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PADMAKAR- IVAN INDEX OF Y-JUNCTION NANOTUBES

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The Padmakar-Ivan (PI) index of a graph G is defined as $PI(G) = \sum[n_{e_u}(e|G) + n_{e_v}(e|G)]$, where for edge e=(u,v) are $n_{e_u}(e|G)$ is the number of edges of G lying closer to u than v, $n_{e_v}(e|G)]$ is the number of edges of G lying closer to v than u and summation goes over all edges of G. In this paper we describe a method of computing PI index of some types of Y-Junction carbon nanotubes using orthogonal cuts.

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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 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, refered to as the Szeged index, Sz is putforward by Gutman [10-12]. 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, P.V.Khadikar introduced yet another index called Padmakar-Ivan (PI) index [13,14]. The PI index of a graph G is defined as:

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

where for edge e = (u,v) neu (e|G) is the number of edges of G lying closer to u than v, nev (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 consider for the calculation of PI index.

In series of papers,the authors [15- 18] investigated the structure and topological indices of some nanotubes and nanotori.In this paper we compute the PI index of , symmetric Y-Junctin carbon nanotubes, see Figure 1. Throughout this paper, our notation is standard. They are appearing as in the same way as in [19].

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2. Main results and discussion

A Y-junction is named symmetric if the three carbon nanotubes joining each other in the Y have identical chirality and the distribution of the n-H rings around the Y is symmetric. Such a junction will be constituted from identical branches oriented at 120°, like in Fig.1.

In this section the PI index of Structural models of symmetric Y-junctions carbon nanotube (fig.1) is determined. For this computation, Suppose that G=YJSN[r,r,t] is the molecular graph of symmetric Y-Junctions carbon nanotubes (fig.1).

In the following theorem we compute the Padmakar-Ivan index of G, Fig. 1.

Theorem1.

$$\mathrm{PI(G)} = 2\times t\times r\times(r^5\times t^2+2\times t\times r^5+t\times r^3+r^5+r^3+r^2\times t^5+2\times r^3\times t^3+r\times t^3+t\times r^4+t\times r^2+$$

$$128\times p\times t^2\times r^4+64\times t\times r^2\times p^3+16\times p\times t\times r^2+8\times p^5+4\times p^3),\ \text{where}\ \mathrm{p}=\min\{\mathrm{r}^2\times\mathrm{t},\mathrm{r}\times\mathrm{t}^2\}.$$

Proof . To compute the PI Index of G, it is enough to calculate $A=[n_{eu}(e|G)+n_{ev}(e|G)]$for every edges e=uv of G=YJN[r,r,t].To do this, we consider three cases where e=uv is vertical, horizontal or oblique. If e is horizontal or vertical, a similar proof as in [15] shows that $A = 4r^2t$, $4rt^2$, respectively. And similarly if e is one oblique edge then A=8rtp; where $p=\min\{r^2t,rt^2\}$.Thus we have:

$$PI(G)=\sum_{e\ is\ Horizontal}[n_{e_u}(e|G)+n_{e_v}(e|G)]+\sum_{e\ is\ vertical}[n_{e_u}(e|G)+n_{e_v}(e|G)]+\sum_{e\ is\ oblique}[n_{e_u}(e|G)+n_{e_v}(e|G)]$$

$$\alpha=2\times t^3\times r^6+4\times t^2\times r^6+2\times t^2\times r^4+2\times t\times r^6+2\times t\times r^4$$

$$\beta=2\times r^3\times t^6+4\times r^4\times t^4+2\times r^2\times t^4+2\times r^5\times t^2+2\times r^3\times t^2$$

$$\chi=4\times r\times t\times p\times(8\times t\times r^2+2\times p^2+1)^2-4\times r\times t\times p\times(8\times t\times r^2+2\times p^2+1)$$

$$PI(G)=\alpha+\beta+\chi\ .$$

Thus:

$$\mathrm{PI(G)} = 2\times t\times r\times(r^5\times t^2+2\times t\times r^5+t\times r^3+r^5+r^3+r^2\times t^5+2\times r^3\times t^3+r\times t^3+t\times r^4+t\times r^2+$$

$$128\times p\times t^2\times r^4+64\times t\times r^2\times p^3+16\times p\times t\times r^2+8\times p^5+4\times p^3),\ \text{where}\ \mathrm{p}=\min\{\mathrm{r}^2\times\mathrm{t},\mathrm{r}\times\mathrm{t}^2\}.$$

, which completed the proof. ▲

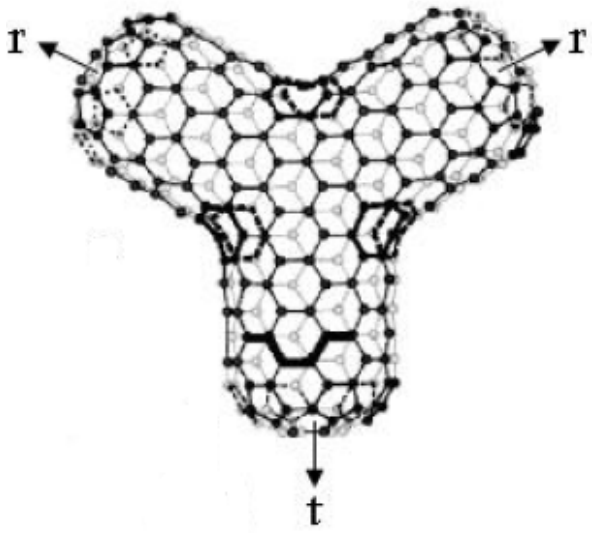

Fig.1 . Structural models of Symetric Y-junctions carbon nanotubes.

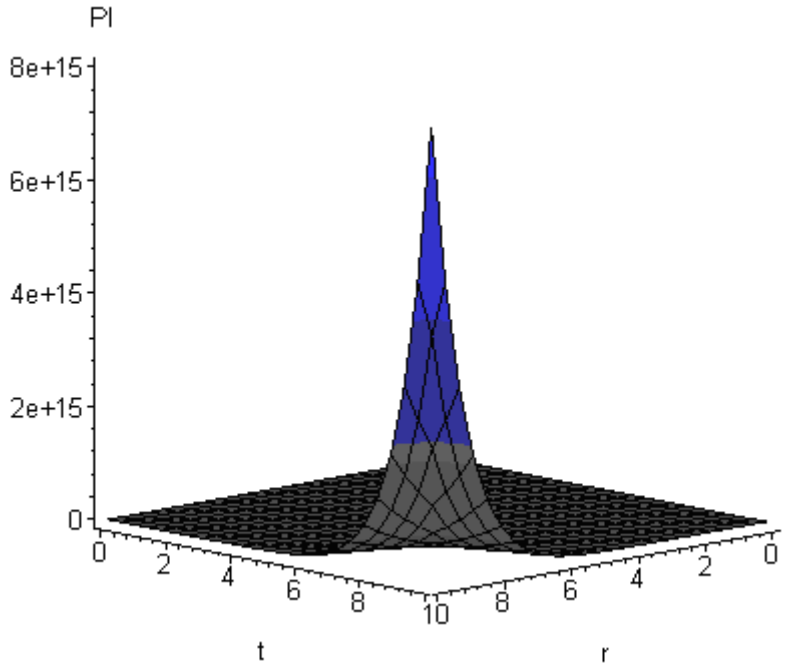

Fig. 2 . Graph of PI(YJN[r,r,t]).

3. Conclusions

Y- junction nanotubes can be formed from chemical vapor deposition, welding two crossed nanotubes with an electron beam at high temperature, or using irradiation techniques on touching tubes to form a Y- tube. In this paper, the Padmakar-Ivan (PI) index of structural models of carbon nanotube Y-junctions are determined.

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