© 2018 IJSRSET | Volume 4 | Issue 10 | Print ISSN: 2395-1990 | Online ISSN : 2394-4099
Themed Section : Engineering and Technology

# Topological Indices of Nanotubes : An Overview

**Sufia Aziz**
*Department of Applied Sciences (Mathematics), Institute of Engineering and Technology,
Devi Ahilya University, Indore, Madhya Pradesh, India

**ABSTRACT**

The study of topological indices of graphs and therefore of carbon nanotubes is a very important part of graph theory and thus nanotechnology. A topological index is a real number related to a graph. There are several topological indices used in chemical graph theory, however, a very few of them are found useful in nanotechnology for solving structural problems related to carbon nanotubes. In this article a brief summary on the development of Wiener, Szeged and Padmakar-Ivan indices for carbon nanotubes is given.

**Keywords :** Topological index, Benzenoid graph, Carbon Nanotubes, Wiener index, Szeged index, Padmakar–Ivan index.

## I. INTRODUCTION

Carbon nanotubes (CNT) have become the subject of intense investigation since their discovery [21]. This is due to the unique behaviour of CNT along with their remarkable electrical, chemical, biomedical, medicinal, mechanical and structural properties. A topological index is a numeric quantity derived on the structural graph of a molecule i.e., a nanostructure. Recent studies of the application of graph theory and subsequent methods for the estimation of topological indices, not only helped the nanotechnologists to investigate aforementioned versatile properties of carbon nanotubes but helped them in preparing unknown carbon nanotubes with still better properties. This is due to the fact that most of the carbon nanotubes that are build, have polycyclic benzenoid hydrocarbon as their basic units.

The literature survey has shown that topological indices like Weiner [25], Szeged [14, 15, 20, 22, 23], Balaban [5] and Pardmakar-Ivan (PI) [1-4, 6-8, 13, 24, 26] indices have been used in solving the problems related to carbon nanotubes. Thus, in the next section of the paper, we give a brief survey of few of these indices for a variety of carbon nanotubes, beginning with basic definitions, properties and the graph theoretical notations used for the calculations of these indices.

## II. MAIN RESULTS AND DISCUSSIONS

### A. *Weiner Index (W):*

The Wiener index W, introduced in 1947 by the chemist Harold Wiener [25]. In graph theoretical language, it is equal to the count of all shortest distances in a graph. Thus, the Wiener index W = W (G) was first defined, for a tree G = T, by the following expression:

$$W = W(T) = 1/2 * \Sigma\, d(i, j), \quad (1)$$

Where d(i, j) is the distance between the vertices u and v in G and the summation going over all pairs (i, j) of vertices $i, j \in V(G)$, or by

$$W = W(T) = \Sigma n(i(e)) * n(j(e)), \quad (2)$$

Where, n(i(e)) and n(j(e)) are the number of vertices of G lying on two sides of the edge e.

1) *Weiner index of Armchair Polyhex Nanotubes*:

Diudea, Stefu, Parr and John [9] have described a method for computing Weiner index of arm chair nanotubes. In doing so, they have considered single-walled nanotubes (SWNTs). They considered hexagonal armchair lattice $TUVC_6[c, n]$ as shown in the Fig. 1:

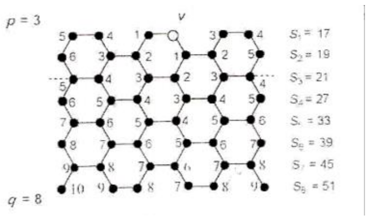


**Figure 1:** An armchair polyhex lattice

and choose a reference vertex v from which the topological distances to all other vertices are evaluated. The sum of such distances, on each level, is given in Fig. 1 as $S_i$. Then, the Weiner index of armchair nanotubes, having $q \geq p$ is given by the following expression:

$$W_{TUVC6}(p, q, z) = \frac{p}{12}[12(-1)^{(p-z)}pq+3(-1)^{(p-z+1)}+3(-1)^{-z}-12q^2z^2 +12q^2z+12(-1)^{(p-z)}p+12z^2q+6(-1)^{(p-z+1)}p^2+8pq^3 -28pq+6q^2+18q+8p^3q+12p^2q^2-12(-1)^{(p-z)}q +6(-1)^{(p-z+1)}q^2-24qz-12p+14p^2+6(-1)^{(1-z)}q-2p^4$$

2) *Weiner index of zig-zag $TUHC_6[c, n]$ Nanotubes*:

Following the methodology given above, the Diudea and John computed Weiner index of zig-zag $TUHC_6$ [c, n] [8], the lattice of which is shown in the Fig. 2:

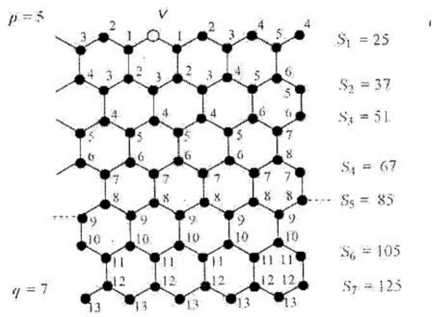


**Figure 2 :** A zig-zag polyhex lattice

In this case they have computed (a) Weiner index of long tubes $q \geq p$ as well as (b) short tubes $q \leq p$. The expressions used for these calculations are mentioned below:

(a) Long Tubes

$$W_{TUHC6}(p, q) = \frac{p^2}{6}[8q^3+4p^2q-6q-p^3+p]$$

(b) Short Tubes

$$W_{TUHC6}(p, q) = \frac{pq}{6}[q^3+4pq^2+6p^2q-q-4p]$$

For q = 1 and $p \geq 2$, the formula for simple cycles on 2p vertices is given as $W(C_{2p}) = p^3$.

**B.** ***Szeged Index (Sz):***

The Szeged index (Sz) is another topological index, in acquaintance with Gutman [11] and Gutman-Khadikar [14]. The Szeged index Sz (G) of graph G is defined as:

$$Sz(G) = \sum_{e=uv\in E(G)}[n_u(e).n_v(e)] \qquad (3)$$

Where, $n_u(e)$ is the number of vertices of G lying closer to u and $n_v(e)$ is the number of vertices of G lying closer to v. Note that vertices equidistant from u and v are not taken into account. The main advantage of the Szeged index is that it is a modification of Wiener index for cyclic graphs; otherwise, it coincides with the Wiener index. The Szeged index of some nanostructures is discussed in the following sub-section:

1) *Szeged index of Armchair Polyhex Nanotubes*:

Eliasi and Taeri [10] have computed an exact expression for Szeged index of $TUVC_6[2p, q]$, the armchair polyhex nanotubes, using a theorem of Dobrynin and Gutman [12]. This tube is as shown in the Fig. 3:

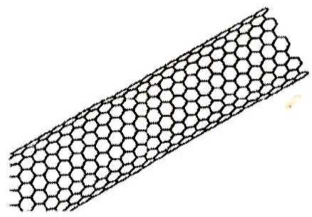

**Figure 3 :** An armchair polyhex nanotube

The lattice of $TUVC_6[2p, q]$ with p = 5 and q = 7 is shown in the Fig. 4:

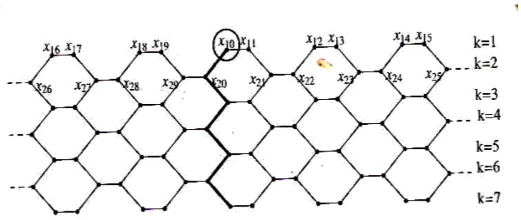


**Figure 4 :** A $TUVC_6[2p, q]$ lattice with p = 5 and q = 7.

The Sz index is given by the following expression:

$Sz(TUVC_6[2p, q])$ =

$$\frac{1}{60}p(12p^5+30p^4-80pq^4-120qp^3+160q^2p^3+60q^3p^2+80p^2q$$
$$-120q^2p+30p(-1)^q+18p+20q^4p-33q-2q^5+15(-1)^{q+1}q+20q^3)$$

if $p < q < 2p - 2$ and p is even. Here, 2p is circumference and q is length.

2) *Szeged index of $HC_5C_7$ [r, p] Nanotube*:

A $C_5C_7$ net is a trivalent decoration made by alternating pentagons $C_5$ and heptagons $C_7$. It can cover either a cylinder or a torus. Iranmanesh and Takravesh [13] have computed Szeged index of the nanotube shown in Fig.5:

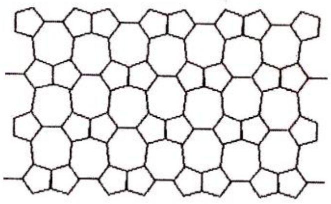

**Figure 5 :** A $HC_5C_7$ [4, 8] nanotube with p = 8, r = 4.

They have given a computer program for computing Szeged index of this nanotube.

### C. *Padmakar Ivan Index (PI)*:

For the reason of the coincidence of Wiener and Szeged indices in case of trees Khadikar [16] introduced another Szeged / Wiener –like index and named it Padmakar-Ivan index and abbreviated as PI.

The Padmakar-Ivan index (PI) index of the graph G is defined as:

$$PI = PI(G) = \sum [n_{eu}(e|G) + n_{ev}(e|G)] \qquad (4)$$

Where, $n_{eu}(e|G)$ is the number of edges lying closer to the vertex u than the vertex v; $n_{ev}(e|G)$, is the number of edges lying closer to the vertex v than the vertex u. Edges equidistant from both ends of the edge e = uv are not counted. And the summation goes over all the edges of G.

Or, the PI index of a bipartite *sco* graph G is defined by (s = 1, 2, …, c)

$$PI(G) = m(G)^2 - \Sigma m_s(G)^2 \qquad (5)$$

Large amount of work has been done on the application of PI index in nanotubes since then. The PI index of some nanostructures is discussed in the following sub-section:

1) *PI index of zig-zag Polyhex Nanotubes*:

Ashrafi and Loghman [2] have computed PI index of zig-zag polyhex nanotubes T = $TUHC_6$ [2p, q] as shown in the Fig. 6:

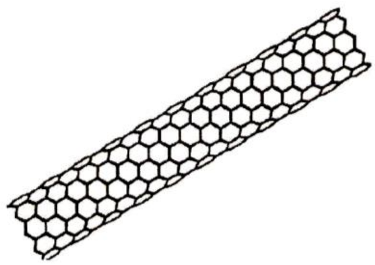

**Figure 6:** A zig-zag $TUHC_6$ [2p, q]

The polyhex lattice of this tube is given in Fig. 7:

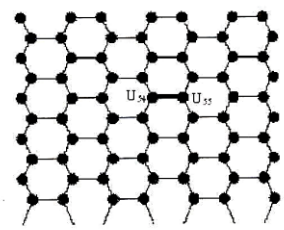


**Figure 7:** A zig-zag polyhex lattice

The PI index of the zig-zag polyhex nanotubes is computed by using the following expression:

$PI(TUHC_6\ (2p, q))$ =

$$\begin{cases} p^2(9q^2-7q+2)-4pq^2, & \text{if } q \le p \\ p^2(9q^2-15q+4p-2)+4pq, & \text{if } q \ge p \end{cases}$$

2) *PI index of $TUC_4H_8$ (S) Carbon Nanotubes*:

Ashrafi and Loghman [3] have also computed PI index of $TUC_4H_8(S)$ carbon nanotubes given in Fig. 8:

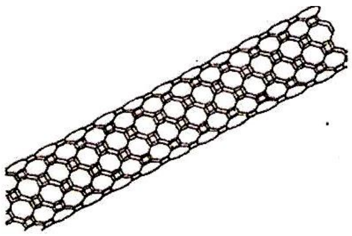

**Figure 8:** A $TUC_4H_8(S)$ carbon nanotube

Lattice with p = 4 and q = 8 is given in Fig. 9 below:

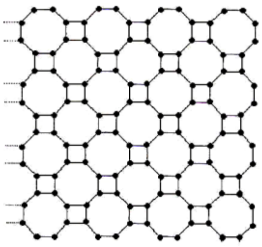

**Figure 9:** A $TUC_4H_8(S)$ lattice with p = 4 and q = 8.

The following expression is proposed for the computation of PI index of $TUC_4H_8$ (S) [4p, q]:

$$PI(TUC_4H_8\,(S)\,[4p, q]) = \begin{cases} X, & \text{if } q \le p \\ Y, & \text{if } q \ge p \end{cases}$$

where, $X = 36p^2q^2 - 28p^2q + 8p^2 - 8pq^2$

and $Y = 36p^2q^2 - 36p^2q - 4pq^2 + 4pq + 4p^3 + 4p^2$.

3) *PI index of Armchair Polyhex Nanotubes*:

Once again, the same authors, namely Ashrafi and Loghman [4] have computed PI index of armchair polyhex nanotubes. These authors have considered T = $TUVC_6$ [2p, q] as arbitrary armchair polyhex nanotubes, as shown in the Fig. 10:

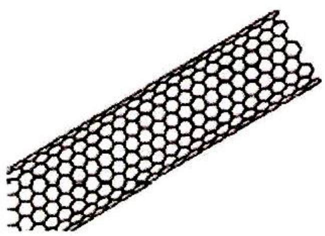

**Figure 10:** An armchair $TUVC_6$ [20, n]

The PI index of this nanotube is computed as:

$$PI(TUVC_6\,[2p, q]) = \begin{cases} \begin{cases} X - p, & \text{if } q \le p+1 \\ Y - p, & \text{if } q \ge p+1 \end{cases}, & 2\,|\,p \;\&\; 2\,|\,q-1 \\ \begin{cases} X, & \text{if } q \le p+1 \\ Y, & \text{if } q \ge p+1 \end{cases}, & \text{otherwise} \end{cases}$$

where, $X = 9p^2q^2 - 12p^2q - 5pq^2 + 8pq + 4p^2 - 4p$

and $Y = 9p^2q^2 - 20p^2q - pq^2 + 4pq + 4p^3 + 8p^2 - 4p$.

4) *PI index of $HAC_5C_6C_7$ Nanotubes*:

Yousefi-Azari, Bahrami and Ashrafi [26] have computed PI index of $HAC_5C_6C_7$ nanotubes and nanotori. The two-dimensional lattice of $HAC_5C_6C_7$ [16, q] nanotube is shown in Fig. 11:

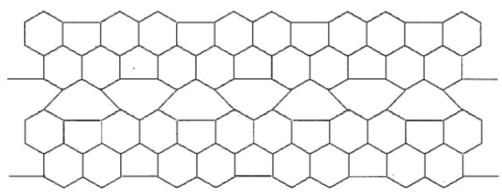

**Figure 11:** The 2-Dimensional lattice of the $HAC_5C_6C_7$ [16, 8] nanotube

The PI index of this tube is computed as:

$$PI\,(HAC_5C_6C_7) = \begin{cases} 2080q^2 - 160q & 2 \nmid q \\ 2080q^2 - 376q & 2\,|\,q \end{cases}$$

5) *PI index of a nanotube $SC_4C_8[q, 2p]$*:

Deng and Ilou [6] have computed PI index of a nanotube G = $SC_4C_8$ [q, 2p], with q rows and 2p columns. They considered three types of G:

Type I: G = $SC_4C_8$ [q, 2p]

Type II: If all the edges on the open ends are the edges of $C_8$ or $C_4$

Type III: Otherwise.

Note that G = $SC_4C_8$ [q, 2p] is a Type III nanotube if and only if q is odd. Nanotubes of Type I and III are shown in Fig. 12:

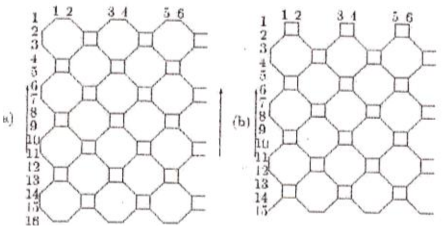

**Figure 12:** (a) A Type-I Nanotube and (b) A Type-III Nanotube

If G is a Type I, then we have

$$PI(G) = \begin{cases} 9p^2q^2 - 14p^2q + 8p^2 - 2pq^2, & \text{if } q \le 2p \\ 9p^2q^2 - 18p^2q + 4p^2 + 2pq - pq^2 + 4p^2, & \text{if } q \ge 2p+2 \end{cases}$$

If G is a Type II, then

PI(G) =

$$\begin{cases} 9p^2q^2 - 14p^2q - 2pq^2 - 4pq + 4p^2 - 4p, \text{ if } q \le 2p+2, q \equiv 0 \\ 9p^2q^2 - 14p^2q - 2pq^2 - 4pq + 4p^2 - 4p, \text{ if } q \le 2p+2, q \equiv 2p \text{ is odd.} \\ 9p^2q^2 - 14p^2q - 2pq^2 - 4pq + 4p^2 - 8p, \text{ if } q \le 2p+2, q \equiv 2p \text{ is even.} \\ 9p^2q^2 - 18p^2q - pq^2 + 4p^3 + 2pq - 8p^2 - 4p, \text{ if } q \ge 2p+4, q \equiv 0. \\ 9p^2q^2 - 18p^2q - pq^2 + 4p^3 + 2pq - 8p^2 - 4p, \text{ if } q \ge 2p+4, q \equiv 2p \text{ is odd.} \\ 9p^2q^2 - 18p^2q - pq^2 + 4p^3 + 2pq - 8p^2 - 4p, \text{ if } q \ge 2p+4, q \equiv 2p \text{ is even.} \end{cases}$$

If G is a Type III, then

PI(G) =

$$\begin{cases} 9p^2q^2 - 14p^2q - pq^2 + 2pq + 6p^2 - p, \text{ if } q \le 2p+1, p \text{ is odd.} \\ 9p^2q^2 - 14p^2q - pq^2 + 2pq + 6p^2 - 2p, \text{ if } q \le 2p+1, p \text{ is even.} \\ 9p^2q^2 - 18p^2q - pq^2 + 4p^3 + 2pq + 6p^2 - 2p, \text{ if } q \ge 2p+3, p \text{ is odd.} \\ 9p^2q^2 - 18p^2q - pq^2 + 4p^3 + 2pq + 6p^2 - 3p, \text{ if } q \ge 2p+3, p \text{ is odd.} \end{cases}$$

6) *PI index of $TUVC_6$ [2p, q]*:

A formula for calculating PI index of $TUVC_6$[2p, q] is given by Deng [7]. In the following Fig. 13, G = $TUVC_6$[2p, q] denotes an armchair polyhex nanotube with p = 6 and q = 9.

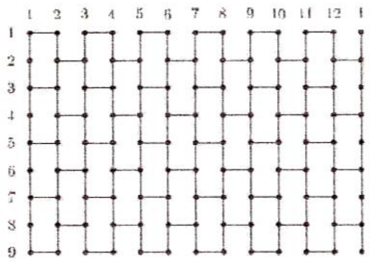

**Figure 13:** G = $TUVC_6$[2p, q] with p = 6 and q = 9

The PI index of G = $TUVC_6$[2p, q] is given as:

(i) If q is even, then

$$PI(G) = \begin{cases} 9p^2q^2 - 12p^2q + 4p^2 - 5pq^2 + 8pq - 4p, & \text{if } q \le p \\ 9p^2q^2 - 20p^2q + 4p^3 - pq^2 + 8p^2 - 4pq - 4p, & \text{if } q \ge p+1 \end{cases}$$

(ii) If q is odd, then

PI(G) =

$$\begin{cases} 9p^2q^2 - 12p^2q - 4p^2 - 5pq^2 - 8pq - 4p, & \text{if } q \le p \text{ and p is odd.} \\ 9p^2q^2 - 20p^2q - 4p^3 - pq^2 + 8p^2 - 4pq - 4p, & \text{if } q \ge p-1 \text{ and p is odd.} \\ 9p^2q^2 - 12p^2q - 4p^2 - 5pq^2 - 8pq - 3p, & \text{if } q \le p \text{ and p is even.} \\ 9p^2q^2 - 20p^2q - 4p^3 - pq^2 + 8p^2 - 6pq - 5p, & \text{if } q \ge p-1 \text{ and p is even} \end{cases}$$

7) *PI indices of $VC_5C_7$ [p, q] and $HC_5C_7$ [p, q] Nanotubes*:

Iranmanesh and Alizadeh [13] have proposed GAP program for computing PI indices of any graph, based on an algorithm and given expressions for the calculation of the same, for graphs $VC_5C_7$[p, q] and $HC_5C_7$[p, q] acting as nanotubes. The nanotube $VC_5C_7$[p, q] is depicted in the Fig. 14:

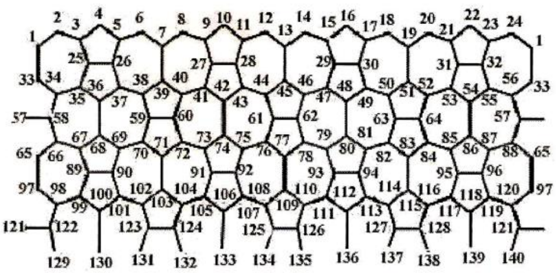

**Figure 14:** A $VC_5C_7$ [4, 2] nanotube

Similarly, the nanotube $HC_5C_7$ [p, q] is shown in the Fig. 15:

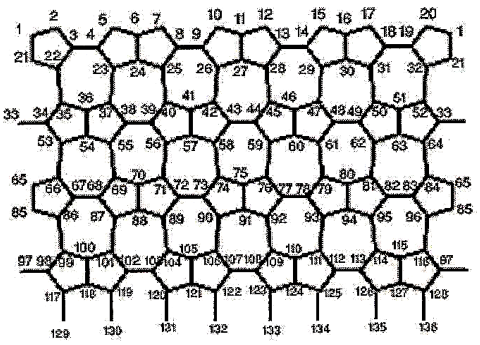

**Figure 15:** A $HC_5C_7$ [4, 2] nanotube

8) *Vertex PI index of $TUC_4C_8(S)$, $TUC_4C_8(R)$ and $HAC_5C_7$[r, p] Nanotubes*:

Sousaraei, Mahmiani and Khormali [24] have computed vertex PI indices of three nanotubes viz $TUC_4C_8$(S), $TUC_4C_8$(R) and $HAC_5C_7$[r, p]:

(i) Vertex PI index of $TUC_4C_8$ (S):

$$PI_v(TUC_4C_8\,(S)) = \sum_{e\in E(G)} 4pk$$

$$= (4pk)(4pk)$$

(ii) Vertex PI index of $TUC_4C_8$ (R):

(a) If p is even, $PI_v(TUC_4C_8\,(R)) = \sum_{e\in E(G)} 4pk$

$$= (4pk)(6pk - p)$$

(b) If p is odd, $PI_v(TUC_4C_8\,(R))$ =

$$= \sum_{e\in E(G)/\{e\in S_{ij}|1\le i\le k,\ 1\le j\le p\}} 4pk + \sum_{\{e\in S_{ij}|1\le i\le k, 1\le j\le p\}} (4pk - p)$$

$$= (4pk)(2pk - p) + (4pk - p)(4pk)$$

(iii) Vertex PI index of $HAC_5C_7$ [r, p]:

For even p ≥ 6

$PI_v(HAC_5C_7\,[r, p])$ =

$$= \begin{cases} \sum_{m=1}^{k} S_1 + \sum_{m=1}^{k-1} p(z_2+t_2), & k \le \frac{p}{2} \\ \sum_{m=1}^{p/2} S_2 + \sum_{m=p/2}^{k} S_3 + \sum_{m=1}^{p/2} p(z_2+t_2) + \sum_{m=p/2+1}^{k-1} p(z_2+t_2), & \frac{p}{2} < k < p \\ \sum_{m=1}^{p/2} S_2 + \sum_{m=k-p/2+1}^{k} S_3 + \sum_{m=p/2+1}^{k-p/2} p(z_2+t_2) + \sum_{m=k-p/2+1}^{k-1} p(z_2+t_2), & k > p \end{cases}$$

For odd p ≥ 7,

$PI_v(G)$ =

$$\begin{cases} \sum_{m=1}^{k} S_1 + \sum_{m=1}^{k-1} p(z_2+t_2), & k \le \left[\frac{p}{2}\right] \\ \sum_{m=1}^{[p/2]} S_2 + \sum_{m=[p/2]+1}^{k} S_3 + \sum_{m=1}^{[p/2]} p(z_2+t_2) + \sum_{m=[p/2]+1}^{k-1} p(z_2+t_2), & \left[\frac{p}{2}\right] < k < p \\ \sum_{m=1}^{[p/2]} S_2 + \sum_{m=k-[p/2]+1}^{k} S_3 + \sum_{m=[p/2]+1}^{k-[p/2]} S_4 + \sum_{m=1}^{[p/2]} p(z_2+t_2) + \sum_{m=[p/2]+1}^{k-[p/2]} p(z_2+t_2) + \sum_{m=k-[p/2]+1}^{k-1} p(z_2+t_2), & k > p \end{cases}$$

## III. CONCLUSION

The paper describes the basic definitions, properties and calculations of the topological indices these for a variety of carbon nanotubes. We surveyed nearly all results related to Weiner, Szeged and PI-indices for carbon nanotubes. It was found that a large amount of work has been done using PI-Index as compared to W- and Sz-index. In recent years, several papers on methods for computing these indices of molecular graphs have been published.

## REFERENCES


1) Ashrafi, A.R., Computing the PI Index of Some Chemical Graphs Related to Nanostructures, The Third Conference of the Asian Consortium for Computational Materials Science, ACCMS-3, Institute of Physics, Chinese Academy of Science, 2005.
2) Ashrafi, A.R.; Loghman, A., PI Index of Zig-Zag Polyhex Nanotubes, MATCH Commun. Math. Comput. Chem., 2006, 55, 447-452.
3) Ashrafi, A.R.; Loghman, A., PI Index of TUC4C8 Carbon Nanotubes, J. of Theo. And Comp. Nanoscience, 2006, 3(3), 378-381.
4) Ashrafi, A.R.; Loghman, A., PI Index of Armchair Polyhex Nanotubes, Ars Combinatoria, 2006, 80, 193-199.
5) Balaban, A.T. Highly discriminating distance-based Ttopological index, Chem. Phys. Lett., 1982, 89, 399-404.
6) Deng, H.; IIou, J., PI Indices of Nanotubes SC4C8 [q, 2p], MATCH Communication Math. Comput. Chem., 2006, 57.
7) Deng, H., The PI Index of TUV C6 [2p; q], MATCH Commun. Math. Comput. Chem., 2006, 55, 461-476.
8) Diudea, M.V.; John, P.E., Wiener Index of Zig-Zag Polyhex Nanotubes, Croat. Chem. Acta 2004, 77, 127-132.
9) Diudea, M.V.; Stefu, M.; Prav, B.; John, P.E., Wiener Index of Armchair Polyhex Nanotubes, Croat. Chem. Acta 2004, 77, 111-115.
10) Eliasi M.; Taeri B. Szeged index of armchair polyhex nanotubes, Communications in Mathematical and in Computer Chemistry, 2008, 59, 437 – 450.
11) Gutman, I. Formula for the Wiener Number of Trees and Its Extension to Graphs Containing Cycles, Graph Theory Notes New York, 1994, 27, 9-15.

12) Gutman, I., Dobrynin, A. On a Graph invariant related to the sum of all distances in a graph, Publ. Inst. Math., 1994, 56, 18-22.
13) Iranmanesh, A.; Alizadeh, Y., Computing the Szeged and PI Indices of VC5C7 [p, q] and HC5C7 [p, q] Nanotubes, Int. J. Mol. Sci., 2008, 9, 141-144.
14) Khadikar, P.V.; Deshpande, N.V.; Kale, P.P.; Dobrynin, A.; Gutman, I.; Domotor, G., The Szeged Index and an Analogy with the Wiener Index, J. Chem. Inf. Comput Sci., 1995, 35, 547-550.
15) Khadikar, P.V.; Kale, P.P.; Deshpande, N.V.; Karmarkar, S.; Agrawal V.K., Szeged Indices of Hexagonal Chains, Commun. Math. Comput. Chem. (MATCH), 2001, 43, 7-15.
16) Khadikar, P.V., On a Novel Structural Descriptor PI, Nat. Acad. Sci. Lett. 2000, 23, 113-118.
17) Khadikar, P.V.; Karmarkar, S.; Agrawal, V.K. A Novel PI Index And Its Applications to QSPR / QSAR Studies, J.Chem. Inf. Comput. Sci. 2001, 41.
18) Khadikar, P.V.; Kale, P.P.; Deshpande, N.V.; Karmarkar, S.; Agrawal, V.K., Novel PI Indices of Hexagonal Chains, J. Math. Chem., 2001, 29, 143-150.
19) Khadikar, P.V.; Diudea, M.V.; Singh. John, P.E.; Shrivastava, A.; Singh, S.; Karmakar, S.; Lakhwani, M.; Thakur, P. Use of PI Index In Computer-Aided Designing Of Bioactive Compounds, Curr. Bioact. Comp. 2006, 2, 19-56.
20) Klavzar, S., Rajapakst, A., Gutman, I. The Szeged and Weiner Index of Graphs, Appl. Math. Lett., 1996, 9, 45-59.
21) Lijima, S., Helical Micromolecules of Graphitic Carbon, Nature, 1991, 354, 56- 58.
22) Minailinc, G.M., Katona, G., Diudea, M. V., Strunje, M., Graovac, A., Gutman, I. Szeged Fragmental Indices, Croat. Chem. Acta., 1998, 71, 473-488.
23) Simic, S., Gutman, I., Baltic, V. Some graphs with extremel Szeged Index, Maths Slovaka, 2000, 50, 1-15.
24) Sousararaei, A., Mahmiani, A., Khormali, O. Vertex PI Index of some Nanotubes, Iranian J. of Mathematical Sc. And Informatics, 2008, 3(1), 49-62.
25) Wiener, H., Structural Determination of Paraffin Boiling Points, J. Amer. Chem. Soc. 1947, 69, 17-20.
26) Yousefi-Azari, H. ; Bahrami, A.; Ashrafi, A.R., Computing PI Index of HAC5C6C7 Nanotubes and Nanotori, J. Comput. Theoret. Nanosci. (In Press).