H, \dots ,H; v, v, \dots v)$,

(n times) which is the special case of bridge graph [12,13].

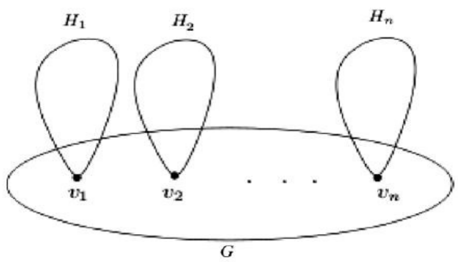

Fig. 1. The extended bridge graph.

Thus, $G_1(H,v)=H$ for any vertex v of H. Let G be a graph with vertex set $V(G)=\{v_1, v_2, \cdots , v_n\}$ and $\{H_i\}$ a sequence of finite connected pairwise disjoint graphs such that $V(G)\bigcap V(H_i)=\{v_i\}$. The extended bridge graph $EB(G;H_1, \cdots ,H_n; v_1, \cdots v_n)$ of G and $\{H_i\}$ with respect to $\{v_i\}$ is constructed by identifying the vertex v_i in G and Hi, by connecting the vertices vi and v_{i+1} by an edge for all $i\in N$ and (i mod n), see [16]. An example is shown in Figure 1. In special case of extended bridge graph, if G a path graph then $EB(G;H_1, \cdots , H_n; v_1, \cdots v_n)=B(H_1,H_2, \dots ,H_n; v_1, v_2, \dots , v_n)$.

MAIN RESULTS AND DISCUSSION

In this section we derive a formula for the PI index of the extended bridge graph when G is a cycle graph. First we denote the set of all edges uu' such that d(u,v)=d(u',v) by $M_v(G)$. The cardinality of $M_v(G)$ is denoted by $m_v(G)$.

Theorem 1. The PI index of the extended bridge graph $K=EB(C_n;H_1, ...,H_n; v_1, v_2, \cdots , v_n)$ of cycle graph C_n and $\{H_i\}$ with respect to $\{v_i\}$ is given by where $e_i =v_iv_{i+1}$ and we have:

$$PI(K)=\sum_{i=1}^{n} PI(H_i)-m(H)|E(K)|-\lambda_e(H)$$
$$+\mu_e(H)+\begin{cases} |E(K)|^2-2n & 2|n \\ |E(K)|^2-|E(K)| & other \end{cases}$$

Where $m(H)=\sum_{i=1}^{n} m_{v_i}(H_i)$,

$\lambda_e(H)=\sum_{i=1}^{n}|E(H_i)|^2$ and

$\mu_e(H)=\sum_{i=1}^{n} m_{v_i}(H_i)|E(H_i)|$

Proof. Let $K=EB(C_n;H_1,\dots,H_n;v_1,\dots,v_n)$ of G and $\{H_i\}$. From the definitions we have that

$$E(K)=\sum_{i=1}^{n} M_{v_i}(H_i)\bigcup\sum_{i=1}^{n}(|E(H_i)|\setminus M_{v_i}(H_i))\bigcup\{v_iv_{i+1}\}_{i=1}^{n}$$

where $v_{n+1}=v_1$ then

$$PI(K)=$$
$$\sum_{e\in E(K)} m_e(K)=\sum_{i=1}^{n}\sum_{e\in E(H_i)} m_e(K)+\sum_{i=1}^{n} m_{v_iv_{i+1}}(K)$$
$$=\sum_{i=1}^{n}\sum_{e\in M_{v_i}(H_i)} m_e(K)+\sum_{i=1}^{n}\sum_{e\in E(H_i)-M_{v_i}(H_i)} m_e(K)+\sum_{i=1}^{n} m_{v_iv_{i+1}}(K)$$

(a) If e is the edge $v_i v_{i+1}$ in K, then there exists the following two cases:
Case(i) If G is a even cycle graph then there exists only a edge which is equidistant from the ends of the edge *e*

$$\sum_{i=1}^{n} m_e(K)=\sum_{i=1}^{n} m_{v_iv_{i+1}}(K)=\sum_{i=1}^{n}(|E(K)|-2)=n(|E(K)|-2)$$

Case(ii) If G is a odd cycle graph then there exists only a vertex such as v_j which is equidistant from the ends of the edge e, thus edges set $E(H_j)$ is equidistant from the ends of the edge *e*

$$\sum_{i=1}^{n} m_e(K) = \sum_{i=1}^{n} m_{v_i v_{i+1}}(K) = \sum_{i=1}^{n} \left(|E(K)| - |E(H_i)| - 1\right) = (n-1)|E(K)|$$

(b) If $e \in M_{vi}(H_i)$ then all the edges in $E(K)\backslash E(H_i)$ are equidistant from the ends of the edge *e*

$$\sum_{i=1}^{n} m_e(K) = \sum_{i=1}^{n} m_e(H_i)$$

(c) If $e \in E(H_i)\backslash M_{vi}(Hi)$ then each edge in $E(K)\backslash E(H_i)$ is not equidistant from the ends of the edge *e*.

$$\sum_{i=1}^{n} m_e(K) = \sum_{i=1}^{n} \left(m_e(H_i) + |E(K)| - |E(H_i)|\right)$$

This can be equivalent to

$$PI(K) = \sum_{i=1}^{n} \sum_{e \in E(H_i)} m_e(H_i) + \sum_{i=1}^{n} (|E(K)| - |E(H_i)|) + n(|E(K)| - 2)$$

$$= \sum_{i=1}^{n} PI(H_i) + \sum_{i=1}^{n} (|E(H_i)| - m_{v_i}(H_i))(|E(K)| - |E(H_i)|) + n|E(K)| - 2n$$

$$= \sum_{i=1}^{n} PI(H_i) + (n + \sum_{i=1}^{n} (|E(H_i)| - m_{v_i}(H_i))|E(K)| - \sum_{i=1}^{n} |E(H_i)|^2 + \sum_{i=1}^{n} |E(H_i)| m_{v_i}(H_i) - 2n$$

when C_n is an even cycle graph , and when C_n is an odd cycle graph, we can:

$$PI(K) = \sum_{i=1}^{n} \sum_{e \in E(H_i)} m_e(H_i) + \sum_{i=1}^{n} (|E(K)| - |E(H_i)|) + (n-1)|E(K)|$$

$$= \sum_{i=1}^{n} PI(H_i) + \sum_{i=1}^{n} m_{v_i}(H_i))|E(H_i)| + (|E(K) - m(H) - 1)|E(K)|$$

We define,

EBn(G,H,v)=EB(G;H,H,…,H;v,…,v}),

(n times and $n \geq 3$) which is the special case of extended bridge graph are built from several copies of the same graph was consider. As a corollary of Theorem 1, we have the following result.

Corollary 1. Let H be any graph with fixed vertex v. Then the PI index of the extended bridge graph $EBn(C_n,H, v)$ is given by

$$PI(EB_n(C_n, H, v)) = nPI(H) + (n^2 - n)|E(H)|^2 + (n - n^2)m_v(H)|E(H)| - n^2 m_v(H) + \begin{cases} 2n^2|E(H)| + n^2 - 2n & 2|n \\ (2n^2 - n)|E(H) + n^2 - n & other \end{cases}$$

Proof. By use of the definitions and Theorem 1 this proof is straightforward.

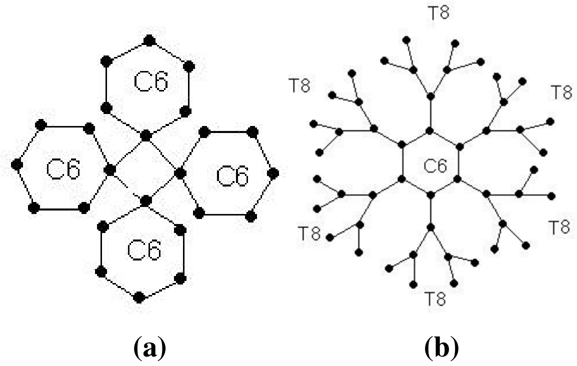

Fig. 2. The extended bridge graph (a)- Γ 4,6 , (b)- Δ 6,8.

Example 1. Let P_m be the path graph on m vertices, Clearly $PI(P_m)=(m-1)(m-2)$, $|V(P_m)|$, $|E(P_m)|=m-1$ and $m_{v1}(P_m)=0$, defined $\delta_{n,m,1} = EB_n(C_n, P_m, v_1)$

Then $PI(\delta_{n,m,1}) = \begin{cases} n^2m^2 - 2n & 2|n \\ n^2m^2 - n(m-2) & other \end{cases}$

We use a path Pm of arbitrary length m and choose a (fixed) vertex v_l with $1 \leq l \leq m$, and define $\delta_{n,m,l} = EB_n(C_n, P_m, v_l)$. It is easy to check that the vertex PI index of the graph $\delta_{n,m,l}$ does not depend on the vertex l which we choose in each path (as long as it is the same in each path). However, checking the formula given in Theorem 1, we see that $m_{vl}(P_m) = 0$ for any vertex v in Pm the resulting formula is the same for any choice of vertices in the paths. We describe the result more precisely in the following corollary.

Corollary 2. For a tree T_m with m vertices, we have

$$PI(\Delta_{n,m,l}) = \begin{cases} n^2m^2 & 2|n \\ n^2m^2 - n(m-2) & other \end{cases}$$

Proof. By use of the definitions, we have $|V(T_m)|=|E(T_m)| + 1=m$, $m_{vi}(T_m) = 0$ for $1 \leq i \leq m$ and Clearly $PI(T_m)=(m-1)(m-2)$, then this proof is straightforward.

Corollary 2. The PI index for $\Gamma_{n,m}=EB_n(C_n,C_m, v)$ is given by

$$PI(\Gamma_{n,m}) = \begin{cases} nm(nm+2n-2)+n(n-2) & 2|n,\ 2|m \\ nm(nm+n)-2n & 2|n,\ 2\nmid m \\ nm(nm+2n-3)+n(n-1) & 2\nmid n,\ 2|m \\ nm(nm+n-1)-n & 2\nmid n,\ 2\nmid m \end{cases}$$

Proof. Let C_m be the cycle graph on m vertices,

$$PI(C_m)=\begin{cases} m(m-2) & 2|m \\ m(m-1) & other \end{cases}$$ and

$$m_v(C_m)=\begin{cases} 0 & 2|m \\ 1 & other \end{cases}$$

Example 2. The PI index for $\Gamma_{n,n}$ = EBn(Cn,Cn,v) is given by

$$PI(\Gamma_{n,n})=\begin{cases} (n^3-n)(n+2) & 2|n \\ (n^3-n)(n+1) & other \end{cases}$$

Dendrimers are highly branched macromolecules. They are being investigated for possible uses in nanotechnology, gene therapy, and other fields. Each dendrimer consists of a multifunctional core molecule with a dendritic wedge attached to each functional site. The core molecule without surrounding dendrons is usually referred to as zeros generation. Each successive repeat unit along all branches forms the next generation, 1st generation and 2nd generation and so on until the terminating generation. The topological study of these macromolecules is the aim in investigations mathematical chemistry see [1-4] for details. In this example we will consider a two classes of dendrimer nanostars and find their PI indices.

NS[r] denotes the molecular graph of a nanostar dendrimer with exactly r generations depicted in Figure 3. In [3] we have:

$$|V(NS[r])| = 24+\sum_{i=1}^{r-1} 18\cdot 2^i = 18\cdot 2^r - 12$$

and

$$|E(NS[r])| = 27+\sum_{i=1}^{r-1} 21\cdot 2^i = 21\cdot 2^r - 15.$$

This dendrimer contains three branches $B_1NS[r]$, $B_2NS[r]$ and $B_3NS[r]$. Hence by use of Theorem 1 one can write:

$$|V(B_iNS[r])| = 6\cdot 2^r - 5$$

and

$$|E(B_iNS[r])| = 7\cdot 2^r - 7 \text{ for } i=1,2,3.$$

Also,

$$m(NS[r]) = \sum_{i=1}^{3} m_{v_i}(B_iNS[r]) = 0,$$
$$\mu_e(BNS[r]) = \sum_{i=1}^{3} m_{v_i}(B_iNS[r])|V(B_iNS[r])| = 0,$$
$$\lambda_e(BNS[r]) = \sum_{i=1}^{3} |E(B_iNS[r])|^2 = 3(7\cdot 2^r - 7)^2.$$

Therefore,

$$PI(NS[r]) = 441\cdot 2^{2r} - 630\cdot 2^r + 213$$

We now consider PI index for NS4[r] class of nanostar dendrimers with exactly r generations depicted in Figure 4. In center of Figure 4, the core of dendrimer nanostar NS4[r] is depicted. Thus, we can check that the vertices set and edges set of NS4[n]. In [4],

$$|V(NS_4[r])| = 96\cdot 2^{r-1} - 60$$ and
$$|E(NS_4[r])| = 105\cdot 2^{r-1} - 66$$

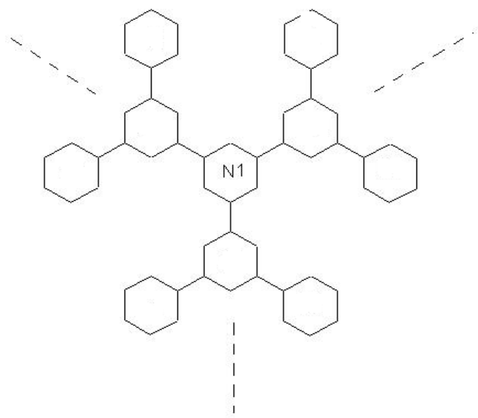

Fig. 3. The nanostar dendrimer NS[n].

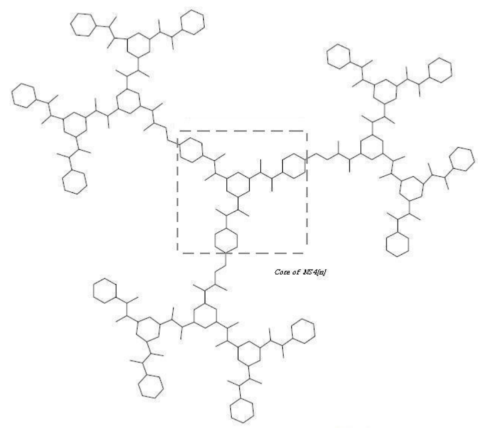

Fig. 4. The Molecular Graph of NS4[n].

Also,

$$|V(B_iNS_4[r])| = 32 \cdot 2^{r-1} - 21$$
$$|E(B_iNS_4[r])| = 35 \cdot 2^{r-1} - 24 \text{ for } i = 1, 2, 3.$$

Thus,

$$\lambda_e(BNS_4[r]) = 3(35 \cdot 2^{r-1} - 24)^2$$

and

$$\mu_e(BNS_4[r]) = 0.$$

Therefore,

$$PI(NS_4[r]) = 11025 \cdot 2^{2r-2} - 6930 \cdot 2^r + 4344.$$

ACKNOWLEDGEMENT

This research is supported by the research council of the Islamic Azad University of Miyaneh.

REFERENCES

1. A.R. Ashrafi, A. Loghman, PI index of zig-zag polyhex nanotubes, MATCH Commun. Math. Comput. Chem. 55 (2006) 447-452.
2. A.R. Ashrafi, A. Loghman, PI index of armchair polyhex nanotubes, Ars Combin. 80 (2006) 193-199.
3. A. R. Ashrafi, M. Saheli, The eccentric connectivity index of a new class of nanostar dendrimers, OAM–RC Vol. 4, No. 6, June 2010, p. 898– 899.
4. A.R. Ashrafi and P. Nikzad, Kekle index and bounds of energy for nanostar dendrimers, Digest Journal of Nanomaterials and Biostructures, Vol. 4, No.2, June 2009,p. 383 388.
5. N. Alon, E. Lubetzky, Independent set in tensor graph powers, J. Graph Theory 54 (2007) 73-87.
6. M.R. Darafsheh, Computation of topological indices of some graphs, Acta Appl Math (2010) 110: 12251235 DOI 10.1007/s10440-009-9503-8.
7. Dobrynin, A.A., Entringer, R., Gutman, I.: Wiener index of trees: Theory and applications. Acta Appl. Math. 66, 211249 (2001).
8. Dobrynin, A.A., Gutman, I.: Congruence relations for the Szeged index of hexagonal chains. Univ. Beogr. Publ. Elektrotehn. Fak. Ser. Mat. 8, 106113 (1997).
9. Entringer, R.C., Jackson, D.E., Snyder, D.A.: Distance in graphs. Czechoslav. Math. J. 26, 283296 (1976).
10. I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, Graph Theory Notes N.Y. 27 (1994) 9-15.
11. W. Imrich, S. Klavar, Product Graphs: Structure and Recognition, Wiley, 2000.
12. M. H. Khalifeh, H. Yousefi-Azari, A.R. Ashrafi, Vertex and edge PI indices of Cartesian product graphs, Discrete Appl. Math. 156 (2008) 1780-1789.
13. T. Mansour, M. Schork, The PI index of bridge and chain graphs, Camillo-Sitte-Weg 25, Frankfurt, Germany, Received May 5, (2008).
14. T. Mansour, M. Schork, The vertex PI index and Szeged index of bridge,Discrete Applied Mathematics 157 (2009) 1600-1606.
15. T. Mansour and M. Schork, Wiener, hyper-Wiener, detour and hyper-detour indices of bridge and chain graphs, J Math Chem (2010) 47;7298 DOI 10.1007/s10910-009- 9531-7.
16. Z. Yarahmadia, T. Doli , A.R. Ashrafi, The bipartite edge frustration of composite graphs, Discrete Applied Mathematics 158 (2010) 1551-1558.
17. H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons. Bull. Chem. Soc. Jpn. 4, 2332-2339 (1971).
18. H. Wiener, Structural determination of paraffin boiling points. J. Am. Chem. Soc. 69, 1720 (1947).