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An algorithm for computing Hosoya polynomial of $TUC_4C_8(R)$ nanotubes

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The Hosoya polynomial of a molecular graph G is defined as $H(G,x)=\sum_{\{u,v\}\subseteq V(G)} x^{d(u,v)}$, where the sum is over all unordered pairs {u,v} of distinct vertices in G. Xu and Zhang in some research papers computed this polynomial for polyhex and $TUC_4C_8(S)$ nanotubes. In this paper, we continue this program and present an algorithm for computing the Hosoya polynomial of $TUC_4C_8(R)$ nanotubes.

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1. Introduction

A topological index is a real number that is derived from molecular graphs of chemical compounds. Such numbers based on the distances in a graph are widely used for establishing relationships between the structure of molecules and their physico-chemical properties. It is easy to see that the number of atoms and the number of bonds in a molecular graph are topological index. The first non trivial topological index was introduced early by Wiener [1]. He defined his index as the sum of distances between any two carbon atoms in the molecules, in terms of carbon-carbon bonds. We encourage the reader to consult papers [2,3]and references therein, for further study on the topic.

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge sets of which are represented by V(G) and E(G), respectively. If e is an edge of G, connecting the vertices u and v then we write e = uv. The distance between a pair of vertices u and w of G is denoted by d(u,w). Thus, we can redefine the Wiener index of a graph G as $W(G)=\sum_{\{x,y\}\subseteq V(G)} d(x,y)$.

The Hosoya polynomial of a molecular graph G is defined as $H(G,x)=\sum_{\{u,v\}\subseteq V(G)} x^{d(u,v)}$, where the sum is over all unordered pairs {u,v} of distinct vertices in G [4,5]. Suppose $D = [d_{ij}]$ denotes the distance matrix of G, where d_{ij} is the length of a minimal path connecting the ith and jth vertices of G. Then one can see that $W(G) = 1/2\sum_{i,j} d_{ij}$ and $H(G,x) = 1/2\sum_{i,j} x^{d_{ij}}$.

In recent years, some authors computed the Hosoya polynomial of some chemical graphs applicable in nano-science [6-10]. One of us (ARA) also computed the Wiener index of a polyhex and $TUC_4C_8(R/S)$ nanotori [11-15]. In this paper we continue this program to present a new algorithm for computing the Hosoya polynomial of $TUC_4C_8(R)$ nanotube. Our notation is standard and mainly taken from the book of Trinajestic [16].

2. Algorithm

In this section an exact formula for the Hosoya polynomial of $TUC_4C_8(R)$ nanotube is derived, Fig. 1. Since $d/dx(H(G,x))|_{x=1}=W(G)$, the Wiener index of this nanotube is also computed.

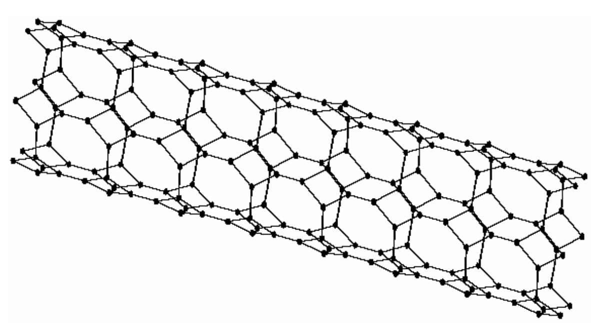

Fig. 1. 3D-Representation of a $TUC_4C_8(R)$ Nanotube.

Suppose T_1 is 2–dimensional lattice of $TUC_4C_8(R)[m,n]$, where m is the number of rows and n is the number of columns, Fig. 2. Choose four base vertices a(1,1), b(1,1), c(1,1) and d(1,1) from the molecular graph of T_1, Figs. 3 and 4.

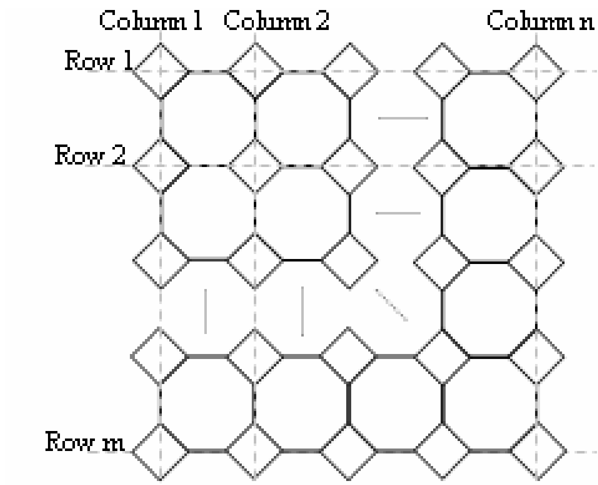

Fig. 2. The 2–dimensional fragments of a $TUC_4C_8(R)$ nanotube.

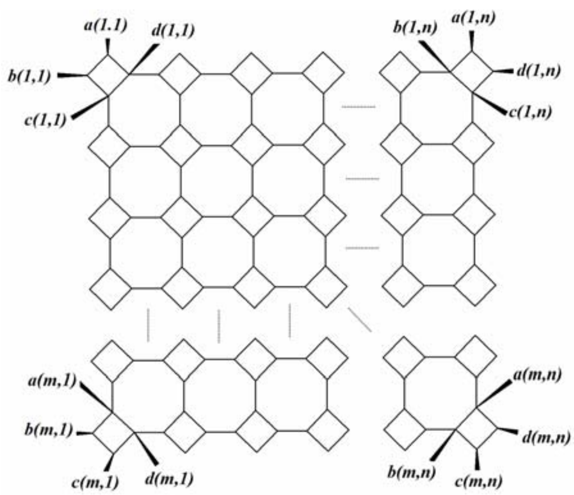

Fig. 3. A labeling of $TUC_4C_8(R)$.

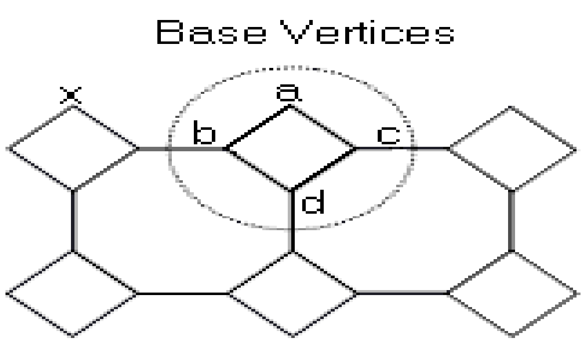

Fig. 4. The base vertices of $TUC_4C_8(R)$.

For computing $D(T_1)$, we first define the following 16 matrices:

$$\begin{array}{l} D_{a(1,1)}^{a(i,j)}, D_{a(1,1)}^{b(i,j)}, D_{a(1,1)}^{c(i,j)}, D_{a(1,1)}^{d(i,j)} \\ D_{b(1,1)}^{a(i,j)}, D_{b(1,1)}^{b(i,j)}, D_{b(1,1)}^{c(i,j)}, D_{b(1,1)}^{d(i,j)} \\ D_{c(1,1)}^{a(i,j)}, D_{c(1,1)}^{b(i,j)}, D_{c(1,1)}^{c(i,j)}, D_{c(1,1)}^{d(i,j)} \\ D_{d(1,1)}^{a(i,j)}, D_{d(1,1)}^{b(i,j)}, D_{d(1,1)}^{c(i,j)}, D_{d(1,1)}^{d(i,j)} \end{array}.$$

To define these matrices, we first partition the vertex set of T_1, into four sets A, B, C and D. A is the set of all vertices with the same position in the rhombs. For example from Fig. 4, one can see that $a, x \in A$. The sets B, C and D are defined similarly. Define $D_{a(1,1)}^{a(i,j)}$ as the distance matrix for the base vertex a(1,1) from other vertices of the set A. The entries of this matrix are distances between a(1,1) and $a(i,j) \in A$ of the graph T_1. We notice that by symmetry of T_1, it is enough to compute eight of these matrices. Remark that four matrices $D_{a(1,1)}^{a(i,j)}$, $D_{b(1,1)}^{b(i,j)}$, $D_{c(1,1)}^{c(i,j)}$ and $D_{d(1,1)}^{d(i,j)}$ are equal. Consider the permutation $\mu = \begin{pmatrix} 1 & 2 & 3 & \dots & n-1 & n \\ 1 & n & n-1 & \dots & 3 & 2 \end{pmatrix}$. It is easy to see that the matrices $D_{a(1,1)}^{b(i,j)}$ and $D_{c(1,1)}^{b(i,j)}$ are obtained from $D_{a(1,1)}^{d(i,j)}$ and $D_{c(1,1)}^{d(i,j)}$. By symmetry of Fig. 3, it is possible to compute the distance matrix evaluated at the base vertex d from the same matrix for the vertex b. On the other hand, the matrices $D_{b(1,1)}^{d(i,j)}$, $D_{d(1,1)}^{c(i,j)}$ and $D_{d(1,1)}^{a(i,j)}$ is computed from $D_{d(1,1)}^{b(i,j)}$, $D_{b(1,1)}^{c(i,j)}$ and $D_{b(1,1)}^{a(i,j)}$ by trace of μ.

In Table 1, some blocks of eight matrices are defined. To complete our definition, we assume that on for other entries of this matrix, we have.

- For other entries of the matrix $D_{a(1,1)}^{c(i,j)}$, $\beta_{ij} = \beta_{i(n-j+2)}$,
- For other entries of the matrix $D_{b(1,1)}^{a(i,j)}$, $\pi_{ij} = \pi_{i(n-j+1)} + 1$,
- For other entries of the matrix $D_{b(1,1)}^{c(i,j)}$, $\rho_{ij} = \rho_{i(n-j+2)} + 1$,
- For other entries of the matrix $D_{b(1,1)}^{a(i,j)}$, $\eta_{ij} = \eta_{i(n-j+1)} + 1$,
- For other entries of the matrix $D_{c(1,1)}^{d(i,j)}$, $\gamma_{ij} = \gamma_{i(n-j+2)} + 1$,
- For other entries of the matrix $D_{a(1,1)}^{a(i,j)}$, $\alpha_{ij} = \alpha_{i(n-j+2)}$,
- For other entries of the matrix $D_{c(1,1)}^{a(i,j)}$, $\delta_{11}=2$ and $\delta_{1j}=\delta_{2j}-1$ for $1<j\le n$. One the other hand, $\delta_{ij} = \delta_{i(n-j+1)}$, where $n/2+1< j \le n$ for $(n|2)$ or $(n+1)/2< j \le n$ $(n\nmid 2)$.

Table 1. Some distance matrices.

The Distance Matrix $D_{a(1,1)}^{a(i,j)}$ between the Base Vertex a(1,1) and Vertices of the Set A.				
For i = 1	j = 1	$2 \le j \le n/2+1$ $(n \mid 2)$ $2 \le j \le (n+1)/2$ $(n \exists 2)$	and for i>1	$1 \le j \le n/2+1$ $(n \mid 2)$ $1 \le j \le (n+1)/2$ $(n \exists 2)$
	$\alpha_{11} = 0$	$\alpha_{1j} = \alpha_{1(j-1)} + 3$		$i \le j$ $\alpha_{ij} = \alpha_{(i-1)j} + 1$ $i > j$ $\alpha_{ij} = \alpha_{(i-1)j} + 3$

The Distance Matrix $D_{a(1,1)}^{c(i,j)}$ between the Base Vertex a(1,1) and Vertices of the Set C.					
For i = 1	j = 1	j = 2	$3 \le j \le n/2+1$ $(n \mid 2)$ $3 \le j \le (n+1)/2$ $(n \exists 2)$	and for i>1	$1 \le j \le n/2+1$ $(n \mid 2)$ $1 \le j \le (n+1)/2$ $(n \exists 2)$
	$\beta_{11} = 2$	$\beta_{12} = 3$	$\beta_{1j} = \beta_{1(j-1)} + 3$		$i < j$ $\beta_{ij} = \beta_{(i-1)j} + 1$ $i \ge j$ $\beta_{ij} = \beta_{(i-1)j} + 3$

The Distance Matrix $D_{a(1,1)}^{d(i,j)}$ between the Base Vertex a(1,1) and Vertices of the Set D.				
For i = 1	j = 1	$2 \le j \le n/2$ $(n \mid 2)$ $2 \le j \le (n+1)/2$ $(n \exists 2)$	and for i>1	$1 \le j \le n/2$ $(n \mid 2)$ $1 \le j \le (n+1)/2$ $(n \exists 2)$
	$\eta_{11} = 1$	$\eta_{1j} = \eta_{1(j-1)} + 3$		$i \le j$ $\eta_{ij} = \eta_{(i-1)j} + 1$ $i > j$ $\eta_{ij} = \eta_{(i-1)j} + 3$

The Distance Matrix $D_{b(1,1)}^{a(i,j)}$ between the Base Vertex b(1,1) and Vertices of the Set A.				
For i = 1	j = 1	$2 \le j \le n/2$ $(n \mid 2)$ $2 \le j \le (n+1)/2$ $(n \exists 2)$	and for i>1	$1 \le j \le n/2$ $(n \mid 2)$ $1 \le j \le (n+1)/2$ $(n \exists 2)$
	$\pi_{11} = 1$	$\pi_{1j} = \pi_{1(j-1)} + 3$		$i+1 \le j$ $\pi_{ij} = \pi_{(i-1)j} + 1$ else $\pi_{ij} = \pi_{(i-1)j} + 3$

The Distance Matrix $D_{b(1,1)}^{c(i,j)}$ between the Base Vertex b(1,1) and Vertices of the Set C.				
For i = 1	j = 1	$2 \le j \le n/2$ $(n \mid 2)$ $2 \le j \le (n+1)/2$ $(n \exists 2)$	and for i>1	$1 \le j \le n/2$ $(n \mid 2)$ $1 \le j \le (n+1)/2$ $(n \exists 2)$
	$\rho_{11} = 1$	$\rho_{1j} = \rho_{1(j-1)} + 3$		$i \le j$ $\rho_{ij} = \rho_{(i-1)j} + 1$ $i > j$ $\rho_{ij} = \rho_{(i-1)j} + 3$

The Distance Matrix $D_{b(1,1)}^{d(i,j)}$ between the Base Vertex b(1,1) and Vertices of the Set D.				
For i = 1	j = 1	j = n	$2 \le j \le n/2$ $(n \mid 2)$ $2 \le j < (n+1)/2$ $(n \exists 2)$	$n/2 < j \le n-1$ $(n \mid 2)$ $(n+1)/2 \le j \le n-1$ $(n \exists 2)$
	$\tau_{11} = 2$	$\tau_{1n} = 1$	$\tau_{1j} = \tau_{1(j-1)} + 3$	$\tau_{1j} = \tau_{1(j+1)} + 3$
For i > 1	$1 \le j \le n/2$ $(n \mid 2)$ $1 \le j < (n+1)/2$ $(n \exists 2)$		$n/2 < j \le n$ $(n \mid 2)$ $(n+1)/2 \le j \le n$ $(n \exists 2)$	
	$i < j+1$ $\tau_{ij} = \tau_{(i-1)j} + 1$ $i > j$ $\tau_{ij} = \tau_{(i-1)j} + 3$		$i \ge n-j$ $\tau_{ij} = \tau_{(i-1)j} + 1$ otherwise $\tau_{ij} = \tau_{(i-1)j} + 3$	

The Distance Matrix $D_{c(1,1)}^{a(i,j)}$ between the Base Vertex c(1,1) and Vertices of the Set A.				
For i = 2	j = 1	$2 \le j \le n/2+1$ $(n \mid 2)$ $2 \le j \le (n+1)/2$ $(n \exists 2)$	and for i>2	$1 \le j \le n/2+1$ $(n \mid 2)$ $1 \le j \le (n+1)/2$ $(n \exists 2)$
	$\delta_{21} = 1$	$\delta_{2j} = \delta_{2(j-1)} + 3$		$i < j+1$ $\delta_{ij} = \delta_{(i-1)j} + 1$ else $\delta_{ij} = \delta_{(i-1)j} + 3$

The Distance Matrix $D_{c(1,1)}^{d(i,j)}$ between the Base Vertex c(1,1) and Vertices of the Set D.				
For i = 1	j = 1	$2 \le j \le n/2$ $(n \mid 2)$ $2 \le j \le (n+1)/2$ $(n \exists 2)$	and for i>1	$1 \le j \le n/2$ $(n \mid 2)$ $1 \le j \le (n+1)/2$ $(n \exists 2)$
	$\gamma_{11} = 1$	$\gamma_{1j} = \gamma_{1(j-1)} + 3$		$i < j+1$ $\gamma_{ij} = \gamma_{(i-1)j} + 1$ $i \ge j+1$ $\gamma_{ij} = \gamma_{(i-1)j} + 3$

In what follows, the row representations of these matrices are considered. Define:

$$D^{a(i,j)}_{a(1,1)} = \begin{bmatrix} A^a_1 \\ \vdots \\ A^a_m \end{bmatrix},\ D^{c(i,j)}_{a(1,1)} = \begin{bmatrix} A^c_1 \\ \vdots \\ A^c_m \end{bmatrix},\ D^{d(i,j)}_{a(1,1)} = \begin{bmatrix} A^d_1 \\ \vdots \\ A^d_m \end{bmatrix},\ D^{a(i,j)}_{b(1,1)} = \begin{bmatrix} B^a_1 \\ \vdots \\ B^a_m \end{bmatrix},$$

$$D^{c(i,j)}_{b(1,1)} = \begin{bmatrix} B^c_1 \\ \vdots \\ B^c_m \end{bmatrix},\ D^{d(i,j)}_{b(1,1)} = \begin{bmatrix} B^d_1 \\ \vdots \\ B^d_m \end{bmatrix},\ D^{a(i,j)}_{c(1,1)} = \begin{bmatrix} C^a_1 \\ \vdots \\ C^a_m \end{bmatrix},\ D^{d(i,j)}_{c(1,1)} = \begin{bmatrix} C^d_1 \\ \vdots \\ C^d_m \end{bmatrix}.$$

To compute the distance matrix of the molecular graph of this nanotube, we define also distance matrices for to the ij[th] rhomb of T_1, Fig. 4. For the rhombs of the first column, we define:

$$D^{a(i,j)}_{a(t,1)} = \begin{bmatrix} A^a_t \\ \vdots \\ A^a_2 \\ A^a_1 \\ \vdots \\ A^a_{m-t+1} \end{bmatrix}, D^{c(i,j)}_{a(t,1)} = \begin{bmatrix} C^a_t \\ \vdots \\ C^a_2 \\ A^c_1 \\ \vdots \\ A^c_{m-t+1} \end{bmatrix}, D^{d(i,j)}_{a(t,1)} = \begin{bmatrix} C^d_t \\ \vdots \\ C^d_2 \\ A^d_1 \\ \vdots \\ A^d_{m-t+1} \end{bmatrix}, D^{a(i,j)}_{b(t,1)} = \begin{bmatrix} B^c_t \\ \vdots \\ B^c_2 \\ B^a_1 \\ \vdots \\ B^a_{m-t+1} \end{bmatrix},$$

$$D^{c(i,j)}_{b(t,1)} = \begin{bmatrix} B^a_t \\ \vdots \\ B^a_2 \\ B^c_1 \\ \vdots \\ B^c_{m-t+1} \end{bmatrix}, D^{d(i,j)}_{b(t,1)} = \begin{bmatrix} B^d_t \\ \vdots \\ B^d_2 \\ B^d_1 \\ \vdots \\ B^d_{m-t+1} \end{bmatrix}, D^{a(i,j)}_{c(t,1)} = \begin{bmatrix} A^c_t \\ \vdots \\ A^c_2 \\ C^a_1 \\ \vdots \\ C^a_{m-t+1} \end{bmatrix}, D^{d(i,j)}_{c(t,1)} = \begin{bmatrix} A^d_t \\ \vdots \\ A^d_2 \\ C^d_1 \\ \vdots \\ C^d_{m-t+1} \end{bmatrix}$$

We claim that the distance matrices of other entries are computable from the matrices of the first column. For example, we assume that $D^{a(i,j)}_{a(t,1)} = [\,{}^1A^a \ \cdots \ {}^nA^a\,]$, where ${}^iA^a$ is the i[th] column of $D^{a(i,j)}_{a(t,1)}$. Then $D^{a(i,j)}_{a(t,s)} = [\,{}^{n-s+2}A^a \ \dots \ {}^nA^a \ \ {}^1A^a \ \cdots \ {}^{n-s+1}A^a\,]$. We now count the repeated entries of these matrices to find the following equation:

$$W^{a(i,j)}_{a(1,1)}(T_1, x) = \frac{1}{2} n\left[\left(m\sum_{j=1}^{n} x^{d_{1j}}\right) + \left(\sum_{i=2}^{m} 2(m-i+1)\left(\sum_{j=1}^{n} x^{d_{ij}}\right)\right)\right],$$

where $D^{a(i,j)}_{a(1,1)} = [d_{ij}]$. Other polynomials are similar and so the Hosoya polynomial of this nanotube is computed as follows:

$$\begin{aligned} W(TUC_4C_8(R), x) = {} & 4W^{a(i,j)}_{a(1,1)}(TUC_4C_8(R), x) + 2W^{d(i,j)}_{a(1,1)}(TUC_4C_8(R), x) \\ & + W^{c(i,j)}_{a(1,1)}(TUC_4C_8(R), x) + W^{a(i,j)}_{c(1,1)}(TUC_4C_8(R), x) \\ & + 2W^{d(i,j)}_{c(1,1)}(TUC_4C_8(R), x) + 2W^{a(i,j)}_{b(1,1)}(TUC_4C_8(R), x) \\ & + 2W^{c(i,j)}_{b(1,1)}(TUC_4C_8(R), x) + 2W^{d(i,j)}_{b(1,1)}(TUC_4C_8(R), x). \end{aligned}$$

3. Conclusions

We have given an efficient algorithm for computing Hosoya polynomial of nanotubes. It is possible to compute the Hosoya polynomial of other nanotubes by using the similar methods. Our calculations in this paper can be performed by applying the Software package MATLAB and our programs are accessible from the authors upon request.

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