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HYPER-WIENER INDEX OF SYMMETRIC Y-JUNCTION NANOTUBES

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Let G be a molecular graph. The distance $d(u,v)$ between the vertices u and v of the graph G is equal to the length of a shortest path that connects u and v. The Wiener index $W(G)$ is the sum of all distances between vertices of G, whereas the hyper-Wiener index $WW(G)$ is defined as WW(G)=1/2W(G)+$\sum_{\{u,v\}\subseteq V(G)} d^2\ (u,v)$. In this paper, Hyper-Wiener index of carbon nanotube Y-junctions is determined.

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1. Introduction

Throughout this paper we consider graphs means simple connected graphs, without loops and multiple edges. Suppose G is a graph with vertex set $V(G)$. The distance between the vertices u and v of $V(G)$ is denoted by $d(u,v)$ and it is defined as the number of edges in a minimal path connecting the vertices u and v. The Wiener index is one of the most studied topological indices, both from a theoretical point of view and applications. It is equal to the sum of distances between all pairs of vertices of the respective graph; see for details [1-5].

The hyper-Wiener index of acyclic graphs was introduced in 1993 [6], generalized Randic's definition for all connected graphs, as a generalization of the Wiener index. It is defined as :

$$WW(G) = \frac{1}{2}W(G) + \sum_{\{u,v\}\subseteq V(G)} d^2\ (u,v)$$

where $d^2(u,v)=d(u,v)^2$. We encourage the reader to consult [7-17] for the properties of hyper-Wiener index and its applications in chemistry. In Refs[18-21] the authors compute some topological indices of nanotubes.In this paper, we continue this program to compute the Hyper-Wiener index of symmetric Y-junctions carbon nanotube (Fig.1). Throughout this paper, all graphs considered are finite and simple. Our notation is standard and taken mainly from [22].

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2. Main Results and discussion

Nanoscale junctions create the intriguing possibility of forming active device elements whose characteristic length scale is determined solely by the intrinsic size of the junction region.A promising type of nanoscale junction which has been attracting increasing interest is the Y-branch or Y-junction structure, consisting of three intersecting low-dimensional electronic transport paths. In this section the Hyper-Wiener index of Structural models of symmetric Y-junctions carbon nanotube (fig.1) is determined.

For this computation, Suppose that G=YJN[r,r,t] be the molecular graph of symmetric Y-Junctions carbon nanotube (fig.1).

In the next theorem Hyper Wiener index of G=YJN[r,r,t] is computed.

Theorem . Suppose that G=YJN[r,r,t].Thus

$$WW(G) = \begin{cases} 1/48(r^4t^2 + 2r^3t^3 + 2r^2t^4 + 4r^2t^3 - 2r^2t^2 - 2r^3t - 4r^2t + 2t^2) & ; if \ r \equiv 0 \ (\mathrm{mod}\ 2) \\ 1/96(2r^4t^2 + 3r^3t^3 + 6r^3t^2 + 8r^2t^2 + 6r^2t^3 + 2r^2t^4) & ; if \ r \equiv 1 \ (\mathrm{mod}\ 2) \end{cases}$$

Proof . The molecular graph of Y-Junction nanotube G can be separated to G_1 ,G_2, G_3 ,such that G_1 ,G_2, G_3 are three intersecting paths of G. But we know that for molecular graphs $G_1, G_2, \ldots, G_n$ *with* $V_i = V(G_i)$, $1 \le i \le n$:

$$WW(G) = |V|^2 \left(\sum_{i=1}^{n} \frac{WW(G_i)}{|V_i|^2} + \left(\sum_{i=1}^{n} \frac{W(G_i)}{|V_i|^2}\right)^2 - \sum_{i=1}^{n} \frac{W^2(G_i)}{|V_i|^4}\right).$$

In particular, $WW(G^n)=n|V(G)|^{2n-4}(|V(G)|^2 WW(G)+(n-1)W^2(G))$.

By this formula and definition of Wiener index the proof is completed.

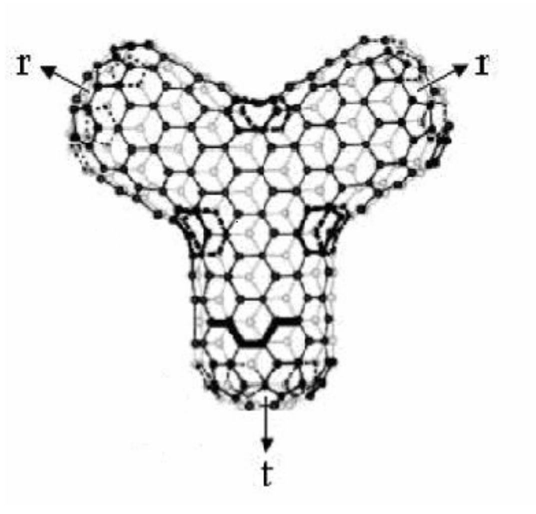

Fig. 1. Structural models of Symetric Y-junctions carbon nanotubes.

3. Conclusion

This paper belongs to our continuous efforts to construct graph invariants of chemical interest and to use them in the structure-property-activity modeling. In the present article, by simulation, one topological index (Hyper-Wiener) for symmetric Y-Junction nanotubes is computed.

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