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A survey on Hosoya polynomial of some nanotubes and nanotori

HOSSEIN SHABANAI

Department of Pure Mathematics, Faculty of Mathematical Sciences,

University of Kashan, Kashan 87317–51167, I R Iran

Email: Shabani.hsh@gmail.com

ABSTRACT. 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. In this paper we arrange the main result about the Hosoya polynomial of armchair polyhex, Zig-Zag, TUC_4C_8(R/S) nanotubes and nanotorus according to Ref.s [23-27].

Keywords: Hosoya polynomial, nanotube, nanotori.

1. INTRODUCTION

Nanotubes and nanotorus are an important category of nanostructured materials can be prepared from carbon [1]. These materials are usually represented as molecular graph where the vertices of graph correspond to the atoms and the edges correspond to the chemical bonds. A topological index of a chemical compound is a number related to the molecular graph of compound, describing some of its physic-chemical properties. 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 [2,3].

We now recall some graph theoretical notations that will be used in this paper. Let G be a simple molecular graph without directed and multiple edges without loops and with vertex and edge sets V(G) and $E(G)$, respectively. Suppose u and v are two vertices of G. A path between u and v is a sequence of vertices and edges where connect this vertices and the length of path is the number of edges of it. The distance between u and v is a path with minimum cardinality and denoted by $d(u,v)$. The

function d(-,-) is a metric function on vertex set of G. The diameter of G is the maximum distance between any pair of vertices, and it is denoted by diam(G) [4].

Hosoya polynomial is a counting polynomial introduced by Hosoya in [5] and he proposed the Wiener polynomial for given molecular graph G for the first time. The roots and coefficients of this polynomial are used for the characterization of topological nature of some chemical compounds. Eventually, it was renamed into "Hosoya polynomial" [6], which name is nowadays most frequently used in the mathematical and mathematico-chemical literature; for further details and references see [7]. The Hosoya polynomial $W(G,x)$ in the variable x, is defined as the summation of all terms $d(G,k)x^k$, where d(G,k) denotes the number of pairs of vertices of the graph G whose distance is k. Evidently, d(G,0) and d(G,1) are, respectively, equal to the number of vertices and edges of G, and therefore Hosoya polynomial is a polynomial of degree diam(G) [8].

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Suppose G is a molecular graph with vertex set $V(G)=\{v_1,v_2,\dots,v_n\}$. Let $D=\left[d_{i,j}\right]_{n\times n}$ denotes the distance matrix of G, where $d_{i,j}=d(v_i,v_j)$. Another equivalent way to write the Hosoya polynomial is

$$W(G,x)=\frac{1}{2}\sum_{j=1}^{n}\sum_{i=1}^{n}x^{d_{i,j}}.$$

The Hosoya polynomial of G satisfies in the following conditions: $\left(W(G,x)\right)'\Big|_{x=1}=W(G)$, $\left(xW(G,x)\right)''\Big|_{x=1}=2WW(G)$ and $\left(x^2W(G,x)\right)'''\Big|_{x=1}=6TSZ(G)$, where W(G), WW($G$) and TSZ($G$) are Wiener index [9], hyper-Wiener index [10] and Tratch–Stankevich–Zefirov index [11].

Diudea and his co-authors introduced firstly the problem of computing topological indices of nanomaterials [12-17] and he takes the armchair, zig-zag and TUC4C_8(R/S) nanotubes into consideration and computed the Wiener index of these nanostructures. Ashrafi and co-authors computed the Wiener index of a polyhex and TUC_4C_8(R/S) nanotori [18-22]. In this paper, we arrange the main results about the computing the Wiener polynomial of armchair polyhex, zig-zag, TUC_4C_8(R/S) nanotubes and nanotori [23-27].

2. Main Results and Discussions

In this section we present the Hosoya polynomial of four classes of carbon nanotubes depicted in Figure 1.

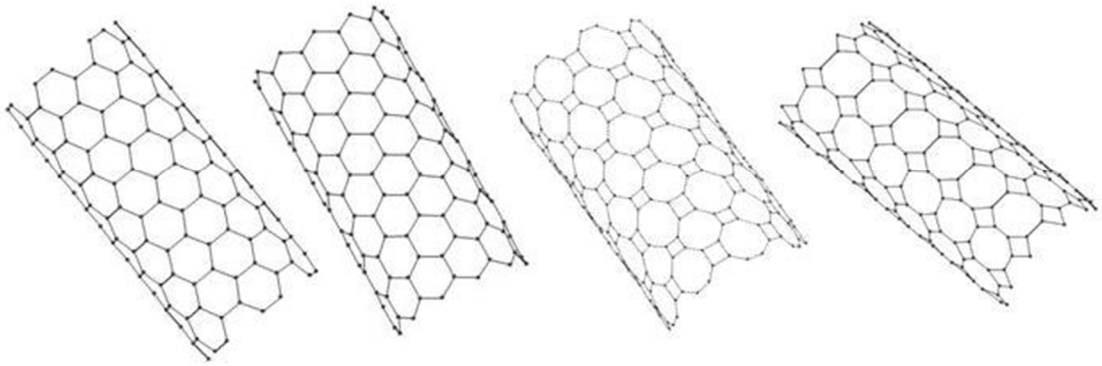

Figure 1. The Armchair Polyhex, Zig-Zag Polyhex, $TUC_4C_8(S)$ and $TUC_4C_8(R)$ Nanotubes.

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2.1 Armchair polyhex carbon nanotube and nanotori

Let TUVC6$[m, n]$ be the 2–dimensional lattice of Armchair polyhex nanotube, where m is the number of rows and n is the number of zig-zags, and $V(\text{TUVC6}[m, n]) = \{v(i, j): 1 \leq i \leq m, 1 \leq j \leq n\}$ Figure 2. Define a distance matrix $D_{v(1,1)} = [d_{i,j}^{v(1,1)}]$ related to vertex $v(i, j)$ as a base vertex, where $d_{i,j}^{v(1,1)}$ is the distance between the base vertex $v(1,1)$ and $v(i, j)$.

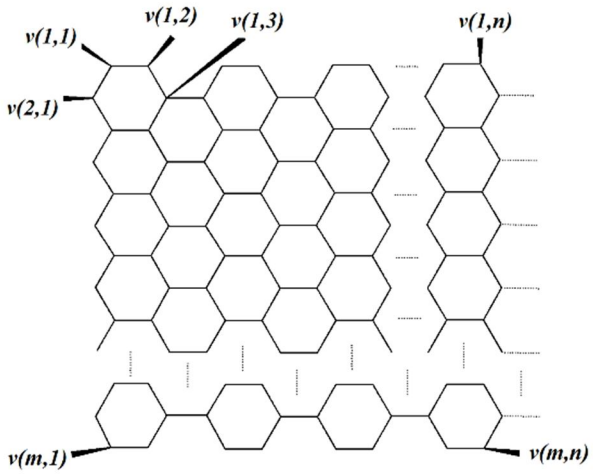

Figure 2. The 2–Dimensional Fragment of an Armchair Polyhex Nanotube.

Now, we consider two new matrices as follows:

Matrix A) The first matrix is $A_{\left(\frac{n}{2}+1\right)\times n}=[a_{i,j}]$, where $a_{1,1}=0$, $a_{2,1}=1$,$a_{2,2}=2$, $a_{1,n}=3$, $a_{2,n}=2$, $a_{1,j}=\begin{cases}a_{1,j-1}+3, & 2\nmid j\\ a_{1,j-1}+1, & 2|j\end{cases}\left(2\le j\le\frac{n}{2}+1\right)$, $a_{1,j}=\begin{cases}a_{1,j-1}+1, & 2\nmid j\\ a_{1,j-1}+3, & 2|j\end{cases}\left(\frac{n}{2}+2\le j\le n-1\right)$, $a_{2,j}=\begin{cases}a_{2,j-1}+1, & 2\nmid j\\ a_{2,j-1}+3, & 2|j\end{cases}\left(2\le j\le\frac{n}{2}+1\right)$, $a_{1,j}=\begin{cases}a_{1,j-1}+3, & 2\nmid j\\ a_{1,j-1}+1, & 2|j\end{cases}\left(\frac{n}{2}+2\le j\le n-1\right)$. Other entries of matrix A is obtained from the first and second rows by equations $a_{i,j}=a_{1,j}$ where $2\nmid i$, and $a_{i,j}=a_{2,j}$, otherwise.

Matrix B) The second matrix is $B_{\left(\frac{n}{2}+1\right)\times n}=[b_{i,j}]$, where $b_{\frac{n}{2}+1,j}=\begin{cases}\frac{n}{2}+j-1, & j\le\frac{n}{2}+1\\ \frac{3n}{2}-j+1, & j>\frac{n}{2}+1\end{cases}$ and $b_{i,j}=b_{i+1,j}-1\ \left(1\le i\le\frac{n}{2}\right)$.

Then the entries of distance matrix of TUVC6$[m,n]$ related to the base vertex $v(1,1)$ is equals to $d_{i,j}^{v(1,1)}=\begin{cases}\max\{a_{i,j},b_{i,j}\}, & j\le\frac{n}{2}+1\\ d_{i-1,j}, & j>\frac{n}{2}+1\end{cases}$. Suppose Δ_1, Δ_2, ..., Δ_m are rows of $D_{v(1,1)}$ and Define permutation functions α_i and β_j as follow:

$$\alpha_i=\begin{pmatrix}1 & 2 & \dots & i & i+1 & \dots & m\\ i & i-1 & \dots & 1 & 2 & \dots & m-i+1\end{pmatrix},$$

$$\beta_j=\begin{pmatrix}1 & 2 & \dots & j-1 & j & \dots & n\\ n-j+2 & n-j+3 & \dots & n & 1 & \dots & n-j+1\end{pmatrix};\ j \text{ is odd},$$

$$\beta_j=\begin{pmatrix}1 & 2 & \dots & j & j+1 & j+2 & \dots & n\\ j & j-1 & \dots & 1 & n & n-1 & \dots & j+1\end{pmatrix};\ j \text{ is even}.$$

It is easy to see that, for an arbitrary vertex $v(i,j)$ of TUVC6$[m,n]$, the distance matrix $D_{v(i,j)}$ related to this vertex is obtained by the equation $D_{v(i,j)}=\beta_j\alpha_i D_{v(1,1)}$. By

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this equation, we enumerate the entries of distance matrix $D_1 = D(\text{TUVC6}[m,n])$. The entries of Δ_1 are appear mn times in D_1 and the entries of Δ_i are appear $2n(m-i+1)$ times where $2 \le i \le m$. Therefore the Hosoya polynomial of $T_1 = \text{TUVC6}[m,n]$ is equals to:

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

Now, consider the distance matrix D_2 of an armchair polyhex carbon nanotorus S_1. By apply a similar algorithm as above, we obtain $D_{v(i,j)} = \beta_j \alpha_{\frac{m}{2}} D_{v(1,1)}$. By this equation the Wiener polynomial of S_1 is as follows:

$$W(S_1,x) = \frac{mn}{2}\left(\sum_{j=1}^{n} x^{d_{1,j}^{v(1,1)}} + 2\left(\sum_{i=2}^{\frac{m}{2}}\sum_{j=1}^{n} x^{d_{i,j}^{v(1,1)}}\right) + \sum_{j=1}^{n} x^{d_{\frac{m}{2}+1,j}^{v(1,1)}}\right)$$

2.2 Zig-zag polyhex carbon nanotube

Let $T_2 = \text{TUVC}_6[m,n]$ be the zig–zag polyhex carbon nanotube, where m is the number of rows and n is the number of zig-zags and it is an even integer, Figure 3.

Choose two base vertices $v(1,1)$ and $u(1,1)$ from the 2–dimensional lattice of T_2. Let $D_{u(1,1)} = \left[d_{i,j}^{u(1,1)}\right]$ and $D_{v(1,1)} = \left[d_{i,j}^{v(1,1)}\right]$ are distance matrices between vertex $u(1,1)$ and vertex $v(1,1)$ and all vertices of T_2, respectively. Define three matrices as follows:

$A_{m\times(\frac{n}{2}+1)}^{u(1,1)} = [a_{i,j}]$:

$$a_{1,1} = 0, a_{1,2} = 1, a_{i,1} = \begin{cases} a_{i-1,1} + 1, & 2|i \\ a_{i,2} + 1, & 2 \nmid i \end{cases}, a_{i,2} = \begin{cases} a_{i-1,1} + 1, & 2|i \\ a_{i-1,2} + 1, & 2 \nmid i \end{cases} \text{ and } a_{i,j} = \begin{cases} a_{i,1}, & 2 \nmid j \\ a_{i,2}, & 2|j \end{cases}.$$

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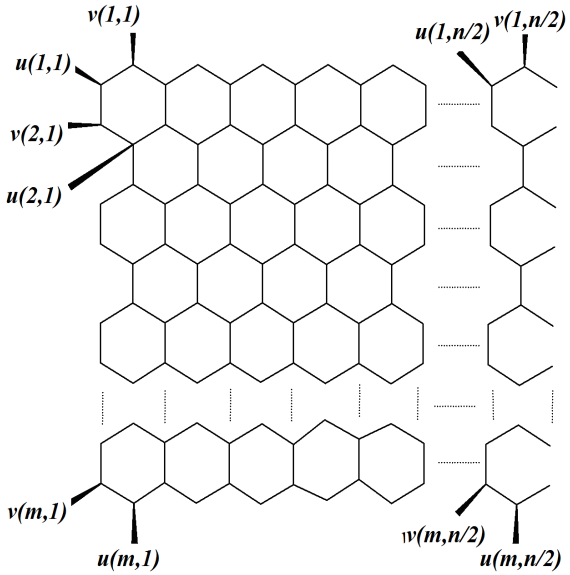

Figure 3. The 2–Dimensional Fragment of an Zig–Zag Polyhex Carbon Nanotube.

$A^{v(1,1)}_{m\times(\frac{n}{2}+1)} = [c_{i,j}]$:

$$c_{1,1} = 0, c_{1,2} = 1, c_{i,1} = \begin{cases} c_{i,1} + 1, & 2|i \\ c_{i-1,1} + 1, & 2 \nmid i \end{cases}, c_{i,2} = \begin{cases} c_{i-1,2} + 1, & 2|i \\ c_{i,1} + 1, & 2 \nmid i \end{cases} \text{ and } c_{i,j} = \begin{cases} c_{i,1}, & 2 \nmid j \\ c_{i,2}, & 2|j \end{cases}.$$

$B_{m\times\left(\frac{n}{2}+1\right)} = [b_{i,j}]$: $b_{i,1} = i - 1$ where $1 \le i \le m$ and $b_{i,j} = b_{i,j-1} + 1$ for other entries.

From these matrices, one can easily compute matrices $D_{u(1,1)}$ and $D_{v(1,1)}$ as follows:

$$d_{ij}^{u(1,1)} = \begin{cases} \max(a_{ij}, b_{ij}) & 1 \le j \le n/2+1 \\ d_{i(n-j+2)}^{u(1,1)} & j > n/2+1 \end{cases}, \quad d_{ij}^{v(1,1)} = \begin{cases} \max(a_{ij}, c_{ij}) & 1 \le j \le n/2+1 \\ d_{i(n-j+2)}^{v(1,1)} & j > n/2+1 \end{cases}.$$

Now, set $D_{u(1,1)} = [\Delta_i^{u(1,1)}]_{1\le i\le m}$ and $D_{v(1,1)} = [\Delta_i^{v(1,1)}]_{1\le i\le m}$, such that Δ_i denotes the ith row of the matrix. We also assume that the first row of $D_{u(1,1)}$ and $D_{v(1,1)}$ are as follows:

$$[d_{u(1,1)}^{u(1,1)}, d_{v(1,2)}^{u(1,1)}, d_{u(1,2)}^{u(1,1)}, \cdots, d_{v(1,n/2)}^{u(1,1)}, d_{u(1,n/2)}^{u(1,1)}, d_{v(1,1)}^{u(1,1)}],$$

$$[d^{v(1,1)}_{v(1,1)}, d^{v(1,1)}_{u(1,1)}, d^{v(1,1)}_{v(1,2)}, d^{v(1,1)}_{u(1,2)} \cdots, d^{v(1,1)}_{v(1,n/2)}, d^{v(1,1)}_{u(1,n/2)}].$$

Suppose $D_{u(i,1)}$ and $D_{v(i,1)}$ are distance matrices associated to the ith row of T_2. Then,

$$D_{u(i,1)} = \begin{bmatrix} \Delta_i^{v(1,1)} \\ \vdots \\ \Delta_2^{v(1,1)} \\ \Delta_1^{u(1,1)} \\ \\ \Delta_{m-i+1}^{u(1,1)} \end{bmatrix}, \quad D_{v(i,1)} = \begin{bmatrix} \Delta_i^{u(1,1)} \\ \vdots \\ \Delta_2^{u(1,1)} \\ \Delta_1^{v(1,1)} \\ \\ \Delta_{m-i+1}^{v(1,1)} \end{bmatrix}.$$

Notice that, two matrices $D_{u(i,j)}$ and $D_{v(i,j)}$ are obtained by replacement of the columns of $D_{u(i,1)}$ and $D_{v(i,1)}$, respectively. Now, by applying above discussion we can enumerate the entries of the distance matrix $D(T_2)$ and To compute the Hosoya polynomial, it is enough to count the equal entries of $D(T_2)$. The entries of the ith row of these matrices ($1 < i \leq m$) are appear $2n(m - i+1)$ times, and the entries of the first row are appear nm times. We achieve two polynomials for vertices u and v, as follows:

$$W_u(T,x) = \frac{1}{2} n \left[\left(m \sum_{j=1}^{n} x^{d_{i,j}^{u(1,1)}} \right) + \left(\sum_{i=2}^{m} 2(m-i+1) \left(\sum_{j=1}^{n} x^{d_{i,j}^{u(1,1)}} \right) \right) \right]$$

$$W_v(T,x) = \frac{1}{2} n \left[\left(m \sum_{j=1}^{n} x^{d_{i,j}^{v(1,1)}} \right) + \left(\sum_{i=2}^{m} 2(m-i+1) \left(\sum_{j=1}^{n} x^{d_{i,j}^{v(1,1)}} \right) \right) \right]$$

Therefore the Hosoya polynomial of T_2 is as follows:

$$W(T,x) = W_u(T,x) + W_v(T,x)$$

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2.3 $TUC_4C_8(S)$ carbon nanotube and nanotori

Suppose T_3 is 2–dimensional lattice of $TUC_4C_8(S)[m,n]$, where m is the number of rows and n is the number of columns. Choose eight base vertices $x_k(1,1)$, $x_k \in \{a_1, b_1, c_1, d_1, a_2, b_2, c_2, d_2\}$, Figure 4. Consider partition $P = \{A_1, A_2, B_1, B_2, C_1, C_2, D_1, D_2\}$ of $V(T_3)$ in which if $X_j \in P$ then $X_j = \{x_k(i,t): 1 \le i \le m, 1 \le t \le n, k = j\}$. The matrix $D^{X_j}_{x_k(1,1)}$ is a matrix in which its entries are the distance from $x_k(1,1)$ to all of vertices in X_i. To compute distance matrix of T_3, we must find all of these matrices. The first row of $D(T_3)$ is the all entries of eight matrices of vertex $a_1(1,1)$, and other rows are obtained similarly. By using the symmetry of T_3, we don't need to investigate the vertices with subscript 2. Hence the computation of sixty four matrices presented above, decreases to thirty two matrices.

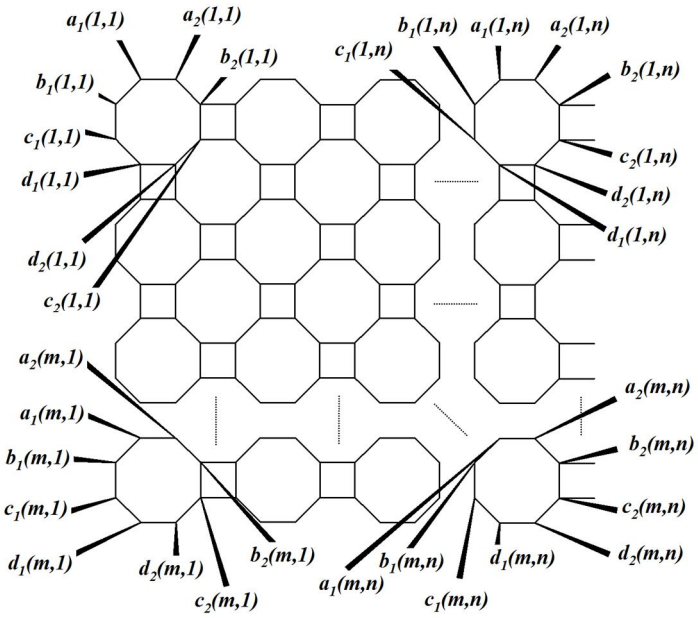

Figure 4. The 2–Dimensional Fragment of an $TUC_4C_8(S)$ Carbon Nanotube.

Let $D^{X_j}_{x_k(1,1)} = [(X_j^{x_k})_i]_{1 \le i \le m}$ where $(X_j^{x_k})_i$ is ith row of the matrix and $k \in \{1,2\}$. We can obtain other matrices for the tth row ($2 \le t \le m$) and first column of T_3. Now we enumerate the entries of distance matrix $D(T_3)$. For this, define α_i, ($1 \le i \le m$), by

$\alpha_i = \begin{pmatrix} 1 & 2 & \dots & i & i+1 & \dots & m \\ i & i-1 & \dots & 1 & 2 & \dots & m-i+1 \end{pmatrix}$, then we can see that the times of repeating s-th row matrix $D^{X_j}_{x_1(1,1)}$ is the number of columns in T_3 multiplied by the number of members of the set $\{\alpha_j(j+s-1), \alpha_j(j-s+1) : j, j+s-1, j-s+1 \le m\}$. Therefore, for this matrix we obtain the following polynomial:

$$W^{X_j}_{x_k(1,1)}(T_3, x) = \frac{1}{2} \times 2n \left[\left(m \sum_{j=1}^{n} x^{d_{1,j}} \right) + \left(\sum_{i=2}^{m} 2(m-i+1) \left(\sum_{j=1}^{n} x^{d_{i,j}} \right) \right) \right]$$

So the Wiener polynomial of T_3 is $W(T_3, x) = \sum_{X_j, x_1} W^{X_j}_{x_1(1,1)}(T_3, x)$.

Now consider the molecular graph of a S_3 = $TUC_4C_8(S)[m,n]$ nanotorus, where m is the number of rows and n is the number of columns. As similar way, choose eight base vertices $x_k(1,1)$, $x_k \in \{a_1, b_1, c_1, d_1, a_2, b_2, c_2, d_2\}$, Figure 5.

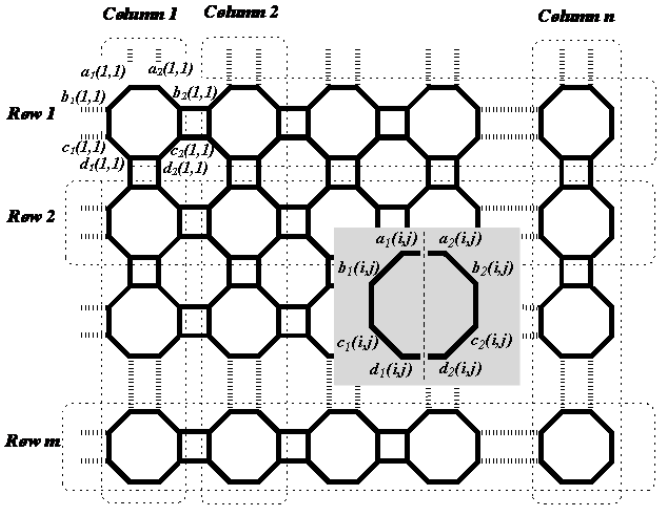

Figure 4. The 2–Dimensional Fragment of an $TUC_4C_8(S)$ Carbon Nanotori.

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Also, partition $V(S_3)$ into eight parts $P = \{A_1, A_2, B_1, B_2, C_1, C_2, D_1, D_2\}$ where $X_j \in P$ and $X_j = \{x_k(i,t) \mid 1 \le i \le m, 1 \le t \le n, k = j\}$. To compute $D(S_3)$, it is enough to calculate matrices $D^{X_j}_{x_k(1,1)}$. By a similar argument as above, we obtain the following polynomial as $W^{X_j}_{x_k(1,1)}(S_3, x) = \frac{1}{2}nm\sum_{i,j} x^{d_{i,j}}$ for matrix $D^{X_j}_{x_k(1,1)}$. Therefore the Hosoya polynomial of S_3 is equals to $W(S_3, x) = 2 \times \sum_{X_j, x_1} W^{X_j}_{x_1(1,1)}(S_3, x)$.

2.4 $TUC_4C_8(R)$ nanotube and nanotori

Let T_4 be 2–dimensional lattice of $TUC_4C_8(R)[m,n]$, where m is the number of rows and n is the number of columns of it. Similar as last section, choose four base vertices $x(1,1)$, $x \in \{a, b, c, d\}$ from the molecular graph of T_4, Figures 5.

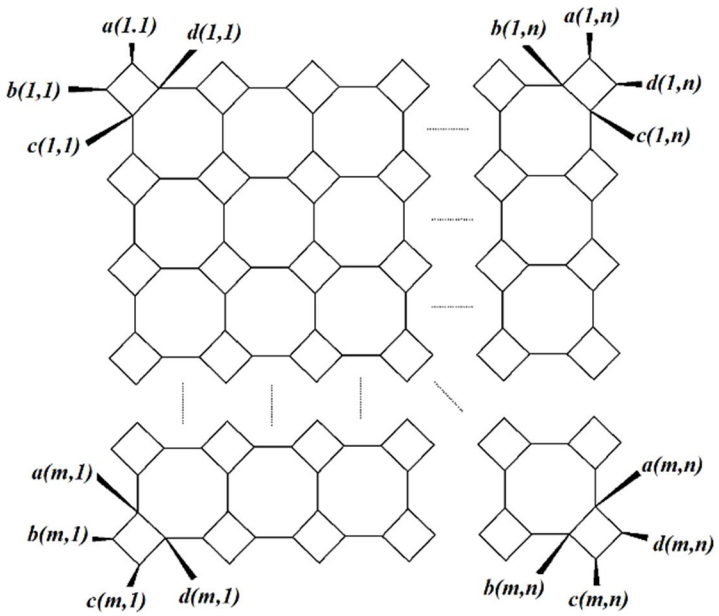

Figure 5. The 2–Dimensional Fragment of $TUC_4C_8(R)$ Carbon Nanotube.

Partition the vertex set of T_4 into four sets A, B, C, and D such that all vertices with label a are in the set A, and so on. Define matrix $D^{a(i,j)}_{a(1,1)}$ as the matrix for the base

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vertex $a(1,1)$ in which the entries of this matrix are distances between $a(1,1)$ and $a(i,j) \in A$. For computing $D(T_1)$, we first define the following 16 matrices:

$$D^{A}_{a(1,1)}, D^{B}_{a(1,1)}, D^{C}_{a(1,1)}, D^{D}_{a(1,1)}, D^{A}_{b(1,1)}, D^{B}_{b(1,1)}, D^{C}_{b(1,1)}, D^{D}_{b(1,1)},$$
$$D^{A}_{c(1,1)}, D^{B}_{c(1,1)}, D^{C}_{c(1,1)}, D^{D}_{c(1,1)}, D^{A}_{d(1,1)}, D^{B}_{d(1,1)}, D^{C}_{d(1,1)}, D^{D}_{d(1,1)}.$$

By using the symmetry of T_4, it is enough to compute eight of these matrices. Remark that four matrices $D^{a(i,j)}_{a(1,1)}$, $D^{b(i,j)}_{b(1,1)}$, $D^{c(i,j)}_{c(1,1)}$ and $D^{d(i,j)}_{d(1,1)}$ are equal. Consider the permutation $\mu = \begin{pmatrix} 1 & 2 & 3 & \dots & n-1 & n \\ 1 & n & n-1 & \dots & 3 & 2 \end{pmatrix}$. One can easily see that the matrices $D^{b(i,j)}_{a(1,1)}$ and $D^{b(i,j)}_{c(1,1)}$ are obtained from $D^{d(i,j)}_{a(1,1)}$ and $D^{d(i,j)}_{c(1,1)}$. By symmetry of T_4, it is possible to compute the matrix evaluated at the base vertex d from the same matrix for the vertex b. On the other hand, the matrices $D^{d(i,j)}_{b(1,1)}$, $D^{c(i,j)}_{d(1,1)}$ and $D^{a(i,j)}_{d(1,1)}$ is computed from $D^{b(i,j)}_{d(1,1)}$, $D^{c(i,j)}_{b(1,1)}$ and $D^{a(i,j)}_{b(1,1)}$ by trace of μ.

We now count the repeated entries of these matrices to find the following equation:

$$W^{a(i,j)}_{a(1,1)}(T_4, x) = \frac{1}{2} n \left[m \left(\sum_{j=1}^{n} x^{d_{1,j}} \right) + \left(\sum_{i=2}^{m} 2(m-i+1) \left(\sum_{j=1}^{n} x^{d_{i,j}} \right) \right) \right],$$

where $D^{a(i,j)}_{a(1,1)} = [d_{i,j}]$.

Other polynomials are similar and so the Hosoya polynomial of this nanotube is computed as follows:

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

Now consider the molecular graph of a S_4 = $TUC_4C_8(R)$ nanotorus. For this molecular graph, choose four base vertices $a(i,j)$, $b(i,j)$, $c(i,j)$ and $d(i,j)$, Figure 6.

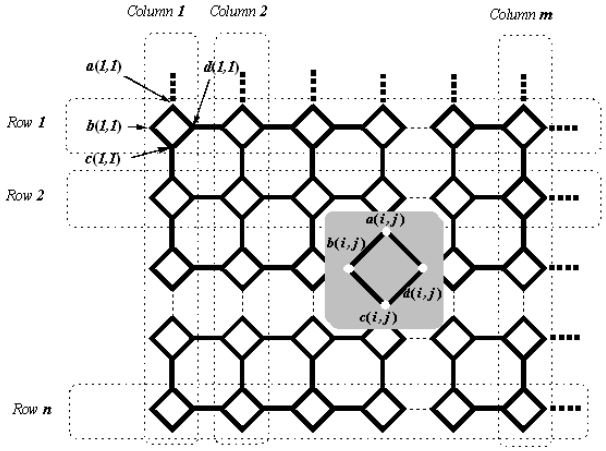

Figure 6. The 2–Dimensional Fragment of $TUC_4C_8(R)$ Carbon Nanotori.

By apply similar argument and consider partition A, B, C and D for vertices, we found the polynomial $W_a^A(T_4,x) = \frac{1}{2}nm\sum_{j=1}^{n}\sum_{i=1}^{m}x^{d_{i,j}}$, where $D^A_{a(1,1)}$ = $[d_{i,j}]$. Other polynomials are similar and so the Hosoya polynomial of this nanotorus is computed as follows:

$$
\begin{aligned}
\boldsymbol{H(T,q)} \quad & = \boldsymbol{4H^A_a(T,q)+2H^D_a(T,q)+H^C_a(T,q)+H^A_c(T,q)+2H^D_c(T,q)}\\
& \quad \boldsymbol{+2H^A_b(T,q)+2H^C_b(T,q)+2H^D_b(T,q).}
\end{aligned}
$$

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