Computation of the Wiener index of a new class of carbon nanojunctions

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Let G be a molecular graph. The Wiener index of G is defined as the sum of the shortest paths between vertices of G. In this paper exact formulae for the Wiener index of ($Le_{2,2}$(Op($Q_{2.0}$(T))) –TU(6,6) is given .

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1. Introduction

A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted. By IUPAC terminology, a topological index is a numerical value associated with a chemical constitution purporting for correlation of chemical structure with various physical properties, chemical reactivity or biological activity [1-3]. This concept was first proposed by Hosoya [4] for characterizing the topological nature of a graph. Such graph invariants are usually related to the distance function d(-,-). To explain, assume that G is a molecular graph with vertex set V(G) and edge set E(G). The mapping d(-,-): $V(G) \times V(G) \rightarrow V(G)$ in which d(x,y) is the length of a minimum path connecting x and y, will be called "*distance function*" on G. Recently, this part of Mathematical Chemistry was named "Metric Graph Theory". The first topological index of this type was proposed in 1947 by the chemist Harold Wiener [5]. It is defined as the sum of all distances between vertices of the graph under consideration. Suppose G is a graph with the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. The distance matrix of G is defined as D(G) = [dij], where dij = d(vi,vj). It is easy to see that the Wiener index of G is the half sum of entries of this matrix.

Recently many researchers were interested in the problem of computing topological indices of nanostructures. There are more than 200 published papers after 2000, but a few of them devoted to the Wiener index. On the other hand, there are not many methods to compute the Wiener index of molecular graphs and most of them are related to bipartite or planar graphs. Since the molecular graphs of nanostructures are usually non-planar and most of them are not bipartite, every author applied a method designed for his/her problem.

In some research papers [6-11] one of present authors (MVD) applied some computer programs to compute the Wiener index of nanotubes and nanotori. In this method, we must decompose the problem in some cases and then prove that the Wiener index in each case is a polynomial of a given order. Finally, we compute the Wiener index in some case and find the coefficients of our polynomials. There is also a numerical method given in [12] for estimating the Wiener index.

In some papers [13-19], the authors presented a matrix method for computing Wiener index of nanotubes and nanotori. This method is appropriate for high symmetry objects and it is not general. The most general methods for computing Wiener index of nanostructures are those given in [20-25]. These methods are useful for graphs constructible by a few numbers of subgraphs. The aim of this paper is to apply the new method on the carbon nanojunction ($Le_{2,2}$(Op($Q_{2.0}$(T))) –TU(6,6) and to compute its Wiener index.

2. Main results and discussion

Throughout this paper G[n] denotes the molecular graph of carbon nano-junction that show by ($Le_{2,2}$(Op($Q_{2.0}$(T)))–TU(6,6), Fig. 1. At first, we introduce two notions. Suppose G and H are graphs such that $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. Then we call H to be a subgraph of G. H is called isometric if for each vertex x, y $\in V(H), d_H(x,y)=d_G(x,y)$. In Figs. 2-5, four isometric subgraphs of G[n] are depicted. Define n to be the number of rows in each arm tube (Fig. 1, n=3). Then by a simple calculation, one can show that $|V(G)| = 144n + 120$.

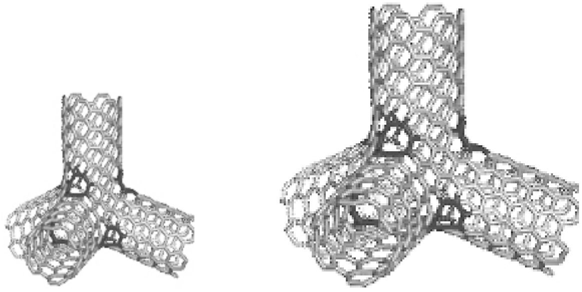

Fig. 1. The Molecular Graph of $Le_{2,2}$(Op($Q_{2.0}$(T))) –TU(6,6).

To compute the Wiener index of $(Le_{2,2}(Op(Q_{2.0}(T))) - TU(6,6)$, we first calculate the Wiener matrices of these subgraphs. Suppose $S_1,..,S_4$ are defined as follows:

- S_1 is the summation of distances between the vertices of core, Fig. 2.
- S_2 is the summation of distances between vertices of a tube and the vertices of the core, Fig. 3.
- S_3 is the summation of distances between two vertices of a tube, Fig. 4.
- S_4 is the summation of distances between vertices of two different tubes, Fig. 5.

We notice that the core has exactly 120 vertices and so its distance matrix is 120 × 120. By using HyperChem [26] and TopoCluj [27], one can see that S_1 =63192. We consider the isometric subgraphs K, L and M depicted in Figs. 3 to 5. To compute S_2, we consider the Fig. 3. Suppose C denotes the subgraph core and D_i, $1 \le i \le n$, are the set of vertices in the i^{th} row of a tube in G[n]. By TopoCluj, we calculate that the summation of distances between vertices of the core and the set D_1 is 43776. In what follows, we obtain a recursive formula for computing S_2.

Fig. 2. The Core.

- The summation of distances between vertices of the core and the set D_1 is 43776,
- The summation of distances between vertices of the core and the set $D_1 U D_2$ is 43776+ 54768,
- The summation of distances between vertices of the core and the set D_1 U D_2U D_3 is 43776+ 54768+67680,
- The summation of distances between vertices of the core and the set D_1 U D_2U D_3U D_4 is 43776+ 54768+67680+12960

Therefore**,**

$$S_2 = 98544 + \sum_{i=0}^{n-3}(67680 + i.12960) = -23856 + 61200n + 6480(n-2)^2$$

Table 1. The Number of R_iR_j in Computing S_3.

Row	The number of R_iR_j	Wiener index
1	R_1R_1	3936
2	$2R_1R_1+R_1R_2$	2.3936 +8832
3	$3R_1R_1+2R_1R_2+R_1R_3$	3.3936+2.8832+11712
⋮	⋮	⋮
n	n R_1R_1+(n-1) R_1R_2+…+ R_1R_n	n.3936+(n-1).8832+(n-2).11712+…

Notice that for computing the Wiener index, we should compute $4S_2$.

We now calculate the quantity S_3.To do this , we assume that R_iR_j denote the summation of distances between vertices of D_i and D_j in subgraph L, Fig. 4. For computing S_3 it is enough to compute R_iR_j, for $1 \le i,j \le n$. In Table 1, the occurrence of R_iR_j in S_3 is computed.

From Table 1, one can compute S_3 as follows:

$$S_3 = n.3936 + (n-1).8832 + (n-2).11712 + (n-3).15552 + (n-4)19440 + \sum_{i=1}^{n-5}(19440 + i.3888) = 1944(n-4)^2 + 76968n - 246096$$

Fig. 3. The Subgraph K.

Notice that in computing the Wiener index of G[n], we should consider $4S_3$, Fig. 1. To compute S4, we assume that Di and Ei, $1 \le i \le n$, denote the set of vertices in the i^{th} row of two different arm tubes in G[n]. Using a similar argument as above, we assume that RiSj denote the summation of distances between vertices of D_i and E_j, $1 \le i,j \le n$. For computing S_4 it is enough to compute the wiener matrix for RiRj, for $1 \le i,j \le n$ and RiRi, for i=j. In Table 2 the occurrence of R_iR_j in S_4 is computed.

Table 2. The wiener index of R_iR_j i=j in Computing S_4.

# Rows	The Number of R_iR_j
R_1R_1	350576
R_2R_2	749696
R_3R_3	1389872
R_4R_4	2333312
R_5R_5	3642224
:	:
R_nR_n	749696+(n-2)(399120+241056)+∑∑241056+i.(62208)

Therefore $\sum R_iR_i$ is equal

$$\sum_{i=1}^{n-5} R_i R_j = 749696 + (n-2)(399120 + 241056) + \sum_{j=1}^{n-3}\sum_{i=1}^{j} 241056 + i.(62208) = 10368(n-2)^3 + 120528(n-2)^2 + 509280n - 268864$$

So S_4=$\sum R_iR_i$ - 63192- $4S_2$-$2S_3$. By attention to figure of graph we should compute $6S_4$ for wiener index. We are now ready to state our main result.

$\sum_{i=1}^{n-5} R_i R_j = 74969$ $\sum_{i=1}^{j} 241056 + i.(62208)$ $= 10368(n-2)^3 + 1$

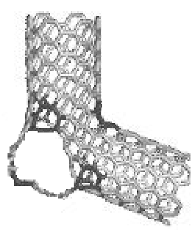

Fig. 4. The Subgraph M.

Theorem. The Wiener index of the molecular graph of nanojunction G[n] is computed as follows:

$$Win(G) = 1011144 + (n-2).(657072 + 526176) + \sum_{j=1}^{n-3}\sum_{i=1}^{j}[526176 + i.(155520) = 67656 + 152928n + 107568n^2 + 25920n$$

Proof. By above calculations

$$W(G[n]) = S_1 + 4S_2 + 4S_3 + 6S_4 = 63192 + 4[-23856 + 61200n + 6480(n-2)^2] + 4[1944(n-4)^2 + 76968n - 246096] + 6[10368(n-2)^3 + 120528(n-2)^2 + 509280n - 268864]$$

Thus, a simple calculation will prove the result.

3. Conclusion

In this paper the Wiener index of a new class of carbon nanojunction is computed. To the best of our knowledge it is the first paper considering the Wiener index of such nanostructures into account. A powerful method for this calculation is presented which is extendable to other nanojunctions.

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