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DISTANCE MATRIX AND WIENER INDEX OF ARMCHAIR POLYHEX NANOTUBES

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ABSTRACT. The Wiener index of a molecular graph G is defined as the sum of all distances between distinct vertices of G, where the distance between two atoms is the minimum number of bonds connecting them in G. In this paper an algorithm for computing distance matrix of an armchair polyhex nanotube is introduced. As a consequence, the Wiener index of this type of nanotubes is computed.

Keywords: *Armchair polyhex nanotube, distance matrix, Wiener index.*

INTRODUCTION

A large number of chemical and physical properties of various small molecules are closely related to the topological nature of their skeletal structure. Thus, some quantitative measures reflecting the essential features of a given topological structure have been introduced for the prediction of their properties. Such measures are called topological indices [1,2]. Topological indices are graph invariants and are used for Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies. The QSAR and QSPR studies are the active areas of chemical research that focus structure-dependent chemical behavior of molecules, [3].

Among topological indices, the Wiener index [4] is probably the most important one. This index was introduced by the chemist H. Wiener to demonstrate correlations between physicochemical properties of organic compounds and the topological structure of their molecular graphs. He defined his index as the sum of distances between any two carbon atoms in the molecules, in terms of carbon-carbon bonds. Next Hosoya named such a graph invariant, topological index, [5]. We encourage the reader to consult papers [6,7] and references therein, for further study on the topic.

The problem of computing topological indices of nanostructures raised by Diudea and his co-authors, [8-14]. The presented authors computed the distance matrix of a polyhex and TUC_4C_8(R/S) nanotori as well as zig-zag

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polyhex nanotube, [15-19]. In this paper we continue this program to find an algorithm for computing distance matrix of an armchair polyhex nanotube, Figure 1. As an immediate consequence, the Wiener index of this type of nanotubes is computed.

Throughout this paper our notation is standard and taken mainly from [20].

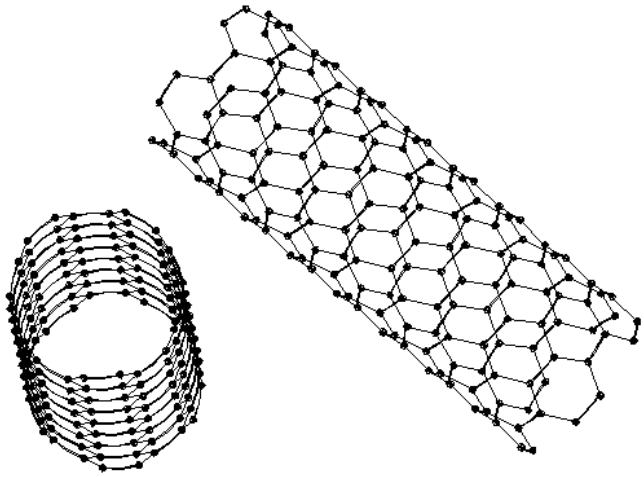

Figure 1. An Armchair Polyhex Nanotube.

RESULTS AND DISCUSSION

Carbon nanotubes form an interesting class of carbon nanomaterials. These can be imagined as rolled sheets of graphite about different axes. There are three types of nanotubes: armchair, chiral and zigzag structures. Further nanotubes can be categorized as single-walled and multi-walled nanotubes and it is very difficult to produce the former.

Diudea, Stefu, Pârv and John [9] computed the Wiener index of an armchair polyhex nanotube $T = TUVC_6[n,m]$, for the first times. Here n is twice the number of vertical crenels and m is the number of rows, see Figure 2. It is obvious that n is even and $|V(T)| = mn$. In this section, distance matrices of these nanotubes are computed.

We first choose a base vertex b from the 2–dimensional lattice of $T = TUVC_6[m,n]$, Figure 2 and assume that $x_{i,j}^{(1,1)}$ is distance between (1,1) and (i,j). This defines a matrix

$$X_{m\times n}^{(1,1)} = [x_{i,j}^{(1,1)}], \text{where } x_{1,1}^{(1,1)} = 0, \quad x_{1,2}^{(1,1)} = x_{2,1}^{(1,1)} = 1. \tag{1}$$

It is clear that by choosing different base vertices, we find different distance matrices of T. Suppose $s_k^{(p,q)}$ is the sum of k^{th} row of $X_{m\times n}^{(p,q)}$, where (p,q) is the base vertex. Then $s_k^{(p,1)} = s_k^{(p,q)}$, $1 \le k \le m$, $1 \le p \le m$ and $1 \le q \le n$. On the other hand, by Eq. (1) and choosing a fixed column, we have:

$$s_k^{(i,j)} = \begin{cases} s_{i-k+1}^{(1,1)} & 1 \le k \le i \le m,\ 1 \le j \le n \\ s_{k-i+1}^{(1,1)} & 1 \le i \le k \le m,\ 1 \le j \le n \end{cases}. \qquad (2)$$

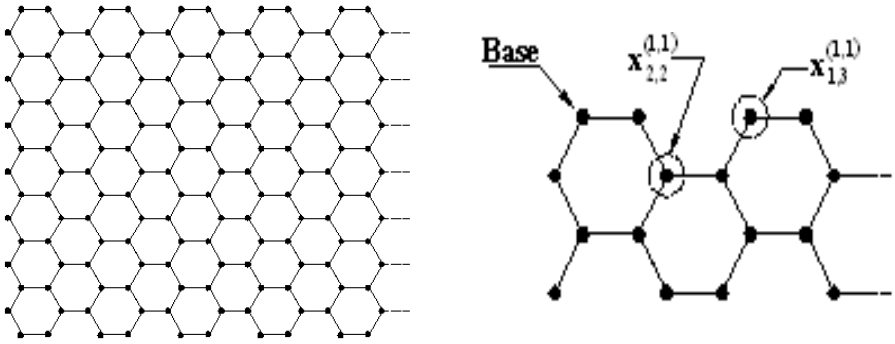

Figure 2. The 2–Dimensional Fragments of an Armchair Polyhex Nanotube.

We now define two matrices $A_{(n/2+1)\times n}$ and $B_{(n/2+1)\times n}$ by the following equations:

$$a_{1,j} = \begin{cases} a_{1,j-1}+1 & j \le (n/2)+1 \\ a_{1,j-1}-1 & j > (n/2)+1 \end{cases}; \quad a_{2,j} = \begin{cases} a_{1,j}+1 & j \le (n/2)+1 \\ a_{1,j}-1 & j > (n/2)+1 \end{cases} \quad 2 \mid j,$$

$$a_{2,j} = \begin{cases} a_{2,j-1}+1 & j \le (n/2)+1 \\ a_{2,j-1}-1 & j > (n/2)+1 \end{cases}; \quad a_{1,j} = \begin{cases} a_{2,j}+1 & j \le (n/2)+1 \\ a_{2,j}-1 & j > (n/2)+1 \end{cases} \quad 2 \nmid j,$$

$$a_{i,j} = \begin{cases} a_{1,j} & 2 \nmid i \\ a_{2,j} & 2 \mid i \end{cases};\ a_{1,1} = 0;\ a_{2,1} = 1, \qquad (3)$$

$$b_{n/2+1,j} = \begin{cases} n/2+j-1 & j \le n/2+1 \\ 3n/2-j+1 & j > n/2+1 \end{cases};\ b_{i,j} = b_{i+1,j}-1, i < n/2+1.$$

By Eqs. 1-3, one can prove:

$$x_{i,j}^{(1,1)} = \begin{cases} c_{i,j} & i \le (n/2)+1 \\ x_{i-1,j}^{(1,1)} + 1 & i > (n/2)+1 \end{cases},\ c_{i,j} = \mathrm{Max}\{a_{i,j},\ b_{i,j}\}. \qquad (4)$$

We now apply Eqs. 2-4 to compute the distance matrix $X_{m\times n}^{(p,q)}$ related to vertex (p,q) is computed. Suppose $s_i^{(p,q)}$ is the sum of i^{th} row of $X_{m\times n}^{(p,q)}$. Then, we have:

$$s_i^{(1,q)} = \begin{cases} (n^2/2)+i^2-2i+(1/2)\left(1-(-1)^{(n/2-1)}\right) & i \le n/2+1 \\ (n^2/4)+n(i-1) & i > n/2+1 \end{cases}, 1 \le i \le m; 1 \le q \le n. \quad (5)$$

Suppose S_p is the sum of all entries of distance matrix $X_{m\times n}^{(p,q)}$. Then

$S_1 = \sum_{i=1}^{m} s_i^{(1,q)}$ and $S_p = S_1 + \sum_{i=2}^{p} s_i^{(1,q)} - \sum_{i=m-p+2}^{m} s_i^{(1,q)}$. Thus

$$S_1 = \begin{cases} (m/6)\left(3n^2+2m^2-3m-2\right)+\left[(-1)^{(n/2)}/4\right]\left[1-(-1)^m\right] & m \le n/2+1 \\ (n/24)\left(n^2+12m^2+6mn+3n-12m-4\right)+(1/4)\left[(-1)^{(n/2)}-1\right] & m > n/2+1 \end{cases}. \quad (6)$$

If $m \le n/2+1$ then a direct calculation shows that

$$S_p = (m/6)\left(3n^2+2m^2+3m-2\right)-mp(m-p+1)-(1/4)\left[(-1)^{(n/2+p)}\right]\left[1-(-1)^m\right]. \qquad (7)$$

Hence it is enough to consider case that m > n/2 + 1. To complete this case, we consider three sub cases as follows:

I) $p \le n/2+1$, $p \le m-n/2+1$. In this case, we have:

$$S_p = (n/24)\left(n^2+12m^2+6mn-3n+12m-4\right)+(p^2/2)(n-1)+(p/12)\left(3n^2-6n-12mn-4\right)$$
$$+(p^3/3)+(1/4)\left[1-(-1)^{(n/2+p)}\right].$$

II) $m-n/2+1 < p \le n/2+1$. In this case, we have: (8)

$$S_p = (m/6)\left(3n^2+2m^2+3m-2\right)-mp(m+1)+mp^2-(1/4)\left[(-1)^{(n/2+p)}\right]\left[1-(-1)^m\right].$$

III) $p > n/2+1$. In this case, $S_p = (n^3/12)-(n/3)+(mn/4)(n+2m+2)-np(m+1)+np^2$.

We now apply Eqs. 5-8 to compute Wiener index of this nanotube. Therefore,

$$W_{m\times n} = \begin{cases} n\left(\sum_{i=1}^{(m-1)/2} S_i + (1/2)S_{(m+1)/2}\right) & 2 \mid m \\ n\sum_{i=1}^{m/2} S_i & 2 \nmid m \end{cases}$$

$$= \begin{cases} (m^2 n/12)\left(3n^2+m^2-4\right)+(n/8)(-1)^{(n/2)}\left[1-(-1)^m\right] & m \le n/2+1 \\ (mn^2/24)\left(n^2+4m^2+3mn-8\right)-(n^3/192)\left(n^2-16\right)+(n/8)\left[(-1)^{(n/2)}-1\right] & m > n/2+1 \end{cases}$$

This completes our arguments.

CONCLUSIONS

Our method for computing distance matrix of armchair polyhex nanotube is general and can be extended to every regular or near to regular graph. Here, a near to regular graph is a graph with exactly two distinct numbers as the degree of vertices. In such graphs, it is possible to consider a base vertex and then compute the distance matrix as a function of base matrix.

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