

Estimating some topological indices for $C_4C_8(S)$ nanotorus

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The newly developed topological indices A_{m1} , A_{m2} and A_{m3} were applied to multivariate analysis in structure–property correlation studies. In this paper the topological indices A_{m1} , A_{m2} and A_{m3} of $C_4C_8(S)$ nanotori are estimated with high accuracy by approximating functions $f_i(p, q)$, $i = 1, 2, 3$, where p and q represent the number of polyhexs in one row and the number of rows in the nanotorus respectively. These functions are obtained using numerical analysis approach. The predictive ability of suggested functions are evaluated according to their Sum of Residuals Squared (SSE) and Coefficient of Determination (r^2).

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1. Introduction

A nanostructure is an object of intermediate size between molecular and microscopic structures. One of the most important of these new materials are carbon nanotubes [1, 2]. A nanotorus is theoretically described as carbon nanotube bent into a torus (doughnut shape). Nanotori are predicted to have many unique properties, such as magnetic moments 1000 times larger than previously expected for certain specific radii [3]. The electronic properties of such structures are less well understood and some of its mathematical properties are determined. Therefore, it is of interest to study the mathematical properties of these materials. For this purpose, the form of molecule must be coded according to numbers. A common method for coding the molecule structure, is to assign a graph to the molecule, where the vertices are atoms of molecule and edges are chemical bonds between the atoms. According to this graph, we can assign various numeral values (topological indices), polynomials, matrices and extra to the molecules which are usually invariant under automorphism of graphs. The topological indices are the basis of the mathematical models for quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies. Such indices based on the distances in graph are widely used for establishing relationships between the structure of nanomolecular and their physicochemical properties [4-6]. The newly developed topological indices A_{m1} , A_{m2} , A_{m3} based on the augmented path matrices have been successfully employed in the studies on structure-property relationships. They describe some molecular properties, such as lipophilicity and branching better than other kinds of topological indices [7].

In this paper we obtain functions accurately estimating the topological indices A_{m1} , A_{m2} and A_{m3} of the $C_4C_8(S)$ $[p, q]$ polyhex nanotorus, where p indicates the number of polyhexs in the row and q is the number of rows (Fig. 1).

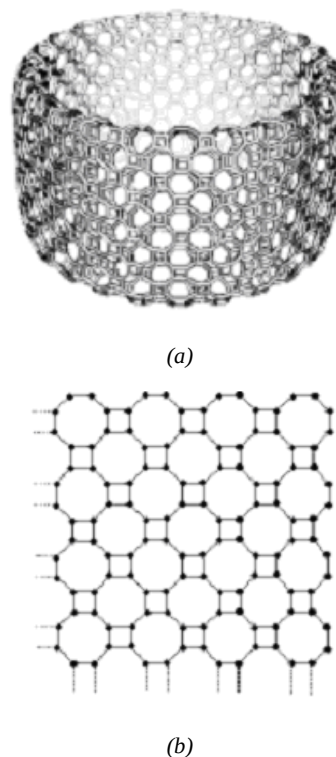


Fig. 1. (a) The 3D representation of the $C_4C_8(S)$ nanotorus; (b) the $C_4C_8(S)$ nanotorous lattice.

2. Main results and discussion

Let A be an adjacency matrix of molecular graph of nanostructures. The newly developed topological indices A_{m1} , A_{m2} and A_{m3} are generated from path matrices A , B and C , respectively [8-9]. The elements of these three matrices are defined as follows:

$$A(i, j) = \begin{cases} 1 & \text{path}(i, j) = 1 \\ 0 & \text{otherwise} \end{cases} \quad i, j = 1, 2, \dots, n,$$

$$B(i, j) = \begin{cases} 2 & \text{path}(i, j) = 2 \\ 0 & \text{otherwise} \end{cases} \quad i, j = 1, 2, \dots, n,$$

$$C(i, j) = \begin{cases} 3 & \text{path}(i, j) = 3 \\ 0 & \text{otherwise} \end{cases} \quad i, j = 1, 2, \dots, n,$$

where n is the number of atoms in the corresponding molecules and by $\text{path}(i, j)$ we mean the length of the shortest path between vertex i and vertex j . By adding two columns into matrices A , B and C , augmented path matrices G_1 , G_2 and G_3 are constructed respectively. The elements in

the first column of matrices G_1 , G_2 and G_3 are square roots of vertex degrees, and those in the second column are the square roots of the Van derWaals radius of atoms [10-11]. Matrices Z_1 , Z_2 and Z_3 can be calculated respectively from matrices G_1 , G_2 and G_3 according to the following formula:

$$Z_1 = G_1 \times G_1^t, \quad Z_2 = G_2 \times G_2^t, \quad Z_3 = G_3 \times G_3^t,$$

where G_1^t , G_2^t and G_3^t are the transposed matrices of G_1 , G_2 and G_3 , respectively. The three topological indices are defined as:

$$A_{m1} = \frac{\lambda_{\max 1}}{2}, \quad A_{m2} = \frac{\lambda_{\max 2}}{2}, \quad A_{m3} = \frac{\lambda_{\max 3}}{2},$$

where $\lambda_{\max 1}$, $\lambda_{\max 2}$ and $\lambda_{\max 3}$ are respectively the largest eigenvalues of matrices Z_1 , Z_2 and Z_3 .

To obtain the adjacency matrix A of $C_4C_8(S)[p, q]$ nanotorus, the nodes of k th row, $0 \leq k \leq q$, are labeled as follow (Fig. 2):

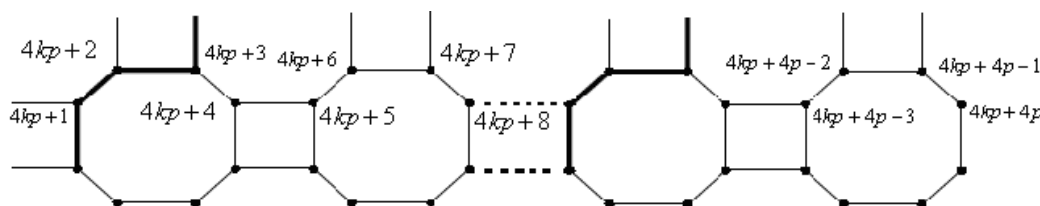


Fig. 2. Labeling of the k th row of $C_4C_8(S)[p, q]$.

Now according to the recommended labeling, the following lemma gives the form of adjacency matrix of $C_4C_8(S)$ nanotorus.

Lemma 1. Let A be an adjacency matrix of $C_4C_8(S)[p, q]$ nanotorus with q rows and p hexagons in a row. Then A is a matrix of order $4p(q+1)$, and

$$A(4kp+l, j) = \begin{cases} 1 & \text{if } j = 4kp + (m-1) \text{ or } j = 4kp + (n+1) \text{ or } (l, j) \in X \cup Y \\ 0 & \text{Otherwise} \end{cases}$$

where $0 \leq k \leq q$, $1 \leq l \leq 4p$ and

$$X = \{(l, j) | l \equiv 0, j = 4(k+(-1)^k)p+l\} \cup \{(l, j) | l \equiv 1, j = 4(k+(-1)^k)p+l\}$$

$$Y = \{(l, j) | l \equiv 2, j = 4(i+(-1)^{k+1})p+l\} \cup \{(l, j) | l \equiv 3, j = 4(i+(-1)^{k+1})p+l\}$$

$$m = \begin{cases} 4p+1 & l=1 \\ l & \text{otherwise} \end{cases}, \quad n = \begin{cases} 0 & l=4p \\ l & \text{otherwise} \end{cases}, \quad i = \begin{cases} q+1 & k=0 \\ -1 & k=q \\ k & \text{otherwise} \end{cases}.$$

The above relations indicate the adjacency between nodes in corresponding molecular graph.

Proof. Suppose x_{kl} be an arbitrary vertex in k th row and l th column, $0 \leq k \leq q, 1 \leq l \leq 4p$. It can be seen easily that $\deg(x_{kl}) = 3$ and according to our recommended labeling, its label is $4kp+l$. This vertex is adjacent with two vertices in k th row and with a vertex in l th column. The adjacent vertices which are in the same row as x_{kl} are determined as follow:

If $l=1$ then $x_{k,l+1}$ and $x_{k,4p}$ with

respectively $4kp+l+1$ and $4kp+4p$ labels, are x_{kl} 's adjacent vertices in the k th row. Therefore

$$A(4kp+l, 4kp+(m-1)) = A(4kp+l, 4kp+(n+1)) = 1, \\ m = 4p+1, \quad n = l.$$

Else if $1 < l < 4p$ then two adjacent vertices of x_{kl} in the k th row are $x_{k,l-1}$ and $x_{k,l+1}$. Hence according to these two vertices labeling, $4kp+l-1$ and $4kp+l+1$, we can write:

$$A(4kp + l, 4kp + (m-1)) = A(4kp + l, 4kp + (n+1)) = 1, \quad m = n = l.$$

Finally, if $l = 4p$ then x_{kl-1} and x_{kl} are x_{kl} 's adjacent vertices which their labels are $4kp + l - 1$ and $4kp + 1$ respectively. So again we have

$$A(4kp + l, 4kp + (m-1)) = A(4kp + l, 4kp + (n+1)) = 1,$$

where $m = l$ and $n = 0$. Now what is discussed above can be summarize as follow:

$$A(4kp + l, j) = 1 \quad \text{if} \quad j = 4kp + (m-1) \quad \text{or} \quad 4kp + (n+1), \quad (0 \leq k \leq q), (1 \leq l \leq 4p),$$

where

$$m = \begin{cases} 4p+1 & l=1 \\ l & \text{otherwise} \end{cases}, \quad n = \begin{cases} 0 & l=4p \\ l & \text{otherwise} \end{cases}.$$

For determining the x_{kl} 's adjacent vertex in the l th column we consider four following cases:

Case1: k is even and l 's residual on 4 is either 0 or 1, which can be restated in mathematical notation as $l \equiv 0 \text{ or } l \equiv 1$. In this case x_{kl} 's adjacent vertex is x_{k+1l} which is labeled with $4(k+1)p + l$.

Case 2: Otherwise if k is odd and $l \equiv 0 \text{ or } l \equiv 1$ then based on the labeling, x_{kl} 's adjacent vertex is x_{k-1l} .

So according to these two cases we can write:

$$A(4kp + l, j) = 1 \quad \text{if} \quad (l, j) \in X, \quad (0 \leq k \leq q), (1 \leq l \leq 4p),$$

where

$$X = \left\{ (l, j) \mid l \equiv 0, j = 4(k + (-1)^k)p + l \right\} \cup \left\{ (l, j) \mid l \equiv 1, j = 4(k + (-1)^k)p + l \right\}.$$

Case 3: k is even and $l \equiv 2 \text{ or } l \equiv 3$. Here x_{k-1l} is x_{kl} 's adjacent vertex in the l th column. Notice that if $k = 0$ then x_{ql} with $4qp + l$ label, is its adjacent vertex.

Case 4: k is odd and $l \equiv 2 \text{ or } l \equiv 3$. Therefore x_{k+1l} is the adjacent vertex of x_{kl} . Regarding that q can be only odd, in this case if $k = q$ then x_{0l} in 0 th row, is its adjacent vertex. As a result of the third and forth case we have:

$$A(4kp + l, j) = 1 \quad \text{if} \quad (l, j) \in Y \\ (0 \leq k \leq q), (1 \leq l \leq 4p)$$

where

$$Y = \left\{ (l, j) \mid l \equiv 2, j = 4(i + (-1)^{k+1})p + l \right\} \cup \left\{ (l, j) \mid l \equiv 3, j = 4(i + (-1)^{k+1})p + l \right\}$$

and

$$i = \begin{cases} q+1 & k=0 \\ -1 & k=q \\ k & \text{otherwise} \end{cases},$$

and this complete the proof.

Now having adjacent matrix at disposal, the element of B is determined as follow:

$$B(i, j) = \begin{cases} 2 & (i, j) \in S \\ 0 & \text{otherwise} \end{cases} \quad 1 \leq i, j \leq 4p(q+1),$$

where

$$S = \{(i, j) \mid \text{there exist } h \text{ such that } A(i, h) = 1 \text{ and } A(h, j) = 1\},$$

and similarly,

$$C(i, j) = \begin{cases} 3 & (i, j) \in R \\ 0 & \text{otherwise} \end{cases}$$

where

$$R = \{(i, j) \mid \text{there exist } h \text{ such that } B(i, h) = 1 \text{ and } A(h, j) = 1\}.$$

3. Numerical experiment

In this section, we apply a MATLAB program to compute the topological indices A_{m1} , A_{m2} and A_{m3} of $C_4C_8(S)[p, q]$ nanotorus for different values of p and q , Table 1.

Table 1. Topological indices of $C_4C_8(S)[p, q]$ nanotorus.

Compounds	A_{m1}	A_{m2}	A_{m3}
$C_4C_8(1,1)$	696.5	710	696.5
$C_4C_8(5,1)$	3464.5	3492	3532
$C_4C_8(7,1)$	4848.5	4876	4916
$C_4C_8(12,1)$	8308.5	8336	8376
$C_4C_8(20,1)$	13800	13872	13912
$C_4C_8(4,3)$	5540.5	5586	5824
$C_4C_8(7,3)$	9692.5	9738	9976
$C_4C_8(11,3)$	15228.5	15274	15512
$C_4C_8(16,3)$	22148.5	22194	22432
$C_4C_8(19,3)$	26300.5	26346	26584
$C_4C_8(20,3)$	27684.5	27730	27968
$C_4C_8(3,5)$	6232.5	6278	6516
$C_4C_8(7,5)$	14536.5	14582	14820
$C_4C_8(14,5)$	29068.5	29114	29352
$C_4C_8(17,5)$	35296.5	35342	35580
$C_4C_8(19,5)$	39448.5	39494	39732
$C_4C_8(2,9)$	6924.5	6970	7208
$C_4C_8(8,9)$	27684.5	27730	27968
$C_4C_8(15,9)$	51904.5	51950	52188
$C_4C_8(20,9)$	69204.5	69250	69488
$C_4C_8(4,15)$	22148.5	22194	22432
$C_4C_8(8,15)$	44292.5	44338	44576
$C_4C_8(13,15)$	71972.5	72018	72256
$C_4C_8(17,15)$	94116.5	94162	94400
$C_4C_8(18,15)$	99652.5	99698	99936

It is clear that the size of matrices A, B and C become extremely large for big values of p and q , therefore computing these topological indices even by using a powerful computing software such as MATLAB is not time consuming

at all. Therefore we continue our progress applying *surface fitting approach* to find two-dimension fitting functions estimating the topological indices A_{m1} , A_{m2} and A_{m3} of $C_4C_8(S)$ nanotorus.

4. Approximating functions

In many kinds of numerical computations, it is convenient to introduce approximate functions. Approximate functions used to express dependent variable z as a function of the two independent variables x and y within the range of the data.

An extensively used criterion that evaluates function fitting performance is *coefficient of determination* (r^2) which is defined according to the following formula:

$$r^2 = 1 - \frac{SSE}{\sum_{i=1}^n w_i (z_i - \bar{z})^2},$$

where SSE is the actual least squares measure of fit. It is a weighted (w_i) sum of the squared residual:

$$SSE = \sum_{i=1}^n w_i (z_i - \hat{z}_i)^2,$$

where z_i , $\hat{z}_i$, $\bar{z}$ and n are z data value, the estimated z value, the mean of the z data value and the number of data points, respectively.

The coefficient of determination is a calculation of the accuracy of the model in explaining the data. It shows how good or bad the prediction was, in comparison with the actual values [12-15].

Techniques discussed above are utilized to discover the possible relationship between the input descriptors p and q and output bioactivities A_{m1} , A_{m2} and A_{m3} .

In Table 1 shown 25 nanotori were used as source data. The result is the following equation, expressing A_{m1} , A_{m2} and A_{m3} as a function of two dependent variables p and q :

$$f(p, q) = a + bp + cq + dp^2 + eq^2 + fpq + gp^3 + hq^3 + ipq^2 + jp^2q \quad 1 \leq p, q \leq 30$$

where the equation's coefficients value for fitting on the A_{m1} 's data are:

$$\begin{aligned} a &= 4.502657344 & f &= 345.9999344, \\ b &= 346.0002094 & g &= -6.5768e-07, \\ c &= -0.00288476 & h &= -2.0273e-05, \\ d &= 6.96191e-06 & i &= -8.6156e-08, \\ e &= 0.000502439 & j &= 2.62273e-06. \end{aligned}$$

Fitting the above function on the A_{m2} 's data source leads to the following coefficients:

$$\begin{aligned} a &= 10.31340052 & f &= 345.7878874 \\ b &= 349.8185085 & g &= 0.004984608 \\ c &= 9.431041001 & h &= 0.01917032 \\ d &= -0.24283824 & i &= 0.003420406 \\ e &= -0.75601882 & j &= 0.005364316 \end{aligned}$$

And finally here are the coefficients value used for estimating A_{m3} :

$$\begin{aligned} a &= -82.9260494 & f &= 344.5456124 \\ b &= 369.3914493 & g &= 0.026018927 \\ c &= 100.0957517 & h &= 0.215884574 \\ d &= -1.36761051 & i &= 0.023251071 \\ e &= -8.36491308 & j &= 0.035900158, \end{aligned}$$

The values of coefficient of determination (r^2) for above fitting functions are 1.0, 0.9999999931 and 0.9999991589 respectively, which mean there are no or almost no differences between actual and predicting values, so it proves the high predictive ability of suggested functions.

All computation was performed using TableCurve 3D software. More information about this software is available at <http://www.systat.com>.

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