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A new algorithm for computing Hosoya polynomial of TUC_4C_8(R/S) nanotorus

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The Hosoya polynomial of a molecular graph G is defined as $H(G,q)=\sum_{\{u,v\}\subseteq V(G)} q^{d(u,v)}$, 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) nanotorus. In this paper, a new algorithm for these calculations is presented. We also compute the Hosoya polynomial of TUC_4C_8(R) nanotorus.

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1. Introduction

The boiling point of a compound is an important property for the simulation of processes in chemical and petroleum industries. So it is important to find theoretical methods for the estimation of boiling point of compunds that are not yet synthesized or whose boiling point is unknown. One of the most important methods is finding a parameter that correlates the physico-chemical or biological properties of the compound under consideration.

A topological index for a chemical compound is a number related to the molecular graph of compound, G, describing some of its physic-chemical properties. The Wiener index [1] was the first topological index reported in the chemical literature. It is defined as the sum of all distances between vertices of the graph under consideration. Here, the distance between two vertices x and y of G, d(u,v), is defined as the length of a minimal path connecting them.

After several years, Hosoya [2] pointed out that the Wiener index can be computed from the topological distance matrix of the graph representing the hydrogen-depleted molecule. Hosoya [3] also introduced a graph polynomial, which he named the Wiener polynomial of the graph. In recent years, many chemists preferred the name Hosoya polynomial [4] and so we use this name throughout the paper. This polynomial is defined as $H(G,q) = \sum_{i=1}^{l} \gamma_i x^i$, where γ_i is the number of pairs of vertices at distance i and l is the longest distance (diameter) in the graph.

Diudea was the first scientist who considered graph theoretical problems of nanotechnology. In some research papers he and his co-workers [5-10] computed too many distance based topological indices and counting polynomials of nanotubes, nanotori and fullerenes. The first author of the present paper (ARA) [11-20] continued this program and computed the Wiener index and Hosoya polynomial of TUC_4C_8(R/S) nanotubes and TC_4C_8(R/S) nanotori. We also stimulated the papers by Xu [21-23] in which the authors computed Hosoya polynomials of C4C8(R/S) nanostructures. Our notation is standard and mainly taken from the book of Trinajstic[24] and papers by Diudea mentioned above.

2. Main results and discussion

In this section exact formulas for the Hosoya polynomial of TC_4C_8(R/S) nanotori are derived. Since $d/dq(H(G,q))|_{q=1}=W(G)$, the Wiener index of these nanotori are also computed.

2.2 Hosoya polynomial of TC_4C_8(R) nanotorus

Consider the molecular graph of an TC_4C_8(R) nanotorus, Fig. 1, and its 2-dimensional lattice, Fig. 2. To simplify our argument, this nanotorus is denoted by T = TUC_4C_8(R)[m,n], where m is the number of rows and n is the number of columns, (Fig. 2).

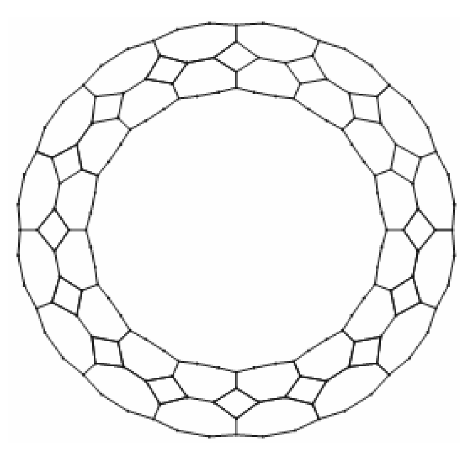

Fig. 1. The 3D-representation of an TC_4C_8(R) nanotorus.

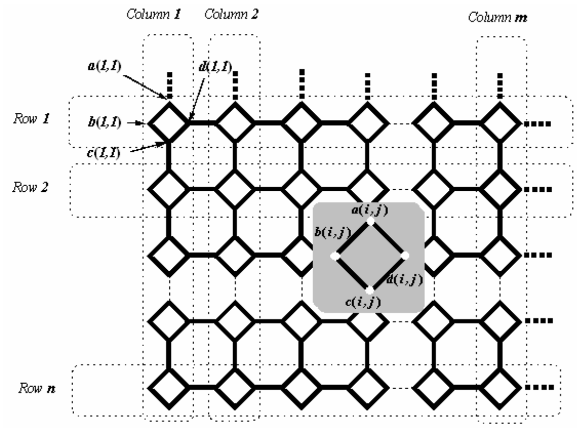

Fig. 2. The 2D-lattice of an $TC_4C_8(S)$ nanotorus.

Choose four base vertices a(i,j), b(i,j), c(i,j) and d(i,j) from the molecular graph of T, Fig. 2. For computing D(T), we must define 16 matrices. To define these matrices, we first make the partition of the vertex set of T, into four sets A, B, C and D. A is the set of all vertices with the same position in the rhombs. The sets B, C and D are defined similarly. Define $D^A_{a(1,1)}$ to be the matrix in which (i,j)-entry is defined as the distance between the vertex a(i,j) of A and the base vertex a(1,1). The other matrices are defined similarly. They are as follows:

$$\begin{array}{l} D^A_{a(1,1)}, D^B_{a(1,1)}, D^C_{a(1,1)}, D^D_{a(1,1)} \\ D^A_{b(1,1)}, D^B_{b(1,1)}, D^C_{b(1,1)}, D^D_{b(1,1)} \\ D^A_{c(1,1)}, D^B_{c(1,1)}, D^C_{c(1,1)}, D^D_{c(1,1)} \\ D^A_{d(1,1)}, D^B_{d(1,1)}, D^C_{d(1,1)}, D^D_{d(1,1)} \end{array} .$$

We notice that by symmetry, it is enough to compute eight of these matrices. Remark that four matrices $D^A_{a(1,1)}$, $D^B_{b(1,1)}$, $D^C_{c(1,1)}$ and $D^D_{d(1,1)}$ are equal. Consider the permutation $\mu = \begin{pmatrix} 1 & 2 & 3 & \dots & n-1 & n \\ 1 & n & n-1 & \dots & 3 & 2 \end{pmatrix}$. It is easy to see that the matrices $D^B_{a(1,1)}$ and $D^B_{c(1,1)}$ are obtained from $D^D_{a(1,1)}$ and $D^D_{c(1,1)}$. By symmetry of Fig. 2, 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 $D^D_{b(1,1)}$, $D^C_{d(1,1)}$ and $D^A_{d(1,1)}$ is computed from $D^B_{d(1,1)}$, $D^C_{b(1,1)}$ and $D^A_{b(1,1)}$ by trace of μ.

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

$$H^A_a(T,q) = \frac{1}{2}mn\sum_{j=1}^{n}\sum_{i=1}^{m} q^{d_{ij}} \qquad (1)$$

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

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

Some distance matrices: Suppose m is even. If m is odd then substitute m/2+1 by (m+1)/2. We first assume that 1≤ i ≤ m/2+1.

Table 1. $D^A_{a(1,1)} = [\alpha_{ij}]$

For i = 1	j = 1	2 ≤ j ≤ n/2+1 (n | 2) 2 ≤ j ≤ (n+1)/2 (n∤ 2)	And for 1< i ≤ m/2+1	1 ≤ j ≤ n/2+1 (n | 2) 1 ≤ j ≤ (n+1)/2 (n∤ 2)
	$\alpha_{11} = 0$	$\alpha_{1j} = \alpha_{1(j-1)} + 3$		i ≤ j $\alpha_{ij} = \alpha_{(i-1)j} + 1$ i > j $\alpha_{ij} = \alpha_{(i-1)j} + 3$
Other entries of this matrix is $\alpha_{ij} = \alpha_{i(n-j+2)}$.				

Table 2. $D^C_{a(1,1)} = [\beta_{ij}]$

For i = 1	j = 1	j = 2	3 ≤ j ≤ n/2+1 (n | 2) 3 ≤ j ≤ (n+1)/2 (n∤ 2)	And for 1< i ≤ m/2+1	1 ≤ j ≤ n/2+1 (n | 2) 1 ≤ j ≤ (n+1)/2 (n∤ 2)
	$\beta_{11} = 2$	$\beta_{12} =$ 3	$\beta_{1j} = \beta_{1(j-1)} + 3$		i < j $\beta_{ij} = \beta_{(i-1)j} + 1$ i ≥ j $\beta_{ij} = \beta_{(i-1)j} + 3$
Other entries of this matrix is $\beta_{ij} = \beta_{i(n-j+2)}$.					

Table 3. $D^D_{a(1,1)} = [\eta_{ij}]$

For i = 1	j = 1	2 ≤ j ≤ n/2 (n | 2) 2 ≤ j ≤ (n+1)/2 (n∤ 2)	And for 1< i ≤ m/2+1	1 ≤ j ≤ n/2 (n | 2) 1 ≤ j ≤ (n+1)/2 (n∤ 2)

	$\eta_{11} = 1$	$\eta_{1j} = \eta_{1(j-1)} + 3$		$i \le j \quad \eta_{ij} = \eta_{(i-1)j} + 1$ $i > j \quad \eta_{ij} = \eta_{(i-1)j} + 3$
Other entries of this matrix is $\eta_{ij} = \eta_{i(n-j+1)} + 1$.				

Table 4. $D^{A}_{b(1,1)} = [\pi_{ij}]$

For i = 1	$j = 1$	$2 \le j \le n/2 \ (n \mid 2)$ $2 \le j \le (n+1)/2 \ (n \nmid 2)$	And for $1 < i \le m/2+1$	$1 \le j \le n/2 \ (n \mid 2)$ $1 \le j \le (n+1)/2 \ (n \nmid 2)$
	$\pi_{11} = 1$	$\pi_{1j} = \pi_{1(j-1)} + 3$		$i+1 \le j \quad \pi_{ij} = \pi_{(i-1)j} + 1$ else $\quad \pi_{ij} = \pi_{(i-1)j} + 3$
Other entries of this matrix is $\pi_{ij} = \pi_{i(n-j+1)} + 1$.				

Table 5. $D^{C}_{b(1,1)} = [\rho_{ij}]$

For i = 1	$j = 1$	$2 \le j \le n/2 \ (n \mid 2)$ $2 \le j \le (n+1)/2 \ (n \nmid 2)$	And for $1 < i \le m/2+1$	$1 \le j \le n/2 \ (n \mid 2)$ $1 \le j \le (n+1)/2 \ (n \nmid 2)$
	$\rho_{11} = 1$	$\rho_{1j} = \rho_{1(j-1)} + 3$		$i \le j \quad \rho_{ij} = \rho_{(i-1)j} + 1$ $i > j \quad \rho_{ij} = \rho_{(i-1)j} + 3$
Other entries of this matrix is $\rho_{ij} = \rho_{i(n-j+2)} + 1$.				

Table 6. $D^{D}_{b(1,1)} = [\tau_{ij}]$

For i = 1	$j = 1$	$j = n$	$2 \le j \le n/2 \ (n \mid 2)$ $2 \le j < (n+1)/2 \ (n \nmid 2)$	$n/2 < j \le n-1 \ (n \mid 2)$ $(n+1)/2 \le j \le n-1 \ (n \nmid 2)$
	$\tau_{11} = 2$	$\tau_{1n} = 1$	$\tau_{1j} = \tau_{1(j-1)} + 3$	$\tau_{1j} = \tau_{1(j+1)} + 3$
For $1 < i \le m/2+1$	$1 \le j \le n/2 \ (n \mid 2)$ $1 \le j < (n+1)/2 \ (n \nmid 2)$		$n/2 < j \le n \ (n \mid 2)$ $(n+1)/2 \le j \le n \ (n \nmid 2)$	
	$i < j+1 \quad \tau_{ij} = \tau_{(i-1)j} + 1$ $i > j \quad \tau_{ij} = \tau_{(i-1)j} + 3$		$i \ge n-j \quad \tau_{ij} = \tau_{(i-1)j} + 1$ otherwise $\ \tau_{ij} = \tau_{(i-1)j} + 3$	

Table 7. $D^{A}_{c(1,1)} = [\delta_{ij}]$

For i = 2	$j = 1$	$2 \le j \le n/2+1 \ (n \mid 2)$ $2 \le j \le (n+1)/2 \ (n \nmid 2)$	And for $2 < i \le m/2+1$	$1 \le j \le n/2+1 \ (n \mid 2)$ $1 \le j \le (n+1)/2 \ (n \nmid 2)$
	$\delta_{21} = 1$	$\delta_{2j} = \delta_{2(j-1)} + 3$		$i < j+1 \quad \delta_{ij} = \delta_{(i-1)j} + 1$ else $\quad \delta_{ij} = \delta_{(i-1)j} + 3$
If i = 1 then $\delta_{11} = 2$ for $j = 1$ & $\delta_{1j} = \delta_{2j} - 1$ for $1 < j \le n$. Other entries of this matrix is $\delta_{ij} = \delta_{i(n-j+1)}$ where $n/2+1 < j \le n \ (n \mid 2)$ or $(n+1)/2 < j \le n \ (n \nmid 2)$				

Table 8. $D^{D}_{c(1,1)} = [\gamma_{ij}]$

For i = 1	$j = 1$	$2 \le j \le n/2 \ (n \mid 2)$ $2 \le j \le (n+1)/2 \ (n \nmid 2)$	And for $1 < i \le m/2+1$	$1 \le j \le n/2 \ (n \mid 2)$ $1 \le j \le (n+1)/2 \ (n \nmid 2)$
	$\gamma_{11} = 1$	$\gamma_{1j} = \gamma_{1(j-1)} + 3$		$i < j+1 \quad \gamma_{ij} = \gamma_{(i-1)j} + 1$ $i \ge j+1 \quad \gamma_{ij} = \gamma_{(i-1)j} + 3$
Other entries of this matrix is $\gamma_{ij} = \gamma_{i(n-j+2)} + 1$.				

If $m/2 + 1 < i \le m$ then we define $\alpha_{ij} = \alpha_{(m-i+2)j}$, $\beta_{ij} = \delta_{(m-i+2)j}$, $\eta_{ij} = \gamma_{(m-i+2)j}$, $\pi_{ij} = \rho_{(m-i+2)j}$, $\rho_{ij} = \pi_{(m-i+2)j}$, $\tau_{ij} = \tau_{(m-i+2)j}$, $\delta_{ij} = \beta_{(m-i+2)j}$ and $\gamma_{ij} = \eta_{(m-i+2)j}$. Applying the same calculations as above completes our algorithm for computing Hosoya polynomial of $TC_4C_8(R)$ nanotorus.

2.3 Hosoya polynomial of $TUC_4C_8(S)$

Consider the molecular graph of an $TC_4C_8(S)$ nanotorus, Fig. 3, and its 2-dimensional lattice, Fig. 4. To simplify our argument, this nanotorus is denoted by $S = TUC_4C_8(S)[m,n]$, where m is the number of rows and n is the number of columns. Choose eight base vertices $x_k(1,1)$, $x_k \in \{a_1, b_1, c_1, d_1, a_2, b_2, c_2, d_2\}$, Fig. 4.

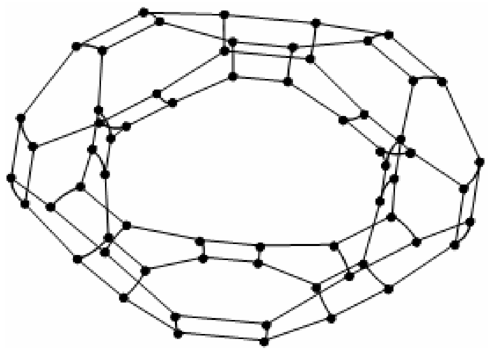

Fig. 3. 3D-Representation of an $TUC_4C_8(S)$ nanotube.

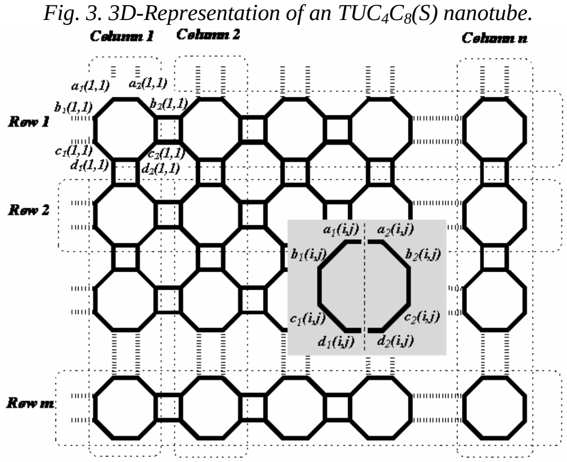

Fig. 4. The 2–dimensional fragments of an $TUC_4C_8(S)$ nanotube.

We partition V(S) into eight parts as 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), we must calculate matrices $D^{X_j}_{x_k(1,1)}$. For example $D^{A_1}_{a_1(1,1)}$ is a matrix in which its entries are the distances from $a_1(1,1)$ to all of vertexes A_1. The first row of D(S) is the all entries of eight matrices of vertex $a_1(1,1)$, and other rows are obtained similarly. We notice that making use of symmetry in S, we don't need to investigate the vertices with subscript 2. This fact has been shown in Fig. 4. Hence the calculation of two hundred fifty six matrices presented above, decreases to thirty two matrices.

Notice that finding the matrices of other rows and columns are the same and is omitted. Now we enumerate the entries of distance matrix D(S).

$$H^{X_j}_{x_k(1,1)}(S,q) = \frac{1}{2} nm \sum_{i,j} q^{d_{ij}} \tag{3}$$

So the Hosoya polynomial of T is $H(S,q) = 2 \times \sum_{X_j, x_1} H^{X_j}_{x_1(1,1)}(S,q)$.

Some distance matrices: Suppose m is even and $1 \le i \le m/2 + 1$ (If m is odd then substitute m/2+1 by (m+1)/2).

Table 1. $D^{A_1}_{a_1(1,1)} = [d_{ij}]$

i = 1	j = 1	$2 \le j \le n/2+1$ (n|2) $2 \le j \le (n+1)/2$ (n∤2)	$1< i \le m/2+1$	$1 \le j \le n/2+1$ (n|2) $1 \le j \le (n+1)/2$ (n∤2)
	d_{11}=0	$d_{ij} = d_{1(j-1)} + 4$		$i \le j$ $d_{ij} = d_{(i-1)j} + 2$ $i > j$ $d_{ij} = d_{(i-1)j} + 4$
$d_{ij} = d_{i(n-j+2)}$ where [n/2+1< j ≤ n & (n|2)] or [(n+1)/2< j ≤ n & (n∤2)]				

- It is clear that four matrices $D^{B_1}_{b_1(1,1)}$, $D^{B_1}_{c_1(1,1)}$, $D^{D_1}_{d_1(1,1)}$ and $D^{A_1}_{a_1(1,1)}$ are the same.
- By adding one to all entries of $D^{A_1}_{a_1(1,1)}$, we obtain $D^{C_1}_{b_1(1,1)}$.
- The second, third, …, m^{th} rows of $D^{A_1}_{d_1(1,1)}$ are the same as the first, …, $(m-1)^{th}$ rows of $D^{A_1}_{a_1(1,1)}$, respectively. Moreover, the first and the second row are equal, except the first entry of first row which is equal to 3.

Table 2. The function $D^{B_1}_{a_1(1,1)} = [s_{ij}]$.

i = 1	j = 1	j = 2	$2 \le j \le n/2+1$ (n|2) $2 \le j \le (n+1)/2+1$ (n∤2)	$1< i \le m/2+1$	j = 1	$2 \le j \le n/2+1$ (n|2) $2 \le j \le (n+1)/2+1$ (n∤2)
	s_{11} = 1	s_{12} = 3	$s_{1j} = s_{1(j-1)} + 4$		$s_{i1} = s_{(i-1)1} + 4$	$i-1 \le j$ $s_{ij} = s_{(i-1)j} + 2$ $i-1 > j$ $sij = s_{(i-1)j} + 4$
Then $s_{ij} = s_{i(n-j+3)}$ where [n/2+1< j ≤ n & (n|2)] or [(n+1)/2< j ≤ n & (n∤2)]						

- By adding one to all entries of $D^{B_1}_{a_1(1,1)}$, we obtain $D^{C_1}_{a_1(1,1)}$.
- The first and second row of $D^{B_1}_{d_1(1,1)}$ are equal; also the rows from 2 to m are equal to the rows from 1 to (m−1) of $D^{B_1}_{a_1(1,1)}$, respectively.
- The first row of $D^{C_1}_{d_1(1,1)}$ and the first row of $D^{B_1}_{a_1(1,1)}$ are the same; the second until mth rows of this matrix, obtained by adding the number two to all entries of the rows from one to (m−1) of $D^{B_1}_{a_1(1,1)}$.
- If for columns $1\le j \le n/2+1$ (n is even) or $1\le j \le (n+1)/2$ (n is odd), we add entries of $D^{B_1}_{a_1(1,1)}$ by 2; and define $v_{ij} = v_{i(n-j+2)}$, where $n/2+1 < j \le n$ (n is even) or $(n+1)/2 < j \le n$ (n is odd). Then $D^{D_1}_{a_1(1,1)} = [v_{ij}]$.
- The rows from two to m of $D^{B_1}_{c_1(1,1)}$ are equal to the rows from one to (m−1) of $D^{D_1}_{a_1(1,1)}$; and the first entry of the first row is one and remaining entries are equal to the second row.
- For columns $1\le j \le n/2$ (n is even) or $1\le j \le (n+1)/2$ (n is odd), we add one to the entries of $D^{D_1}_{a_1(1,1)}$ and for columns $n/2 < j \le n$ (n is even) or $(n+1)/2 < j \le n$ (n is odd) we add -1 to the entries of $D^{D_1}_{a_1(1,1)}$ to obtain $D^{D_2}_{a_1(1,1)}$.
- The first and second rows of $D^{B_2}_{c_1(1,1)} = [w_{ij}]$ are equal, except the last entry of the first row which is equal to 2; and the rows from two to m are calculated from the equation $w_{ij} = s_{(i-1)(n-j+1)}$.

Table 3. $D^{A_2}_{a_1(1,1)} = [r_{ij}]$

i = 1	j = 1	j = n	$2 \le j \le n/2$ (n|2) $2 \le j \le (n+1)/2$ (n∤2)	$n/2 < j < n$ (n|2) $(n+1)/2 < j < n$ (n∤2)
	$r_{11} = 1$	$r_{1n} = 3$	$r_{1j} = r_{1(j-1)} + 4$	$r_{1j} = r_{1(j+1)} + 4$
$1< i \le m/2+1$	$1 \le j \le n/2$ (n|2) $1 \le j \le (n+1)/2$ (n∤2)			$n/2+1 \le j \le n$ (n|2) $(n+1)/2+1 \le j \le n$ (n∤2)
	$i \le j$ $r_{ij} = r_{(i-1)j} + 2$ $i > j$ $r_{ij} = r_{(i-1)j} + 4$			$i \le n-j+2$ $r_{ij} = r_{(i-1)j} + 2$ else $r_{ij} = r_{(i-1)j} + 4$

- The matrix $D^{D_2}_{d_1(1,1)}$ is equals to $D^{A_2}_{a_1(1,1)}$.
- In matrix $D^{A_2}_{d_1(1,1)}$ the first entry is 4, and other entries of the first row are equal to entries in the second row. We also add one to entries in the first row until (m−1)th row of $D^{A_2}_{a_1(1,1)}$ to obtain the rows from two to m of this matrix, respectively.
- The entries of $D^{B_2}_{b_1(1,1)} = [u_{ij}]$ are obtained from $D^{A_2}_{a_1(1,1)}$ by the equation $u_{ij} = r_{i(n-j+1)}$
- The matrix $D^{C_2}_{c_1(1,1)}$ is obtained from above equation.
- If we add one by all entries of $D^{B_2}_{b_1(1,1)}$ then we acquire $D^{C_2}_{b_1(1,1)}$.

Table 4. $D^{B_2}_{a_1(1,1)} = [e_{ij}]$.

i = 1	j = 1	$2 \le j \le n/2$ (n|2) $2 \le j \le (n+1)/2$ (n∤2)	$1< i \le m/2+1$	$1 \le j \le n/2$ (n|2) $1 \le j \le (n+1)/2$ (n∤2)
	$e_{11}=2$	$e_{1j} = e_{1(j-1)} + 4$		$i \le j$ $e_{ij} = e_{(i-1)j} + 2$ $i > j$ $e_{ij} = e_{(i-1)j} + 4$
$e_{ij} = e_{i(n-j+1)}$ where [$n/2 < j \le n$ & (n|2)] or [$(n+1)/2< j \le n$ & (n∤2)]				

- The matrix $D^{D_2}_{c_1(1,1)}$ is equal to $D^{B_2}_{a_1(1,1)}$.
- Two matrices $D^{C_2}_{a_1(1,1)}$ and $D^{D_2}_{b_1(1,1)}$ are achieved by adding 1 to each entry of $D^{B_2}_{a_1(1,1)}$.
- The first and second rows of $D^{A_2}_{b_1(1,1)}$ and $D^{C_2}_{d_1(1,1)}$ are equal and the second until last row of these matrices are computed by adding 2 to the first until (m−1)th row of $D^{B_2}_{a_1(1,1)}$.
- The first and second rows of matrices $D^{A_2}_{c_1(1,1)}$ and $D^{B_2}_{d_1(1,1)}$ are the same and the rows from two to m are equal to the rows from one to (m−1) of $D^{C_2}_{a_1(1,1)}$.

- The matrix $D^{D_1}_{c_1(1,1)} = [z_{ij}]$ obtained from the matrix $D^{B_2}_{a_1(1,1)}$ by the relations below;

if $1 \le j \le n/2$ (n is even) or $1 \le j \le (n+1)/2$ (n is odd) then $z_{ij} = e_{ij} - 1$; and if, $n/2 < j \le n$ (n is even) or $(n+1)/2 < j \le n$ (n is odd) then $z_{ij} = e_{ij} + 1$.

- By adding 1 to all entry of $D^{D_1}_{c_1(1,1)} = [d_{ij}]$ we receive to the matrix $D^{D_1}_{b_1(1,1)} = [d_{ij}]$.
- The first and second rows of $D^{A_1}_{c_1(1,1)}$ are equal; and the second until m[th] row are equal to the first until (m−1)[th] row of $D^{D_1}_{b_1(1,1)}$, respectively.
- The first row of $D^{A_1}_{b_1(1,1)}$ is equal to the first row of $D^{D_1}_{c_1(1,1)}$, and the rows from two to m are obtained by adding 2 to entries of the rows from one to (m−1) of $D^{D_1}_{c_1(1,1)}$.
- If $m/2+1 < i \le m$ then we define $D^{X_j}_{x_k(1,1)} = \left[(X_j^{x_k})_i\right]_{1 \le i \le m}$, where $(X_j^{x_k})_i$ is i[th] row of the matrix and $k \in \{1,2\}$. To compute rows for $m/2+1 < i \le m$, we consider the case of $a_1(1,1)$. Then,

$$D^{A_1}_{a_1(1,1)} = \begin{bmatrix} (A_1^{a_1})_1 \\ \vdots \\ (A_1^{a_1})_{m/2+1} \\ (D_2^{d_2})_{m/2} \\ \vdots \\ (D_2^{d_2})_2 \end{bmatrix}, \quad D^{B_1}_{a_1(1,1)} = \begin{bmatrix} (B_1^{a_1})_1 \\ \vdots \\ (B_1^{a_1})_{m/2+1} \\ (C_2^{d_2})_{m/2} \\ \vdots \\ (C_2^{d_2})_2 \end{bmatrix}, \quad D^{C_1}_{a_1(1,1)} = \begin{bmatrix} (C_1^{a_1})_1 \\ \vdots \\ (C_1^{a_1})_{m/2+1} \\ (B_2^{d_2})_{m/2} \\ \vdots \\ (B_2^{d_2})_2 \end{bmatrix}, \quad D^{D_1}_{a_1(1,1)} = \begin{bmatrix} (D_1^{a_1})_1 \\ \vdots \\ (D_1^{a_1})_{m/2+1} \\ (A_2^{d_2})_{m/2} \\ \vdots \\ (A_2^{d_2})_2 \end{bmatrix}$$

$$D^{A_2}_{a_1(1,1)} = \begin{bmatrix} (A_2^{a_1})_1 \\ \vdots \\ (A_2^{a_1})_{m/2+1} \\ (D_1^{d_2})_{m/2} \\ \vdots \\ (D_1^{d_2})_2 \end{bmatrix}, \quad D^{B_2}_{a_1(1,1)} = \begin{bmatrix} (B_2^{a_1})_1 \\ \vdots \\ (B_2^{a_1})_{m/2+1} \\ (C_1^{d_2})_{m/2} \\ \vdots \\ (C_1^{d_2})_2 \end{bmatrix}, \quad D^{C_2}_{a_1(1,1)} = \begin{bmatrix} (C_2^{a_1})_1 \\ \vdots \\ (C_2^{a_1})_{m/2+1} \\ (B_1^{d_2})_{m/2} \\ \vdots \\ (B_1^{d_2})_2 \end{bmatrix}, \quad D^{D_2}_{a_1(1,1)} = \begin{bmatrix} (D_2^{a_1})_1 \\ \vdots \\ (D_2^{a_1})_{m/2+1} \\ (A_1^{d_2})_{m/2} \\ \vdots \\ (A_1^{d_2})_2 \end{bmatrix}$$

In a similar way we acquire other matrices.

The other cases are calculated in a similar way as above and as in Section 2.1.

3. Conclusions

In this paper algorithms for computing Hosoya polynomials of $TUC_4C_8(R/S)$ are presented. We prepared some MATLAB programs for these algorithms. The running time of our MATLAB codes show that our algorithms are efficient.

References

[1] H. Wiener, J. Am. Chem. Soc. **69,** 17 (1947).
[2] H. Hosoya, Bull. Chem. Soc. Jpn. **44,** 2332 (1971).
[3] H. Hosoya, Discr. Appl. Math. **19,** 239 (1988).
[4] E. Estrada, O. Ivanciuc, I. Gutman, A. Gutierrez, L. Rodriguez, New J. Chem., 819, 1998.
[5] M. V. Diudea, MATCH Commun. Math. Comput. Chem. **45,** 109 (2002).
[6] M. V. Diudea, Bull. Chem. Soc. Japan **75,** 487 (2002).
[7] M. V. Diudea, P. E. John, MATCH Commun. Math. Comput. Chem., **44,** 103 (2001).
[8] M. V. Diudea, B. Pârv, M. I. Topan, J. Serb. Chem. Soc. **62,** 267 (1997).
[9] M. V. Diudea, J. Chem. Inf. Comput. Sci. **37,** 300 (1997).
[10] M. V. Diudea, O. M. Minailiuc, G. Katona, I. Gutman, MATCH Commun. Math. Comput. Chem. **35,** 129 (1997).
[11] A. R. Ashrafi, M. Jalali, M. Ghorbani, M. V. Diudea, MATCH Commun. Math. Comput. Chem. **60,** 905 (2008).
[12] S. Yousefi, A. R. Ashrafi, MATCH Commun. Math. Comput. Chem. **56,** 169 (2006).
[13] A. R. Ashrafi, S. Yousefi, MATCH Commun. Math. Comput. Chem. **57,** 403 (2007).
[14] A. R. Ashrafi, S. Yousefi, Nanoscale Res. Lett. **2,** 202 (2007).
[15] S. Yousefi, A.R. Ashrafi, J. Math. Chem. **42,** 1031 (2007).
[16] S. Yousefi, A. R. Ashrafi, Current Nanoscience **4,** 161 (2008).

[17] S. Yousefi, H. Yousefi-Azari, A. R. Ashrafi, M. H. Khalifeh, J. Sci. Univ. Tehran **33**(3), 7 (2008).
[18] A. R. Ashrafi, S. Yousefi, Digest Journal of Nanomaterials and Biostructures **4,** 407 (2009).
[19] A. R. Ashrafi, H. Shabani, Optoelectron. Adv. Mater.-Rapid Comm. **3**(4)**,** 356 (2009).
[20] A. R. Ashrafi, H. Shabani, Digest Journal of Nanomaterials and Biostructures **4,** 453 (2009).
[21] S. Xu, H. Zhang, Int. J. Quant. Chem. **107,** 586 (2007).
[22] S. Xu, H. Zhang, Discr. Appl. Math. **156**, 2930.
[23] S. Xu, H. Zhang H 2008, J. Math. Chem. In press
[24] N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton, FL, 1992.

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